



Full wwPDB EM Validation Report ⓘ

Oct 8, 2026 – 04:08 PM EDT

PDB ID : 9PDJ / pdb_00009pdj
EMDB ID : EMD-71535
Title : Composite map of open form of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-30
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

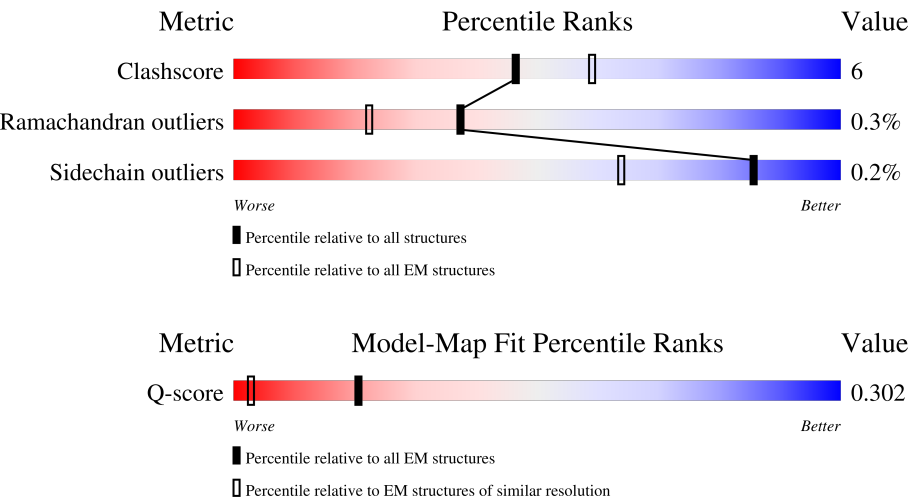
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



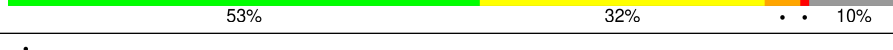
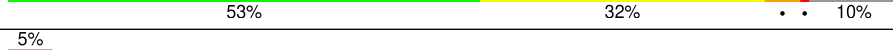
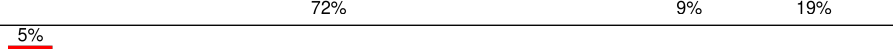
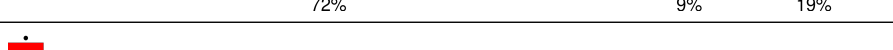
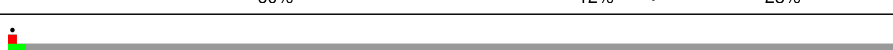
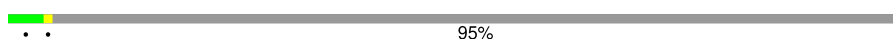
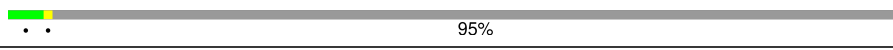
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	778	
1	B0	778	
2	A1	642	
2	B1	642	

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Mol	Chain	Length	Quality of chain
3	A2	513	
3	B2	513	
4	A3	321	
4	B3	321	
5	A4	338	
5	B4	338	
6	A5	72	
6	B5	72	
7	A6	461	
7	B6	461	
8	A7	843	
8	B7	843	
9	A8	905	
9	B8	905	
9	SF	905	
9	sF	905	
10	A9	244	
10	B9	244	
11	AA	1733	
11	BA	1733	
11	MA	1733	
11	mA	1733	
12	AB	1224	
12	BB	1224	
13	AC	318	

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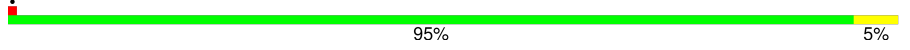
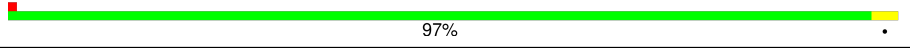
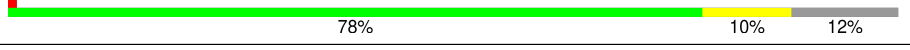
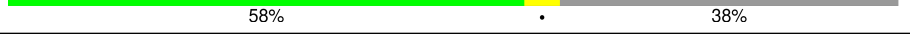
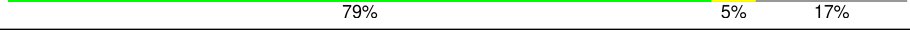
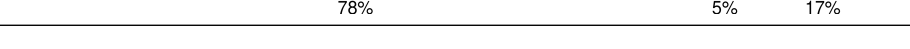
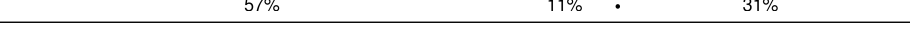
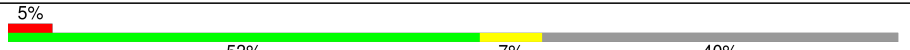
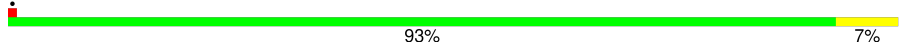
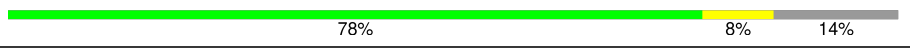
Mol	Chain	Length	Quality of chain
13	BC	318	
14	AD	221	
14	BD	221	
15	AE	215	
15	BE	215	
16	AF	155	
16	BF	155	
17	AG	171	
17	BG	171	
18	AH	146	
18	BH	146	
19	AI	122	
19	BI	122	
20	AJ	70	
20	BJ	70	
21	AK	120	
21	BK	120	
22	AL	70	
22	BL	70	
23	AM	345	
23	BM	345	
24	AN	69	
24	BN	69	
25	AO	240	
25	BO	240	

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Mol	Chain	Length	Quality of chain
26	AQ	735	25% 71%
26	BQ	735	25% 71%
27	AR	400	6% 53% 11% 35%
27	BR	400	6% 54% 11% 35%
28	AS	309	11% 35% 14% 47%
28	BS	309	11% 35% 13% 47%
29	AT	69	83% 7% 10%
29	BT	69	80% 10% 10%
30	AU	286	29% 6% 64%
30	BU	286	29% 6% 64%
31	AV	122	7% 70% 15% 15%
31	BV	122	7% 72% 13% 15%
32	AW	482	7% 41% 6% 53%
32	BW	482	8% 40% 6% 53%
33	AX	328	14% 55% 42%
33	BX	328	14% 55% 42%
34	Ma	295	53% 43%
34	ma	295	54% 43%
35	Mb	223	61% 9% 30%
35	mb	223	61% 9% 30%
36	Mc	115	83% 10% 6%
36	mc	115	83% 10% 6%
37	Md	687	73% 5% 22%
37	md	687	73% 5% 22%
38	Me	307	76% 19%



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Mol	Chain	Length	Quality of chain
38	me	307	
39	Mf	210	
39	mf	210	
40	Mg	121	
40	mg	121	
41	Mh	284	
41	mh	284	
42	Mi	222	
42	mi	222	
43	Mj	149	
43	mj	149	
44	Mk	157	
44	mk	157	
45	MI	1082	
45	T4	1082	
45	ml	1082	
45	t4	1082	
46	Mm	220	
46	mm	220	
47	Mn	140	
47	mn	140	
48	Mo	127	
48	mo	127	
49	Mp	566	
49	mp	566	

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Mol	Chain	Length	Quality of chain
50	SA	566	
50	sA	566	
51	SB	825	
51	SD	825	
51	sB	825	
51	sD	825	
52	SC	332	
52	sC	332	
53	SE	623	
53	sE	623	
54	SG	47	
54	sG	47	
55	SH	1703	
55	sH	1703	
56	SI	1314	
56	sI	1314	
57	SJ	157	
57	sJ	157	
58	SK	477	
58	sK	477	
59	SL	467	
59	sL	467	
60	E3	1132	
60	T3	1132	
60	t3	1132	

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Mol	Chain	Length	Quality of chain
61	E6	974	26% 85% 10% • •
61	T6	974	82% 13% • •
61	t6	974	82% 13% • •
62	T1	431	12% • 85%
62	t1	431	13% • 85%
63	T2	397	23% • • 72%
63	t2	397	23% • • 72%
64	T5	1081	7% • 90%
64	t5	1081	7% • 90%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 319192 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		
1	B0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		
2	B1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		

- Molecule 3 is a protein called General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		
3	B2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		
4	B3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 5 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		
5	B4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		
6	B5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		
7	B6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		
8	B7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		

- Molecule 9 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A8	17	Total	C	N	O	S	0	0
			134	89	22	22	1		
9	SF	411	Total	C	N	O	S	0	0
			3374	2130	571	663	10		
9	B8	17	Total	C	N	O	S	0	0
			134	89	22	22	1		
9	sF	411	Total	C	N	O	S	0	0
			3374	2130	571	663	10		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A9	68	Total	C	N	O	S	0	0
			542	345	82	113	2		
10	B9	68	Total	C	N	O	S	0	0
			542	345	82	113	2		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		
11	MA	79	Total	C	N	O		0	0
			575	361	79	135			
11	BA	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		
11	mA	79	Total	C	N	O		0	0
			575	361	79	135			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		
12	BB	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		
13	BC	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AD	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		
14	BD	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AE	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		
15	BE	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AF	83	Total	C	N	O	S	0	0
			670	428	114	125	3		
16	BF	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AG	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		
17	BG	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AH	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		
18	BH	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AI	116	Total	C	N	O	S	0	0
			944	581	172	181	10		
19	BI	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AJ	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	BJ	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AK	115	Total	C	N	O	S	0	0
			924	593	157	172	2		
21	BK	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 22 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AL	45	Total	C	N	O	S	0	0
			359	221	71	63	4		
22	BL	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	276	Total	C	N	O	S	0	0
			2097	1328	359	393	17		
23	BM	276	Total	C	N	O	S	0	0
			2097	1328	359	393	17		

- Molecule 24 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AN	69	Total	C	N	O	P	0	0
			1413	679	248	417	69		
24	BN	69	Total	C	N	O	P	0	0
			1413	679	248	417	69		

- Molecule 25 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AO	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		
25	BO	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 26 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AQ	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		
26	BQ	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		

- Molecule 27 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AR	261	Total	C	N	O	S	0	0
			2173	1369	383	411	10		
27	BR	261	Total	C	N	O	S	0	0
			2173	1369	383	411	10		

- Molecule 28 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AS	164	Total	C	N	O	S	0	0
			1301	812	230	251	8		
28	BS	164	Total	C	N	O	S	0	0
			1301	812	230	251	8		

- Molecule 29 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AT	69	Total	C	N	O	P	0	0
			1416	679	257	411	69		
29	BT	69	Total	C	N	O	P	0	0
			1416	679	257	411	69		

- Molecule 30 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AU	102	Total	C	N	O	S	0	0
			843	531	142	167	3		
30	BU	102	Total	C	N	O	S	0	0
			843	531	142	167	3		

- Molecule 31 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AV	104	Total	C	N	O	S	0	0
			815	511	136	164	4		
31	BV	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AW	226	Total	C	N	O	S	0	0
			1836	1168	317	344	7		
32	BW	226	Total	C	N	O	S	0	0
			1836	1168	317	344	7		

- Molecule 33 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AX	191	Total	C	N	O	S	0	0
			1530	980	256	289	5		
33	BX	191	Total	C	N	O	S	0	0
			1530	980	256	289	5		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ma	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		
34	ma	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Mb	157	Total	C	N	O	S	0	0
			1295	822	224	246	3		
35	mb	157	Total	C	N	O	S	0	0
			1295	822	224	246	3		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Mc	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
36	mc	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Md	535	Total	C	N	O	S	0	0
			4325	2766	730	816	13		
37	md	535	Total	C	N	O	S	0	0
			4325	2766	730	816	13		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Me	248	Total	C	N	O	S	0	0
			1958	1247	325	376	10		
38	me	248	Total	C	N	O	S	0	0
			1958	1247	325	376	10		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Mf	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		
39	mf	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Mg	106	Total	C	N	O	S	0	0
			847	528	139	175	5		
40	mg	106	Total	C	N	O	S	0	0
			847	528	139	175	5		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Mh	177	Total	C	N	O	S	0	0
			1441	910	242	284	5		
41	mh	177	Total	C	N	O	S	0	0
			1441	910	242	284	5		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Mi	185	Total	C	N	O	S	0	0
			1538	989	259	284	6		
42	mi	185	Total	C	N	O	S	0	0
			1538	989	259	284	6		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Mj	103	Total	C	N	O	S	0	0
			864	539	160	164	1		
43	mj	103	Total	C	N	O	S	0	0
			864	539	160	164	1		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Mk	144	Total	C	N	O	S	0	0
			1157	715	204	235	3		
44	mk	144	Total	C	N	O	S	0	0
			1157	715	204	235	3		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	MI	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		
45	ml	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		
45	T4	220	Total	C	N	O	S	0	0
			1780	1136	302	333	9		
45	t4	220	Total	C	N	O	S	0	0
			1780	1136	302	333	9		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Mm	83	Total	C	N	O	S	0	0
			671	424	111	135	1		
46	mm	83	Total	C	N	O	S	0	0
			671	424	111	135	1		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Mn	140	Total	C	N	O	S	0	0
			1124	701	189	228	6		
47	mn	140	Total	C	N	O	S	0	0
			1124	701	189	228	6		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Mo	109	Total	C	N	O	S	0	0
			914	603	141	164	6		
48	mo	109	Total	C	N	O	S	0	0
			914	603	141	164	6		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Mp	409	Total	C	N	O	S	0	0
			3330	2115	535	669	11		
49	mp	409	Total	C	N	O	S	0	0
			3330	2115	535	669	11		

- Molecule 50 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SA	442	Total	C	N	O	S	0	0
			3552	2231	608	698	15		
50	sA	442	Total	C	N	O	S	0	0
			3552	2231	608	698	15		

- Molecule 51 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
51	SD	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		
51	sB	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
51	sD	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		

- Molecule 52 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		
52	sC	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		

- Molecule 53 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SE	411	Total	C	N	O	S	0	0
			3333	2142	569	617	5		
53	sE	411	Total	C	N	O	S	0	0
			3333	2142	569	617	5		

- Molecule 54 is a protein called unsigned peptide of SWISNF.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	SG	47	Total	C	N	O	0	0
			271	166	56	49		
54	sG	47	Total	C	N	O	0	0
			271	166	56	49		

- Molecule 55 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SH	241	Total	C	N	O	S	0	0
			1958	1227	353	372	6		
55	sH	241	Total	C	N	O	S	0	0
			1958	1227	353	372	6		

- Molecule 56 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	552	Total	C	N	O	S	0	0
			4474	2894	749	820	11		
56	sI	552	Total	C	N	O	S	0	0
			4474	2894	749	820	11		

- Molecule 57 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	82	Total	C	N	O	S	0	0
			711	450	123	135	3		
57	sJ	82	Total	C	N	O	S	0	0
			711	450	123	135	3		

- Molecule 58 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SK	431	Total	C	N	O	S	0	0
			3453	2213	563	658	19		
58	sK	431	Total	C	N	O	S	0	0
			3453	2213	563	658	19		

- Molecule 59 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	406	Total	C	N	O	S	0	0
			3266	2095	533	630	8		
59	sL	406	Total	C	N	O	S	0	0
			3266	2095	533	630	8		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	E3	749	Total	C	N	O	S	0	0
			6069	3916	983	1156	14		
60	T3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		
60	t3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	E6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		
61	T6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		
61	t6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	T1	65	Total	C	N	O	S	0	0
			516	328	82	102	4		
62	t1	65	Total	C	N	O	S	0	0
			516	328	82	102	4		

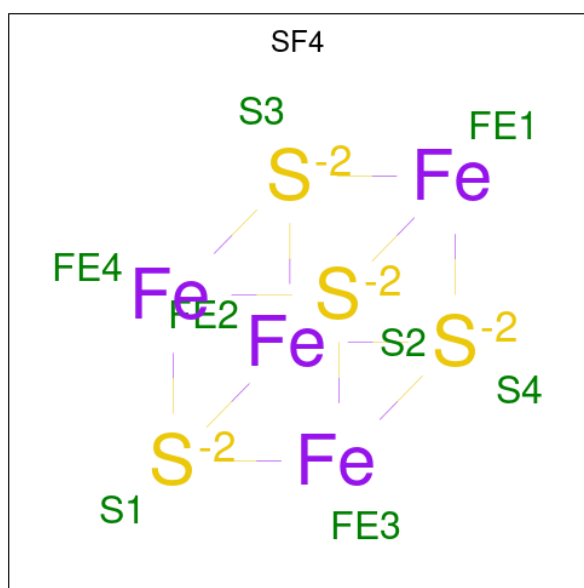
- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	T2	110	Total	C	N	O	S	0	0
			891	560	155	172	4		
63	t2	110	Total	C	N	O	S	0	0
			891	560	155	172	4		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	T5	111	Total	C	N	O	S	0	0
			894	558	161	169	6		
64	t5	111	Total	C	N	O	S	0	0
			894	558	161	169	6		

- Molecule 65 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
65	A0	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
65	B0	1	Total	Fe	S	0
			8	4	4	

- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	A3	2	Total	Zn	0
			2	2	
66	A4	1	Total	Zn	0
			1	1	
66	A6	4	Total	Zn	0
			4	4	
66	AA	2	Total	Zn	0
			2	2	
66	AB	1	Total	Zn	0
			1	1	
66	AC	1	Total	Zn	0
			1	1	
66	AI	2	Total	Zn	0
			2	2	
66	AJ	1	Total	Zn	0
			1	1	
66	AL	1	Total	Zn	0
			1	1	
66	AM	1	Total	Zn	0
			1	1	
66	AS	1	Total	Zn	0
			1	1	
66	AW	1	Total	Zn	0
			1	1	
66	B3	2	Total	Zn	0
			2	2	
66	B4	1	Total	Zn	0
			1	1	
66	B6	4	Total	Zn	0
			4	4	
66	BA	2	Total	Zn	0
			2	2	
66	BB	1	Total	Zn	0
			1	1	
66	BC	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
66	BI	2	Total 2	Zn 2	0
66	BJ	1	Total 1	Zn 1	0
66	BL	1	Total 1	Zn 1	0
66	BM	1	Total 1	Zn 1	0
66	BS	1	Total 1	Zn 1	0
66	BW	1	Total 1	Zn 1	0

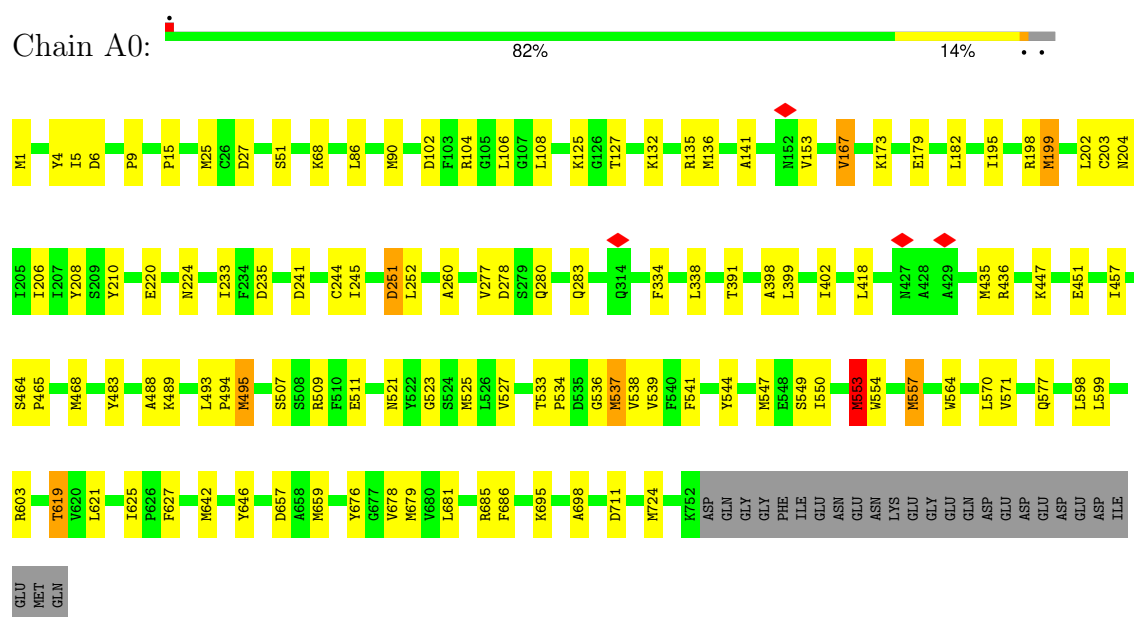
- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	AA	1	Total 1	Mg 1	0
67	BA	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3



- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3



98%

55%



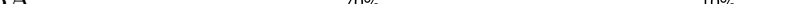


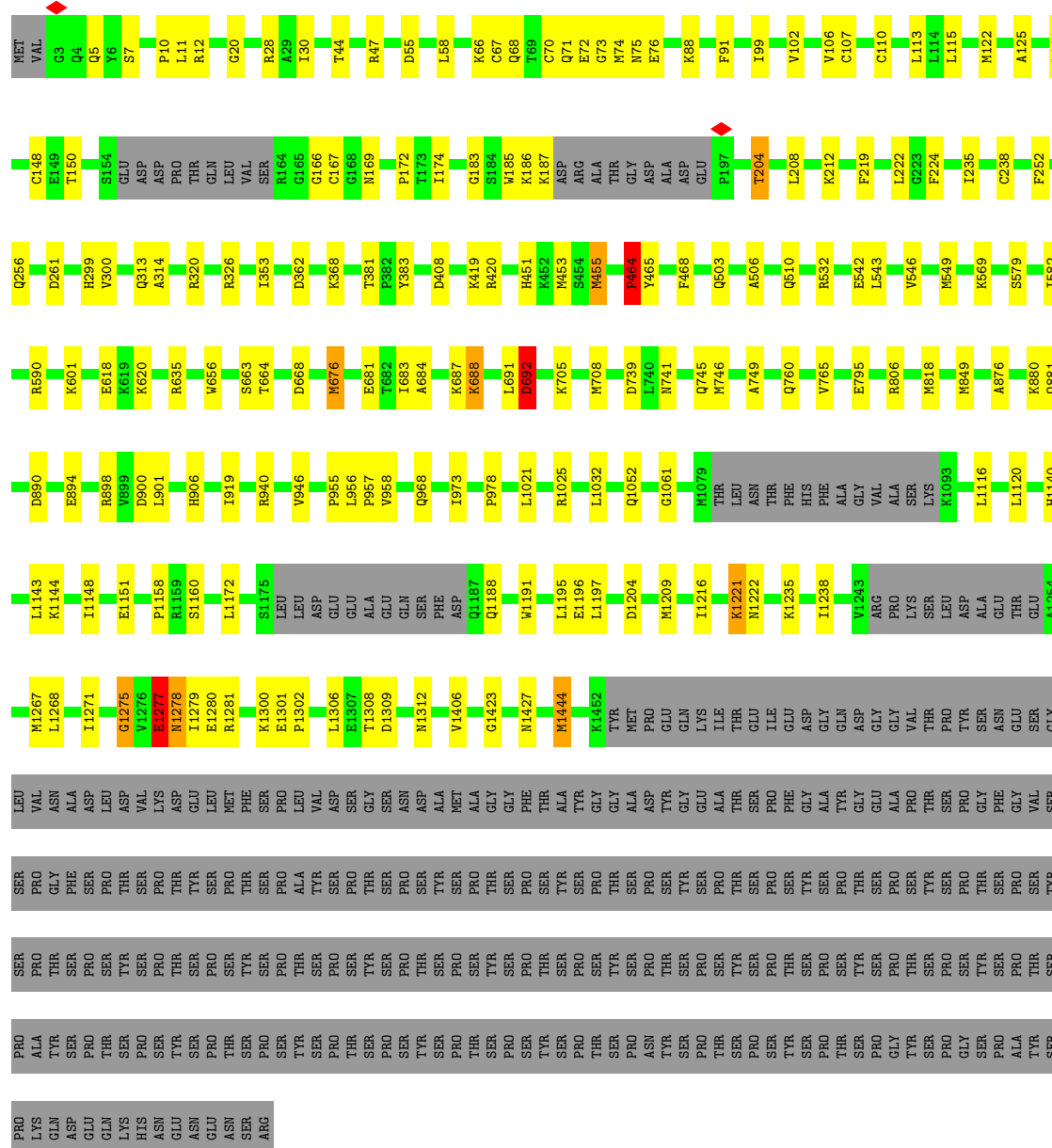




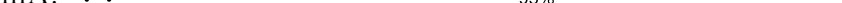


- Molecule 11: DNA-directed RNA polymerase II subunit RPB1

Chain BA:  70% 10% 19%

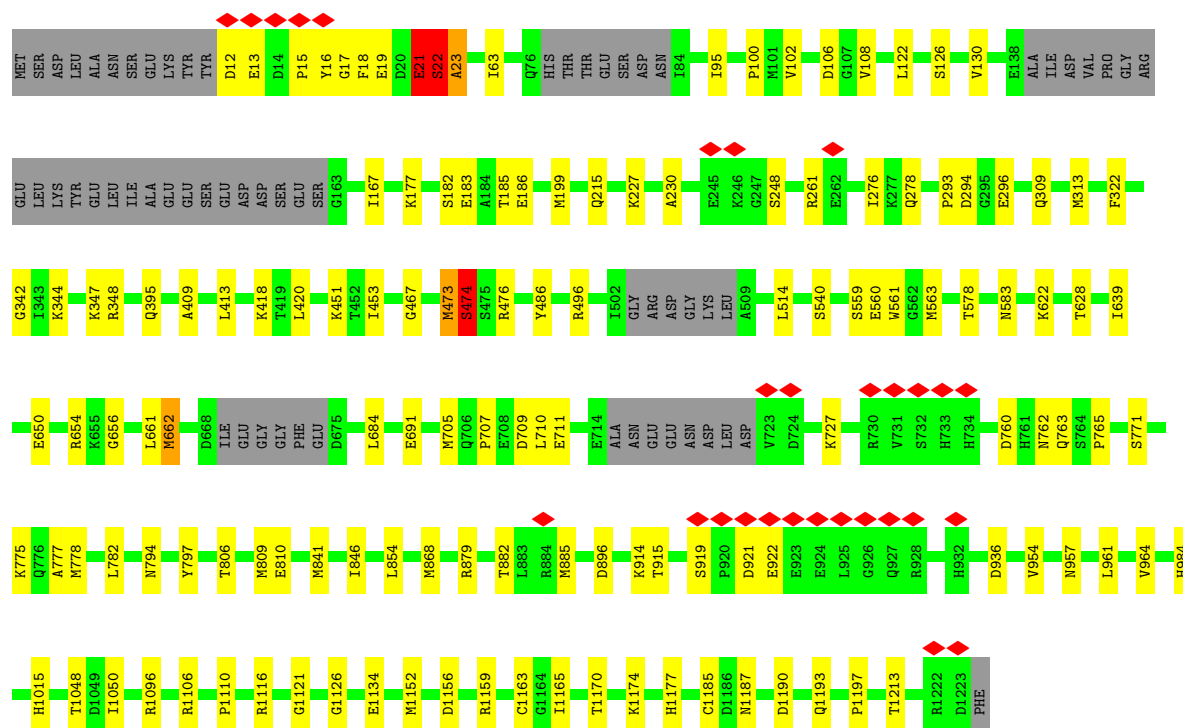


- Molecule 11: DNA-directed RNA polymerase II subunit RPB1

Chain mA:  95%

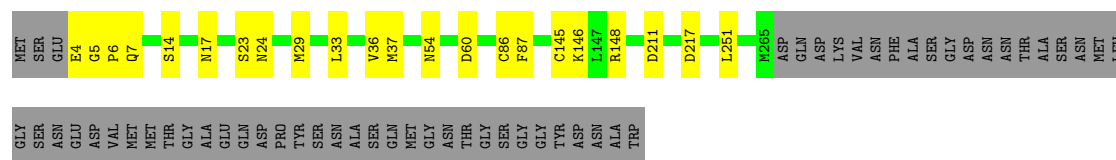






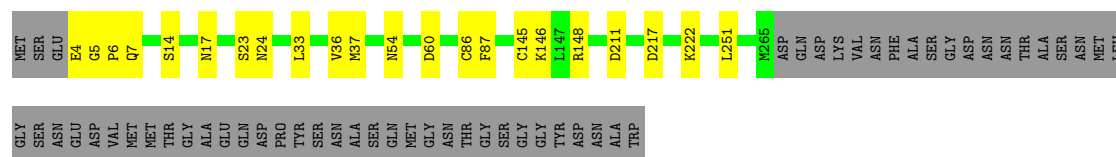
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain AC: 75% 7% 18%



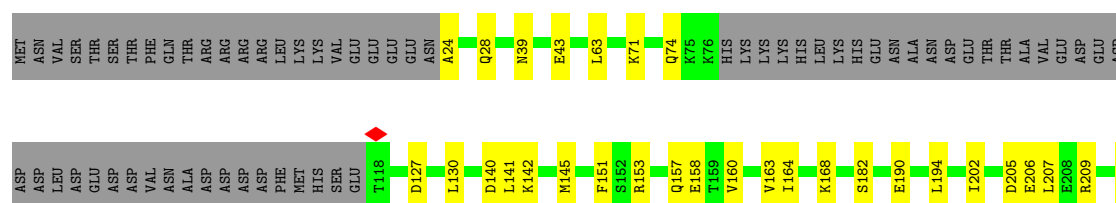
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain BC: 75% 7% 18%



• Molecule 14: DNA-directed RNA polymerase II subunit RPB4

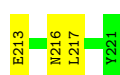
Chain AD: 56% 15% 29%





- Molecule 14: DNA-directed RNA polymerase II subunit RPB4

Chain BD: 56% 15% 29%



- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain AE: 90% 8% ..



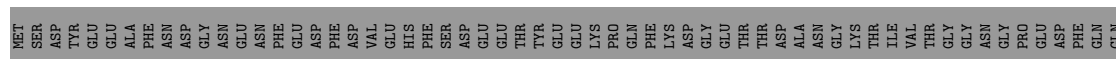
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain BE: 90% 8% ..



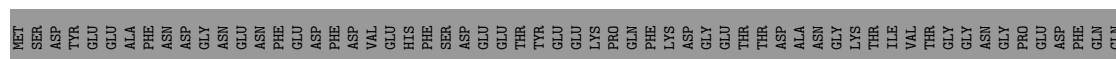
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain AF: 49% 5% 46%

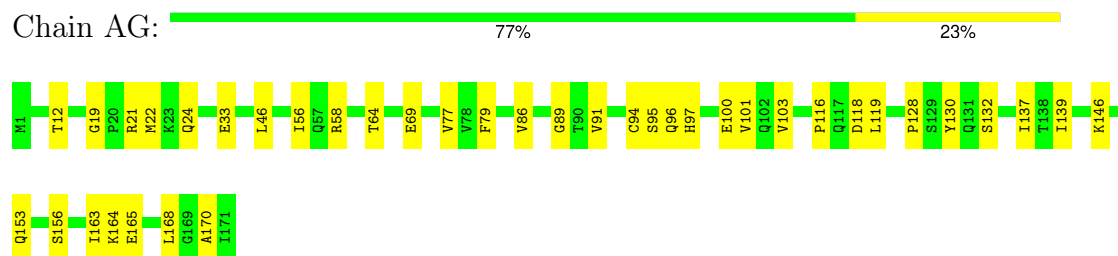


- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

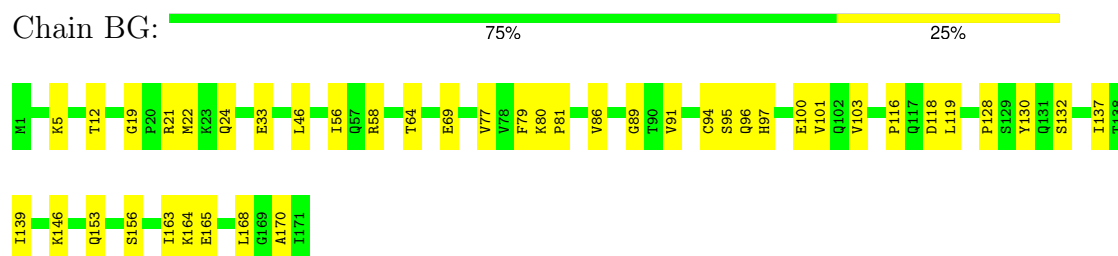
Chain BF: 50% 1% 46%



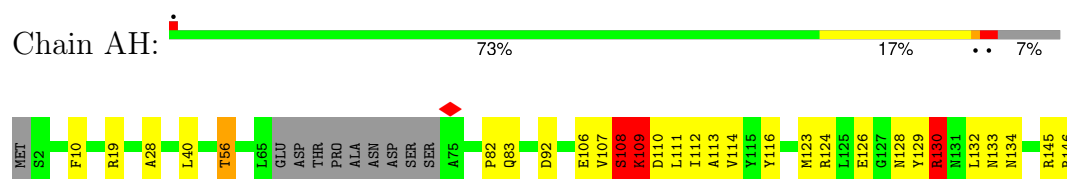
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



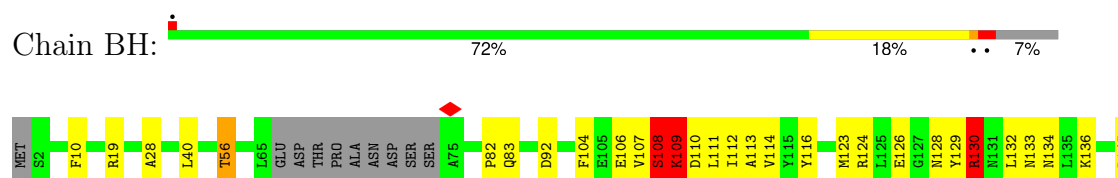
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



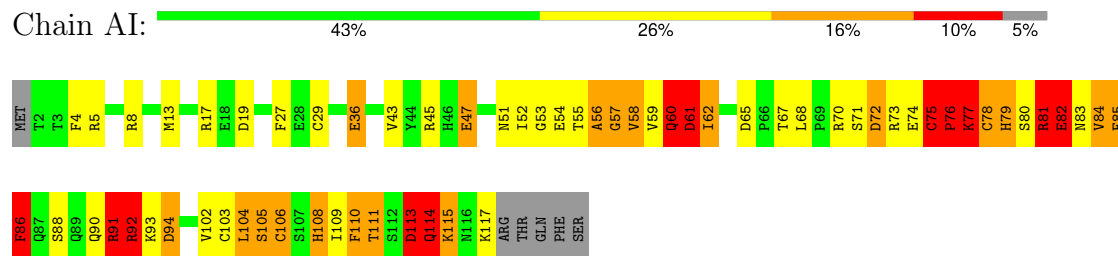
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



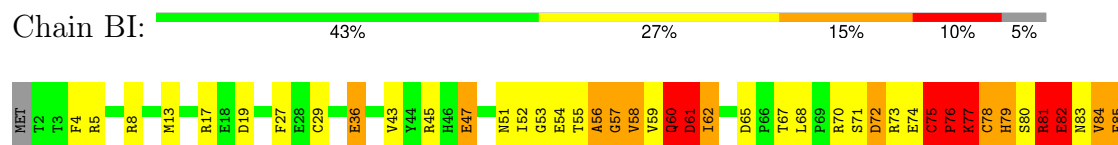
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



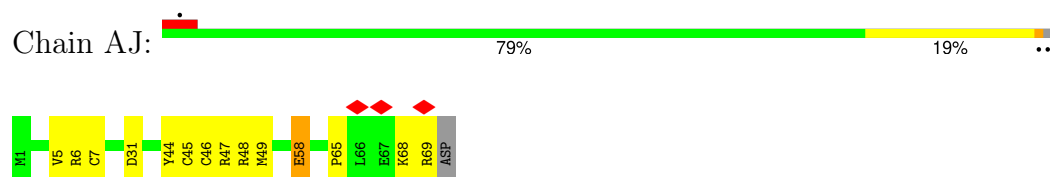
- Molecule 19: DNA-directed RNA polymerase II subunit RPB9



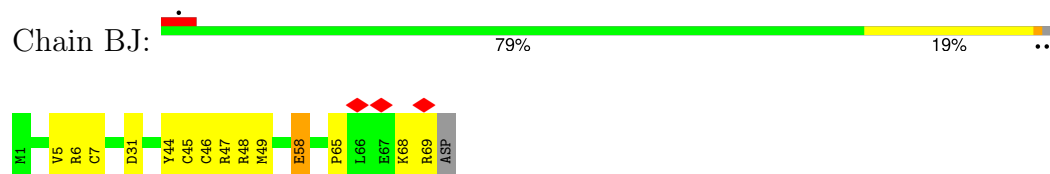
- Molecule 19: DNA-directed RNA polymerase II subunit RPB9



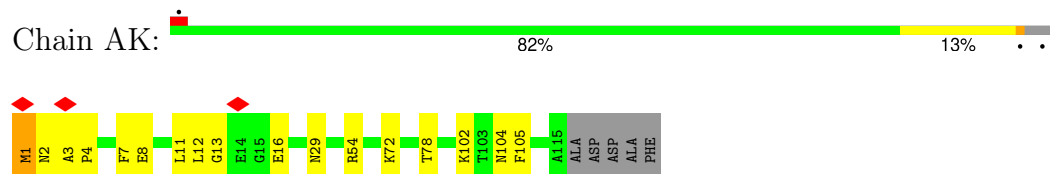
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5



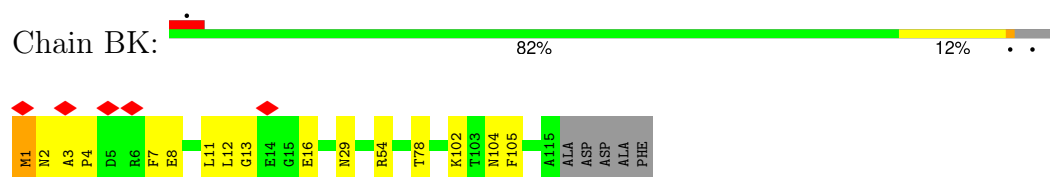
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5



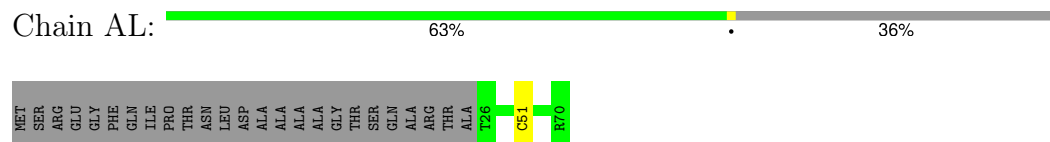
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11



- Molecule 21: DNA-directed RNA polymerase II subunit RPB11

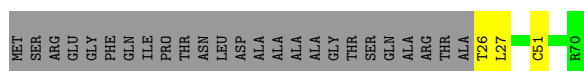


- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

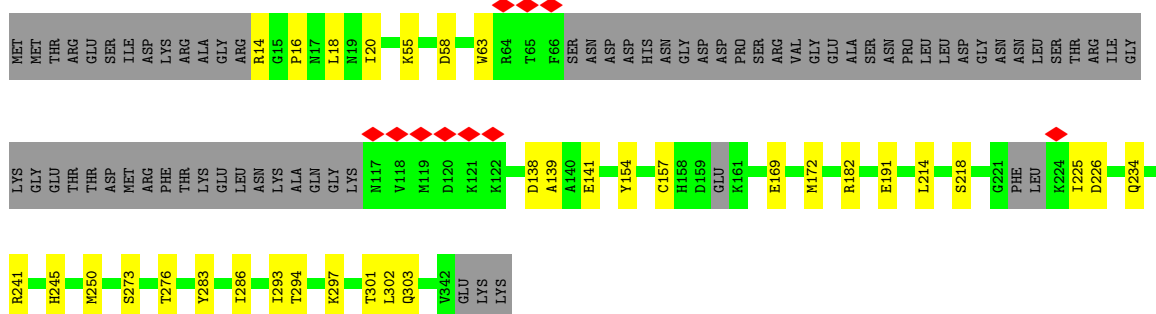


- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

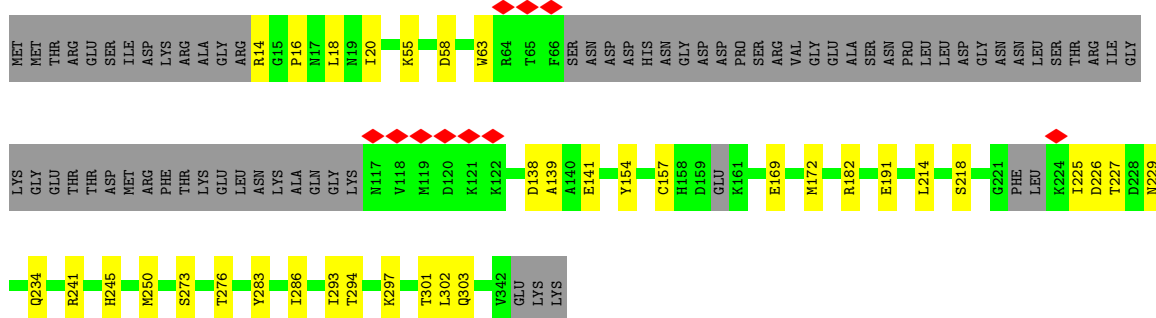




- Molecule 23: Transcription initiation factor IIB



- Molecule 23: Transcription initiation factor IIB



- Molecule 24: promoter DNA

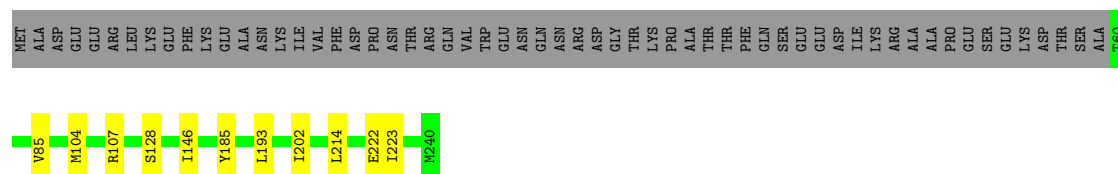


- Molecule 24: promoter DNA

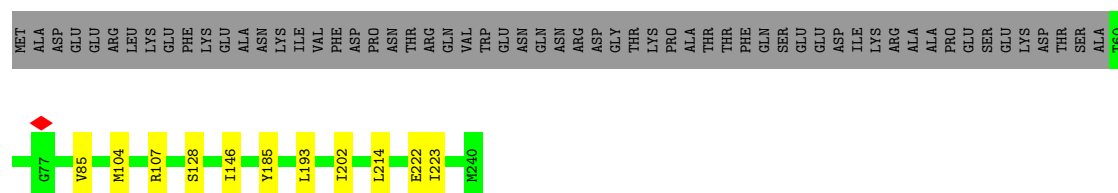


- Molecule 25: TATA-box-binding protein

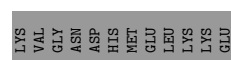
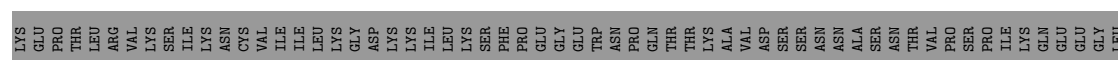
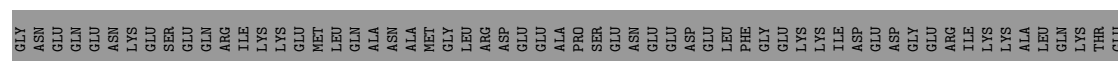
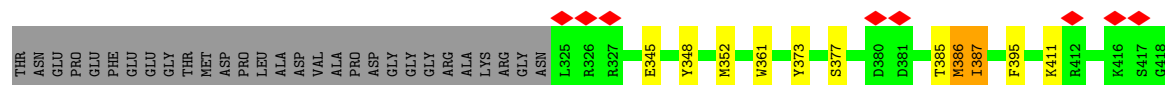
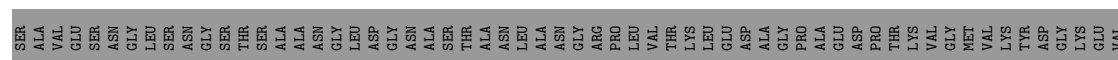
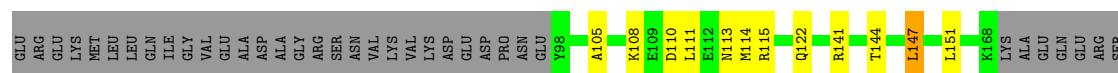
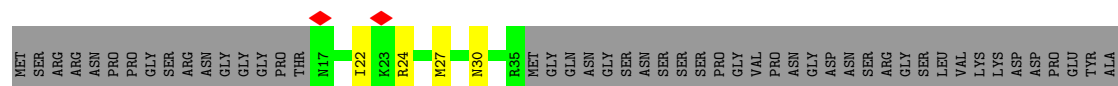




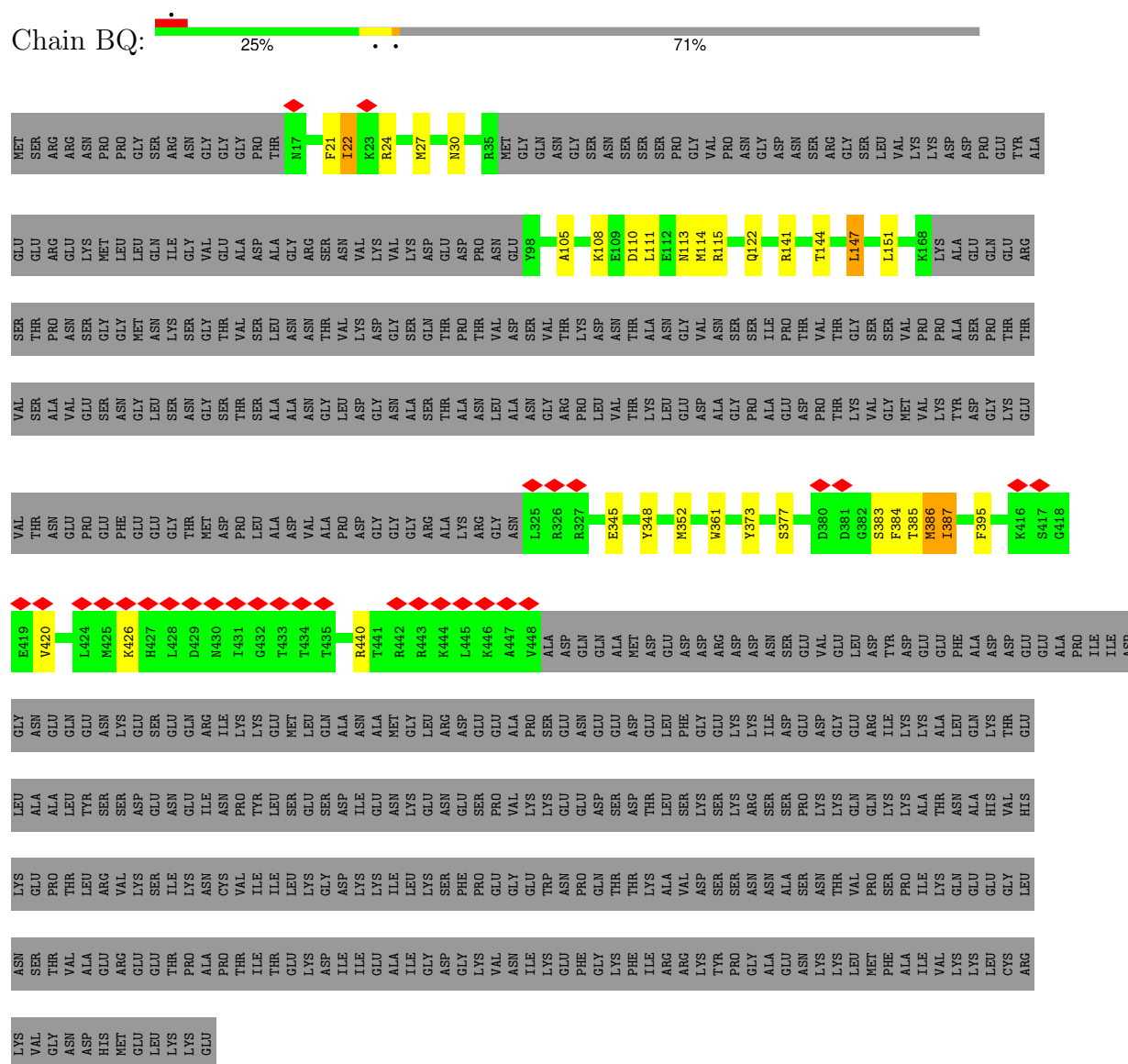
• Molecule 25: TATA-box-binding protein



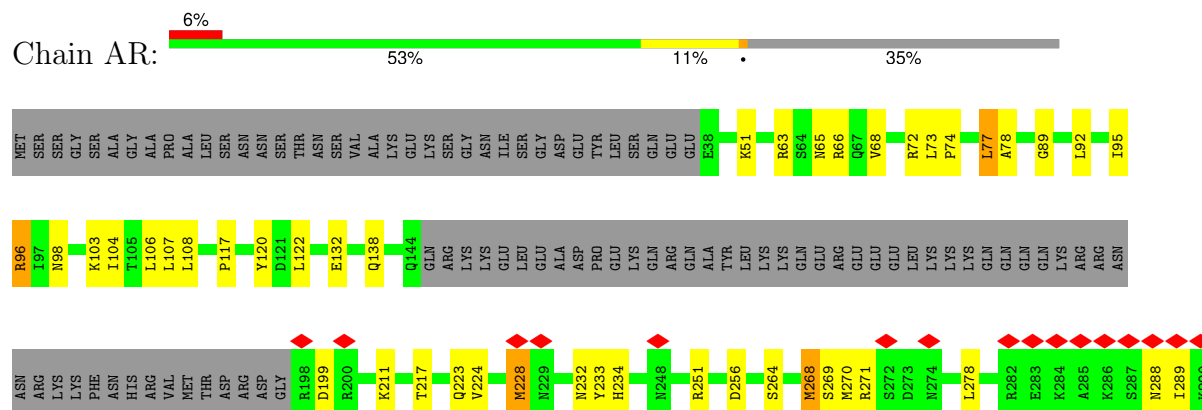
• Molecule 26: Transcription initiation factor IIF subunit alpha



• Molecule 26: Transcription initiation factor IIF subunit alpha



• Molecule 27: Transcription initiation factor IIF subunit beta



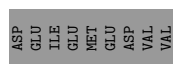
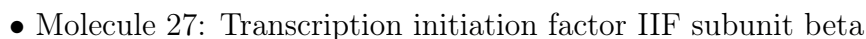
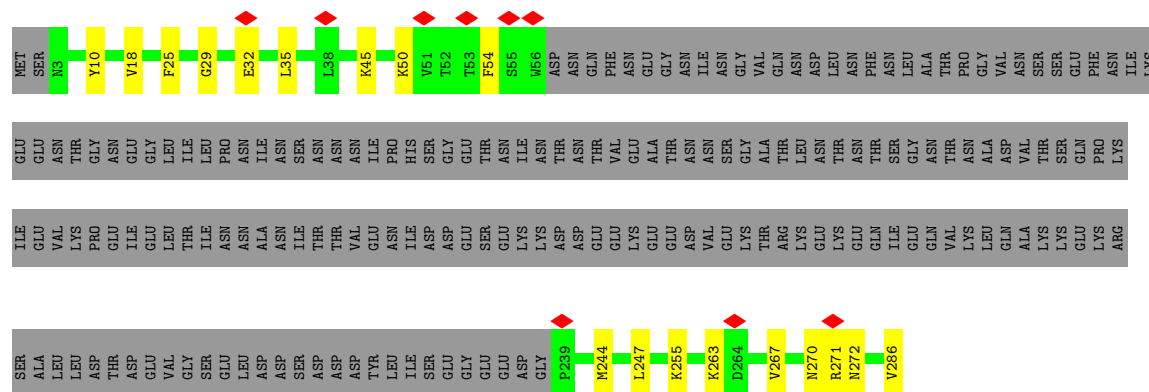
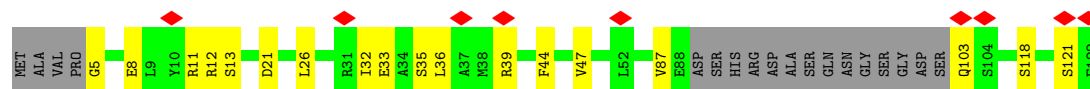


Diagram illustrating a sequence of 18 numbered blocks (R287 to S309) arranged in a row. The blocks are colored in a repeating pattern: yellow (R287, S288, A289, D290, E291, P292, L293, T294, T295, F296), green (E300, A301, C302, G303, N304, R305), and blue (F308, S309). Red diamond shapes are placed above each block. The blocks are connected by horizontal lines, with some blocks having additional lines extending from them.

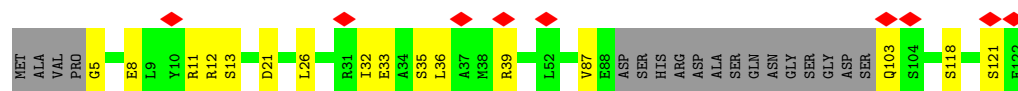
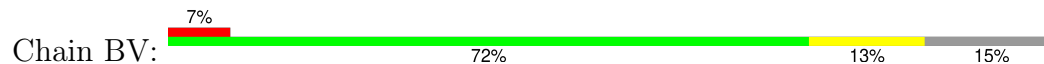
Chain BS:



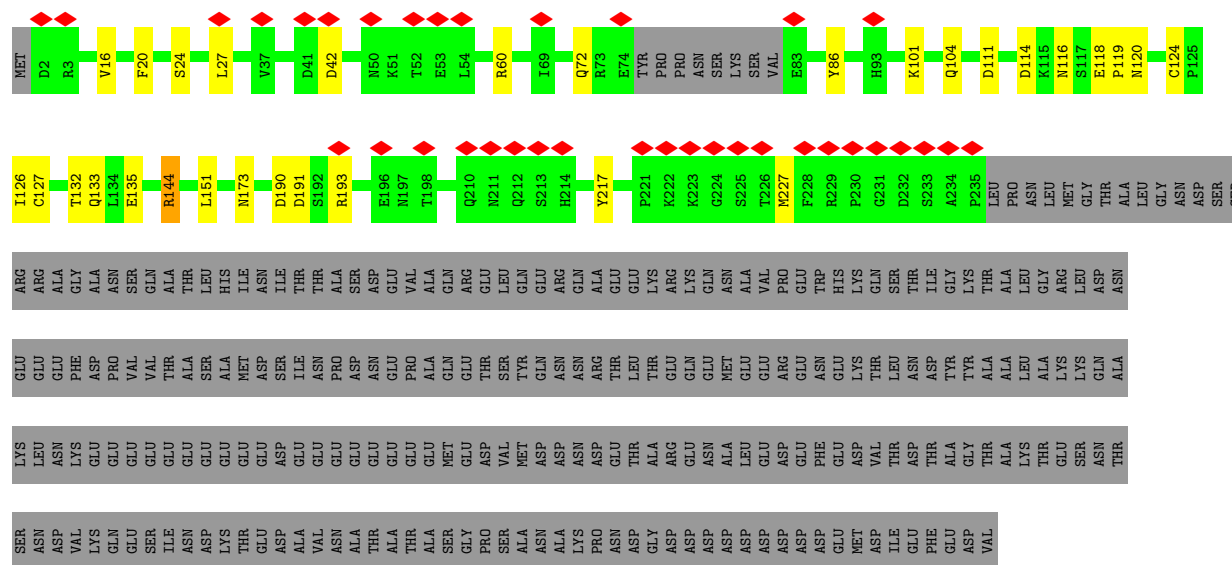
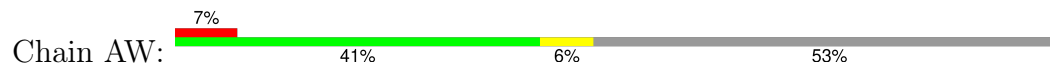
• Molecule 31: Transcription initiation factor IIA subunit 2



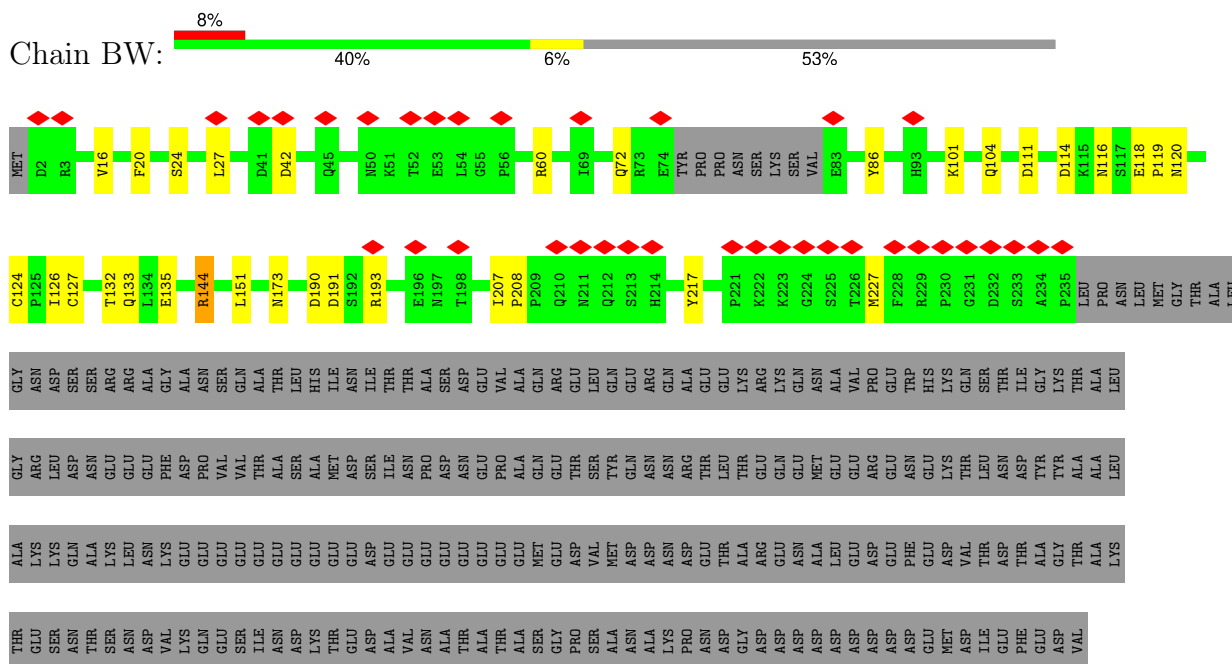
• Molecule 31: Transcription initiation factor IIA subunit 2



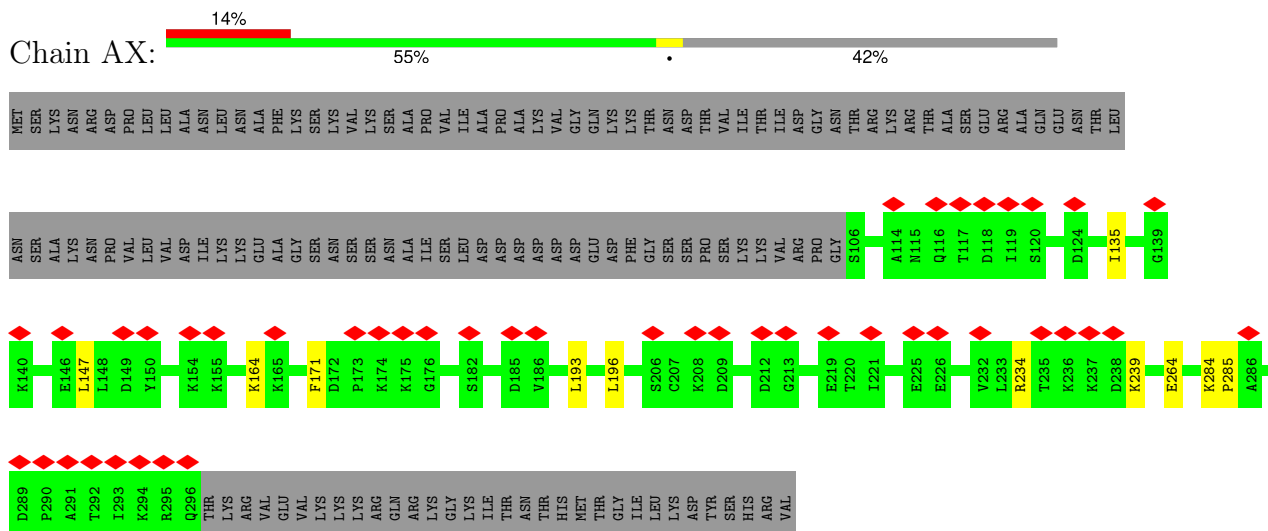
• Molecule 32: Transcription initiation factor IIE subunit alpha



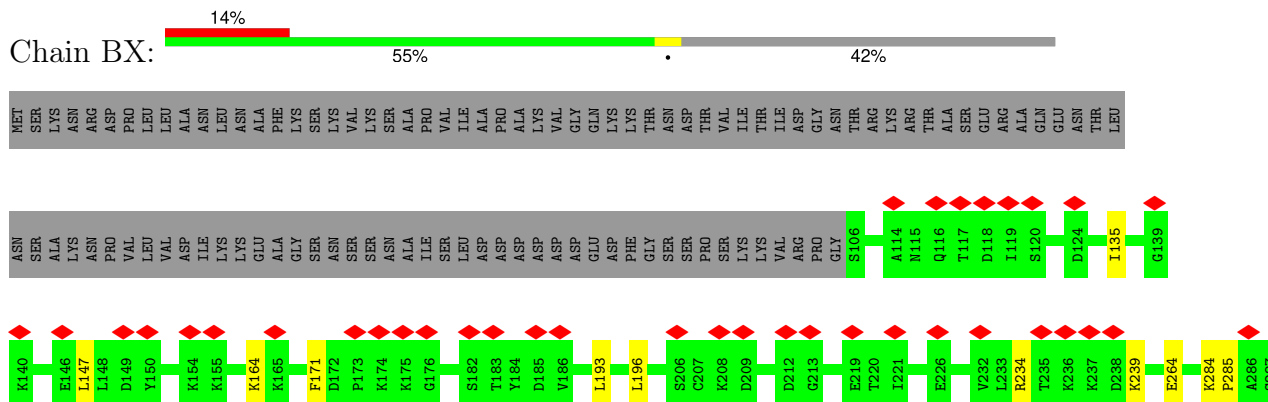
• Molecule 32: Transcription initiation factor IIE subunit alpha

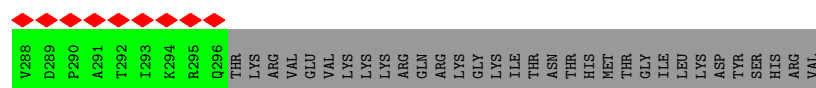


- Molecule 33: Transcription initiation factor IIE subunit beta

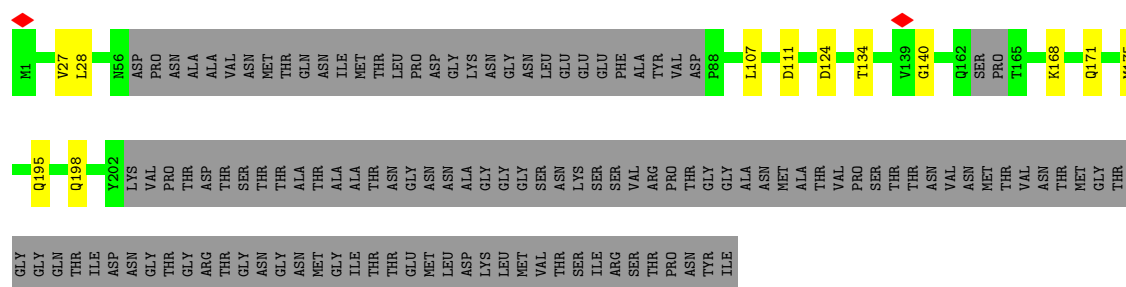


- Molecule 33: Transcription initiation factor IIE subunit beta

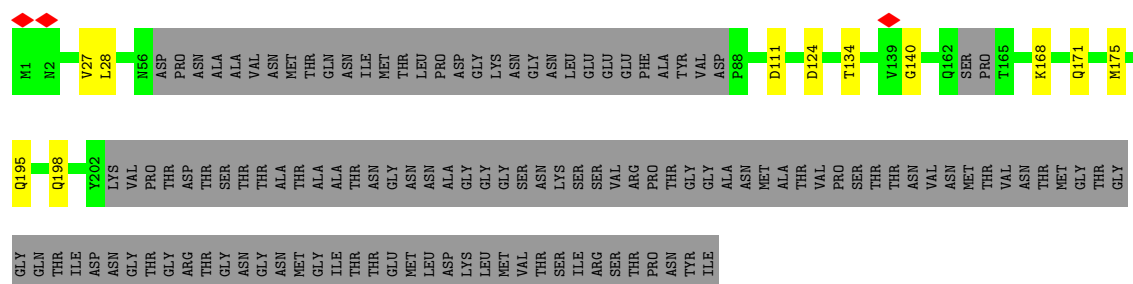




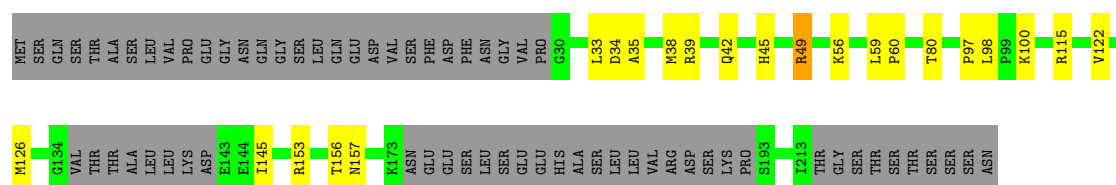
- Molecule 34: Mediator of RNA polymerase II transcription subunit 6



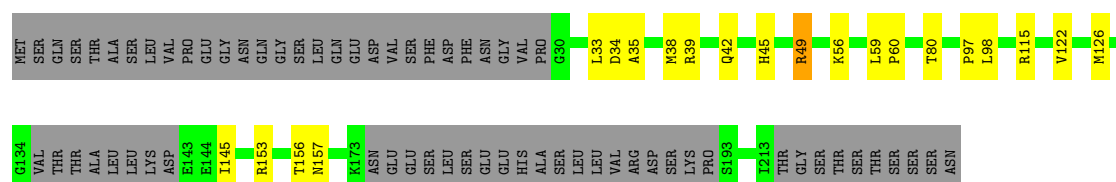
- Molecule 34: Mediator of RNA polymerase II transcription subunit 6



- Molecule 35: Mediator of RNA polymerase II transcription subunit 8



- Molecule 35: Mediator of RNA polymerase II transcription subunit 8



- Molecule 36: Mediator of RNA polymerase II transcription subunit 11

Chain Mc:  83% 10% • 6%



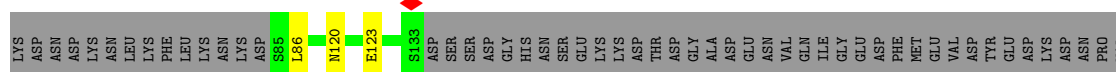
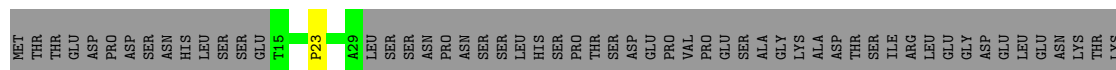
- Molecule 36: Mediator of RNA polymerase II transcription subunit 11

Chain mc:  83% 10% • 6%



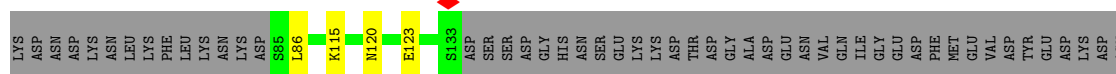
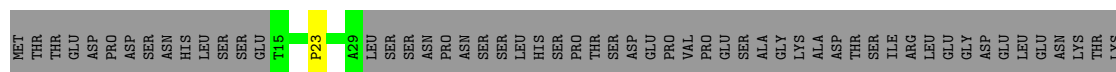
- Molecule 37: Mediator of RNA polymerase II transcription subunit 17

Chain Md:  73% 5% 22%

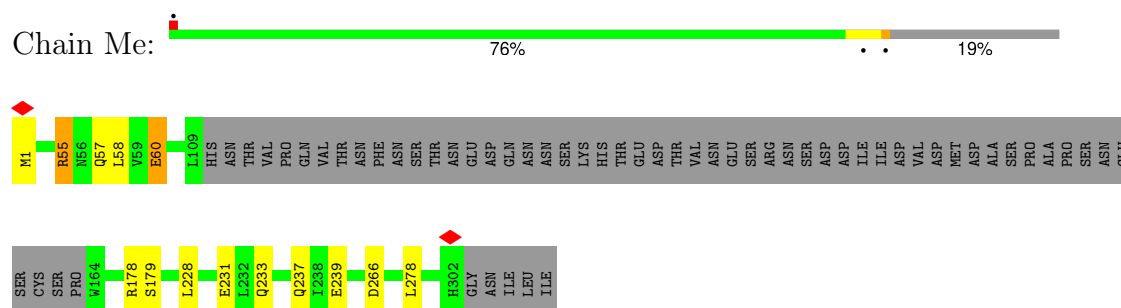


- Molecule 37: Mediator of RNA polymerase II transcription subunit 17

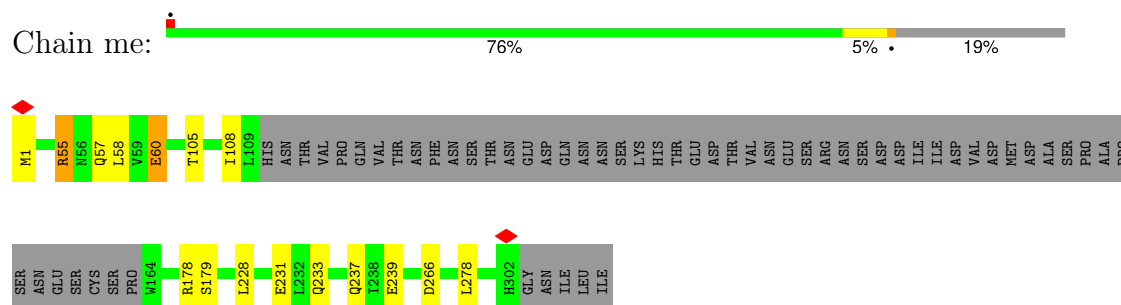
Chain md:  73% 5% 22%



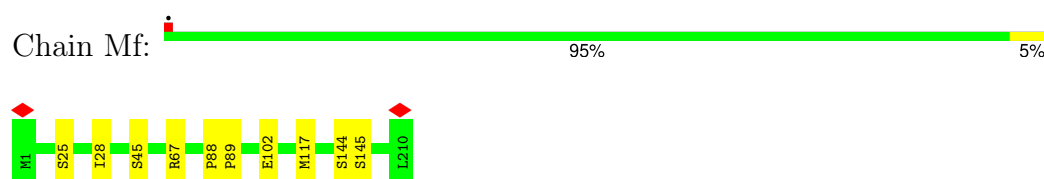
- Molecule 38: Mediator of RNA polymerase II transcription subunit 18



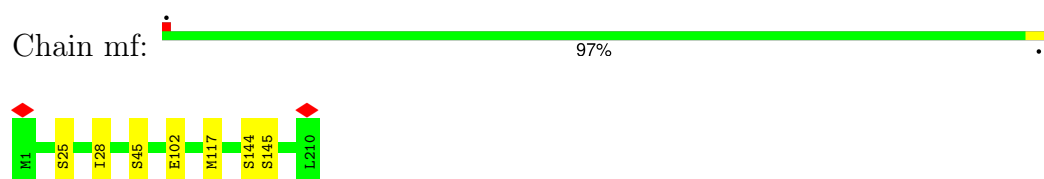
- Molecule 38: Mediator of RNA polymerase II transcription subunit 18



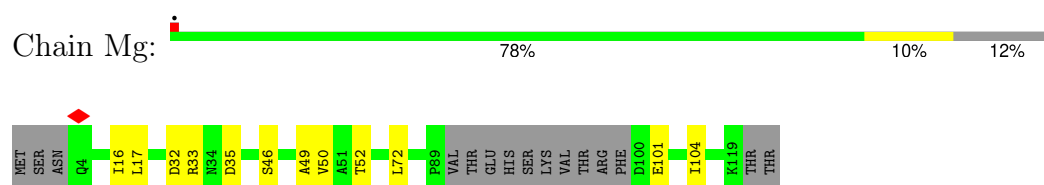
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



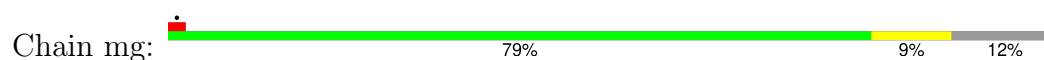
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



- Molecule 40: Mediator of RNA polymerase II transcription subunit 22



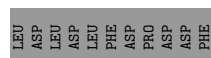
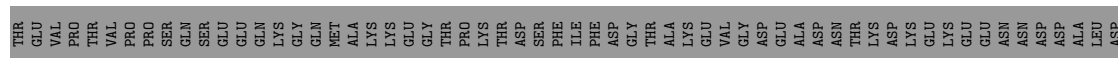
- Molecule 40: Mediator of RNA polymerase II transcription subunit 22





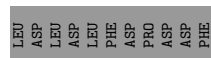
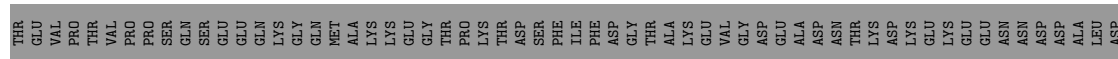
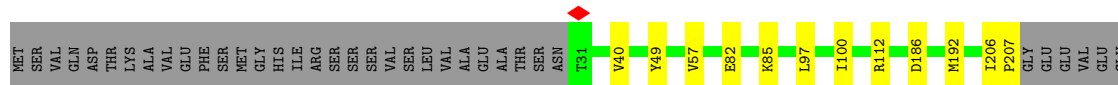
- Molecule 41: Mediator of RNA polymerase II transcription subunit 4

Chain Mh: 58% 38%



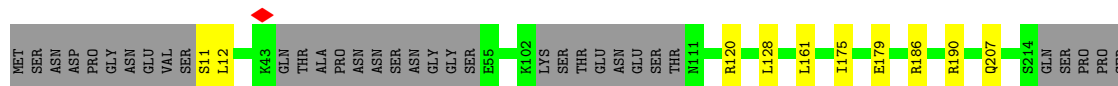
- Molecule 41: Mediator of RNA polymerase II transcription subunit 4

Chain mh: 58% 38%



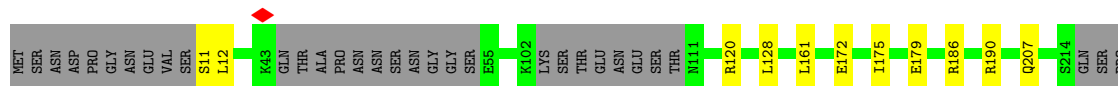
- Molecule 42: Mediator of RNA polymerase II transcription subunit 7

Chain Mi: 79% 5% 17%



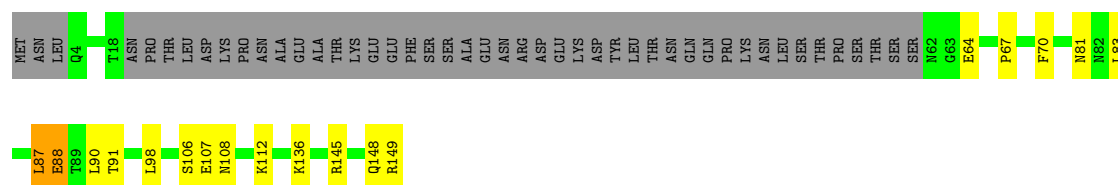
- Molecule 42: Mediator of RNA polymerase II transcription subunit 7

Chain mi: 78% 5% 17%



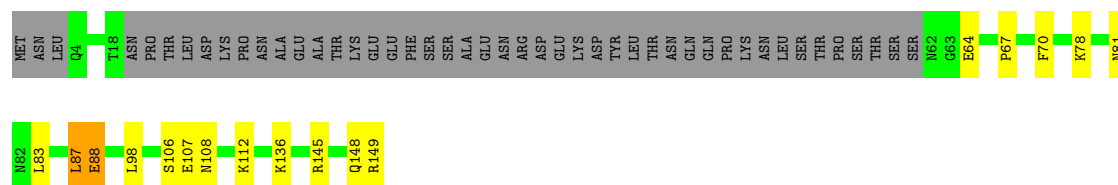
- Molecule 43: Mediator of RNA polymerase II transcription subunit 9

Chain Mj:  57% 11% 31%



- Molecule 43: Mediator of RNA polymerase II transcription subunit 9

Chain mj:  58% 10% 31%



- Molecule 44: Mediator of RNA polymerase II transcription subunit 10

Chain Mk:  5% 80% 11% 8%



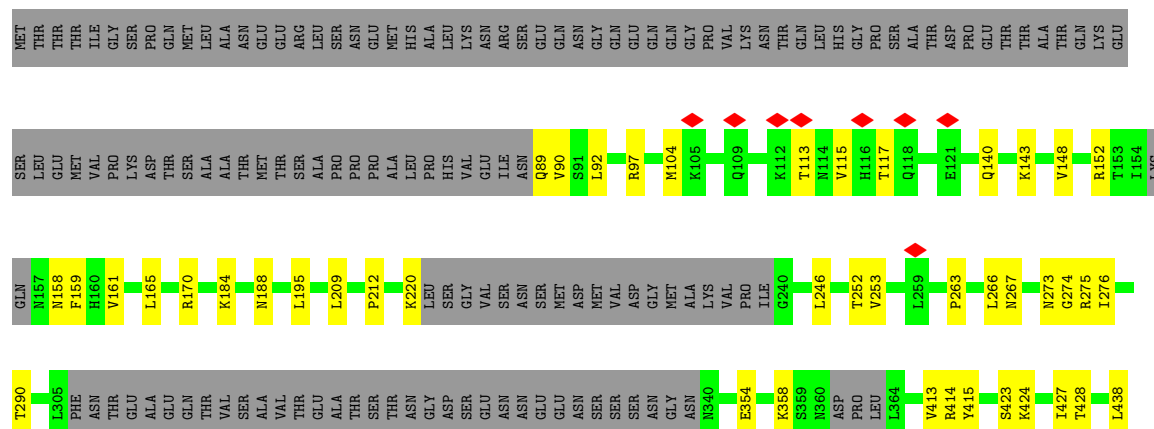
- Molecule 44: Mediator of RNA polymerase II transcription subunit 10

Chain mk:  5% 80% 11% 8%

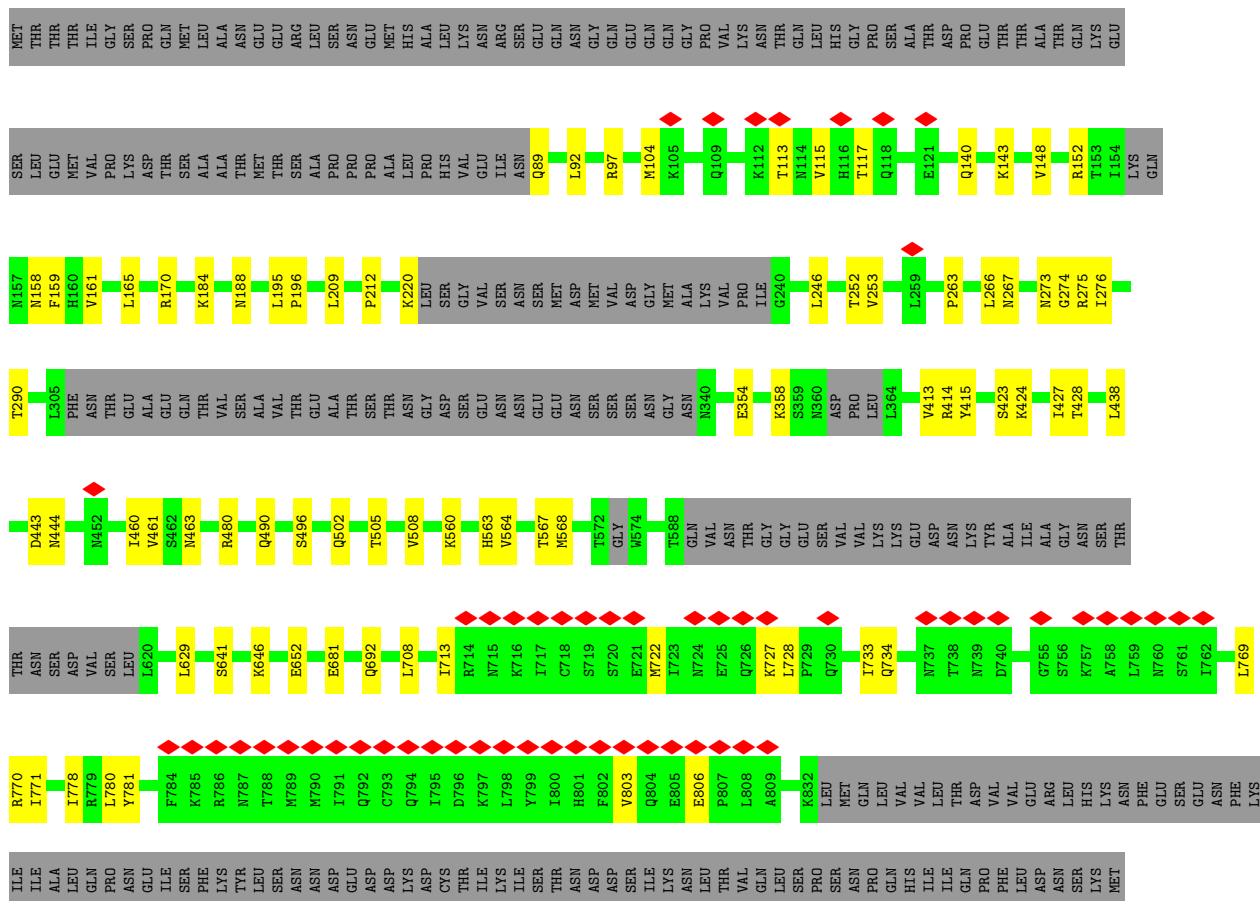


- Molecule 45: Mediator of RNA polymerase II transcription subunit 14

Chain Ml:  5% 53% 7% 40%



- Molecule 45: Mediator of RNA polymerase II transcription subunit 14



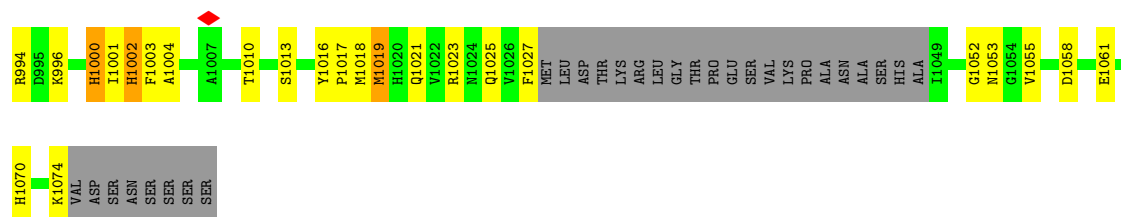
PRO	GLU	SER	VAL	LYS	PRO	ALA	ASN	ALA	SER	HIS	ALA	ILE	ARG	LEU	GLY	ASN	GLY	VAL	ALA	CYS	ASP	PRO	SER	GLU	ILE	GLU	PRO	ILE	LEU	MET	GLU	ILE	HIS	ASN	ILE	LEU	LYS	VAL	ASP	SER	ASN	SER	SER	SER	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 45: Mediator of RNA polymerase II transcription subunit 14

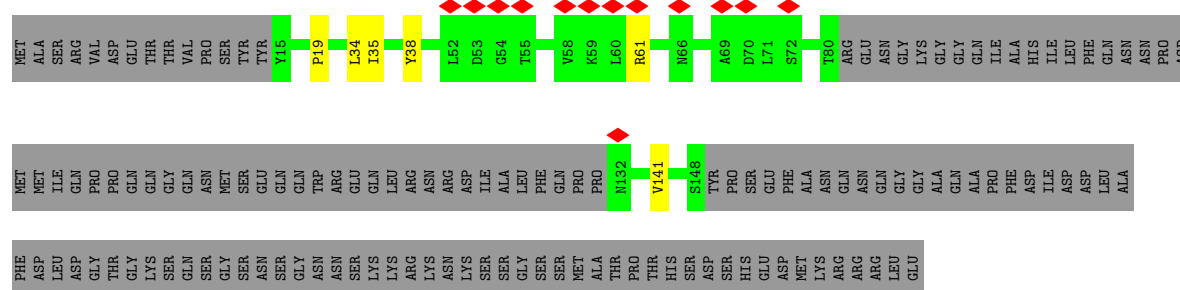


R R A A S S E E S S G G N N R R T T T T E E N N S S N N E E P P S S U U R R E E S S S S L L N N N N U U U U A A E E R R U U U U U U U U E E R R R R N N U U Y Y E E E E L L L L N N R R U U R R S S E E G G N N S S U U 34 35 40 43

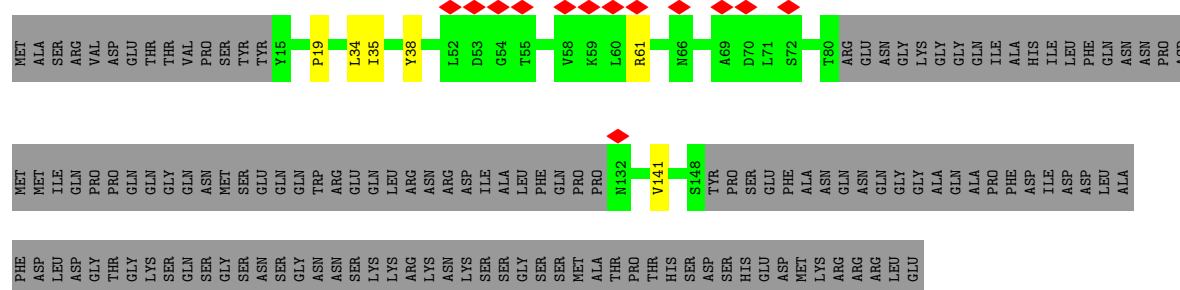




- Molecule 46: Mediator of RNA polymerase II transcription subunit 19



- Molecule 46: Mediator of RNA polymerase II transcription subunit 19



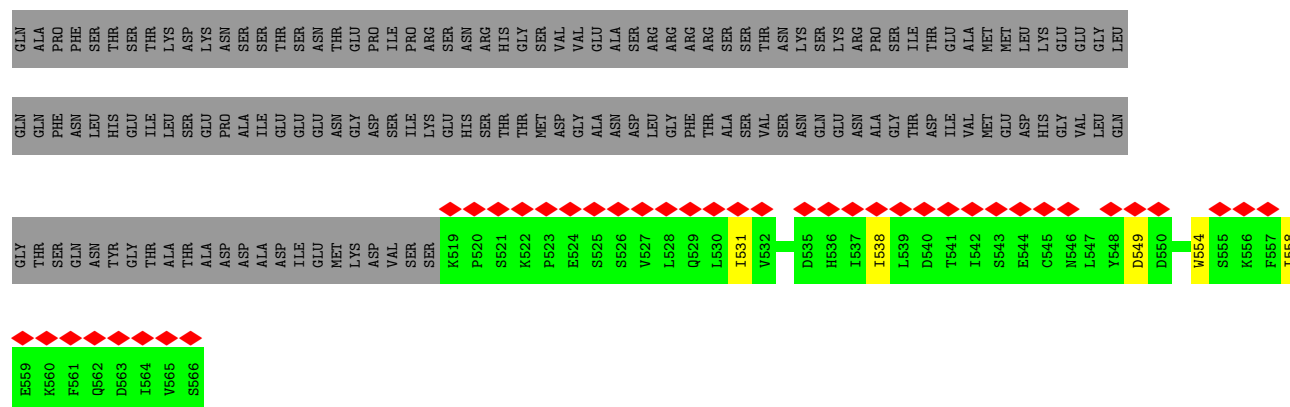
- Molecule 47: Mediator of RNA polymerase II transcription subunit 21



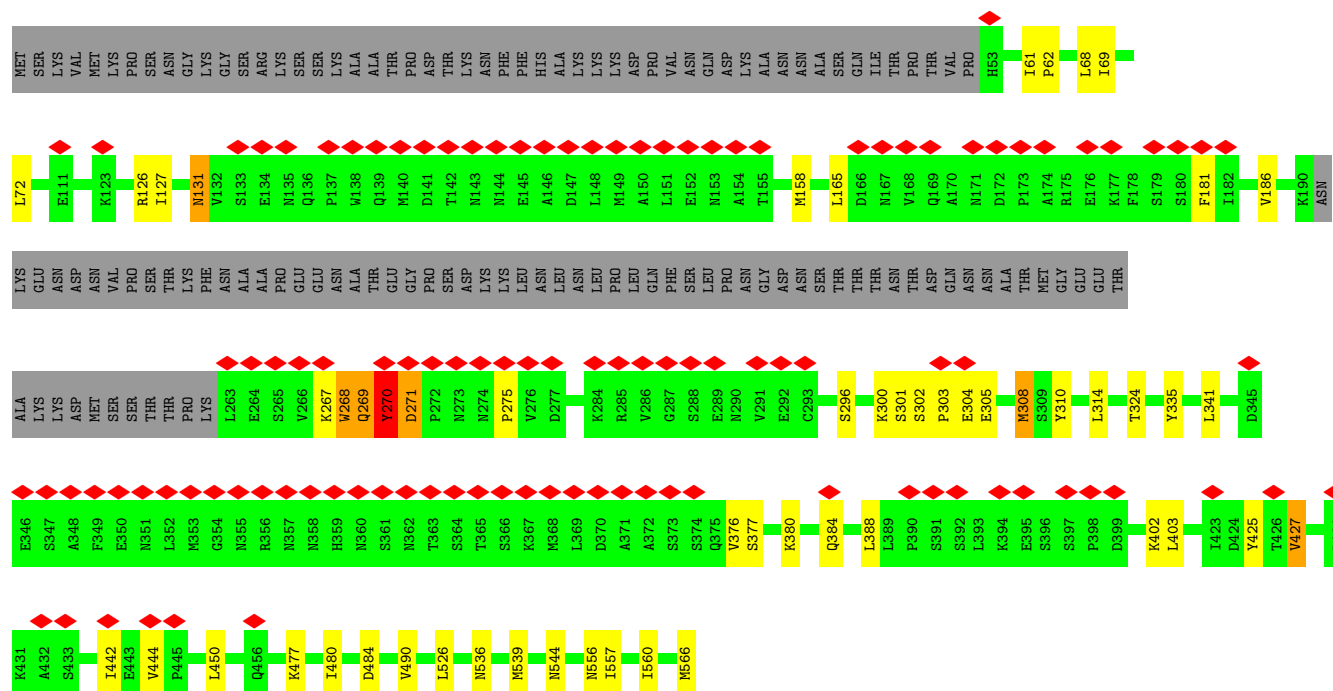
- Molecule 47: Mediator of RNA polymerase II transcription subunit 21



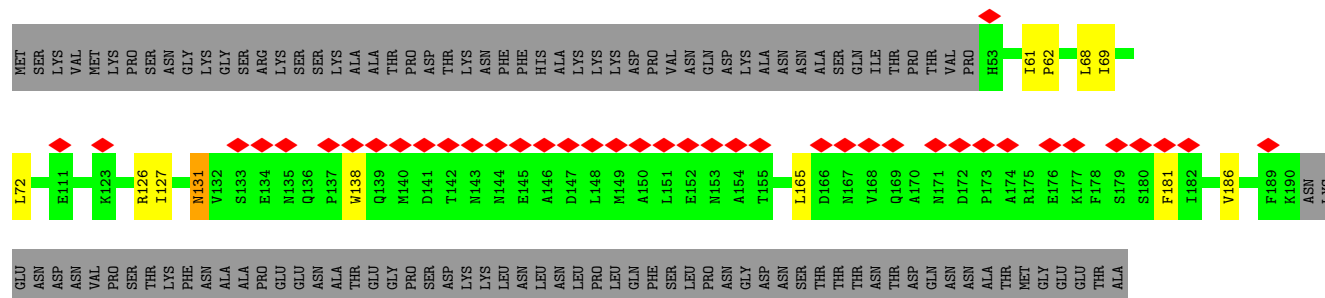
- Molecule 48: Mediator of RNA polymerase II transcription subunit 31



• Molecule 50: Transcription regulatory protein SNF12



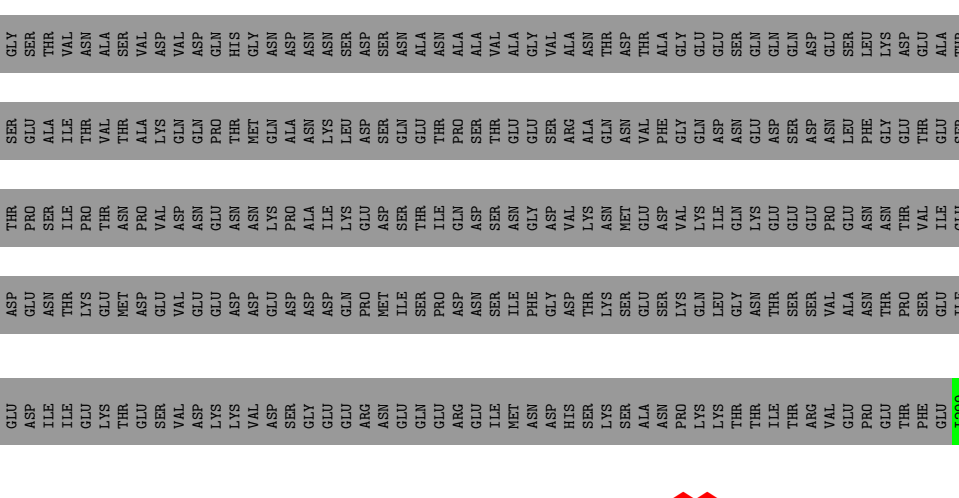
• Molecule 50: Transcription regulatory protein SNF12



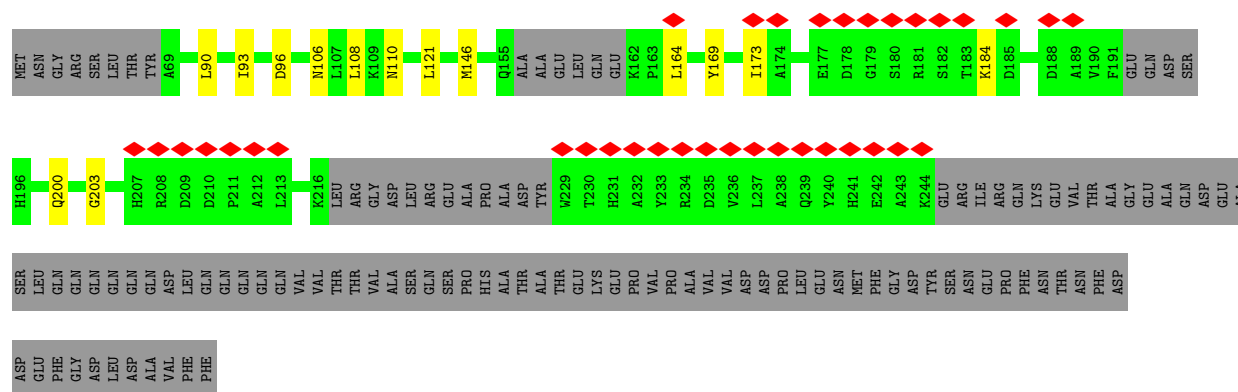


● Molecule 51: SWI/SNF complex subunit SWI3

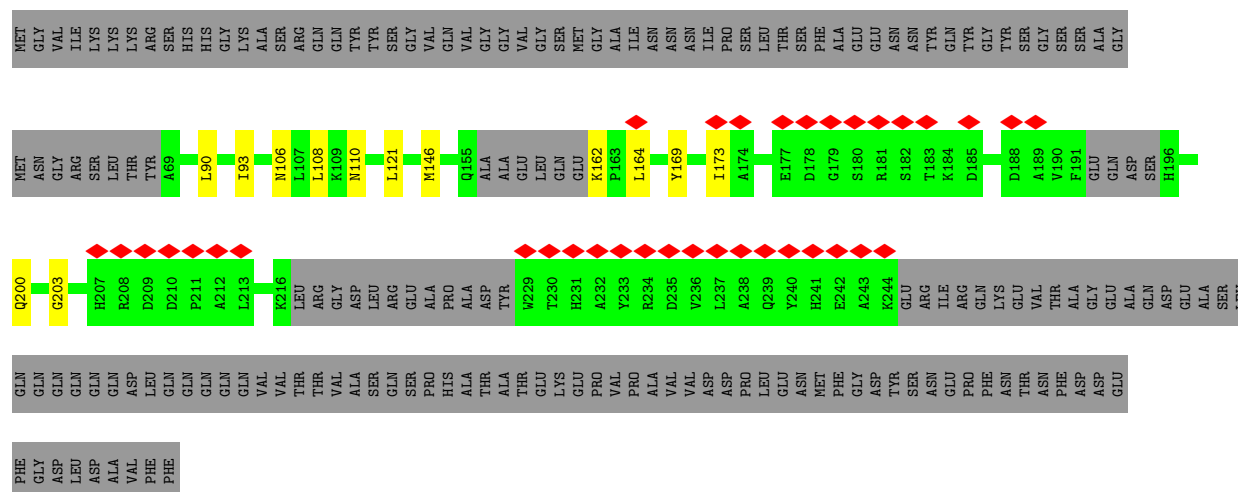
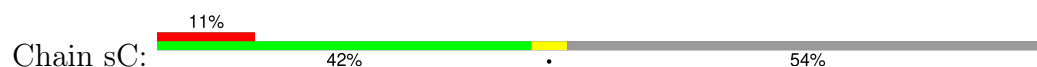
Chain sB: 



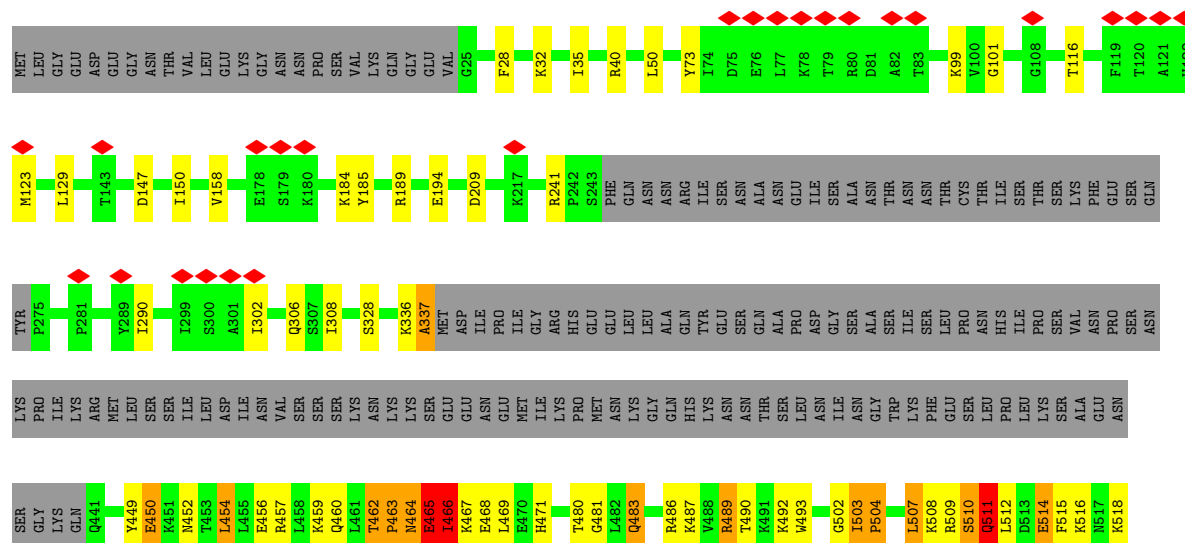
The figure displays a sequence logo for Chain sB, representing the SWI/SNF complex subunit SWI3. The logo is divided into three segments: 41% (green), 6% (yellow), and 52% (grey). The y-axis represents the conservation score, ranging from 0 to 1.0. The x-axis shows the amino acid sequence, with positions 1 to 100. The logo highlights conserved residues, with the most conserved positions (1-41) showing high conservation scores (up to 1.0) for residues like P308, N315, K318, L327, P328, E329, F330, I335, K338, Y343, M344, R347, E360, A377, R380, G389, S397, K398, L399, S431, V432, D436, M437, L440, L443, M444, S447, D448, L453, T468, and G579. The 6% segment (positions 42-47) shows lower conservation, and the 52% segment (positions 48-100) shows the highest conservation, with residues like P513, L514, K515, L566, Q567, G579, and P606 being highly conserved.



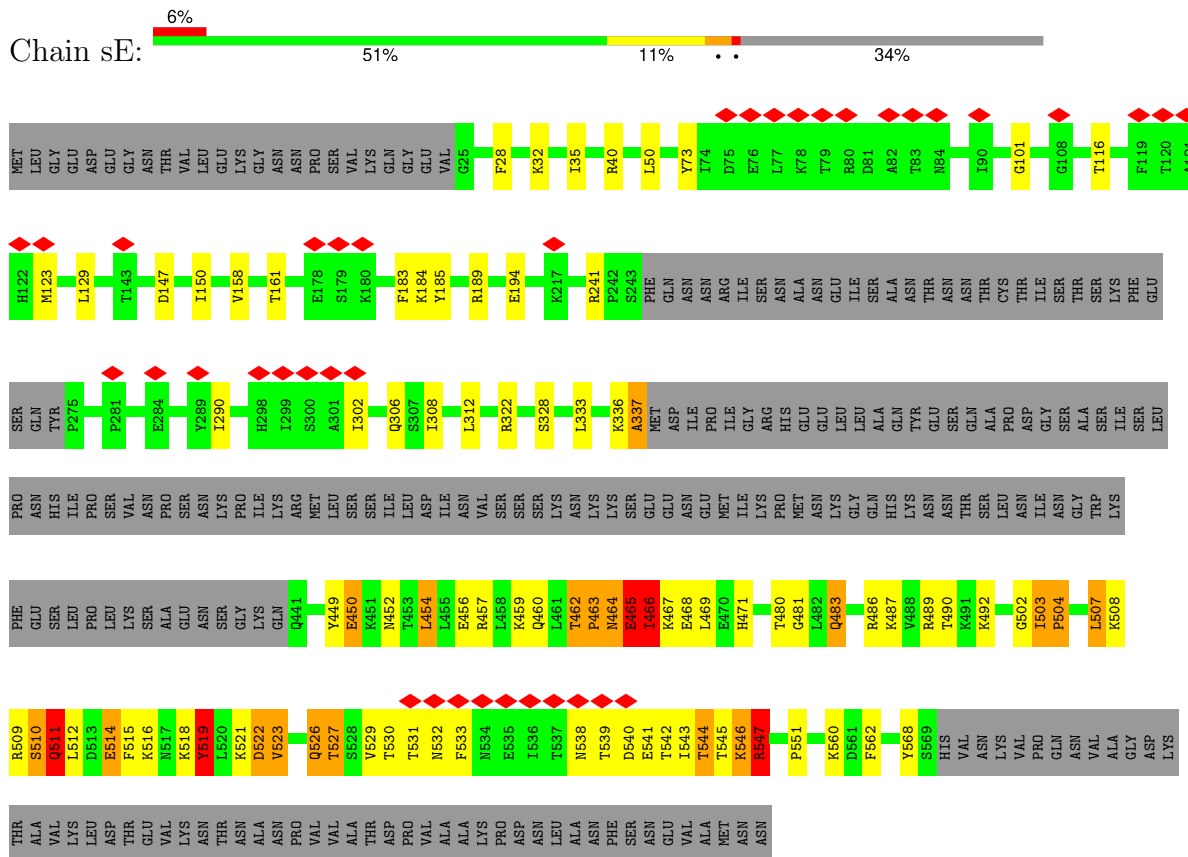
• Molecule 52: Transcription regulatory protein SNF6



• Molecule 53: SWI/SNF global transcription activator complex subunit SWP82



- Molecule 53: SWI/SNF global transcription activator complex subunit SWP82



- Molecule 54: unsigned peptide of SWISNF

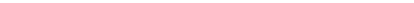


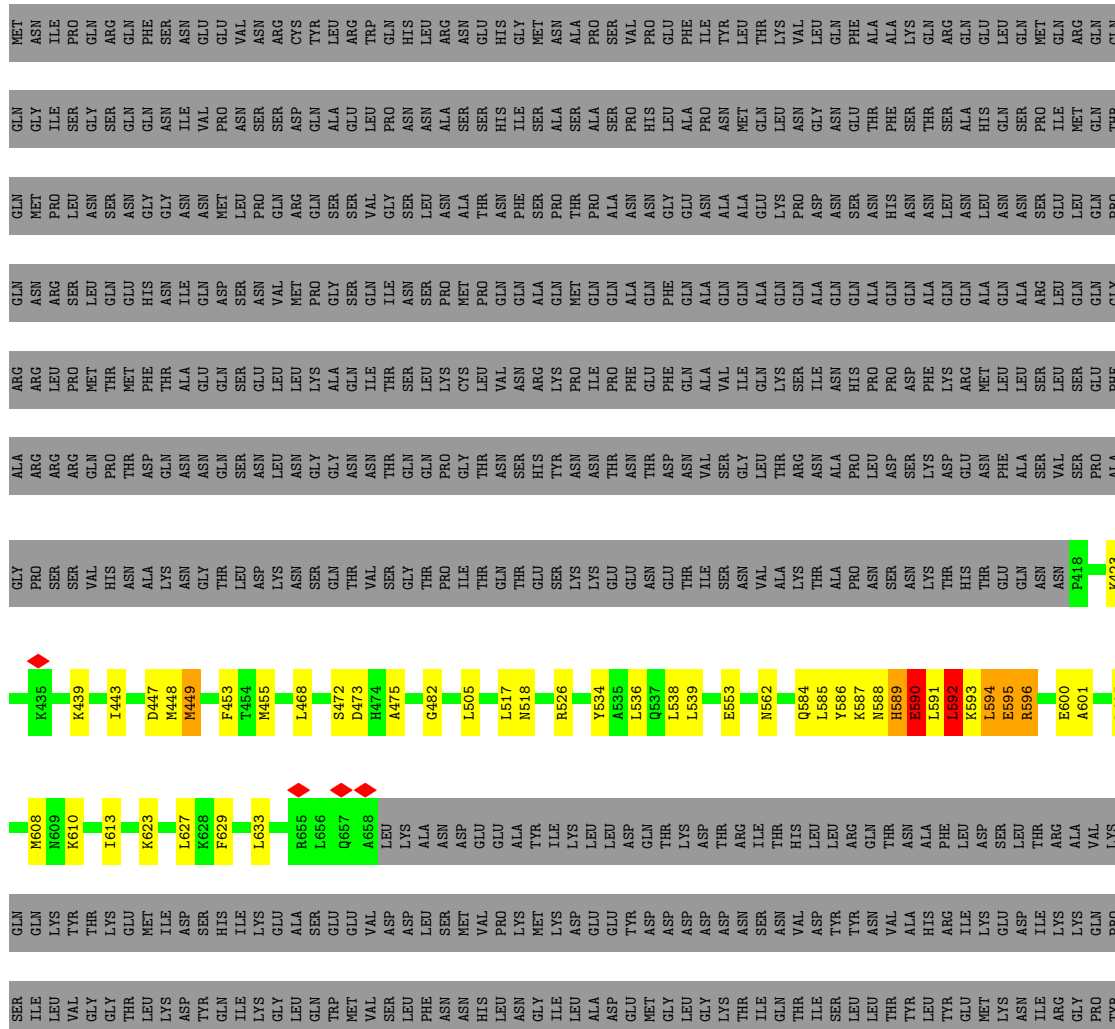
- Molecule 55: Transcription regulatory protein SNF2



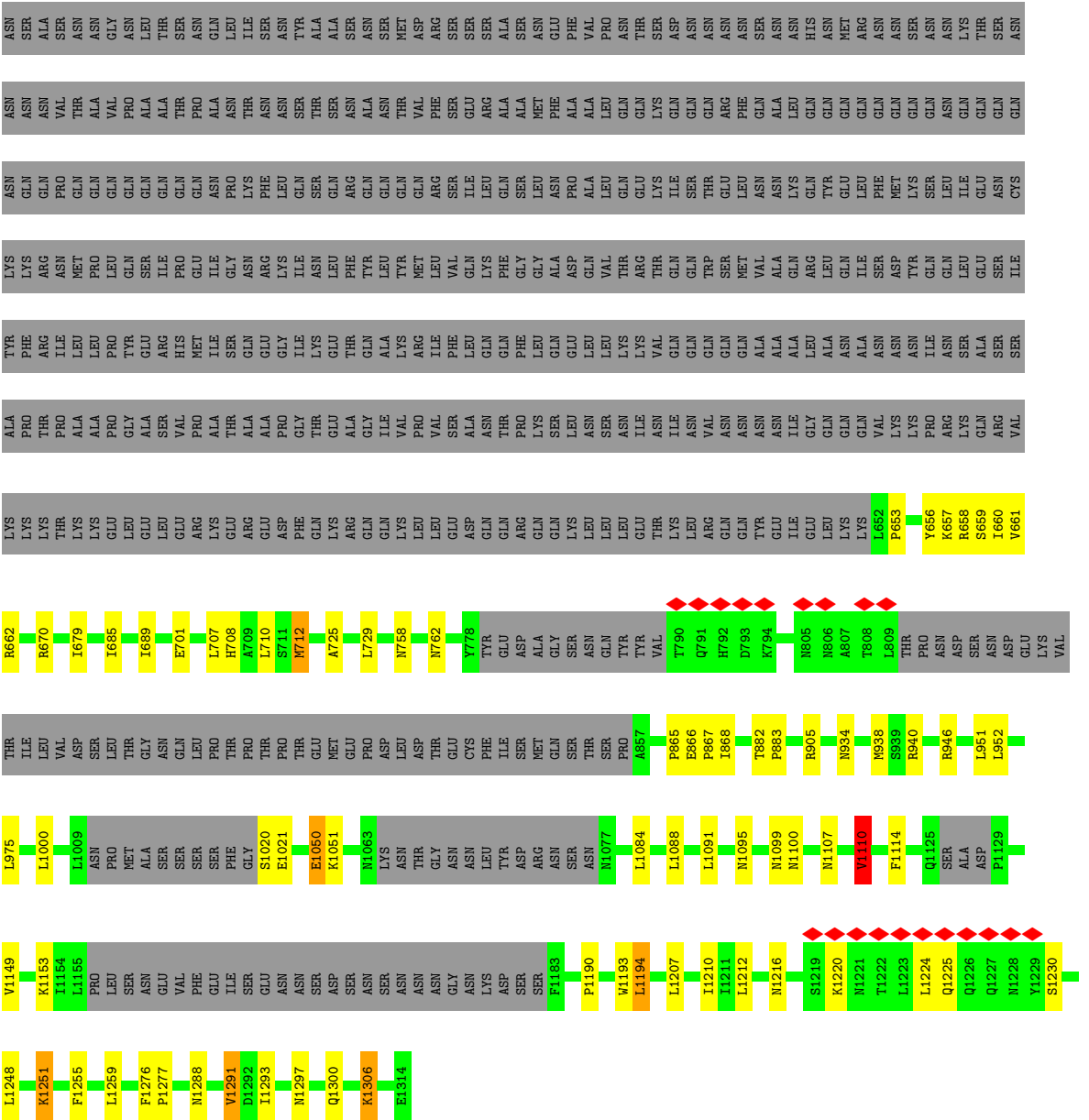


- Molecule 55: Transcription regulatory protein SNF2

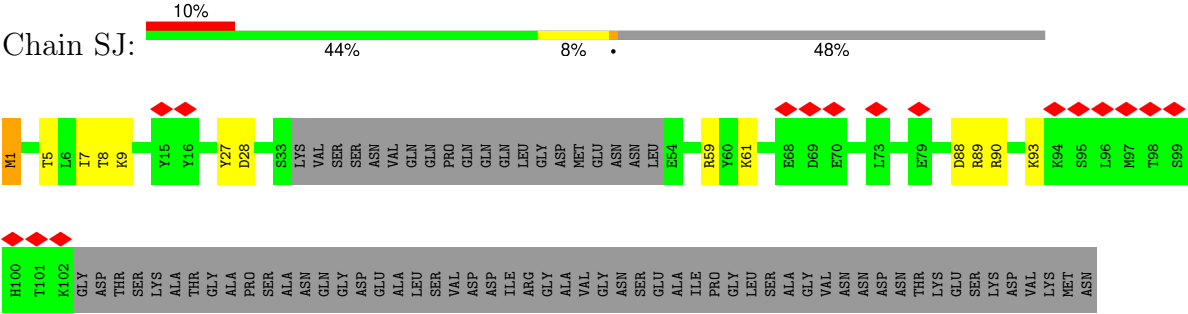
Chain sH:  11% 1% 86%







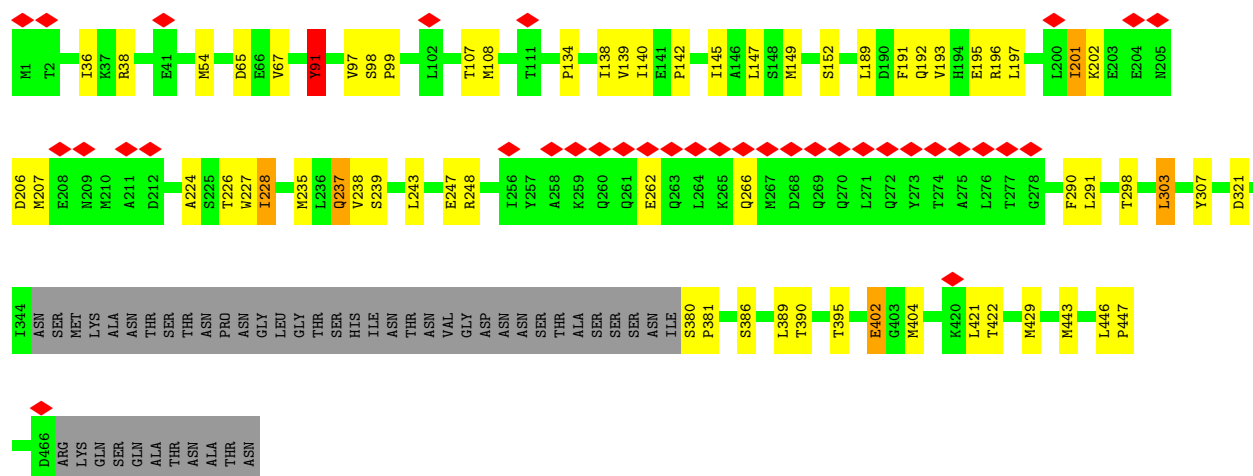
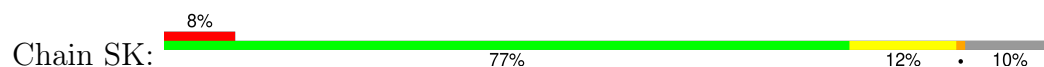
• Molecule 57: Regulator of Ty1 transposition protein 102



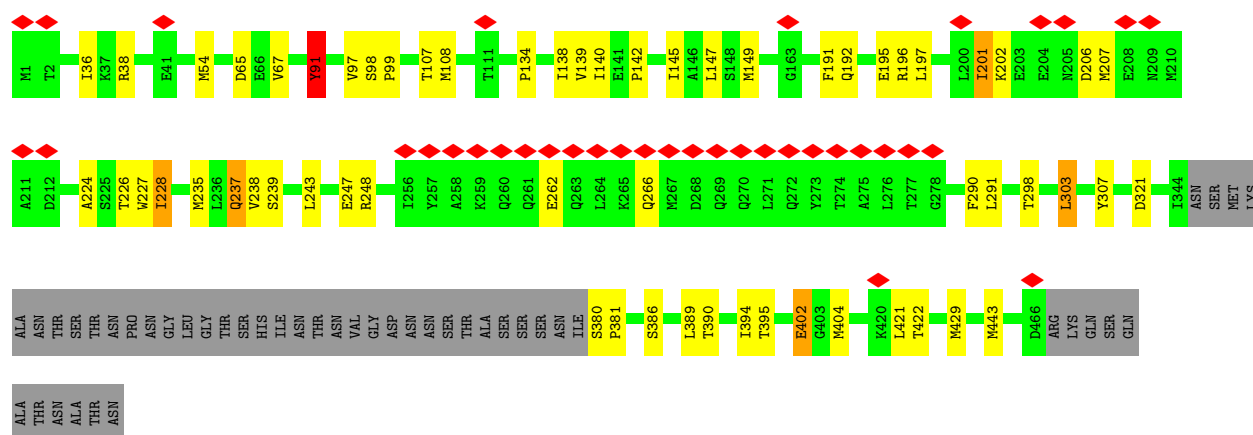
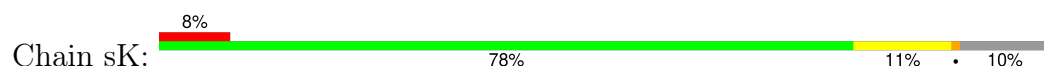
• Molecule 57: Regulator of Ty1 transposition protein 102



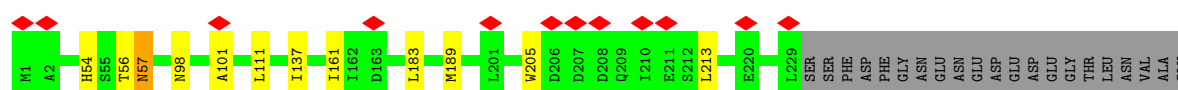
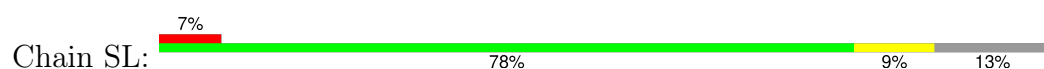
- Molecule 58: Actin-related protein 7

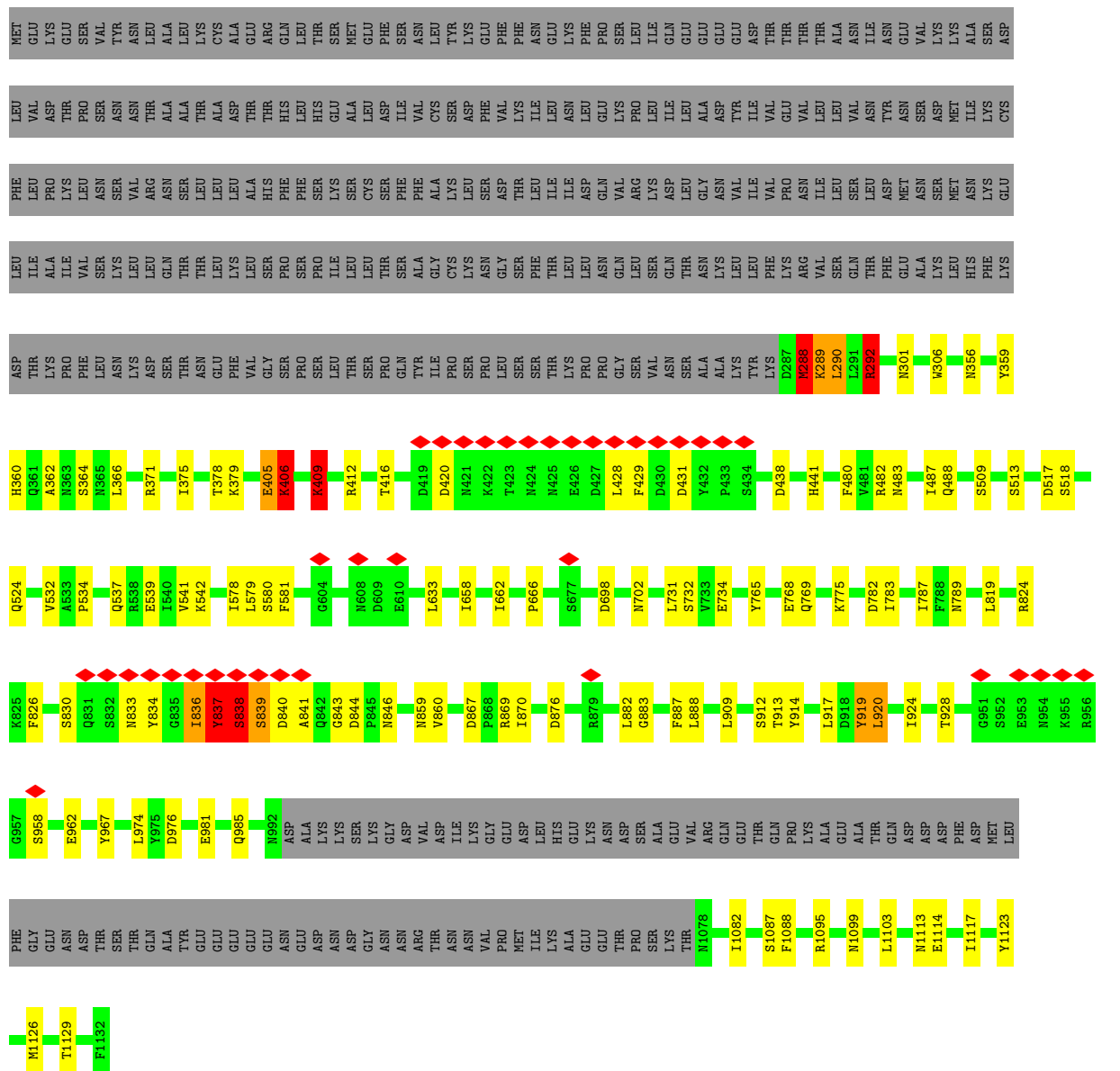


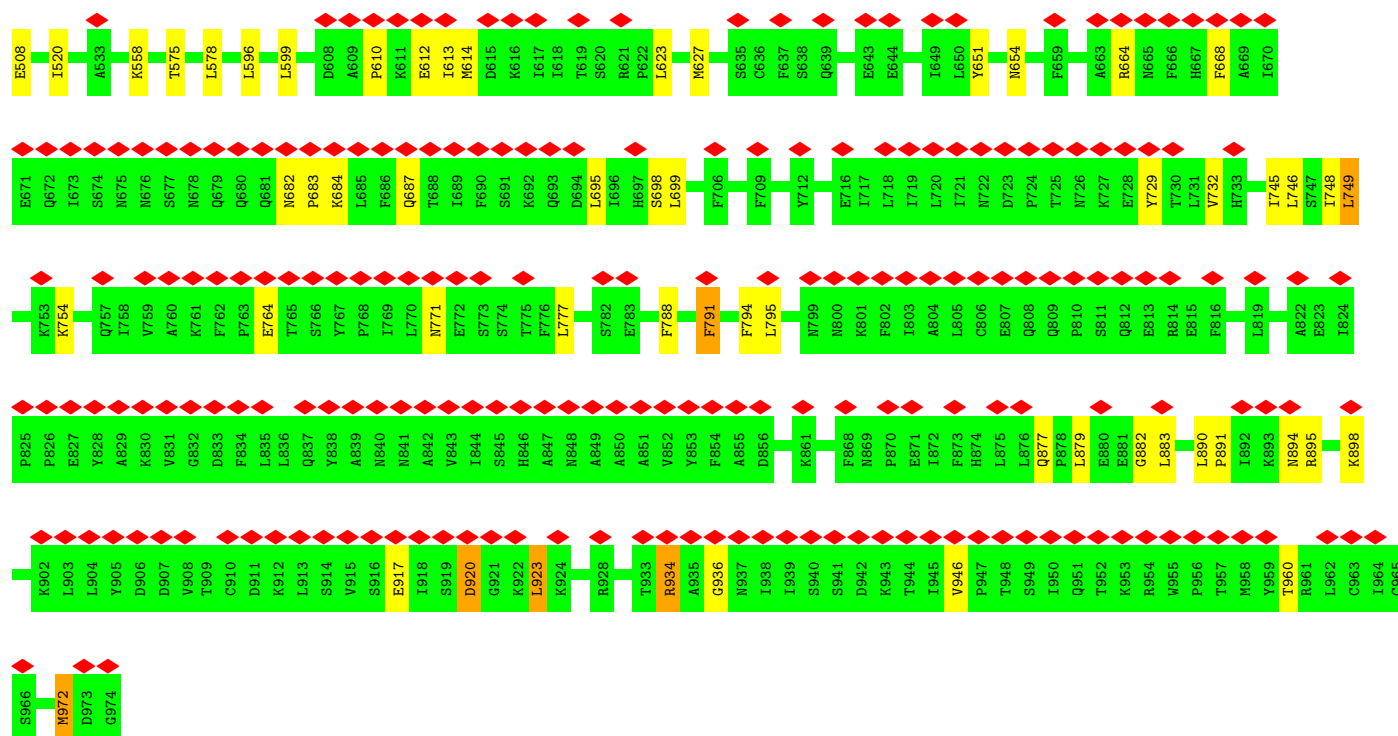
- Molecule 58: Actin-related protein 7



- Molecule 59: Actin-like protein ARP9

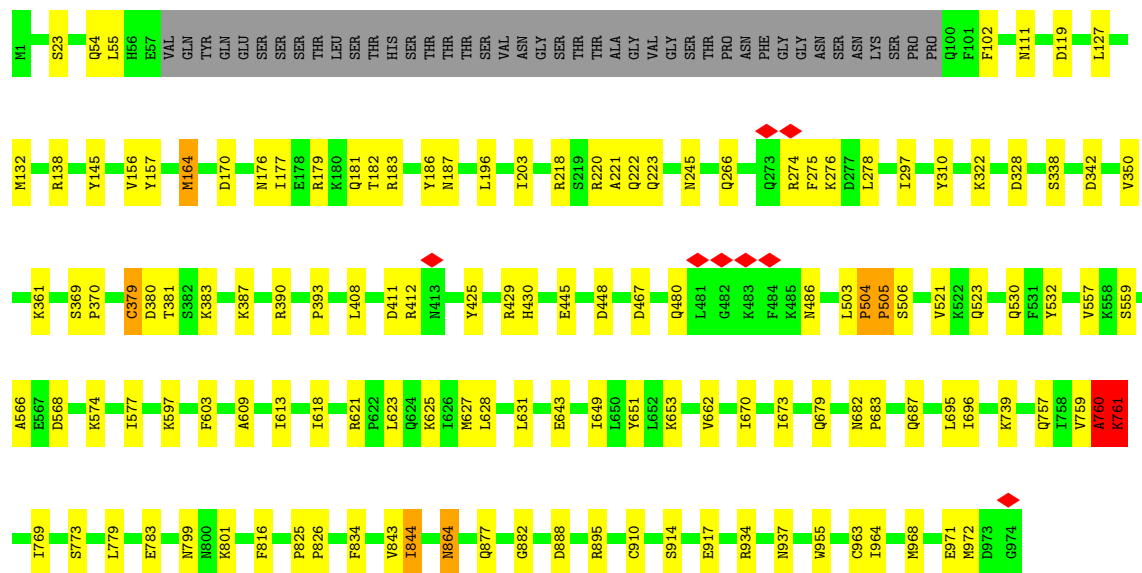






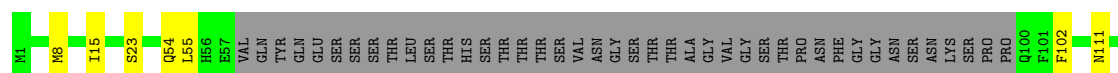
• Molecule 61: Mediator of RNA polymerase II transcription subunit 16

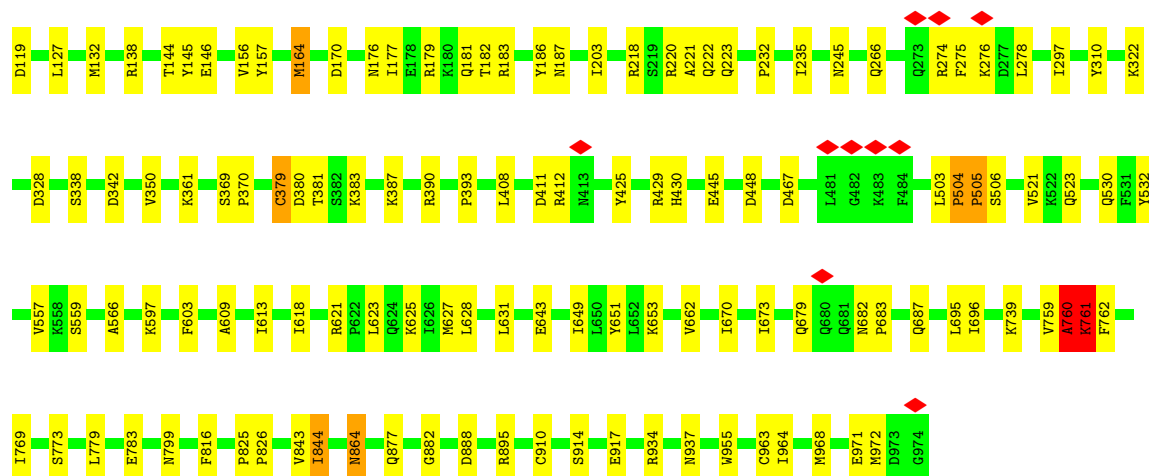
Chain T6: 82% 13% . .



• Molecule 61: Mediator of RNA polymerase II transcription subunit 16

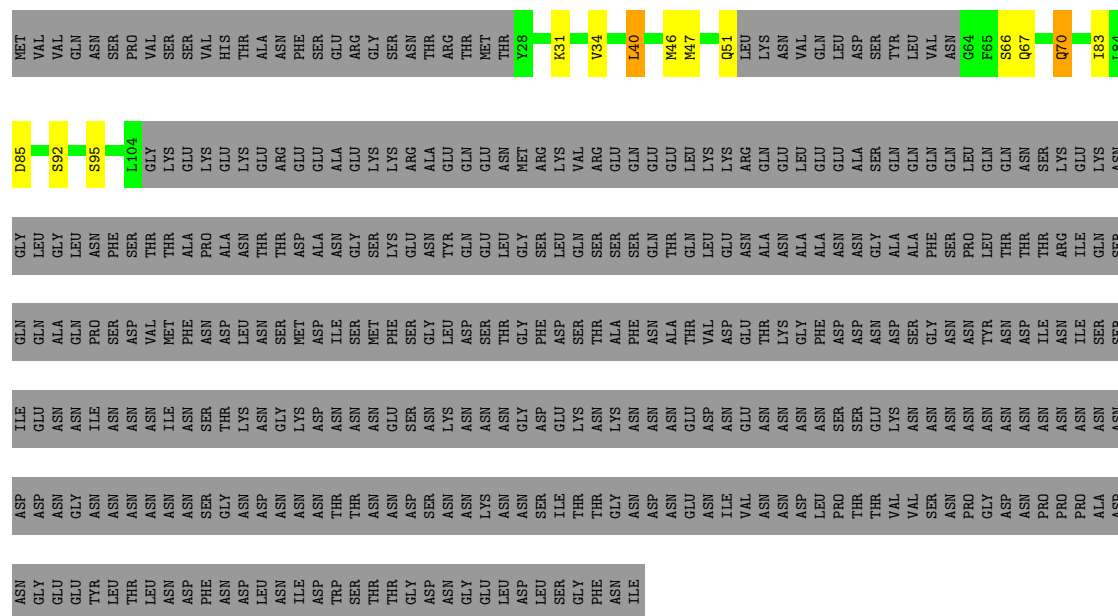
Chain t6: 82% 13% . .





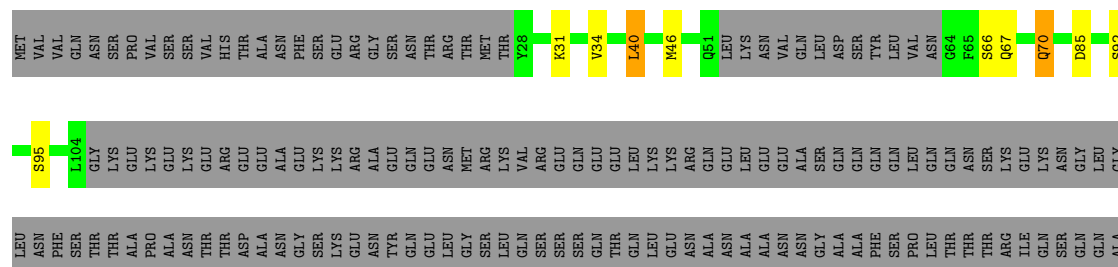
• Molecule 62: Mediator of RNA polymerase II transcription subunit 2

Chain T1: 12% . 85%



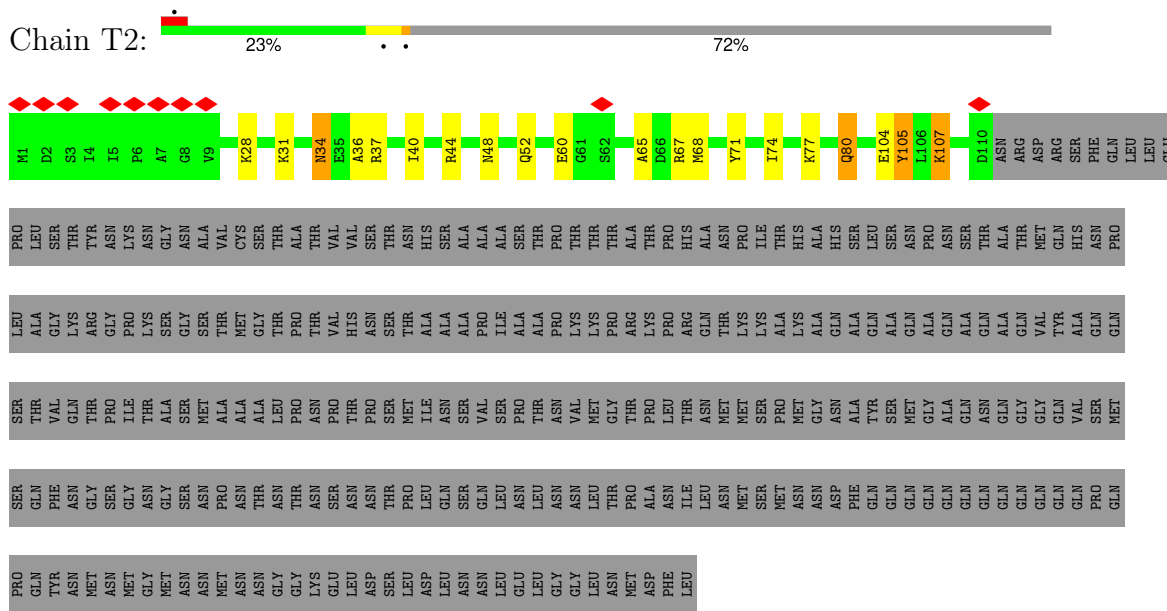
• Molecule 62: Mediator of RNA polymerase II transcription subunit 2

Chain t1: 13% . 85%

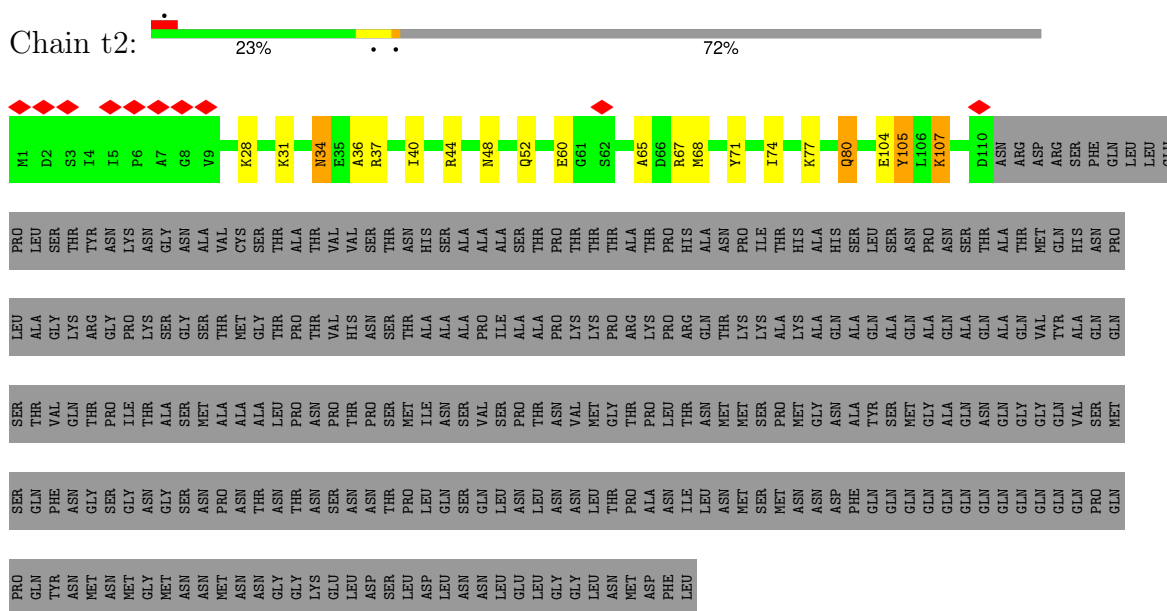


[illegible]

- Molecule 63: Mediator of RNA polymerase II transcription subunit 3



- Molecule 63: Mediator of RNA polymerase II transcription subunit 3



- Molecule 64: Mediator of RNA polymerase II transcription subunit 15





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3090211	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.713	Depositor
Minimum map value	0.000	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.336	Depositor
Map size (Å)	896.0, 896.0, 896.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A0	0.52	10/6209 (0.2%)	0.63	6/8384 (0.1%)
1	B0	0.52	10/6209 (0.2%)	0.63	6/8384 (0.1%)
2	A1	0.35	2/3426 (0.1%)	0.63	5/4613 (0.1%)
2	B1	0.35	2/3426 (0.1%)	0.64	5/4613 (0.1%)
3	A2	0.76	20/3664 (0.5%)	1.51	37/4952 (0.7%)
3	B2	0.76	20/3664 (0.5%)	1.51	37/4952 (0.7%)
4	A3	0.86	6/1109 (0.5%)	1.30	13/1492 (0.9%)
4	B3	0.86	6/1109 (0.5%)	1.30	13/1492 (0.9%)
5	A4	0.31	1/2312 (0.0%)	0.58	0/3127
5	B4	0.32	1/2312 (0.0%)	0.58	0/3127
6	A5	1.29	9/520 (1.7%)	2.38	15/701 (2.1%)
6	B5	1.29	9/520 (1.7%)	2.38	15/701 (2.1%)
7	A6	0.43	4/3007 (0.1%)	0.60	0/4066
7	B6	0.43	4/3007 (0.1%)	0.60	0/4066
8	A7	0.43	5/4985 (0.1%)	0.67	2/6745 (0.0%)
8	B7	0.43	5/4985 (0.1%)	0.67	2/6745 (0.0%)
9	A8	0.72	0/137	1.19	0/185
9	B8	0.72	0/137	1.19	0/185
9	SF	0.85	17/3447 (0.5%)	1.30	40/4671 (0.9%)
9	sF	0.86	17/3447 (0.5%)	1.30	40/4671 (0.9%)
10	A9	1.65	8/549 (1.5%)	2.59	23/743 (3.1%)
10	B9	1.65	8/549 (1.5%)	2.59	23/743 (3.1%)
11	AA	0.43	13/11191 (0.1%)	0.75	34/15127 (0.2%)
11	BA	0.43	13/11191 (0.1%)	0.76	33/15127 (0.2%)
11	MA	0.23	0/606	0.70	0/848
11	mA	0.23	0/606	0.70	0/848
12	AB	0.34	4/9431 (0.0%)	0.58	18/12718 (0.1%)
12	BB	0.34	4/9431 (0.0%)	0.58	18/12718 (0.1%)
13	AC	0.19	0/2099	0.40	0/2845
13	BC	0.19	0/2099	0.40	0/2845
14	AD	0.23	0/1262	0.51	0/1693
14	BD	0.24	0/1262	0.51	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	AE	0.29	1/1780 (0.1%)	0.45	1/2395 (0.0%)
15	BE	0.29	1/1780 (0.1%)	0.45	1/2395 (0.0%)
16	AF	0.31	0/682	0.61	1/922 (0.1%)
16	BF	0.31	0/682	0.61	1/922 (0.1%)
17	AG	0.35	0/1368	0.74	4/1844 (0.2%)
17	BG	0.36	0/1368	0.74	4/1844 (0.2%)
18	AH	0.80	3/1107 (0.3%)	1.15	12/1499 (0.8%)
18	BH	0.80	3/1107 (0.3%)	1.15	12/1499 (0.8%)
19	AI	2.04	31/962 (3.2%)	3.30	102/1295 (7.9%)
19	BI	2.04	32/962 (3.3%)	3.30	102/1295 (7.9%)
20	AJ	0.70	3/578 (0.5%)	0.93	3/775 (0.4%)
20	BJ	0.70	3/578 (0.5%)	0.93	3/775 (0.4%)
21	AK	0.29	0/942	0.58	1/1272 (0.1%)
21	BK	0.29	0/942	0.58	1/1272 (0.1%)
22	AL	0.29	0/361	0.51	0/478
22	BL	0.29	0/361	0.51	0/478
23	AM	0.31	0/2120	0.68	5/2849 (0.2%)
23	BM	0.31	0/2120	0.68	5/2849 (0.2%)
24	AN	1.09	7/1583 (0.4%)	1.23	11/2441 (0.5%)
24	BN	1.09	7/1583 (0.4%)	1.23	11/2441 (0.5%)
25	AO	0.25	0/1449	0.60	0/1952
25	BO	0.26	0/1449	0.60	0/1952
26	AQ	0.42	4/1852 (0.2%)	0.55	1/2480 (0.0%)
26	BQ	0.42	4/1852 (0.2%)	0.55	1/2480 (0.0%)
27	AR	0.51	2/2207 (0.1%)	0.76	11/2963 (0.4%)
27	BR	0.51	2/2207 (0.1%)	0.76	11/2963 (0.4%)
28	AS	1.15	14/1324 (1.1%)	1.69	35/1787 (2.0%)
28	BS	1.15	14/1324 (1.1%)	1.69	35/1787 (2.0%)
29	AT	1.10	5/1589 (0.3%)	1.23	14/2450 (0.6%)
29	BT	1.10	5/1589 (0.3%)	1.23	14/2450 (0.6%)
30	AU	0.31	0/856	0.82	4/1156 (0.3%)
30	BU	0.31	0/856	0.82	4/1156 (0.3%)
31	AV	0.30	0/822	0.83	2/1109 (0.2%)
31	BV	0.30	0/822	0.83	2/1109 (0.2%)
32	AW	0.30	0/1870	0.66	0/2524
32	BW	0.30	0/1870	0.66	0/2524
33	AX	0.20	0/1559	0.51	0/2102
33	BX	0.21	0/1559	0.51	0/2102
34	Ma	0.19	0/1440	0.46	0/1946
34	ma	0.19	0/1440	0.46	0/1946
35	Mb	0.23	0/1320	0.58	3/1785 (0.2%)
35	mb	0.23	0/1320	0.58	3/1785 (0.2%)
36	Mc	0.42	1/885 (0.1%)	0.80	2/1183 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	mc	0.42	1/885 (0.1%)	0.80	2/1183 (0.2%)
37	Md	0.19	0/4389	0.49	3/5901 (0.1%)
37	md	0.20	0/4389	0.49	3/5901 (0.1%)
38	Me	0.20	0/1993	0.59	4/2698 (0.1%)
38	me	0.20	0/1993	0.59	4/2698 (0.1%)
39	Mf	0.19	0/1635	0.49	0/2215
39	mf	0.19	0/1635	0.49	0/2215
40	Mg	0.28	0/851	0.65	0/1148
40	mg	0.28	0/851	0.64	0/1148
41	Mh	0.30	0/1462	0.62	2/1970 (0.1%)
41	mh	0.30	0/1462	0.62	2/1970 (0.1%)
42	Mi	0.28	0/1569	0.59	0/2117
42	mi	0.28	0/1569	0.59	0/2117
43	Mj	0.37	0/877	0.92	8/1180 (0.7%)
43	mj	0.37	0/877	0.92	8/1180 (0.7%)
44	Mk	0.28	0/1172	0.62	1/1581 (0.1%)
44	mk	0.28	0/1172	0.62	1/1581 (0.1%)
45	Ml	0.22	0/5460	0.52	0/7373
45	T4	0.55	5/1817 (0.3%)	0.86	9/2456 (0.4%)
45	ml	0.22	0/5460	0.52	0/7373
45	t4	0.55	5/1817 (0.3%)	0.86	9/2456 (0.4%)
46	Mm	0.24	0/684	0.67	3/928 (0.3%)
46	mm	0.24	0/684	0.68	3/928 (0.3%)
47	Mn	0.30	0/1135	0.63	0/1526
47	mn	0.30	0/1135	0.63	0/1526
48	Mo	0.36	0/941	0.71	3/1282 (0.2%)
48	mo	0.36	0/941	0.70	3/1282 (0.2%)
49	Mp	0.15	0/3394	0.40	0/4589
49	mp	0.16	0/3394	0.40	0/4589
50	SA	0.59	10/3617 (0.3%)	0.90	13/4895 (0.3%)
50	sA	0.59	10/3617 (0.3%)	0.90	13/4895 (0.3%)
51	SB	0.56	5/3318 (0.2%)	0.73	9/4465 (0.2%)
51	SD	0.40	2/3517 (0.1%)	0.69	5/4735 (0.1%)
51	sB	0.56	5/3318 (0.2%)	0.73	9/4465 (0.2%)
51	sD	0.41	2/3517 (0.1%)	0.69	5/4735 (0.1%)
52	SC	0.37	0/1287	0.74	1/1729 (0.1%)
52	sC	0.37	0/1287	0.74	1/1729 (0.1%)
53	SE	1.05	24/3399 (0.7%)	1.21	42/4584 (0.9%)
53	sE	1.05	24/3399 (0.7%)	1.21	42/4584 (0.9%)
54	SG	0.20	0/101	0.50	0/123
54	sG	0.20	0/101	0.50	0/123
55	SH	1.16	21/1991 (1.1%)	1.36	26/2692 (1.0%)
55	sH	1.16	21/1991 (1.1%)	1.36	26/2692 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
56	SI	0.53	6/4552 (0.1%)	0.70	11/6163 (0.2%)
56	sI	0.53	6/4552 (0.1%)	0.70	11/6163 (0.2%)
57	SJ	0.52	1/728 (0.1%)	0.64	0/978
57	sJ	0.52	1/728 (0.1%)	0.64	0/978
58	SK	0.59	9/3525 (0.3%)	0.74	9/4769 (0.2%)
58	sK	0.59	10/3525 (0.3%)	0.74	9/4769 (0.2%)
59	SL	0.33	2/3333 (0.1%)	0.55	1/4517 (0.0%)
59	sL	0.33	2/3333 (0.1%)	0.55	1/4517 (0.0%)
60	E3	0.61	15/6190 (0.2%)	1.03	34/8398 (0.4%)
60	T3	0.64	17/6293 (0.3%)	0.97	36/8534 (0.4%)
60	t3	0.64	17/6293 (0.3%)	0.97	35/8534 (0.4%)
61	E6	0.58	13/7725 (0.2%)	0.66	13/10461 (0.1%)
61	T6	0.46	9/7725 (0.1%)	0.71	10/10461 (0.1%)
61	t6	0.46	9/7725 (0.1%)	0.71	9/10461 (0.1%)
62	T1	0.68	2/520 (0.4%)	0.79	0/693
62	t1	0.68	2/520 (0.4%)	0.79	0/693
63	T2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
63	t2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
64	T5	1.28	16/904 (1.8%)	2.16	31/1202 (2.6%)
64	t5	1.28	16/904 (1.8%)	2.16	31/1202 (2.6%)
All	All	0.56	632/325317 (0.2%)	0.87	1320/440531 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	B0	0	1
2	A1	0	1
2	B1	0	1
3	A2	0	5
3	B2	0	5
4	A3	0	2
4	B3	0	2
5	A4	0	1
5	B4	0	1
6	A5	0	2
6	B5	0	2
8	A7	0	4
8	B7	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	A8	0	1
9	B8	0	1
9	SF	1	6
9	sF	1	6
10	A9	1	2
10	B9	1	2
11	AA	0	7
11	BA	0	7
12	AB	0	3
12	BB	0	3
17	AG	0	1
17	BG	0	1
18	AH	0	3
18	BH	0	3
19	AI	0	13
19	BI	0	13
20	AJ	0	1
20	BJ	0	1
28	AS	1	4
28	BS	1	4
31	AV	0	1
31	BV	0	1
32	AW	0	1
32	BW	0	1
37	Md	0	1
37	md	0	1
38	Me	0	2
38	me	0	2
45	T4	0	1
45	t4	0	1
47	Mn	0	1
47	mn	0	1
50	SA	1	2
50	sA	1	2
51	SB	0	1
51	sB	0	1
53	SE	0	10
53	sE	0	10
55	SH	0	2
55	sH	0	2
56	SI	0	4
56	sI	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
58	SK	0	3
58	sK	0	3
60	E3	0	6
60	T3	1	6
60	t3	1	6
61	E6	0	3
61	T6	0	1
61	t6	0	1
63	T2	0	1
63	t2	0	1
64	T5	1	2
64	t5	1	2
All	All	12	201

All (632) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SE	547	ARG	CZ-NH1	-29.68	0.91	1.32
53	sE	547	ARG	CZ-NH1	-29.66	0.91	1.32
19	BI	86	PHE	CG-CD2	21.75	1.84	1.38
19	AI	86	PHE	CG-CD2	21.73	1.84	1.38
55	SH	608	MET	SD-CE	-19.93	1.29	1.79
55	sH	608	MET	SD-CE	-19.91	1.29	1.79
60	T3	837	TYR	CG-CD2	19.69	1.80	1.39
60	t3	837	TYR	CG-CD2	19.68	1.80	1.39
9	sF	401	LYS	CB-CG	-18.94	0.95	1.52
9	SF	401	LYS	CB-CG	-18.94	0.95	1.52
61	E6	972	MET	SD-CE	-18.45	1.33	1.79
9	sF	485	LEU	CG-CD1	-17.27	0.95	1.52
9	SF	485	LEU	CG-CD1	-17.27	0.95	1.52
64	T5	920	LYS	CB-CG	-16.18	1.03	1.52
64	t5	920	LYS	CB-CG	-16.18	1.03	1.52
4	A3	64	ARG	CG-CD	-16.11	1.04	1.52
4	B3	64	ARG	CG-CD	-16.09	1.04	1.52
28	BS	206	VAL	CA-C	16.06	1.73	1.52
28	AS	206	VAL	CA-C	16.05	1.73	1.52
1	A0	553	MET	SD-CE	-16.01	1.39	1.79
1	B0	553	MET	SD-CE	-16.01	1.39	1.79
18	AH	109	LYS	CA-C	15.78	1.73	1.52
18	BH	109	LYS	CA-C	15.72	1.73	1.52
29	AT	61	DA	C3'-O3'	-15.66	1.23	1.44
29	BT	61	DA	C3'-O3'	-15.61	1.23	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AN	-43	DA	C3'-C2'	-15.41	1.39	1.52
24	BN	-43	DA	C3'-C2'	-15.38	1.39	1.52
10	B9	199	GLN	CA-CB	-15.16	1.27	1.53
10	A9	199	GLN	CA-CB	-15.13	1.27	1.53
1	A0	557	MET	CG-SD	-15.05	1.43	1.80
1	B0	557	MET	CG-SD	-15.03	1.43	1.80
58	SK	91	TYR	CZ-OH	-15.00	1.06	1.38
58	sK	91	TYR	CZ-OH	-14.98	1.06	1.38
11	BA	688	LYS	CB-CG	-14.97	1.07	1.52
11	AA	688	LYS	CB-CG	-14.97	1.07	1.52
55	sH	590	GLU	CA-C	14.93	1.72	1.52
55	SH	590	GLU	CA-C	14.92	1.72	1.52
19	BI	61	ASP	CA-C	14.81	1.73	1.52
19	AI	61	ASP	CA-C	14.81	1.73	1.52
10	B9	217	GLU	CD-OE2	14.70	1.53	1.25
10	A9	217	GLU	CD-OE2	14.70	1.53	1.25
51	sB	432	VAL	CB-CG1	-14.47	1.04	1.52
51	SB	432	VAL	CB-CG1	-14.46	1.04	1.52
50	SA	269	GLN	CA-C	-14.15	1.40	1.53
50	sA	269	GLN	CA-C	-14.08	1.40	1.53
4	A3	49	LEU	CB-CG	-13.98	1.25	1.53
4	B3	49	LEU	CB-CG	-13.98	1.25	1.53
28	BS	198	ARG	CG-CD	-13.62	1.11	1.52
28	AS	198	ARG	CG-CD	-13.61	1.11	1.52
53	SE	514	GLU	CD-OE2	-13.50	0.99	1.25
53	sE	514	GLU	CD-OE2	-13.49	0.99	1.25
3	B2	490	LYS	CB-CG	-13.36	1.12	1.52
3	A2	490	LYS	CB-CG	-13.34	1.12	1.52
55	SH	594	LEU	CG-CD2	13.31	1.96	1.52
55	sH	594	LEU	CG-CD2	13.30	1.96	1.52
28	BS	206	VAL	CA-CB	-13.18	1.36	1.54
28	AS	206	VAL	CA-CB	-13.13	1.36	1.54
55	sH	595	GLU	CD-OE2	-12.61	1.01	1.25
55	SH	595	GLU	CD-OE2	-12.60	1.01	1.25
10	A9	200	MET	CB-CG	-12.51	1.15	1.52
10	B9	200	MET	CB-CG	-12.49	1.15	1.52
55	SH	590	GLU	CB-CG	-12.40	1.15	1.52
55	sH	590	GLU	CB-CG	-12.40	1.15	1.52
20	AJ	58	GLU	CB-CG	-12.17	1.16	1.52
60	T3	289	LYS	CG-CD	-12.17	1.16	1.52
20	BJ	58	GLU	CB-CG	-12.15	1.16	1.52
60	t3	289	LYS	CG-CD	-12.15	1.16	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A9	209	MET	CB-CG	-12.12	1.16	1.52
10	B9	209	MET	CB-CG	-12.09	1.16	1.52
60	T3	289	LYS	CB-CG	11.99	1.88	1.52
60	t3	289	LYS	CB-CG	11.97	1.88	1.52
19	AI	86	PHE	CG-CD1	-11.66	1.14	1.38
19	BI	86	PHE	CG-CD1	-11.62	1.14	1.38
63	t2	34	ASN	CG-OD1	-11.61	1.01	1.23
60	E3	939	THR	CA-C	11.61	1.68	1.52
12	AB	22	SER	C-N	11.60	1.50	1.33
63	T2	34	ASN	CG-OD1	-11.59	1.01	1.23
12	BB	22	SER	C-N	11.55	1.49	1.33
11	AA	688	LYS	CA-C	11.47	1.68	1.52
11	BA	688	LYS	CA-C	11.43	1.68	1.52
18	AH	109	LYS	N-CA	-11.38	1.31	1.46
55	sH	594	LEU	CB-CG	-11.38	1.30	1.53
18	BH	109	LYS	N-CA	-11.36	1.31	1.46
55	SH	594	LEU	CB-CG	-11.35	1.30	1.53
27	BR	228	MET	SD-CE	-11.35	1.51	1.79
27	AR	228	MET	SD-CE	-11.35	1.51	1.79
55	sH	590	GLU	CD-OE2	11.32	1.46	1.25
55	SH	590	GLU	CD-OE2	11.31	1.46	1.25
50	sA	269	GLN	N-CA	-11.26	1.33	1.47
50	SA	269	GLN	N-CA	-11.23	1.33	1.47
53	SE	464	ASN	CG-OD1	-11.20	1.02	1.23
53	sE	464	ASN	CG-OD1	-11.19	1.02	1.23
6	B5	5	ARG	CA-CB	-11.17	1.26	1.53
6	A5	5	ARG	CA-CB	-11.16	1.26	1.53
19	AI	82	GLU	CG-CD	-11.09	1.24	1.52
19	BI	82	GLU	CG-CD	-11.08	1.24	1.52
12	AB	23	ALA	N-CA	11.01	1.63	1.45
12	BB	23	ALA	N-CA	10.98	1.63	1.45
6	A5	50	VAL	CB-CG1	-10.74	1.17	1.52
6	B5	50	VAL	CB-CG1	-10.74	1.17	1.52
10	B9	199	GLN	CD-NE2	10.71	1.55	1.33
60	E3	939	THR	CB-CG2	10.70	1.87	1.52
10	A9	199	GLN	CD-NE2	10.69	1.55	1.33
9	sF	448	GLN	CD-OE1	-10.65	1.03	1.23
9	SF	448	GLN	CD-OE1	-10.62	1.03	1.23
19	AI	92	ARG	CG-CD	-10.57	1.20	1.52
19	BI	92	ARG	CG-CD	-10.56	1.20	1.52
53	sE	523	VAL	CB-CG2	-10.56	1.17	1.52
55	sH	455	MET	SD-CE	-10.55	1.53	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SE	523	VAL	CB-CG2	-10.55	1.17	1.52
55	SH	455	MET	SD-CE	-10.52	1.53	1.79
61	E6	791	PHE	CD2-CE2	-10.44	1.07	1.38
55	sH	600	GLU	CD-OE1	-10.37	1.05	1.25
55	SH	600	GLU	CD-OE1	-10.36	1.05	1.25
11	BA	688	LYS	CA-CB	10.29	1.72	1.53
56	sI	712	MET	SD-CE	-10.28	1.53	1.79
11	AA	688	LYS	CA-CB	10.27	1.72	1.53
56	SI	712	MET	SD-CE	-10.25	1.53	1.79
6	B5	3	ARG	CG-CD	-10.20	1.21	1.52
6	A5	3	ARG	CG-CD	-10.19	1.21	1.52
1	B0	537	MET	CG-SD	-10.11	1.55	1.80
1	A0	537	MET	CG-SD	-10.11	1.55	1.80
19	AI	92	ARG	CD-NE	-10.06	1.32	1.46
19	BI	92	ARG	CD-NE	-10.03	1.32	1.46
11	BA	688	LYS	CD-CE	-10.00	1.22	1.52
11	AA	688	LYS	CD-CE	-9.99	1.22	1.52
56	SI	1248	LEU	CG-CD1	-9.97	1.19	1.52
56	sI	1248	LEU	CG-CD1	-9.95	1.19	1.52
8	A7	349	ASN	CG-ND2	-9.81	1.12	1.33
8	B7	349	ASN	CG-ND2	-9.80	1.12	1.33
61	E6	923	LEU	CA-C	-9.74	1.39	1.53
19	AI	93	LYS	CE-NZ	-9.69	1.20	1.49
19	BI	93	LYS	CE-NZ	-9.68	1.20	1.49
26	BQ	386	MET	SD-CE	-9.62	1.55	1.79
26	AQ	386	MET	SD-CE	-9.61	1.55	1.79
12	AB	662	MET	CG-SD	-9.55	1.56	1.80
12	BB	662	MET	CG-SD	-9.55	1.56	1.80
9	sF	401	LYS	CE-NZ	-9.52	1.20	1.49
9	SF	401	LYS	CE-NZ	-9.50	1.20	1.49
56	sI	1110	VAL	CB-CG1	-9.45	1.21	1.52
56	SI	1110	VAL	CB-CG1	-9.44	1.21	1.52
19	AI	61	ASP	N-CA	-9.43	1.35	1.46
51	sB	770	PHE	CE2-CZ	-9.41	1.10	1.38
19	BI	61	ASP	N-CA	-9.41	1.35	1.46
51	SB	770	PHE	CE2-CZ	-9.40	1.10	1.38
19	AI	82	GLU	CD-OE1	-9.35	1.07	1.25
19	BI	82	GLU	CD-OE1	-9.32	1.07	1.25
10	A9	199	GLN	CD-OE1	-9.21	1.06	1.23
10	B9	199	GLN	CD-OE1	-9.19	1.06	1.23
45	t4	1018	MET	CB-CG	-9.05	1.25	1.52
45	T4	1018	MET	CB-CG	-9.04	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SK	303	LEU	CG-CD1	-9.02	1.22	1.52
60	T3	836	ILE	C-N	9.01	1.46	1.33
58	sK	303	LEU	CG-CD1	-9.01	1.22	1.52
60	t3	836	ILE	C-N	8.99	1.46	1.33
3	B2	69	ASN	CG-OD1	-8.97	1.06	1.23
7	B6	384	MET	SD-CE	-8.97	1.57	1.79
19	BI	104	LEU	CG-CD2	8.96	1.82	1.52
7	A6	384	MET	SD-CE	-8.96	1.57	1.79
50	sA	269	GLN	CB-CG	-8.96	1.25	1.52
50	SA	269	GLN	CB-CG	-8.96	1.25	1.52
3	A2	69	ASN	CG-OD1	-8.96	1.06	1.23
19	AI	104	LEU	CG-CD2	8.95	1.82	1.52
19	BI	62	ILE	CA-C	8.92	1.66	1.52
19	AI	62	ILE	CA-C	8.91	1.66	1.52
28	AS	198	ARG	CB-CG	-8.83	1.25	1.52
53	SE	483	GLN	CD-OE1	-8.83	1.06	1.23
28	BS	198	ARG	CB-CG	-8.83	1.25	1.52
53	sE	483	GLN	CD-OE1	-8.82	1.06	1.23
60	T3	289	LYS	CA-CB	8.81	1.67	1.53
60	t3	289	LYS	CA-CB	8.80	1.67	1.53
3	B2	195	GLU	CD-OE1	-8.79	1.08	1.25
3	A2	195	GLU	CD-OE1	-8.78	1.08	1.25
28	BS	183	ASN	C-O	-8.68	1.13	1.24
61	T6	864	ASN	CG-ND2	-8.67	1.15	1.33
60	t3	288	MET	C-N	8.66	1.45	1.33
61	t6	864	ASN	CG-ND2	-8.66	1.15	1.33
28	AS	183	ASN	C-O	-8.62	1.13	1.24
50	SA	308	MET	SD-CE	-8.62	1.57	1.79
50	sA	308	MET	SD-CE	-8.60	1.58	1.79
60	T3	288	MET	C-N	8.59	1.45	1.33
29	BT	45	DT	P-O5'	8.59	1.68	1.59
61	E6	934	ARG	CG-CD	-8.58	1.26	1.52
29	AT	45	DT	P-O5'	8.58	1.68	1.59
50	sA	131	ASN	CG-ND2	-8.54	1.15	1.33
58	sK	201	ILE	CG1-CD1	-8.53	1.18	1.51
58	SK	201	ILE	CG1-CD1	-8.52	1.18	1.51
50	SA	131	ASN	CG-ND2	-8.50	1.15	1.33
19	AI	84	VAL	CA-CB	-8.49	1.44	1.54
19	BI	84	VAL	CA-CB	-8.49	1.44	1.54
55	SH	590	GLU	N-CA	-8.47	1.35	1.46
55	sH	590	GLU	N-CA	-8.46	1.35	1.46
3	A2	352	ASN	CG-OD1	-8.45	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A2	408	MET	SD-CE	-8.45	1.58	1.79
53	SE	507	LEU	CG-CD2	-8.44	1.24	1.52
11	BA	455	MET	SD-CE	-8.44	1.58	1.79
11	AA	455	MET	SD-CE	-8.44	1.58	1.79
3	B2	408	MET	SD-CE	-8.43	1.58	1.79
53	sE	507	LEU	CG-CD2	-8.42	1.24	1.52
3	B2	352	ASN	CG-OD1	-8.42	1.07	1.23
19	AI	62	ILE	CG1-CD1	-8.39	1.19	1.51
19	BI	62	ILE	CG1-CD1	-8.38	1.19	1.51
8	A7	545	GLN	CD-OE1	-8.37	1.07	1.23
8	B7	545	GLN	CD-OE1	-8.36	1.07	1.23
6	A5	3	ARG	CB-CG	-8.35	1.27	1.52
6	B5	3	ARG	CB-CG	-8.33	1.27	1.52
9	sF	524	PHE	CE1-CZ	-8.32	1.13	1.38
9	SF	524	PHE	CE1-CZ	-8.31	1.13	1.38
11	AA	683	ILE	C-N	8.29	1.45	1.33
64	t5	919	ARG	NE-CZ	-8.28	1.24	1.33
64	T5	919	ARG	NE-CZ	-8.28	1.24	1.33
64	t5	943	LEU	CG-CD1	-8.24	1.25	1.52
64	T5	943	LEU	CG-CD1	-8.23	1.25	1.52
61	t6	132	MET	SD-CE	-8.22	1.58	1.79
61	T6	132	MET	SD-CE	-8.22	1.59	1.79
50	SA	271	ASP	C-N	8.21	1.53	1.33
50	sA	271	ASP	C-N	8.20	1.53	1.33
1	A0	251	ASP	CG-OD1	-8.18	1.09	1.25
19	BI	82	GLU	CD-OE2	8.17	1.40	1.25
1	B0	251	ASP	CG-OD1	-8.16	1.09	1.25
19	AI	82	GLU	CD-OE2	8.16	1.40	1.25
19	BI	94	ASP	CG-OD2	8.16	1.40	1.25
19	AI	94	ASP	CG-OD2	8.12	1.40	1.25
3	B2	97	MET	CG-SD	-8.07	1.60	1.80
3	A2	97	MET	CG-SD	-8.07	1.60	1.80
53	SE	454	LEU	CG-CD2	-8.05	1.25	1.52
53	sE	454	LEU	CG-CD2	-8.05	1.25	1.52
60	E3	734	GLU	CG-CD	-8.04	1.31	1.52
53	SE	523	VAL	CB-CG1	8.03	1.79	1.52
53	sE	523	VAL	CB-CG1	8.02	1.79	1.52
27	BR	268	MET	SD-CE	-8.00	1.59	1.79
27	AR	268	MET	SD-CE	-8.00	1.59	1.79
19	BI	77	LYS	CE-NZ	-8.00	1.25	1.49
19	AI	77	LYS	CE-NZ	-7.99	1.25	1.49
55	sH	592	LEU	CG-CD1	7.98	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	SH	592	LEU	CG-CD1	7.98	1.78	1.52
9	SF	401	LYS	CA-CB	-7.97	1.40	1.53
11	BA	683	ILE	C-N	7.96	1.45	1.33
9	sF	401	LYS	CA-CB	-7.94	1.40	1.53
19	BI	75	CYS	CB-SG	7.89	2.07	1.81
19	AI	75	CYS	CB-SG	7.89	2.07	1.81
10	A9	199	GLN	CB-CG	-7.84	1.28	1.52
19	AI	93	LYS	CB-CG	-7.83	1.28	1.52
10	B9	199	GLN	CB-CG	-7.82	1.29	1.52
19	BI	93	LYS	CB-CG	-7.81	1.29	1.52
55	SH	592	LEU	CG-CD2	-7.80	1.26	1.52
55	sH	592	LEU	CG-CD2	-7.80	1.26	1.52
29	AT	60	DT	C1'-N1	7.74	1.58	1.47
29	BT	60	DT	C1'-N1	7.69	1.58	1.47
6	A5	3	ARG	CD-NE	-7.63	1.35	1.46
57	SJ	1	MET	SD-CE	-7.63	1.60	1.79
6	B5	3	ARG	CD-NE	-7.63	1.35	1.46
57	sJ	1	MET	SD-CE	-7.62	1.60	1.79
61	E6	749	LEU	CG-CD1	7.60	1.77	1.52
50	sA	427	VAL	CB-CG2	-7.60	1.27	1.52
50	SA	427	VAL	CB-CG2	-7.59	1.27	1.52
9	SF	389	ASN	CG-ND2	7.59	1.49	1.33
60	T3	289	LYS	CA-C	-7.59	1.43	1.52
64	T5	920	LYS	CA-C	-7.59	1.42	1.52
60	t3	289	LYS	CA-C	-7.59	1.43	1.52
64	t5	920	LYS	CA-C	-7.57	1.42	1.52
9	sF	389	ASN	CG-ND2	7.55	1.49	1.33
19	AI	78	CYS	CA-C	-7.55	1.42	1.52
19	BI	78	CYS	CA-C	-7.53	1.42	1.52
19	BI	91	ARG	CG-CD	-7.53	1.29	1.52
19	AI	91	ARG	CG-CD	-7.52	1.29	1.52
3	A2	506	LYS	CB-CG	-7.51	1.29	1.52
3	B2	506	LYS	CB-CG	-7.50	1.29	1.52
29	BT	44	DC	O3'-P	7.50	1.70	1.61
29	AT	44	DC	O3'-P	7.48	1.70	1.61
5	A4	109	ILE	CB-CG2	-7.44	1.27	1.52
5	B4	109	ILE	CB-CG2	-7.43	1.28	1.52
60	T3	290	LEU	N-CA	-7.41	1.37	1.46
60	t3	290	LEU	N-CA	-7.37	1.37	1.46
1	B0	537	MET	SD-CE	-7.37	1.61	1.79
1	A0	537	MET	SD-CE	-7.37	1.61	1.79
10	B9	217	GLU	CD-OE1	-7.37	1.11	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A9	217	GLU	CD-OE1	-7.35	1.11	1.25
64	t5	923	LYS	CE-NZ	-7.34	1.27	1.49
60	E3	939	THR	CA-CB	-7.34	1.42	1.53
64	T5	923	LYS	CE-NZ	-7.34	1.27	1.49
9	sF	401	LYS	N-CA	7.32	1.55	1.46
2	A1	197	GLU	CD-OE1	-7.31	1.11	1.25
28	AS	205	ASN	C-N	-7.31	1.23	1.33
3	B2	69	ASN	N-CA	-7.31	1.37	1.46
28	BS	205	ASN	C-N	-7.31	1.23	1.33
2	B1	197	GLU	CD-OE1	-7.31	1.11	1.25
60	E3	409	LYS	CE-NZ	-7.30	1.27	1.49
24	BN	-45	DA	N9-C4	-7.29	1.33	1.37
55	sH	592	LEU	CB-CG	-7.28	1.38	1.53
9	sF	524	PHE	CG-CD1	-7.27	1.23	1.38
55	SH	592	LEU	CB-CG	-7.26	1.39	1.53
11	BA	684	ALA	N-CA	7.26	1.55	1.46
9	SF	401	LYS	N-CA	7.26	1.55	1.46
9	SF	524	PHE	CG-CD1	-7.26	1.23	1.38
24	AN	-45	DA	N9-C4	-7.24	1.33	1.37
3	A2	69	ASN	N-CA	-7.22	1.37	1.46
19	AI	104	LEU	CG-CD1	-7.22	1.28	1.52
19	BI	104	LEU	CG-CD1	-7.22	1.28	1.52
51	sB	770	PHE	CG-CD1	-7.21	1.23	1.38
11	AA	684	ALA	N-CA	7.20	1.55	1.46
51	SB	770	PHE	CG-CD1	-7.19	1.23	1.38
45	t4	1019	MET	CB-CG	-7.18	1.30	1.52
1	B0	199	MET	SD-CE	-7.17	1.61	1.79
1	A0	199	MET	SD-CE	-7.17	1.61	1.79
45	T4	1019	MET	CB-CG	-7.16	1.30	1.52
19	BI	82	GLU	N-CA	-7.16	1.37	1.46
19	AI	82	GLU	N-CA	-7.12	1.37	1.46
61	E6	749	LEU	CG-CD2	7.12	1.76	1.52
3	B2	69	ASN	CB-CG	-7.12	1.34	1.52
3	A2	69	ASN	CB-CG	-7.10	1.34	1.52
64	t5	920	LYS	CE-NZ	-7.09	1.28	1.49
53	sE	547	ARG	CG-CD	-7.09	1.31	1.52
59	SL	183	LEU	CG-CD1	-7.08	1.29	1.52
64	T5	920	LYS	CE-NZ	-7.08	1.28	1.49
53	SE	547	ARG	CG-CD	-7.08	1.31	1.52
59	sL	183	LEU	CG-CD1	-7.07	1.29	1.52
61	T6	972	MET	SD-CE	-6.96	1.62	1.79
8	A7	338	LEU	C-O	-6.96	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	SA	269	GLN	C-O	6.96	1.29	1.23
61	t6	972	MET	SD-CE	-6.96	1.62	1.79
50	sA	269	GLN	C-O	6.95	1.29	1.23
51	sD	607	VAL	CB-CG2	-6.94	1.29	1.52
51	SD	607	VAL	CB-CG2	-6.94	1.29	1.52
55	SH	592	LEU	CA-C	-6.93	1.43	1.52
53	SE	337	ALA	CA-CB	-6.91	1.29	1.52
8	B7	338	LEU	C-O	-6.91	1.15	1.24
18	AH	109	LYS	CA-CB	-6.91	1.43	1.53
53	sE	337	ALA	CA-CB	-6.89	1.29	1.52
18	BH	109	LYS	CA-CB	-6.89	1.43	1.53
55	sH	592	LEU	CA-C	-6.89	1.43	1.52
61	E6	151	VAL	CB-CG1	-6.88	1.29	1.52
63	T2	80	GLN	CD-OE1	-6.86	1.10	1.23
53	SE	527	THR	CB-OG1	-6.86	1.32	1.43
63	t2	80	GLN	CD-OE1	-6.84	1.10	1.23
62	t1	40	LEU	CG-CD1	-6.84	1.29	1.52
53	sE	527	THR	CB-OG1	-6.83	1.32	1.43
62	T1	40	LEU	CG-CD1	-6.82	1.30	1.52
1	B0	557	MET	CB-CG	-6.82	1.31	1.52
1	A0	557	MET	CB-CG	-6.81	1.32	1.52
15	AE	121	MET	SD-CE	-6.80	1.62	1.79
15	BE	121	MET	SD-CE	-6.80	1.62	1.79
60	T3	919	TYR	CD2-CE2	-6.80	1.18	1.38
60	t3	919	TYR	CD2-CE2	-6.79	1.18	1.38
6	A5	3	ARG	CZ-NH2	-6.79	1.24	1.33
58	SK	402	GLU	CD-OE2	-6.78	1.12	1.25
58	sK	402	GLU	CD-OE2	-6.78	1.12	1.25
6	B5	3	ARG	CZ-NH2	-6.76	1.24	1.33
60	T3	838	SER	CA-C	6.75	1.61	1.52
56	sI	1114	PHE	CG-CD2	-6.75	1.24	1.38
53	SE	526	GLN	CD-OE1	-6.74	1.10	1.23
53	sE	526	GLN	CD-OE1	-6.73	1.10	1.23
60	t3	838	SER	CA-C	6.72	1.61	1.52
1	A0	495	MET	SD-CE	-6.72	1.62	1.79
1	B0	495	MET	SD-CE	-6.72	1.62	1.79
56	SI	1114	PHE	CG-CD2	-6.71	1.24	1.38
4	B3	64	ARG	CB-CG	-6.70	1.32	1.52
4	A3	64	ARG	CB-CG	-6.68	1.32	1.52
36	mc	45	LYS	C-N	6.66	1.43	1.33
53	sE	519	TYR	CD2-CE2	-6.66	1.18	1.38
36	Mc	45	LYS	C-N	6.65	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SE	519	TYR	CD2-CE2	-6.64	1.18	1.38
61	T6	971	GLU	CD-OE1	-6.62	1.12	1.25
11	AA	683	ILE	CA-C	6.59	1.62	1.52
7	A6	214	LEU	CG-CD1	-6.58	1.30	1.52
61	t6	971	GLU	CD-OE1	-6.58	1.12	1.25
7	B6	214	LEU	CG-CD1	-6.58	1.30	1.52
11	BA	683	ILE	CA-C	6.58	1.62	1.52
55	sH	590	GLU	CA-CB	-6.55	1.42	1.53
55	SH	590	GLU	CA-CB	-6.53	1.42	1.53
19	AI	78	CYS	CB-SG	-6.50	1.59	1.81
19	BI	78	CYS	CB-SG	-6.49	1.59	1.81
61	E6	923	LEU	CG-CD1	-6.48	1.31	1.52
55	sH	453	PHE	CE2-CZ	-6.45	1.19	1.38
55	SH	453	PHE	CE2-CZ	-6.45	1.19	1.38
50	SA	269	GLN	CD-OE1	-6.44	1.11	1.23
4	B3	64	ARG	CA-C	-6.44	1.44	1.52
4	A3	64	ARG	CA-C	-6.43	1.44	1.52
50	sA	269	GLN	CD-OE1	-6.43	1.11	1.23
9	sF	603	MET	CG-SD	-6.42	1.64	1.80
53	sE	462	THR	C-N	6.41	1.48	1.33
53	SE	462	THR	C-N	6.41	1.48	1.33
9	SF	603	MET	CG-SD	-6.40	1.64	1.80
4	B3	85	ARG	CB-CG	-6.39	1.33	1.52
4	A3	85	ARG	CB-CG	-6.38	1.33	1.52
7	A6	234	ILE	CG1-CD1	-6.38	1.26	1.51
55	sH	455	MET	CA-C	-6.38	1.46	1.52
28	AS	182	MET	SD-CE	-6.37	1.63	1.79
7	B6	234	ILE	CG1-CD1	-6.37	1.26	1.51
24	BN	-63	DA	P-O5'	6.36	1.66	1.59
28	BS	182	MET	SD-CE	-6.36	1.63	1.79
61	E6	791	PHE	CE1-CZ	-6.34	1.19	1.38
55	SH	455	MET	CA-C	-6.34	1.46	1.52
3	A2	258	LEU	CG-CD2	-6.32	1.31	1.52
28	AS	206	VAL	N-CA	-6.30	1.38	1.46
3	B2	22	GLN	CB-CG	-6.30	1.33	1.52
3	B2	258	LEU	CG-CD2	-6.30	1.31	1.52
24	AN	-63	DA	P-O5'	6.30	1.66	1.59
3	A2	22	GLN	CB-CG	-6.29	1.33	1.52
58	SK	195	GLU	CD-OE1	-6.28	1.13	1.25
58	sK	195	GLU	CD-OE1	-6.28	1.13	1.25
3	A2	506	LYS	CE-NZ	6.28	1.68	1.49
3	B2	506	LYS	CE-NZ	6.27	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BQ	147	LEU	CG-CD2	-6.27	1.31	1.52
28	BS	206	VAL	N-CA	-6.26	1.38	1.46
61	E6	791	PHE	CG-CD2	-6.26	1.25	1.38
26	AQ	147	LEU	CG-CD2	-6.25	1.31	1.52
53	sE	511	GLN	CB-CG	6.24	1.71	1.52
53	SE	511	GLN	CB-CG	6.22	1.71	1.52
28	AS	209	LYS	CG-CD	-6.21	1.33	1.52
24	AN	-42	DT	C5-C6	6.21	1.38	1.34
51	sB	770	PHE	CD1-CE1	-6.20	1.20	1.38
51	SB	770	PHE	CD1-CE1	-6.20	1.20	1.38
24	BN	-42	DT	C5-C6	6.20	1.38	1.34
28	BS	209	LYS	CG-CD	-6.19	1.33	1.52
9	SF	321	LEU	CG-CD2	-6.17	1.32	1.52
9	sF	321	LEU	CG-CD2	-6.17	1.32	1.52
51	SD	626	MET	SD-CE	-6.16	1.64	1.79
60	t3	837	TYR	CB-CG	-6.16	1.38	1.51
51	sD	626	MET	SD-CE	-6.15	1.64	1.79
60	T3	837	TYR	CB-CG	-6.14	1.38	1.51
19	AI	84	VAL	CB-CG2	-6.14	1.32	1.52
19	BI	84	VAL	CB-CG2	-6.13	1.32	1.52
53	SE	519	TYR	CD1-CE1	-6.12	1.20	1.38
53	sE	519	TYR	CD1-CE1	-6.11	1.20	1.38
60	E3	372	LYS	CD-CE	-6.09	1.34	1.52
60	T3	837	TYR	N-CA	6.09	1.54	1.46
60	t3	837	TYR	N-CA	6.09	1.54	1.46
53	sE	511	GLN	CD-OE1	-6.07	1.12	1.23
53	SE	511	GLN	CD-OE1	-6.05	1.12	1.23
64	T5	923	LYS	CG-CD	-6.04	1.34	1.52
20	AJ	58	GLU	CD-OE1	-6.03	1.13	1.25
64	t5	923	LYS	CG-CD	-6.03	1.34	1.52
4	B3	49	LEU	CA-CB	-6.01	1.42	1.54
4	A3	49	LEU	CA-CB	-6.01	1.42	1.54
20	BJ	58	GLU	CD-OE1	-6.01	1.14	1.25
60	T3	920	LEU	CG-CD1	-6.00	1.32	1.52
60	t3	920	LEU	CG-CD1	-6.00	1.32	1.52
60	E3	306	TRP	CE3-CZ3	-6.00	1.20	1.38
60	T3	406	LYS	CA-C	5.98	1.60	1.52
9	SF	393	LYS	CB-CG	-5.96	1.34	1.52
9	sF	393	LYS	CB-CG	-5.96	1.34	1.52
28	AS	182	MET	N-CA	5.96	1.53	1.46
11	AA	542	GLU	CD-OE1	-5.96	1.14	1.25
58	sK	237	GLN	CG-CD	-5.96	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SK	237	GLN	CG-CD	-5.95	1.37	1.52
64	t5	877	LYS	CD-CE	-5.95	1.34	1.52
28	BS	182	MET	N-CA	5.95	1.53	1.46
64	T5	877	LYS	CD-CE	-5.94	1.34	1.52
60	t3	406	LYS	CA-C	5.94	1.60	1.52
12	BB	22	SER	CA-C	5.92	1.60	1.52
45	t4	1016	TYR	C-N	5.92	1.41	1.33
11	BA	542	GLU	CD-OE1	-5.92	1.14	1.25
8	A7	723	GLN	CD-OE1	-5.92	1.12	1.23
8	B7	723	GLN	CD-OE1	-5.90	1.12	1.23
45	T4	1016	TYR	C-N	5.89	1.41	1.33
60	E3	436	SER	CA-CB	-5.89	1.37	1.54
53	sE	503	ILE	CB-CG2	-5.89	1.33	1.52
12	AB	22	SER	CA-C	5.88	1.60	1.52
53	SE	503	ILE	CB-CG2	-5.87	1.33	1.52
58	sK	228	ILE	CG1-CD1	-5.87	1.28	1.51
58	SK	228	ILE	CG1-CD1	-5.87	1.28	1.51
28	BS	209	LYS	CD-CE	-5.85	1.34	1.52
53	sE	519	TYR	CE2-CZ	-5.84	1.24	1.38
28	AS	209	LYS	CD-CE	-5.84	1.34	1.52
1	A0	167	VAL	CB-CG2	-5.83	1.33	1.52
11	BA	688	LYS	N-CA	-5.83	1.38	1.46
3	B2	464	THR	CB-CG2	5.83	1.71	1.52
53	SE	519	TYR	CE2-CZ	-5.82	1.24	1.38
3	A2	464	THR	CB-CG2	5.81	1.71	1.52
1	B0	167	VAL	CB-CG2	-5.81	1.33	1.52
11	AA	688	LYS	N-CA	-5.81	1.38	1.46
62	T1	70	GLN	CD-OE1	-5.80	1.12	1.23
24	BN	-62	DG	O3'-P	5.80	1.68	1.61
53	sE	522	ASP	C-N	5.79	1.40	1.33
64	T5	872	ARG	CZ-NH2	-5.79	1.25	1.33
24	AN	-62	DG	O3'-P	5.78	1.68	1.61
62	t1	70	GLN	CD-OE1	-5.78	1.12	1.23
53	SE	522	ASP	C-N	5.78	1.40	1.33
55	sH	482	GLY	C-O	-5.77	1.17	1.23
64	t5	872	ARG	CZ-NH2	-5.75	1.25	1.33
19	AI	60	GLN	CD-OE1	-5.75	1.12	1.23
64	T5	877	LYS	CA-C	-5.75	1.45	1.52
19	BI	60	GLN	CD-OE1	-5.75	1.12	1.23
3	B2	463	GLU	CB-CG	-5.74	1.35	1.52
60	E3	409	LYS	CD-CE	-5.73	1.35	1.52
61	t6	955	TRP	C-N	5.73	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	T6	955	TRP	C-N	5.73	1.40	1.34
64	t5	931	GLN	CB-CG	-5.72	1.35	1.52
3	A2	463	GLU	CB-CG	-5.72	1.35	1.52
59	SL	320	ILE	CG1-CD1	-5.71	1.29	1.51
55	SH	482	GLY	C-O	-5.71	1.17	1.23
59	sL	320	ILE	CG1-CD1	-5.71	1.29	1.51
64	t5	877	LYS	CA-C	-5.70	1.45	1.52
64	T5	931	GLN	CB-CG	-5.70	1.35	1.52
60	t3	289	LYS	C-N	-5.70	1.26	1.33
45	t4	1000	HIS	C-O	-5.69	1.15	1.23
6	A5	62	ILE	CG1-CD1	-5.68	1.29	1.51
3	B2	490	LYS	CD-CE	-5.68	1.35	1.52
3	B2	506	LYS	CA-C	5.68	1.60	1.52
3	A2	506	LYS	CA-C	5.68	1.60	1.52
53	SE	511	GLN	C-N	5.68	1.40	1.33
3	A2	490	LYS	CD-CE	-5.67	1.35	1.52
6	B5	62	ILE	CG1-CD1	-5.67	1.29	1.51
29	AT	60	DT	C3'-O3'	-5.66	1.36	1.44
19	AI	111	THR	CA-C	5.66	1.60	1.53
9	SF	389	ASN	CG-OD1	-5.66	1.12	1.23
29	BT	60	DT	C3'-O3'	-5.66	1.36	1.44
9	sF	389	ASN	CG-OD1	-5.66	1.12	1.23
60	T3	289	LYS	C-N	-5.65	1.26	1.33
45	T4	1000	HIS	C-O	-5.64	1.15	1.23
19	AI	111	THR	CB-CG2	5.64	1.71	1.52
56	sI	1306	LYS	CD-CE	-5.64	1.35	1.52
19	BI	111	THR	CB-CG2	5.64	1.71	1.52
56	SI	1306	LYS	CD-CE	-5.63	1.35	1.52
7	B6	128	LEU	CG-CD2	-5.63	1.33	1.52
53	sE	511	GLN	C-N	5.63	1.40	1.33
19	BI	111	THR	CA-C	5.63	1.60	1.53
61	T6	532	TYR	CD1-CE1	-5.62	1.21	1.38
61	t6	532	TYR	CD1-CE1	-5.62	1.21	1.38
3	A2	490	LYS	CG-CD	-5.62	1.35	1.52
7	A6	128	LEU	CG-CD2	-5.62	1.34	1.52
3	B2	490	LYS	CG-CD	-5.62	1.35	1.52
3	A2	253	MET	SD-CE	-5.62	1.65	1.79
64	T5	877	LYS	CE-NZ	-5.62	1.32	1.49
64	t5	877	LYS	CE-NZ	-5.62	1.32	1.49
3	B2	253	MET	SD-CE	-5.61	1.65	1.79
26	BQ	387	ILE	CG1-CD1	-5.60	1.29	1.51
26	AQ	387	ILE	CG1-CD1	-5.58	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AI	60	GLN	CD-NE2	5.58	1.45	1.33
28	AS	228	LEU	CG-CD2	-5.58	1.34	1.52
60	T3	633	LEU	CG-CD1	-5.57	1.34	1.52
28	BS	228	LEU	CG-CD2	-5.57	1.34	1.52
19	BI	60	GLN	CD-NE2	5.56	1.45	1.33
60	t3	633	LEU	CG-CD1	-5.56	1.34	1.52
24	AN	-59	DC	C1'-N1	5.55	1.55	1.47
53	SE	510	SER	C-N	5.53	1.41	1.33
61	T6	761	LYS	CD-CE	-5.53	1.35	1.52
61	t6	761	LYS	CD-CE	-5.53	1.35	1.52
64	T5	923	LYS	CB-CG	-5.51	1.35	1.52
24	BN	-59	DC	C1'-N1	5.51	1.54	1.47
53	sE	510	SER	C-N	5.51	1.41	1.33
60	E3	372	LYS	CG-CD	-5.50	1.35	1.52
64	t5	923	LYS	CB-CG	-5.50	1.35	1.52
64	T5	931	GLN	CG-CD	-5.49	1.38	1.52
9	sF	400	GLN	C-O	-5.48	1.17	1.24
64	t5	931	GLN	CG-CD	-5.48	1.38	1.52
61	t6	164	MET	SD-CE	-5.47	1.65	1.79
19	AI	115	LYS	CG-CD	-5.47	1.36	1.52
28	AS	182	MET	CA-C	-5.47	1.45	1.52
6	B5	3	ARG	CZ-NH1	5.47	1.40	1.32
9	SF	400	GLN	C-O	-5.46	1.17	1.24
61	T6	164	MET	SD-CE	-5.46	1.65	1.79
28	BS	182	MET	CA-C	-5.46	1.45	1.52
19	BI	115	LYS	CG-CD	-5.46	1.36	1.52
55	sH	449	MET	CG-SD	-5.46	1.67	1.80
60	E3	897	LYS	CG-CD	-5.45	1.36	1.52
61	t6	54	GLN	CD-NE2	-5.45	1.21	1.33
60	E3	413	ILE	CA-C	5.45	1.59	1.52
55	SH	449	MET	CG-SD	-5.45	1.67	1.80
6	A5	3	ARG	CZ-NH1	5.42	1.40	1.32
58	sK	91	TYR	CD2-CE2	-5.41	1.22	1.38
11	AA	1444	MET	SD-CE	-5.41	1.66	1.79
61	T6	54	GLN	CD-NE2	-5.41	1.21	1.33
11	BA	1444	MET	SD-CE	-5.40	1.66	1.79
58	SK	91	TYR	CD2-CE2	-5.39	1.22	1.38
45	T4	1018	MET	CG-SD	-5.36	1.67	1.80
28	BS	232	ASP	CG-OD2	5.35	1.35	1.25
28	AS	232	ASP	CG-OD2	5.34	1.35	1.25
64	t5	931	GLN	CD-NE2	5.34	1.44	1.33
6	B5	54	LEU	CG-CD1	-5.33	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	t4	1018	MET	CG-SD	-5.33	1.67	1.80
64	T5	931	GLN	CD-NE2	5.33	1.44	1.33
6	A5	54	LEU	CG-CD1	-5.33	1.34	1.52
9	sF	392	MET	SD-CE	-5.33	1.66	1.79
9	SF	392	MET	SD-CE	-5.31	1.66	1.79
55	SH	594	LEU	CA-CB	-5.31	1.44	1.53
11	AA	692	ASP	CG-OD1	-5.30	1.15	1.25
11	BA	692	ASP	CG-OD1	-5.28	1.15	1.25
58	sK	147	LEU	CB-CG	-5.28	1.42	1.53
55	sH	594	LEU	CA-CB	-5.28	1.44	1.53
60	T3	917	LEU	CG-CD2	-5.28	1.35	1.52
60	t3	917	LEU	CG-CD2	-5.27	1.35	1.52
58	SK	147	LEU	CB-CG	-5.27	1.43	1.53
60	E3	413	ILE	CB-CG2	5.21	1.69	1.52
20	AJ	58	GLU	CD-OE2	5.21	1.35	1.25
55	SH	453	PHE	CG-CD2	-5.20	1.27	1.38
56	SI	1114	PHE	CD2-CE2	-5.18	1.23	1.38
55	sH	453	PHE	CG-CD2	-5.18	1.27	1.38
56	sI	1114	PHE	CD2-CE2	-5.18	1.23	1.38
20	BJ	58	GLU	CD-OE2	5.17	1.35	1.25
50	sA	269	GLN	CD-NE2	-5.17	1.22	1.33
9	sF	341	GLN	CD-OE1	-5.17	1.13	1.23
51	sB	716	GLU	CG-CD	-5.16	1.39	1.52
1	B0	451	GLU	CD-OE1	-5.16	1.15	1.25
53	SE	50	LEU	CG-CD2	-5.16	1.35	1.52
51	SB	716	GLU	CG-CD	-5.16	1.39	1.52
53	sE	50	LEU	CG-CD2	-5.16	1.35	1.52
60	E3	675	GLU	CG-CD	-5.15	1.39	1.52
1	A0	451	GLU	CD-OE1	-5.15	1.15	1.25
24	AN	-60	DA	C3'-C2'	5.14	1.56	1.52
50	SA	269	GLN	CD-NE2	-5.14	1.22	1.33
9	SF	341	GLN	CD-OE1	-5.14	1.13	1.23
9	sF	477	LEU	CG-CD2	-5.14	1.35	1.52
9	SF	477	LEU	CG-CD2	-5.13	1.35	1.52
3	A2	195	GLU	CD-OE2	-5.13	1.15	1.25
3	B2	195	GLU	CD-OE2	-5.13	1.15	1.25
8	B7	224	LYS	CD-CE	-5.13	1.37	1.52
24	BN	-60	DA	C3'-C2'	5.12	1.56	1.52
8	A7	224	LYS	CD-CE	-5.12	1.37	1.52
19	AI	114	GLN	CD-OE1	-5.09	1.13	1.23
3	B2	506	LYS	CG-CD	-5.08	1.37	1.52
19	BI	114	GLN	CD-OE1	-5.08	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	BA	692	ASP	CA-C	5.07	1.59	1.52
61	E6	920	ASP	CB-CG	-5.07	1.39	1.52
3	A2	506	LYS	CG-CD	-5.07	1.37	1.52
11	AA	692	ASP	CA-C	5.07	1.59	1.52
60	E3	406	LYS	CD-CE	-5.07	1.37	1.52
61	E6	795	LEU	CG-CD1	-5.07	1.35	1.52
53	sE	519	TYR	CB-CG	-5.05	1.40	1.51
19	BI	85	PHE	N-CA	5.05	1.51	1.45
61	E6	113	TRP	CE3-CZ3	-5.05	1.23	1.38
2	B1	437	LEU	CG-CD2	-5.03	1.35	1.52
2	A1	437	LEU	CG-CD2	-5.03	1.35	1.52
53	SE	519	TYR	CB-CG	-5.03	1.40	1.51
26	BQ	22	ILE	CG1-CD1	-5.01	1.32	1.51
19	AI	85	PHE	N-CA	5.01	1.51	1.45
26	AQ	22	ILE	CG1-CD1	-5.01	1.32	1.51
64	T5	877	LYS	CG-CD	-5.01	1.37	1.52
64	t5	877	LYS	CG-CD	-5.00	1.37	1.52
19	BI	82	GLU	C-N	5.00	1.40	1.33
58	sK	147	LEU	CG-CD1	5.00	1.69	1.52

All (1320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A2	69	ASN	CA-CB-CG	54.96	167.56	112.60
3	B2	69	ASN	CA-CB-CG	54.95	167.56	112.60
50	sA	269	GLN	CA-CB-CG	32.94	179.98	114.10
50	SA	269	GLN	CA-CB-CG	32.94	179.97	114.10
10	A9	199	GLN	CA-CB-CG	32.92	179.93	114.10
55	SH	590	GLU	CA-CB-CG	32.92	179.93	114.10
10	B9	199	GLN	CA-CB-CG	32.91	179.91	114.10
55	sH	590	GLU	CA-CB-CG	32.89	179.88	114.10
3	B2	69	ASN	CB-CG-ND2	-32.11	68.23	116.40
3	A2	69	ASN	CB-CG-ND2	-32.11	68.24	116.40
64	T5	920	LYS	CB-CG-CD	29.86	179.98	111.30
64	t5	920	LYS	CB-CG-CD	29.86	179.97	111.30
55	sH	590	GLU	N-CA-CB	28.52	158.68	110.49
55	SH	590	GLU	N-CA-CB	28.49	158.64	110.49
50	sA	269	GLN	N-CA-CB	27.58	152.87	110.39
50	SA	269	GLN	N-CA-CB	27.58	152.86	110.39
60	E3	897	LYS	CA-CB-CG	27.05	168.20	114.10
18	BH	109	LYS	N-CA-C	-26.65	81.10	113.88
18	AH	109	LYS	N-CA-C	-26.65	81.10	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B3	64	ARG	CB-CG-CD	26.44	172.12	111.30
4	A3	64	ARG	CB-CG-CD	26.44	172.11	111.30
19	AI	86	PHE	CD1-CG-CD2	-26.24	79.25	118.60
19	BI	86	PHE	CD1-CG-CD2	-26.23	79.25	118.60
6	B5	3	ARG	CA-CB-CG	25.29	164.67	114.10
6	A5	3	ARG	CA-CB-CG	25.28	164.66	114.10
6	B5	3	ARG	CB-CG-CD	25.18	169.22	111.30
6	A5	3	ARG	CB-CG-CD	25.18	169.21	111.30
9	SF	389	ASN	CB-CG-ND2	-24.84	79.14	116.40
10	A9	200	MET	CA-CB-CG	24.83	163.76	114.10
10	B9	200	MET	CA-CB-CG	24.83	163.75	114.10
9	sF	389	ASN	CB-CG-ND2	-24.82	79.17	116.40
3	A2	490	LYS	CB-CG-CD	23.48	165.30	111.30
3	B2	490	LYS	CB-CG-CD	23.47	165.27	111.30
60	E3	406	LYS	CG-CD-CE	23.16	164.57	111.30
60	T3	837	TYR	CB-CG-CD2	-22.98	86.33	120.80
60	t3	837	TYR	CB-CG-CD2	-22.98	86.33	120.80
3	A2	69	ASN	CB-CG-OD1	22.94	166.68	120.80
3	B2	69	ASN	CB-CG-OD1	22.93	166.65	120.80
9	sF	401	LYS	CB-CA-C	22.50	155.20	110.42
9	SF	401	LYS	CB-CA-C	22.48	155.16	110.42
9	sF	401	LYS	CA-CB-CG	22.10	158.29	114.10
9	SF	401	LYS	CA-CB-CG	22.08	158.26	114.10
6	B5	5	ARG	CA-CB-CG	22.00	158.09	114.10
6	A5	5	ARG	CA-CB-CG	21.99	158.09	114.10
11	BA	688	LYS	CB-CG-CD	21.30	160.29	111.30
11	AA	688	LYS	CB-CG-CD	21.30	160.28	111.30
19	BI	77	LYS	CD-CE-NZ	21.28	179.99	111.90
19	AI	77	LYS	CD-CE-NZ	21.27	179.98	111.90
60	E3	409	LYS	CD-CE-NZ	21.27	179.96	111.90
64	t5	919	ARG	CD-NE-CZ	21.04	153.86	124.40
64	T5	919	ARG	CD-NE-CZ	21.03	153.84	124.40
28	AS	205	ASN	CA-C-N	20.88	159.55	121.97
28	AS	205	ASN	C-N-CA	20.88	159.55	121.97
28	BS	205	ASN	CA-C-N	20.84	159.48	121.97
28	BS	205	ASN	C-N-CA	20.84	159.48	121.97
6	A5	3	ARG	CG-CD-NE	20.47	157.03	112.00
6	B5	3	ARG	CG-CD-NE	20.46	157.02	112.00
64	T5	923	LYS	CB-CG-CD	20.43	158.29	111.30
64	t5	923	LYS	CB-CG-CD	20.42	158.26	111.30
19	BI	82	GLU	CB-CG-CD	20.42	147.31	112.60
19	AI	82	GLU	CB-CG-CD	20.40	147.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	92	ARG	CG-CD-NE	20.29	156.64	112.00
19	BI	92	ARG	CG-CD-NE	20.29	156.65	112.00
60	E3	897	LYS	CB-CG-CD	20.17	157.68	111.30
19	AI	93	LYS	CD-CE-NZ	19.87	175.50	111.90
19	BI	93	LYS	CD-CE-NZ	19.86	175.46	111.90
19	AI	92	ARG	CD-NE-CZ	-19.66	96.88	124.40
19	BI	92	ARG	CD-NE-CZ	-19.65	96.89	124.40
60	E3	418	LYS	CG-CD-CE	19.64	156.48	111.30
6	B5	5	ARG	NE-CZ-NH1	-19.37	102.13	121.50
20	AJ	58	GLU	CA-CB-CG	19.34	152.78	114.10
20	BJ	58	GLU	CA-CB-CG	19.34	152.77	114.10
11	BA	692	ASP	N-CA-C	-19.31	90.13	113.88
6	A5	5	ARG	NE-CZ-NH1	-19.30	102.20	121.50
11	AA	692	ASP	N-CA-C	-19.28	90.17	113.88
19	AI	91	ARG	CD-NE-CZ	19.18	151.25	124.40
19	BI	91	ARG	CD-NE-CZ	19.17	151.23	124.40
9	SF	401	LYS	CB-CG-CD	18.91	154.80	111.30
9	sF	401	LYS	CB-CG-CD	18.91	154.79	111.30
64	t5	923	LYS	CG-CD-CE	-18.80	68.07	111.30
64	T5	923	LYS	CG-CD-CE	-18.79	68.08	111.30
11	AA	688	LYS	CA-CB-CG	-18.77	76.56	114.10
11	BA	688	LYS	CA-CB-CG	-18.75	76.59	114.10
28	BS	206	VAL	CG1-CB-CG2	-18.74	69.56	110.80
28	AS	206	VAL	CG1-CB-CG2	-18.74	69.58	110.80
19	AI	93	LYS	CB-CG-CD	18.66	154.23	111.30
19	BI	93	LYS	CB-CG-CD	18.64	154.17	111.30
3	B2	506	LYS	CB-CG-CD	18.61	154.11	111.30
3	A2	506	LYS	CB-CG-CD	18.59	154.04	111.30
10	A9	199	GLN	N-CA-CB	18.55	141.85	110.49
10	B9	199	GLN	N-CA-CB	18.55	141.84	110.49
11	BA	676	MET	CB-CG-SD	18.33	167.69	112.70
11	AA	676	MET	CB-CG-SD	18.33	167.68	112.70
19	AI	78	CYS	CB-CA-C	-18.20	73.24	110.38
19	BI	78	CYS	CB-CA-C	-18.20	73.24	110.38
9	SF	389	ASN	OD1-CG-ND2	-17.98	104.62	122.60
9	sF	389	ASN	OD1-CG-ND2	-17.98	104.62	122.60
11	BA	688	LYS	N-CA-C	-17.32	92.15	113.28
11	AA	688	LYS	N-CA-C	-17.32	92.15	113.28
45	t4	1018	MET	N-CA-CB	17.17	134.97	109.91
45	T4	1018	MET	N-CA-CB	17.16	134.96	109.91
3	A2	463	GLU	CG-CD-OE1	-16.97	79.38	118.40
3	B2	463	GLU	CG-CD-OE1	-16.95	79.41	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B2	97	MET	CB-CG-SD	16.86	163.29	112.70
3	A2	97	MET	CB-CG-SD	16.86	163.27	112.70
19	AI	75	CYS	CB-CA-C	-16.81	84.17	109.56
19	BI	75	CYS	CB-CA-C	-16.81	84.18	109.56
19	BI	61	ASP	N-CA-C	-16.69	92.23	112.59
19	AI	61	ASP	N-CA-C	-16.64	92.28	112.59
28	BS	206	VAL	N-CA-CB	16.47	138.41	111.23
28	AS	206	VAL	N-CA-CB	16.45	138.37	111.23
64	t5	920	LYS	CA-CB-CG	16.44	146.97	114.10
64	T5	920	LYS	CA-CB-CG	16.42	146.94	114.10
19	AI	86	PHE	CG-CD1-CE1	16.22	148.28	120.70
9	SF	389	ASN	CB-CG-OD1	16.20	153.21	120.80
19	BI	86	PHE	CG-CD1-CE1	16.19	148.22	120.70
9	sF	389	ASN	CB-CG-OD1	16.19	153.17	120.80
19	BI	62	ILE	CB-CG1-CD1	16.08	147.56	113.80
19	AI	62	ILE	CB-CG1-CD1	16.08	147.56	113.80
19	AI	86	PHE	CB-CG-CD2	-15.78	93.88	120.70
19	BI	86	PHE	CB-CG-CD2	-15.78	93.88	120.70
11	AA	676	MET	N-CA-CB	-15.61	84.11	110.49
11	BA	676	MET	N-CA-CB	-15.60	84.13	110.49
19	AI	84	VAL	CA-CB-CG2	15.53	136.80	110.40
19	BI	84	VAL	CA-CB-CG2	15.52	136.78	110.40
10	B9	200	MET	CB-CG-SD	15.25	158.46	112.70
10	A9	200	MET	CB-CG-SD	15.25	158.45	112.70
60	E3	412	ARG	CB-CG-CD	15.20	146.25	111.30
60	t3	837	TYR	CD1-CG-CD2	-15.04	95.53	118.10
60	T3	837	TYR	CD1-CG-CD2	-15.03	95.55	118.10
3	B2	490	LYS	CG-CD-CE	14.99	145.77	111.30
3	A2	490	LYS	CG-CD-CE	14.98	145.75	111.30
60	E3	418	LYS	CB-CG-CD	14.96	145.72	111.30
58	sK	91	TYR	CE1-CZ-OH	-14.89	75.23	119.90
58	SK	91	TYR	CE1-CZ-OH	-14.88	75.27	119.90
19	AI	84	VAL	N-CA-CB	14.55	131.04	111.25
19	BI	84	VAL	N-CA-CB	14.52	130.99	111.25
19	AI	82	GLU	CA-CB-CG	14.47	143.04	114.10
19	BI	82	GLU	CA-CB-CG	14.44	142.98	114.10
60	E3	939	THR	N-CA-C	-14.32	94.14	112.90
55	sH	590	GLU	CB-CA-C	-14.30	81.96	110.42
55	SH	590	GLU	CB-CA-C	-14.29	81.98	110.42
9	sF	401	LYS	N-CA-CB	-14.26	86.40	110.49
9	SF	401	LYS	N-CA-CB	-14.23	86.44	110.49
64	t5	877	LYS	CG-CD-CE	14.19	143.94	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	T5	877	LYS	CG-CD-CE	14.17	143.90	111.30
10	A9	200	MET	N-CA-CB	14.07	132.09	110.28
10	B9	200	MET	N-CA-CB	14.07	132.08	110.28
10	A9	209	MET	CA-CB-CG	14.05	142.19	114.10
10	B9	209	MET	CA-CB-CG	14.03	142.16	114.10
11	AA	692	ASP	OD1-CG-OD2	-13.90	89.54	122.90
11	BA	692	ASP	OD1-CG-OD2	-13.90	89.53	122.90
19	AI	75	CYS	CA-CB-SG	13.84	146.22	114.40
19	BI	75	CYS	CA-CB-SG	13.83	146.20	114.40
38	me	55	ARG	CG-CD-NE	13.55	141.81	112.00
38	Me	55	ARG	CG-CD-NE	13.54	141.79	112.00
19	BI	82	GLU	N-CA-CB	13.46	132.80	110.59
19	AI	82	GLU	N-CA-CB	13.45	132.79	110.59
19	AI	86	PHE	CB-CG-CD1	13.40	143.49	120.70
4	B3	49	LEU	N-CA-C	-13.38	96.57	113.43
19	BI	86	PHE	CB-CG-CD1	13.38	143.44	120.70
4	A3	49	LEU	N-CA-C	-13.37	96.58	113.43
3	B2	69	ASN	N-CA-CB	13.28	129.82	110.16
3	A2	69	ASN	N-CA-CB	13.27	129.81	110.16
64	t5	919	ARG	CA-CB-CG	13.26	140.63	114.10
64	T5	919	ARG	CA-CB-CG	13.25	140.60	114.10
4	A3	49	LEU	N-CA-CB	-13.15	88.16	110.51
4	B3	49	LEU	N-CA-CB	-13.14	88.17	110.51
3	A2	463	GLU	CG-CD-OE2	12.91	148.10	118.40
3	B2	463	GLU	CG-CD-OE2	12.89	148.06	118.40
12	BB	19	GLU	CG-CD-OE1	12.88	148.03	118.40
12	AB	19	GLU	CG-CD-OE1	12.87	147.99	118.40
60	T3	837	TYR	CG-CD1-CE1	12.80	140.40	121.20
60	t3	837	TYR	CG-CD1-CE1	12.79	140.39	121.20
10	B9	217	GLU	CG-CD-OE1	12.78	147.79	118.40
10	A9	217	GLU	CG-CD-OE1	12.78	147.79	118.40
64	T5	931	GLN	CB-CG-CD	12.73	134.24	112.60
64	t5	931	GLN	CB-CG-CD	12.72	134.23	112.60
19	AI	113	ASP	CA-CB-CG	12.71	125.31	112.60
19	BI	113	ASP	CA-CB-CG	12.68	125.28	112.60
6	B5	5	ARG	CG-CD-NE	-12.67	84.13	112.00
6	A5	5	ARG	CG-CD-NE	-12.66	84.14	112.00
53	sE	547	ARG	NE-CZ-NH2	12.62	130.56	119.20
28	BS	198	ARG	CD-NE-CZ	-12.60	106.76	124.40
28	AS	198	ARG	CD-NE-CZ	-12.57	106.80	124.40
53	SE	547	ARG	NE-CZ-NH2	12.54	130.49	119.20
64	T5	920	LYS	CG-CD-CE	-12.51	82.52	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	t5	920	LYS	CG-CD-CE	-12.51	82.53	111.30
9	sF	401	LYS	CG-CD-CE	-12.51	82.54	111.30
64	T5	931	GLN	CG-CD-NE2	-12.50	97.64	116.40
10	B9	217	GLU	OE1-CD-OE2	-12.50	92.89	122.90
9	SF	401	LYS	CG-CD-CE	-12.50	82.55	111.30
10	A9	217	GLU	OE1-CD-OE2	-12.50	92.91	122.90
10	B9	217	GLU	CA-CB-CG	12.50	139.10	114.10
10	A9	217	GLU	CA-CB-CG	12.48	139.07	114.10
64	t5	931	GLN	CG-CD-NE2	-12.48	97.68	116.40
10	A9	209	MET	CB-CA-C	12.45	131.00	110.22
10	B9	209	MET	CB-CA-C	12.45	131.00	110.22
51	SB	432	VAL	CG1-CB-CG2	-12.39	83.55	110.80
51	sB	432	VAL	CG1-CB-CG2	-12.38	83.56	110.80
4	A3	64	ARG	N-CA-C	12.38	128.44	110.24
4	B3	64	ARG	N-CA-C	12.37	128.43	110.24
4	A3	49	LEU	CB-CA-C	12.33	130.36	109.65
4	B3	64	ARG	CG-CD-NE	12.32	139.10	112.00
4	A3	64	ARG	CG-CD-NE	12.31	139.09	112.00
4	B3	49	LEU	CB-CA-C	12.30	130.31	109.65
6	B5	3	ARG	CD-NE-CZ	12.29	141.61	124.40
6	A5	3	ARG	CD-NE-CZ	12.29	141.61	124.40
19	AI	62	ILE	CA-CB-CG1	12.25	131.22	110.40
50	SA	269	GLN	CB-CG-CD	-12.24	91.78	112.60
60	T3	837	TYR	N-CA-CB	-12.24	91.88	111.22
60	t3	837	TYR	N-CA-CB	-12.24	91.88	111.22
19	BI	62	ILE	CA-CB-CG1	12.23	131.20	110.40
50	sA	269	GLN	CB-CG-CD	-12.20	91.85	112.60
55	SH	594	LEU	CB-CG-CD2	-12.18	74.17	110.70
55	sH	594	LEU	CB-CG-CD2	-12.16	74.21	110.70
60	E3	939	THR	CA-CB-CG2	-12.12	89.89	110.50
60	t3	837	TYR	CB-CG-CD1	12.09	138.93	120.80
60	T3	837	TYR	CB-CG-CD1	12.08	138.92	120.80
6	B5	5	ARG	NE-CZ-NH2	12.06	130.06	119.20
6	A5	5	ARG	NE-CZ-NH2	12.05	130.04	119.20
3	A2	97	MET	CA-CB-CG	-12.02	90.06	114.10
3	B2	97	MET	CA-CB-CG	-12.02	90.07	114.10
55	SH	594	LEU	CB-CA-C	11.98	132.63	110.70
55	sH	594	LEU	CB-CA-C	11.98	132.63	110.70
53	sE	514	GLU	OE1-CD-OE2	-11.93	94.28	122.90
53	SE	514	GLU	OE1-CD-OE2	-11.92	94.29	122.90
19	AI	60	GLN	CA-C-N	-11.86	103.82	122.67
19	AI	60	GLN	C-N-CA	-11.86	103.82	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BI	60	GLN	CA-C-N	-11.85	103.82	122.67
19	BI	60	GLN	C-N-CA	-11.85	103.82	122.67
61	E6	749	LEU	CD1-CG-CD2	11.69	136.52	110.80
64	t5	920	LYS	CB-CA-C	11.56	125.64	109.92
64	T5	920	LYS	CB-CA-C	11.55	125.62	109.92
12	BB	19	GLU	CB-CG-CD	11.54	132.22	112.60
12	AB	19	GLU	CB-CG-CD	11.52	132.18	112.60
19	BI	115	LYS	CG-CD-CE	11.34	137.38	111.30
19	AI	115	LYS	CG-CD-CE	11.34	137.38	111.30
55	sH	592	LEU	CB-CG-CD2	11.29	144.56	110.70
55	SH	592	LEU	CB-CG-CD2	11.27	144.50	110.70
27	AR	228	MET	CA-CB-CG	-11.22	91.65	114.10
19	BI	60	GLN	OE1-CD-NE2	-11.22	111.38	122.60
27	BR	228	MET	CA-CB-CG	-11.21	91.69	114.10
19	AI	60	GLN	OE1-CD-NE2	-11.20	111.40	122.60
60	t3	406	LYS	CA-C-N	11.20	138.99	120.62
60	t3	406	LYS	C-N-CA	11.20	138.99	120.62
60	T3	406	LYS	CA-C-N	11.18	138.96	120.62
60	T3	406	LYS	C-N-CA	11.18	138.96	120.62
55	SH	594	LEU	CD1-CG-CD2	-11.16	86.26	110.80
55	sH	594	LEU	CD1-CG-CD2	-11.15	86.26	110.80
60	E3	413	ILE	N-CA-C	-11.13	100.02	110.82
60	E3	675	GLU	CG-CD-OE2	-11.11	92.85	118.40
12	AB	19	GLU	CG-CD-OE2	-11.09	92.89	118.40
12	BB	19	GLU	CG-CD-OE2	-11.09	92.91	118.40
20	BJ	58	GLU	CB-CA-C	-11.07	93.50	110.88
20	AJ	58	GLU	CB-CA-C	-11.06	93.52	110.88
6	B5	3	ARG	N-CA-CB	10.96	130.84	111.00
6	A5	3	ARG	N-CA-CB	10.94	130.79	111.00
12	BB	22	SER	CA-C-O	-10.92	104.89	120.51
45	T4	1018	MET	CB-CA-C	-10.92	94.14	110.96
45	t4	1018	MET	CB-CA-C	-10.91	94.15	110.96
12	AB	22	SER	CA-C-O	-10.91	104.91	120.51
61	E6	749	LEU	CB-CG-CD1	-10.91	77.98	110.70
28	AS	232	ASP	CB-CA-C	10.86	128.26	110.88
28	BS	232	ASP	CB-CA-C	10.85	128.24	110.88
64	T5	919	ARG	CG-CD-NE	-10.79	88.25	112.00
28	AS	182	MET	CG-SD-CE	10.79	124.64	100.90
28	BS	182	MET	CG-SD-CE	10.78	124.60	100.90
64	t5	919	ARG	CG-CD-NE	-10.77	88.30	112.00
45	T4	1018	MET	CB-CG-SD	10.76	144.97	112.70
19	BI	93	LYS	CA-CB-CG	-10.75	92.60	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	104	LEU	CD1-CG-CD2	-10.75	87.15	110.80
45	t4	1018	MET	CB-CG-SD	10.75	144.95	112.70
19	BI	104	LEU	CD1-CG-CD2	-10.75	87.16	110.80
19	AI	93	LYS	CA-CB-CG	-10.73	92.65	114.10
61	t6	760	ALA	CA-C-N	10.72	142.03	121.54
61	t6	760	ALA	C-N-CA	10.72	142.03	121.54
53	SE	463	PRO	CA-N-CD	-10.71	97.01	112.00
60	E3	418	LYS	CD-CE-NZ	10.71	146.16	111.90
55	SH	594	LEU	CA-CB-CG	10.70	153.75	116.30
55	sH	594	LEU	CA-CB-CG	10.70	153.76	116.30
61	T6	760	ALA	CA-C-N	10.70	141.98	121.54
61	T6	760	ALA	C-N-CA	10.70	141.98	121.54
53	sE	463	PRO	CA-N-CD	-10.69	97.04	112.00
10	B9	209	MET	N-CA-CB	-10.56	92.42	110.17
10	A9	209	MET	N-CA-CB	-10.56	92.43	110.17
28	AS	206	VAL	CB-CA-C	-10.54	94.01	111.29
28	BS	206	VAL	CB-CA-C	-10.53	94.03	111.29
11	AA	692	ASP	CA-CB-CG	10.52	123.12	112.60
11	BA	692	ASP	CA-CB-CG	10.50	123.10	112.60
3	B2	463	GLU	CB-CG-CD	10.48	130.41	112.60
12	BB	22	SER	CA-C-N	10.47	141.01	122.48
12	BB	22	SER	C-N-CA	10.47	141.01	122.48
3	A2	463	GLU	CB-CG-CD	10.46	130.38	112.60
28	BS	182	MET	CB-CA-C	10.45	128.19	110.84
12	AB	22	SER	CA-C-N	10.44	140.97	122.48
12	AB	22	SER	C-N-CA	10.44	140.97	122.48
19	BI	111	THR	OG1-CB-CG2	-10.43	88.44	109.30
28	AS	182	MET	CB-CA-C	10.42	128.14	110.84
19	AI	111	THR	OG1-CB-CG2	-10.41	88.47	109.30
28	BS	209	LYS	CD-CE-NZ	-10.29	78.96	111.90
28	AS	209	LYS	CD-CE-NZ	-10.29	78.98	111.90
60	E3	939	THR	CB-CA-C	-10.27	89.02	109.67
12	AB	662	MET	CB-CG-SD	10.24	143.43	112.70
12	BB	662	MET	CB-CG-SD	10.24	143.43	112.70
19	AI	62	ILE	CA-CB-CG2	10.24	127.90	110.50
19	BI	62	ILE	CA-CB-CG2	10.23	127.90	110.50
60	E3	372	LYS	CG-CD-CE	-10.23	87.77	111.30
9	SF	389	ASN	N-CA-C	-10.22	99.08	112.68
29	BT	60	DT	O4'-C1'-N1	10.22	115.16	108.00
29	AT	60	DT	O4'-C1'-N1	10.21	115.14	108.00
9	sF	389	ASN	N-CA-C	-10.21	99.10	112.68
24	AN	-43	DA	O4'-C1'-C2'	-10.14	97.78	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BN	-43	DA	O4'-C1'-C2'	-10.14	97.79	105.90
9	SF	393	LYS	CA-CB-CG	10.10	134.31	114.10
9	sF	393	LYS	CA-CB-CG	10.09	134.27	114.10
19	BI	91	ARG	CA-CB-CG	-10.07	93.96	114.10
60	E3	412	ARG	CG-CD-NE	10.07	134.15	112.00
19	AI	91	ARG	CA-CB-CG	-10.06	93.97	114.10
53	sE	547	ARG	NH1-CZ-NH2	-10.05	106.23	119.30
28	AS	209	LYS	CG-CD-CE	10.04	134.39	111.30
28	BS	209	LYS	CG-CD-CE	10.03	134.36	111.30
53	SE	547	ARG	NH1-CZ-NH2	-10.00	106.30	119.30
29	AT	44	DC	P-O3'-C3'	9.98	131.68	119.70
29	BT	44	DC	P-O3'-C3'	9.95	131.64	119.70
61	E6	972	MET	CG-SD-CE	-9.95	79.01	100.90
60	E3	406	LYS	CD-CE-NZ	9.92	143.64	111.90
19	AI	78	CYS	N-CA-CB	9.90	125.55	110.30
19	BI	78	CYS	N-CA-CB	9.89	125.54	110.30
28	BS	182	MET	N-CA-CB	-9.88	92.93	109.72
9	sF	389	ASN	CB-CA-C	9.87	126.72	110.24
28	AS	182	MET	N-CA-CB	-9.87	92.95	109.72
9	SF	389	ASN	CB-CA-C	9.86	126.70	110.24
10	B9	199	GLN	OE1-CD-NE2	-9.83	112.77	122.60
53	SE	547	ARG	NE-CZ-NH1	-9.80	111.70	121.50
10	A9	199	GLN	OE1-CD-NE2	-9.77	112.83	122.60
53	sE	547	ARG	NE-CZ-NH1	-9.77	111.73	121.50
19	BI	113	ASP	N-CA-CB	9.73	126.94	110.49
19	AI	113	ASP	N-CA-CB	9.70	126.88	110.49
60	E3	406	LYS	CB-CG-CD	9.69	133.59	111.30
27	BR	228	MET	CG-SD-CE	9.69	122.22	100.90
27	AR	228	MET	CG-SD-CE	9.67	122.18	100.90
60	T3	836	ILE	N-CA-CB	9.66	131.01	110.64
60	t3	836	ILE	N-CA-CB	9.65	131.01	110.64
10	A9	217	GLU	N-CA-CB	9.61	127.22	111.27
10	B9	217	GLU	N-CA-CB	9.59	127.19	111.27
60	T3	837	TYR	CA-CB-CG	9.59	131.16	113.90
60	t3	837	TYR	CA-CB-CG	9.58	131.15	113.90
53	SE	519	TYR	OH-CZ-CE2	-9.50	91.40	119.90
53	sE	519	TYR	OH-CZ-CE2	-9.48	91.45	119.90
3	A2	490	LYS	N-CA-CB	-9.44	94.19	111.37
9	sF	389	ASN	CA-CB-CG	9.44	122.04	112.60
19	AI	62	ILE	CB-CA-C	-9.42	93.79	111.79
19	BI	62	ILE	CB-CA-C	-9.42	93.79	111.79
3	B2	490	LYS	N-CA-CB	-9.42	94.22	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	E3	412	ARG	N-CA-CB	9.42	126.03	110.39
9	SF	389	ASN	CA-CB-CG	9.41	122.01	112.60
19	BI	77	LYS	CB-CG-CD	9.38	132.87	111.30
19	AI	77	LYS	CB-CG-CD	9.38	132.87	111.30
53	SE	464	ASN	CA-C-N	9.34	139.37	121.54
53	SE	464	ASN	C-N-CA	9.34	139.37	121.54
55	sH	592	LEU	CD1-CG-CD2	-9.33	90.28	110.80
55	SH	592	LEU	CD1-CG-CD2	-9.32	90.29	110.80
53	sE	464	ASN	CA-C-N	9.32	139.35	121.54
53	sE	464	ASN	C-N-CA	9.32	139.35	121.54
60	T3	409	LYS	N-CA-CB	9.32	126.25	110.49
60	t3	409	LYS	N-CA-CB	9.31	126.22	110.49
35	Mb	49	ARG	CD-NE-CZ	-9.22	111.49	124.40
35	mb	49	ARG	CD-NE-CZ	-9.20	111.52	124.40
19	AI	91	ARG	CG-CD-NE	9.19	132.22	112.00
19	BI	91	ARG	CG-CD-NE	9.18	132.20	112.00
28	BS	206	VAL	CA-CB-CG1	-9.16	94.82	110.40
28	AS	206	VAL	CA-CB-CG1	-9.16	94.83	110.40
53	SE	510	SER	CA-C-O	-9.02	110.81	120.92
64	T5	920	LYS	CD-CE-NZ	9.02	140.77	111.90
64	t5	920	LYS	CD-CE-NZ	9.02	140.77	111.90
53	sE	510	SER	CA-C-O	-9.00	110.84	120.92
56	SI	656	TYR	CA-CB-CG	8.99	130.09	113.90
60	E3	897	LYS	N-CA-CB	-8.99	96.80	110.20
56	sI	656	TYR	CA-CB-CG	8.99	130.07	113.90
3	B2	464	THR	OG1-CB-CG2	-8.97	91.36	109.30
3	A2	464	THR	OG1-CB-CG2	-8.96	91.37	109.30
11	BA	676	MET	CB-CA-C	8.96	128.25	110.42
11	AA	676	MET	CB-CA-C	8.96	128.24	110.42
11	AA	1444	MET	CG-SD-CE	-8.94	81.23	100.90
11	BA	1444	MET	CG-SD-CE	-8.94	81.24	100.90
28	BS	198	ARG	CA-CB-CG	8.89	131.89	114.10
28	AS	198	ARG	CA-CB-CG	8.88	131.87	114.10
18	BH	130	ARG	NE-CZ-NH2	-8.88	111.21	119.20
18	AH	130	ARG	NE-CZ-NH2	-8.87	111.22	119.20
10	B9	217	GLU	CG-CD-OE2	-8.86	98.03	118.40
10	A9	217	GLU	CG-CD-OE2	-8.85	98.05	118.40
28	BS	232	ASP	OD1-CG-OD2	-8.80	101.77	122.90
28	AS	232	ASP	OD1-CG-OD2	-8.80	101.78	122.90
3	B2	490	LYS	CA-CB-CG	8.80	131.70	114.10
3	A2	490	LYS	CA-CB-CG	8.79	131.69	114.10
3	B2	506	LYS	N-CA-CB	-8.78	96.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A2	506	LYS	N-CA-CB	-8.78	96.10	110.40
19	BI	78	CYS	CA-CB-SG	8.77	134.58	114.40
19	AI	78	CYS	CA-CB-SG	8.77	134.58	114.40
12	BB	662	MET	CA-CB-CG	8.75	131.61	114.10
60	T3	292	ARG	CD-NE-CZ	8.75	136.65	124.40
12	AB	662	MET	CA-CB-CG	8.75	131.59	114.10
60	t3	292	ARG	CD-NE-CZ	8.72	136.61	124.40
60	T3	289	LYS	N-CA-CB	8.72	122.89	110.07
60	t3	289	LYS	N-CA-CB	8.71	122.87	110.07
19	AI	94	ASP	OD1-CG-OD2	-8.68	102.07	122.90
19	BI	94	ASP	OD1-CG-OD2	-8.67	102.09	122.90
18	AH	109	LYS	N-CA-CB	8.63	122.07	110.59
18	BH	109	LYS	N-CA-CB	8.62	122.05	110.59
29	BT	61	DA	OP2-P-O3'	8.61	133.83	108.00
29	AT	61	DA	OP2-P-O3'	8.61	133.81	108.00
19	BI	94	ASP	CB-CG-OD2	-8.59	98.64	118.40
61	t6	761	LYS	CB-CG-CD	8.58	131.03	111.30
19	AI	94	ASP	CB-CG-OD2	-8.57	98.68	118.40
19	BI	76	PRO	N-CA-C	8.57	130.12	112.47
61	T6	761	LYS	CB-CG-CD	8.56	130.99	111.30
19	AI	76	PRO	N-CA-C	8.54	130.07	112.47
53	SE	519	TYR	CE1-CZ-OH	8.54	145.51	119.90
19	AI	94	ASP	CA-CB-CG	8.53	121.13	112.60
53	sE	519	TYR	CE1-CZ-OH	8.52	145.47	119.90
19	BI	94	ASP	CA-CB-CG	8.49	121.09	112.60
60	E3	897	LYS	CG-CD-CE	8.48	130.81	111.30
19	AI	60	GLN	CG-CD-NE2	-8.47	103.70	116.40
19	BI	60	GLN	CG-CD-NE2	-8.47	103.70	116.40
64	t5	931	GLN	OE1-CD-NE2	-8.44	114.16	122.60
19	BI	114	GLN	CG-CD-NE2	-8.43	103.75	116.40
9	SF	485	LEU	CD1-CG-CD2	-8.43	92.25	110.80
9	SF	321	LEU	CD1-CG-CD2	-8.43	92.26	110.80
9	sF	321	LEU	CD1-CG-CD2	-8.43	92.26	110.80
19	AI	114	GLN	CG-CD-NE2	-8.42	103.77	116.40
9	sF	485	LEU	CD1-CG-CD2	-8.42	92.27	110.80
64	T5	931	GLN	OE1-CD-NE2	-8.41	114.19	122.60
19	AI	111	THR	N-CA-C	-8.40	97.86	109.95
53	SE	454	LEU	CD1-CG-CD2	-8.39	92.34	110.80
19	AI	86	PHE	N-CA-CB	8.38	124.81	111.56
19	BI	86	PHE	N-CA-CB	8.38	124.80	111.56
63	t2	107	LYS	O-C-N	-8.38	110.90	122.46
19	BI	111	THR	N-CA-C	-8.38	97.89	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	sE	454	LEU	CD1-CG-CD2	-8.37	92.38	110.80
60	E3	939	THR	N-CA-CB	8.37	122.88	110.33
63	T2	107	LYS	O-C-N	-8.37	110.91	122.46
9	SF	389	ASN	N-CA-CB	-8.33	96.34	110.33
64	t5	931	GLN	CG-CD-OE1	8.33	137.45	120.80
9	sF	389	ASN	N-CA-CB	-8.32	96.35	110.33
60	E3	939	THR	OG1-CB-CG2	-8.32	92.66	109.30
51	SD	743	CYS	CB-CA-C	-8.32	97.76	110.90
12	AB	21	GLU	CA-C-O	-8.31	108.62	120.51
64	T5	931	GLN	CG-CD-OE1	8.31	137.43	120.80
12	BB	21	GLU	CA-C-O	-8.31	108.62	120.51
51	sD	743	CYS	CB-CA-C	-8.31	97.77	110.90
50	sA	269	GLN	CB-CA-C	-8.26	97.22	112.00
50	SA	269	GLN	CB-CA-C	-8.25	97.23	112.00
19	AI	68	LEU	N-CA-C	8.23	119.06	109.60
53	SE	512	LEU	N-CA-C	8.21	123.58	111.34
19	BI	68	LEU	N-CA-C	8.21	119.04	109.60
53	sE	512	LEU	N-CA-C	8.20	123.56	111.34
45	t4	1018	MET	CG-SD-CE	-8.17	82.93	100.90
45	T4	1018	MET	CG-SD-CE	-8.15	82.96	100.90
9	sF	393	LYS	CB-CA-C	8.07	125.47	110.70
19	AI	77	LYS	CG-CD-CE	-8.07	92.74	111.30
9	SF	393	LYS	CB-CA-C	8.07	125.46	110.70
19	BI	77	LYS	CG-CD-CE	-8.06	92.76	111.30
53	sE	509	ARG	CA-C-N	8.06	132.91	120.82
53	sE	509	ARG	C-N-CA	8.06	132.91	120.82
9	SF	333	ASP	CA-C-N	8.06	136.93	121.54
9	SF	333	ASP	C-N-CA	8.06	136.93	121.54
9	sF	333	ASP	CA-C-N	8.05	136.92	121.54
9	sF	333	ASP	C-N-CA	8.05	136.92	121.54
53	SE	509	ARG	CA-C-N	8.05	132.89	120.82
53	SE	509	ARG	C-N-CA	8.05	132.89	120.82
19	AI	83	ASN	CA-C-N	8.04	133.16	123.19
19	AI	83	ASN	C-N-CA	8.04	133.16	123.19
11	BA	1277	GLU	O-C-N	-8.03	111.91	122.59
11	AA	1277	GLU	O-C-N	-8.02	111.92	122.59
28	BS	227	PHE	N-CA-C	8.01	121.18	111.40
19	BI	94	ASP	CB-CG-OD1	8.01	136.83	118.40
19	AI	94	ASP	CB-CG-OD1	8.00	136.80	118.40
28	AS	227	PHE	N-CA-C	7.98	121.14	111.40
6	A5	5	ARG	CD-NE-CZ	7.97	135.56	124.40
19	BI	83	ASN	CA-C-N	7.97	133.07	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BI	83	ASN	C-N-CA	7.97	133.07	123.19
19	AI	114	GLN	OE1-CD-NE2	-7.97	114.63	122.60
6	B5	5	ARG	CD-NE-CZ	7.96	135.55	124.40
19	BI	114	GLN	OE1-CD-NE2	-7.93	114.67	122.60
11	BA	683	ILE	CA-C-N	7.89	133.88	120.71
11	BA	683	ILE	C-N-CA	7.89	133.88	120.71
6	A5	5	ARG	CB-CG-CD	7.87	129.39	111.30
19	BI	88	SER	CB-CA-C	7.86	122.04	109.61
19	AI	88	SER	CB-CA-C	7.86	122.03	109.61
6	B5	5	ARG	CB-CG-CD	7.86	129.37	111.30
19	AI	92	ARG	N-CA-CB	7.82	122.78	111.05
19	BI	92	ARG	N-CA-CB	7.81	122.77	111.05
60	E3	439	ILE	CA-CB-CG2	7.81	123.78	110.50
28	AS	230	THR	OG1-CB-CG2	7.80	124.89	109.30
64	T5	919	ARG	CB-CG-CD	7.79	129.22	111.30
64	t5	919	ARG	CB-CG-CD	7.79	129.22	111.30
28	BS	230	THR	OG1-CB-CG2	7.79	124.88	109.30
28	AS	206	VAL	N-CA-C	-7.76	93.20	109.34
28	BS	206	VAL	N-CA-C	-7.75	93.21	109.34
53	sE	527	THR	CA-CB-OG1	-7.75	97.98	109.60
53	SE	527	THR	CA-CB-OG1	-7.74	97.99	109.60
19	BI	115	LYS	CD-CE-NZ	-7.74	87.13	111.90
19	AI	115	LYS	CD-CE-NZ	-7.73	87.16	111.90
64	t5	919	ARG	CA-C-N	7.72	136.20	122.08
64	t5	919	ARG	C-N-CA	7.72	136.20	122.08
64	T5	919	ARG	CA-C-N	7.71	136.18	122.08
64	T5	919	ARG	C-N-CA	7.71	136.18	122.08
6	A5	3	ARG	CB-CA-C	-7.70	94.11	109.35
6	B5	3	ARG	CB-CA-C	-7.70	94.10	109.35
36	Mc	44	VAL	CA-C-N	7.70	132.36	120.97
36	Mc	44	VAL	C-N-CA	7.70	132.36	120.97
64	t5	919	ARG	N-CA-C	7.69	121.03	109.95
21	BK	1	MET	CG-SD-CE	-7.69	83.98	100.90
21	AK	1	MET	CG-SD-CE	-7.67	84.02	100.90
56	sI	1248	LEU	CD1-CG-CD2	-7.67	93.92	110.80
60	T3	836	ILE	CB-CG1-CD1	-7.67	97.69	113.80
60	t3	836	ILE	CB-CG1-CD1	-7.67	97.69	113.80
56	SI	1248	LEU	CD1-CG-CD2	-7.67	93.93	110.80
19	BI	60	GLN	CG-CD-OE1	7.66	136.12	120.80
64	T5	919	ARG	N-CA-C	7.66	120.98	109.95
36	mc	44	VAL	CA-C-N	7.66	132.30	120.97
36	mc	44	VAL	C-N-CA	7.66	132.30	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	60	GLN	CG-CD-OE1	7.64	136.09	120.80
60	T3	919	TYR	CZ-CE2-CD2	7.64	133.35	119.60
10	A9	199	GLN	CG-CD-NE2	-7.63	104.95	116.40
60	t3	919	TYR	CZ-CE2-CD2	7.63	133.34	119.60
10	B9	199	GLN	CG-CD-NE2	-7.62	104.96	116.40
10	B9	209	MET	CG-SD-CE	-7.62	84.13	100.90
10	A9	209	MET	CG-SD-CE	-7.62	84.15	100.90
19	AI	104	LEU	CB-CG-CD1	7.61	133.51	110.70
19	BI	104	LEU	CB-CG-CD1	7.61	133.52	110.70
55	SH	600	GLU	CG-CD-OE1	-7.60	100.91	118.40
55	sH	600	GLU	CG-CD-OE1	-7.59	100.93	118.40
28	BS	171	ILE	CA-CB-CG1	7.58	123.29	110.40
28	AS	171	ILE	CA-CB-CG1	7.57	123.26	110.40
9	sF	398	THR	N-CA-C	7.56	126.90	110.80
9	SF	398	THR	N-CA-C	7.55	126.88	110.80
1	A0	537	MET	CG-SD-CE	7.54	117.48	100.90
12	AB	18	PHE	N-CA-C	-7.53	101.17	112.54
12	BB	18	PHE	N-CA-C	-7.52	101.18	112.54
1	B0	537	MET	CG-SD-CE	7.51	117.43	100.90
28	AS	235	ASP	CB-CA-C	-7.50	95.50	110.42
28	BS	235	ASP	CB-CA-C	-7.49	95.51	110.42
19	BI	88	SER	N-CA-C	7.49	120.83	110.35
59	sL	306	ILE	N-CA-C	-7.48	106.02	113.20
59	SL	306	ILE	N-CA-C	-7.48	106.02	113.20
19	AI	88	SER	N-CA-C	7.48	120.82	110.35
19	AI	62	ILE	CG1-CB-CG2	-7.46	88.32	110.70
53	SE	469	LEU	CD1-CG-CD2	-7.46	94.38	110.80
53	sE	452	ASN	N-CA-C	7.46	122.60	111.04
19	BI	62	ILE	CG1-CB-CG2	-7.46	88.33	110.70
53	SE	452	ASN	N-CA-C	7.45	122.58	111.04
19	AI	86	PHE	CD1-CE1-CZ	-7.45	106.60	120.00
53	sE	469	LEU	CD1-CG-CD2	-7.44	94.43	110.80
9	SF	448	GLN	CG-CD-NE2	7.43	127.55	116.40
60	t3	838	SER	CB-CA-C	-7.43	98.36	110.77
9	sF	448	GLN	CG-CD-NE2	7.43	127.54	116.40
60	T3	838	SER	CB-CA-C	-7.42	98.37	110.77
64	T5	877	LYS	CD-CE-NZ	7.42	135.65	111.90
19	BI	86	PHE	CD1-CE1-CZ	-7.41	106.66	120.00
64	t5	877	LYS	CD-CE-NZ	7.41	135.60	111.90
60	E3	413	ILE	CB-CG1-CD1	7.37	129.27	113.80
19	BI	77	LYS	CA-CB-CG	-7.36	99.38	114.10
19	AI	77	LYS	CA-CB-CG	-7.35	99.40	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SF	398	THR	OG1-CB-CG2	7.31	123.92	109.30
9	sF	398	THR	OG1-CB-CG2	7.30	123.91	109.30
27	BR	289	ILE	CA-C-N	7.29	134.26	122.81
27	BR	289	ILE	C-N-CA	7.29	134.26	122.81
9	sF	392	MET	CB-CG-SD	-7.29	90.83	112.70
9	SF	392	MET	CB-CG-SD	-7.29	90.83	112.70
27	AR	289	ILE	CA-C-N	7.28	134.25	122.81
27	AR	289	ILE	C-N-CA	7.28	134.25	122.81
4	A3	49	LEU	CD1-CG-CD2	-7.28	94.78	110.80
4	B3	49	LEU	CD1-CG-CD2	-7.28	94.79	110.80
63	T2	34	ASN	CB-CG-ND2	7.26	127.29	116.40
19	AI	94	ASP	N-CA-CB	-7.26	99.22	111.20
19	BI	94	ASP	N-CA-CB	-7.25	99.24	111.20
63	t2	34	ASN	CB-CG-ND2	7.25	127.27	116.40
3	B2	506	LYS	CD-CE-NZ	-7.24	88.75	111.90
3	A2	506	LYS	CD-CE-NZ	-7.23	88.75	111.90
19	AI	68	LEU	CB-CG-CD1	7.23	132.40	110.70
4	A3	64	ARG	N-CA-CB	7.23	120.68	109.48
19	BI	68	LEU	CB-CG-CD1	7.23	132.38	110.70
10	A9	209	MET	CB-CG-SD	7.22	134.36	112.70
4	B3	64	ARG	N-CA-CB	7.21	120.66	109.48
10	B9	209	MET	CB-CG-SD	7.21	134.34	112.70
26	BQ	22	ILE	CA-CB-CG1	-7.21	98.15	110.40
26	AQ	22	ILE	CA-CB-CG1	-7.21	98.15	110.40
18	AH	109	LYS	CA-C-O	7.16	127.33	119.24
53	sE	527	THR	OG1-CB-CG2	-7.15	95.00	109.30
1	B0	619	THR	CA-CB-CG2	7.14	122.64	110.50
18	BH	109	LYS	CA-C-O	7.14	127.31	119.24
53	SE	527	THR	OG1-CB-CG2	-7.14	95.03	109.30
1	A0	619	THR	CA-CB-CG2	7.13	122.62	110.50
19	AI	67	THR	N-CA-C	7.13	122.24	112.90
61	E6	161	ASN	CB-CA-C	7.12	122.11	109.65
28	AS	183	ASN	CA-C-O	-7.11	111.79	119.97
19	BI	67	THR	N-CA-C	7.11	122.21	112.90
2	B1	197	GLU	CG-CD-OE1	-7.10	102.07	118.40
2	A1	197	GLU	CG-CD-OE1	-7.08	102.12	118.40
28	BS	183	ASN	CA-C-O	-7.07	111.84	119.97
53	SE	514	GLU	CG-CD-OE1	7.05	134.62	118.40
53	sE	514	GLU	CG-CD-OE1	7.05	134.62	118.40
60	t3	836	ILE	CB-CA-C	-7.05	100.72	111.08
60	T3	836	ILE	CB-CA-C	-7.04	100.73	111.08
60	t3	289	LYS	N-CA-C	-7.04	102.16	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B9	200	MET	CB-CA-C	-7.03	97.18	110.67
10	A9	200	MET	CB-CA-C	-7.02	97.19	110.67
60	T3	289	LYS	N-CA-C	-7.02	102.19	111.24
60	E3	439	ILE	CG1-CB-CG2	-6.99	89.73	110.70
28	BS	198	ARG	N-CA-CB	6.98	121.10	110.28
28	AS	198	ARG	N-CA-CB	6.98	121.10	110.28
55	sH	590	GLU	N-CA-C	-6.97	95.95	110.80
19	AI	81	ARG	CA-C-N	-6.97	110.84	121.86
19	AI	81	ARG	C-N-CA	-6.97	110.84	121.86
55	SH	590	GLU	N-CA-C	-6.97	95.96	110.80
11	BA	691	LEU	CA-C-N	-6.96	110.38	122.36
11	BA	691	LEU	C-N-CA	-6.96	110.38	122.36
19	BI	81	ARG	CA-C-N	-6.96	110.86	121.86
19	BI	81	ARG	C-N-CA	-6.96	110.86	121.86
11	AA	691	LEU	CA-C-N	-6.96	110.39	122.36
11	AA	691	LEU	C-N-CA	-6.96	110.39	122.36
58	SK	443	MET	CG-SD-CE	-6.95	85.61	100.90
10	B9	216	GLU	CA-C-N	6.95	133.12	122.08
10	B9	216	GLU	C-N-CA	6.95	133.12	122.08
3	B2	65	TRP	N-CA-C	6.94	120.98	112.23
58	sK	443	MET	CG-SD-CE	-6.94	85.62	100.90
3	A2	65	TRP	N-CA-C	6.94	120.97	112.23
3	A2	490	LYS	CD-CE-NZ	-6.94	89.69	111.90
3	B2	490	LYS	CD-CE-NZ	-6.94	89.70	111.90
60	E3	675	GLU	CG-CD-OE1	6.94	134.35	118.40
58	SK	97	VAL	CA-C-O	-6.93	113.93	121.28
19	AI	104	LEU	CB-CA-C	6.93	121.90	110.81
10	A9	216	GLU	CA-C-N	6.93	133.10	122.08
10	A9	216	GLU	C-N-CA	6.93	133.10	122.08
50	sA	270	TYR	N-CA-C	-6.92	102.96	112.03
4	B3	85	ARG	CG-CD-NE	6.91	127.20	112.00
19	BI	104	LEU	CB-CA-C	6.91	121.86	110.81
4	A3	85	ARG	CG-CD-NE	6.90	127.19	112.00
50	SA	270	TYR	N-CA-C	-6.90	102.99	112.03
56	sI	1291	VAL	CA-C-N	6.89	134.69	121.54
56	sI	1291	VAL	C-N-CA	6.89	134.69	121.54
45	t4	1018	MET	N-CA-C	6.88	118.47	110.97
56	SI	1291	VAL	CA-C-N	6.88	134.68	121.54
56	SI	1291	VAL	C-N-CA	6.88	134.68	121.54
58	sK	97	VAL	CA-C-O	-6.88	113.99	121.28
45	T4	1018	MET	N-CA-C	6.86	118.45	110.97
23	AM	63	TRP	N-CA-C	6.86	118.93	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	SA	427	VAL	CG1-CB-CG2	-6.86	95.71	110.80
64	T5	920	LYS	N-CA-CB	6.85	120.29	110.77
23	BM	63	TRP	N-CA-C	6.84	118.92	110.91
50	sA	427	VAL	CG1-CB-CG2	-6.84	95.76	110.80
64	t5	920	LYS	N-CA-CB	6.83	120.27	110.77
28	AS	223	ILE	CA-CB-CG1	6.81	121.97	110.40
28	BS	223	ILE	CA-CB-CG1	6.81	121.97	110.40
53	sE	466	ILE	CA-C-O	-6.81	112.27	120.78
53	SE	466	ILE	CA-C-O	-6.80	112.28	120.78
19	BI	94	ASP	CB-CA-C	6.79	122.01	111.02
19	AI	94	ASP	CB-CA-C	6.77	121.98	111.02
63	T2	105	TYR	CB-CG-CD2	-6.76	110.65	120.80
24	BN	-64	DG	O3'-P-O5'	6.76	116.84	104.00
24	AN	-64	DG	O3'-P-O5'	6.76	116.84	104.00
63	t2	105	TYR	CB-CG-CD2	-6.75	110.67	120.80
58	SK	195	GLU	CG-CD-OE1	-6.75	102.87	118.40
3	B2	506	LYS	CA-CB-CG	6.75	127.60	114.10
58	sK	195	GLU	CG-CD-OE1	-6.74	102.89	118.40
3	A2	506	LYS	CA-CB-CG	6.74	127.58	114.10
55	SH	590	GLU	CG-CD-OE2	-6.73	102.91	118.40
55	sH	590	GLU	CG-CD-OE2	-6.73	102.93	118.40
19	AI	78	CYS	N-CA-C	6.72	120.70	112.23
19	BI	78	CYS	N-CA-C	6.72	120.70	112.23
28	AS	206	VAL	CA-C-O	6.71	129.17	120.78
55	sH	592	LEU	N-CA-CB	6.71	121.83	110.49
55	SH	592	LEU	N-CA-CB	6.71	121.83	110.49
28	BS	206	VAL	CA-C-O	6.70	129.15	120.78
18	BH	109	LYS	CB-CA-C	-6.70	98.18	109.03
18	AH	109	LYS	CB-CA-C	-6.69	98.19	109.03
51	sB	360	GLU	CG-CD-OE1	-6.68	103.04	118.40
51	SB	360	GLU	CG-CD-OE1	-6.67	103.05	118.40
29	BT	61	DA	O3'-P-O5'	-6.66	91.34	104.00
29	AT	61	DA	O3'-P-O5'	-6.65	91.36	104.00
11	BA	1277	GLU	CA-C-O	-6.65	111.00	120.51
61	E6	160	TYR	CB-CG-CD2	-6.64	110.84	120.80
19	AI	84	VAL	CB-CA-C	-6.63	100.94	110.83
18	BH	56	THR	N-CA-CB	6.63	120.98	110.57
11	AA	1277	GLU	CA-C-O	-6.63	111.03	120.51
18	AH	56	THR	N-CA-CB	6.63	120.98	110.57
12	AB	19	GLU	CB-CA-C	6.62	122.87	110.63
55	SH	455	MET	CG-SD-CE	-6.61	86.35	100.90
12	BB	19	GLU	CB-CA-C	6.61	122.86	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	692	ASP	CB-CG-OD1	6.61	133.60	118.40
11	BA	692	ASP	CB-CG-OD1	6.61	133.59	118.40
19	BI	84	VAL	CB-CA-C	-6.60	101.00	110.83
55	sH	455	MET	CG-SD-CE	-6.59	86.39	100.90
53	SE	483	GLN	CG-CD-NE2	6.59	126.29	116.40
53	sE	483	GLN	CG-CD-NE2	6.59	126.29	116.40
51	SB	431	SER	CA-C-N	6.59	133.83	121.97
51	SB	431	SER	C-N-CA	6.59	133.83	121.97
51	sB	431	SER	CA-C-N	6.59	133.83	121.97
51	sB	431	SER	C-N-CA	6.59	133.83	121.97
27	AR	228	MET	CB-CA-C	6.58	122.60	110.10
27	BR	228	MET	CB-CA-C	6.57	122.57	110.10
51	sB	397	SER	CA-C-N	6.55	134.05	121.54
51	sB	397	SER	C-N-CA	6.55	134.05	121.54
51	SB	397	SER	CA-C-N	6.55	134.05	121.54
51	SB	397	SER	C-N-CA	6.55	134.05	121.54
3	B2	69	ASN	CB-CA-C	-6.53	99.75	110.85
60	T3	837	TYR	CB-CA-C	6.53	124.81	111.11
60	t3	837	TYR	CB-CA-C	6.52	124.81	111.11
3	A2	69	ASN	CB-CA-C	-6.52	99.77	110.85
18	AH	108	SER	CA-C-N	-6.52	111.14	122.36
18	AH	108	SER	C-N-CA	-6.52	111.14	122.36
61	t6	379	CYS	CA-C-N	6.52	133.99	121.54
61	t6	379	CYS	C-N-CA	6.52	133.99	121.54
18	BH	108	SER	CA-C-N	-6.51	111.16	122.36
18	BH	108	SER	C-N-CA	-6.51	111.16	122.36
61	T6	379	CYS	CA-C-N	6.51	133.97	121.54
61	T6	379	CYS	C-N-CA	6.51	133.97	121.54
2	B1	213	ARG	CA-C-N	6.50	124.33	120.24
2	B1	213	ARG	C-N-CA	6.50	124.33	120.24
55	sH	592	LEU	N-CA-C	6.50	124.64	110.80
28	BS	209	LYS	CB-CG-CD	-6.49	96.37	111.30
64	T5	919	ARG	CB-CA-C	6.49	123.88	111.48
55	SH	592	LEU	N-CA-C	6.49	124.61	110.80
28	AS	209	LYS	CB-CG-CD	-6.48	96.40	111.30
60	T3	838	SER	N-CA-C	-6.46	98.66	108.67
64	t5	919	ARG	CB-CA-C	6.46	123.82	111.48
38	me	60	GLU	CA-CB-CG	6.44	126.98	114.10
60	t3	838	SER	N-CA-C	-6.44	98.69	108.67
2	A1	213	ARG	CA-C-N	6.43	124.29	120.24
2	A1	213	ARG	C-N-CA	6.43	124.29	120.24
19	AI	61	ASP	CB-CA-C	-6.42	100.67	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	61	ASP	CA-CB-CG	-6.42	106.18	112.60
19	BI	61	ASP	CA-CB-CG	-6.42	106.18	112.60
55	SH	600	GLU	CG-CD-OE2	6.42	133.16	118.40
38	Me	60	GLU	CA-CB-CG	6.42	126.93	114.10
19	BI	108	HIS	CB-CG-CD2	6.42	139.54	131.20
55	sH	600	GLU	CG-CD-OE2	6.41	133.14	118.40
19	BI	61	ASP	CB-CA-C	-6.41	100.71	111.02
19	AI	67	THR	CA-CB-CG2	6.40	121.38	110.50
51	SD	607	VAL	CG1-CB-CG2	-6.40	96.73	110.80
28	BS	243	GLN	N-CA-C	-6.40	104.92	114.64
19	AI	108	HIS	CB-CG-CD2	6.39	139.51	131.20
51	sD	607	VAL	CG1-CB-CG2	-6.39	96.74	110.80
28	AS	243	GLN	N-CA-C	-6.38	104.94	114.64
19	AI	110	PHE	CA-C-N	-6.37	111.48	123.27
19	AI	110	PHE	C-N-CA	-6.37	111.48	123.27
19	BI	67	THR	CA-CB-CG2	6.37	121.33	110.50
19	BI	110	PHE	CA-C-N	-6.36	111.50	123.27
19	BI	110	PHE	C-N-CA	-6.36	111.50	123.27
1	A0	447	LYS	CA-C-O	-6.36	112.17	118.34
19	BI	114	GLN	CG-CD-OE1	6.35	133.50	120.80
1	B0	447	LYS	CA-C-O	-6.35	112.18	118.34
19	AI	114	GLN	CG-CD-OE1	6.35	133.50	120.80
23	BM	58	ASP	CA-C-N	6.35	133.66	121.54
23	BM	58	ASP	C-N-CA	6.35	133.66	121.54
53	sE	463	PRO	CA-C-N	6.34	133.66	121.54
53	sE	463	PRO	C-N-CA	6.34	133.66	121.54
23	AM	58	ASP	CA-C-N	6.34	133.65	121.54
23	AM	58	ASP	C-N-CA	6.34	133.65	121.54
53	SE	463	PRO	CA-C-N	6.34	133.64	121.54
53	SE	463	PRO	C-N-CA	6.34	133.64	121.54
19	BI	104	LEU	CB-CG-CD2	-6.32	91.73	110.70
19	AI	104	LEU	CB-CG-CD2	-6.32	91.74	110.70
3	A2	506	LYS	CB-CA-C	-6.29	96.83	109.99
24	BN	-43	DA	C4'-C3'-C2'	-6.29	97.44	103.10
3	B2	506	LYS	CB-CA-C	-6.29	96.85	109.99
27	BR	288	ASN	N-CA-C	6.29	124.19	110.80
24	AN	-43	DA	C4'-C3'-C2'	-6.28	97.44	103.10
60	T3	840	ASP	CA-CB-CG	6.28	118.88	112.60
10	B9	199	GLN	CG-CD-OE1	6.28	133.36	120.80
9	sF	310	GLN	CA-CB-CG	6.27	126.65	114.10
58	SK	91	TYR	OH-CZ-CE2	6.27	138.72	119.90
9	SF	310	GLN	CA-CB-CG	6.27	126.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	sD	739	VAL	CB-CA-C	6.27	120.23	112.02
1	A0	557	MET	CB-CG-SD	6.27	131.50	112.70
58	sK	91	TYR	OH-CZ-CE2	6.27	138.70	119.90
60	t3	840	ASP	CA-CB-CG	6.26	118.86	112.60
27	AR	288	ASN	N-CA-C	6.26	124.14	110.80
6	A5	5	ARG	N-CA-CB	-6.25	99.68	111.00
6	B5	5	ARG	N-CA-CB	-6.25	99.69	111.00
51	SD	739	VAL	CB-CA-C	6.25	120.21	112.02
11	BA	688	LYS	CA-C-O	6.25	126.62	119.18
1	B0	557	MET	CB-CG-SD	6.24	131.43	112.70
10	A9	199	GLN	CG-CD-OE1	6.24	133.28	120.80
11	AA	688	LYS	CA-C-O	6.24	126.60	119.18
10	A9	199	GLN	CB-CA-C	-6.24	98.01	110.42
10	B9	199	GLN	CB-CA-C	-6.23	98.03	110.42
11	AA	1275	GLY	CA-C-N	-6.20	110.82	121.97
11	AA	1275	GLY	C-N-CA	-6.20	110.82	121.97
11	BA	1275	GLY	CA-C-N	-6.19	110.83	121.97
11	BA	1275	GLY	C-N-CA	-6.19	110.83	121.97
38	me	55	ARG	CB-CA-C	6.19	122.74	110.42
38	Me	55	ARG	CB-CA-C	6.18	122.72	110.42
35	mb	49	ARG	CG-CD-NE	6.17	125.56	112.00
30	AU	18	VAL	CA-C-N	-6.16	110.59	122.06
30	AU	18	VAL	C-N-CA	-6.16	110.59	122.06
30	BU	18	VAL	CA-C-N	-6.16	110.60	122.06
30	BU	18	VAL	C-N-CA	-6.16	110.60	122.06
64	t5	923	LYS	CA-CB-CG	-6.15	101.79	114.10
12	AB	19	GLU	N-CA-CB	-6.15	100.75	110.22
64	T5	923	LYS	CA-CB-CG	-6.15	101.79	114.10
9	SF	398	THR	N-CA-CB	6.15	120.88	110.49
35	Mb	49	ARG	CG-CD-NE	6.15	125.53	112.00
55	SH	589	HIS	CA-C-N	6.15	133.28	121.54
55	SH	589	HIS	C-N-CA	6.15	133.28	121.54
55	sH	589	HIS	CA-C-N	6.15	133.28	121.54
55	sH	589	HIS	C-N-CA	6.15	133.28	121.54
12	BB	19	GLU	N-CA-CB	-6.14	100.76	110.22
3	B2	489	LYS	CA-C-N	6.14	132.20	122.62
3	B2	489	LYS	C-N-CA	6.14	132.20	122.62
3	A2	489	LYS	CA-C-N	6.13	132.19	122.62
3	A2	489	LYS	C-N-CA	6.13	132.19	122.62
64	t5	922	THR	CA-C-N	6.13	133.26	121.54
64	t5	922	THR	C-N-CA	6.13	133.26	121.54
64	T5	922	THR	CA-C-N	6.13	133.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	T5	922	THR	C-N-CA	6.13	133.25	121.54
9	sF	398	THR	N-CA-CB	6.12	120.83	110.49
27	BR	278	LEU	N-CA-C	6.11	118.06	110.91
51	sD	432	VAL	CA-C-N	6.11	133.22	121.54
51	sD	432	VAL	C-N-CA	6.11	133.22	121.54
61	E6	946	VAL	N-CA-C	-6.11	104.18	109.19
29	BT	61	DA	O4'-C1'-N9	6.11	112.28	108.00
2	B1	197	GLU	CG-CD-OE2	6.11	132.44	118.40
27	AR	278	LEU	N-CA-C	6.10	118.05	110.91
64	t5	877	LYS	N-CA-C	6.10	118.71	111.33
2	A1	197	GLU	CG-CD-OE2	6.10	132.42	118.40
51	SB	770	PHE	CG-CD2-CE2	-6.10	110.34	120.70
19	AI	67	THR	N-CA-CB	-6.09	101.19	110.33
64	T5	877	LYS	N-CA-C	6.09	118.70	111.33
51	sB	770	PHE	CG-CD2-CE2	-6.09	110.35	120.70
53	SE	547	ARG	CG-CD-NE	6.09	125.39	112.00
51	SD	432	VAL	CA-C-N	6.08	133.16	121.54
51	SD	432	VAL	C-N-CA	6.08	133.16	121.54
19	BI	67	THR	N-CA-CB	-6.08	101.21	110.33
53	sE	547	ARG	CG-CD-NE	6.08	125.37	112.00
8	A7	114	ARG	CA-CB-CG	6.06	126.21	114.10
60	t3	405	GLU	CA-C-N	-6.06	112.17	120.28
60	t3	405	GLU	C-N-CA	-6.06	112.17	120.28
3	B2	97	MET	N-CA-CB	-6.05	101.12	110.56
29	AT	61	DA	O4'-C1'-N9	6.05	112.23	108.00
8	B7	114	ARG	CA-CB-CG	6.04	126.19	114.10
18	AH	130	ARG	CD-NE-CZ	6.04	132.86	124.40
18	BH	130	ARG	CD-NE-CZ	6.04	132.86	124.40
12	BB	662	MET	N-CA-C	-6.03	105.00	112.90
12	AB	662	MET	N-CA-C	-6.03	105.00	112.90
3	A2	97	MET	N-CA-CB	-6.02	101.17	110.56
19	AI	62	ILE	N-CA-CB	6.01	122.69	110.78
60	T3	405	GLU	CA-C-N	-6.01	112.22	120.28
60	T3	405	GLU	C-N-CA	-6.01	112.22	120.28
19	BI	62	ILE	N-CA-CB	6.01	122.68	110.78
4	A3	64	ARG	CB-CA-C	-6.00	100.83	109.84
9	sF	448	GLN	CG-CD-OE1	-5.99	108.82	120.80
9	SF	311	THR	CA-C-N	-5.98	117.28	122.96
9	SF	311	THR	C-N-CA	-5.98	117.28	122.96
61	t6	971	GLU	CG-CD-OE2	5.98	132.15	118.40
9	SF	448	GLN	CG-CD-OE1	-5.98	108.85	120.80
4	B3	64	ARG	CB-CA-C	-5.97	100.88	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	T6	971	GLU	CG-CD-OE2	5.97	132.12	118.40
63	t2	34	ASN	CB-CG-OD1	-5.96	108.87	120.80
19	AI	114	GLN	N-CA-CB	-5.95	100.43	110.49
63	T2	34	ASN	CB-CG-OD1	-5.95	108.90	120.80
19	BI	114	GLN	N-CA-CB	-5.94	100.44	110.49
9	sF	311	THR	CA-C-N	-5.94	117.31	122.96
9	sF	311	THR	C-N-CA	-5.94	117.31	122.96
29	BT	61	DA	C3'-C2'-C1'	-5.94	95.37	102.50
19	AI	114	GLN	CB-CG-CD	5.94	122.69	112.60
19	BI	114	GLN	CB-CG-CD	5.93	122.69	112.60
60	T3	836	ILE	CG1-CB-CG2	5.93	128.50	110.70
3	A2	138	TYR	CZ-CE2-CD2	5.93	130.28	119.60
3	B2	138	TYR	CZ-CE2-CD2	5.93	130.27	119.60
29	AT	61	DA	C3'-C2'-C1'	-5.93	95.39	102.50
60	t3	836	ILE	CG1-CB-CG2	5.93	128.48	110.70
48	Mo	107	PRO	CA-N-CD	-5.92	103.71	112.00
55	SH	596	ARG	CA-C-O	-5.92	114.60	120.82
55	sH	596	ARG	CA-C-O	-5.92	114.60	120.82
48	mo	107	PRO	CA-N-CD	-5.92	103.71	112.00
60	E3	412	ARG	CB-CA-C	-5.92	97.94	110.31
19	BI	105	SER	CA-C-N	-5.91	112.94	121.98
19	BI	105	SER	C-N-CA	-5.91	112.94	121.98
64	T5	927	ARG	N-CA-CB	5.91	119.77	109.72
19	AI	105	SER	CA-C-N	-5.91	112.94	121.98
19	AI	105	SER	C-N-CA	-5.91	112.94	121.98
53	sE	502	GLY	CA-C-N	5.91	133.05	122.13
53	sE	502	GLY	C-N-CA	5.91	133.05	122.13
24	BN	-45	DA	OP1-P-O3'	-5.90	90.29	108.00
64	t5	927	ARG	N-CA-CB	5.90	119.75	109.72
19	AI	91	ARG	CB-CG-CD	5.90	124.87	111.30
64	t5	931	GLN	N-CA-CB	-5.90	101.43	110.16
53	SE	502	GLY	CA-C-N	5.89	133.04	122.13
53	SE	502	GLY	C-N-CA	5.89	133.04	122.13
19	BI	91	ARG	CB-CG-CD	5.89	124.86	111.30
4	B3	64	ARG	CA-CB-CG	5.89	125.88	114.10
64	T5	931	GLN	N-CA-CB	-5.89	101.44	110.16
24	AN	-45	DA	OP1-P-O3'	-5.88	90.34	108.00
11	AA	1221	LYS	CA-C-N	5.87	130.81	121.18
11	AA	1221	LYS	C-N-CA	5.87	130.81	121.18
4	A3	64	ARG	CA-CB-CG	5.87	125.84	114.10
9	SF	401	LYS	CA-C-O	-5.87	112.12	120.51
9	sF	401	LYS	CA-C-O	-5.87	112.12	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BA	1221	LYS	CA-C-N	5.86	130.79	121.18
11	BA	1221	LYS	C-N-CA	5.86	130.79	121.18
58	sK	91	TYR	CE1-CZ-CE2	5.86	132.01	120.30
58	SK	91	TYR	CE1-CZ-CE2	5.84	131.98	120.30
3	A2	96	LEU	CA-C-N	5.83	133.35	122.74
3	A2	96	LEU	C-N-CA	5.83	133.35	122.74
60	T3	409	LYS	CB-CA-C	-5.83	98.82	110.42
60	t3	409	LYS	CB-CA-C	-5.83	98.82	110.42
3	B2	66	VAL	N-CA-C	5.83	117.10	108.65
15	BE	116	ILE	CG1-CB-CG2	-5.82	93.23	110.70
3	A2	66	VAL	N-CA-C	5.82	117.09	108.65
3	B2	96	LEU	CA-C-N	5.82	133.33	122.74
3	B2	96	LEU	C-N-CA	5.82	133.33	122.74
15	AE	116	ILE	CG1-CB-CG2	-5.82	93.25	110.70
1	A0	451	GLU	CG-CD-OE1	-5.80	105.06	118.40
1	B0	451	GLU	CG-CD-OE1	-5.80	105.06	118.40
55	sH	536	LEU	CA-C-N	-5.79	111.28	122.06
55	sH	536	LEU	C-N-CA	-5.79	111.28	122.06
55	SH	536	LEU	CA-C-N	-5.78	111.31	122.06
55	SH	536	LEU	C-N-CA	-5.78	111.31	122.06
29	BT	59	DG	O4'-C1'-N9	5.78	112.05	108.00
50	SA	427	VAL	CA-CB-CG2	5.78	120.22	110.40
3	B2	463	GLU	CA-C-N	-5.77	112.44	122.37
3	B2	463	GLU	C-N-CA	-5.77	112.44	122.37
27	BR	96	ARG	CA-CB-CG	5.76	125.62	114.10
43	Mj	106	SER	CA-C-N	-5.76	111.35	122.06
43	Mj	106	SER	C-N-CA	-5.76	111.35	122.06
19	BI	67	THR	OG1-CB-CG2	5.76	120.82	109.30
27	AR	96	ARG	CA-CB-CG	5.76	125.61	114.10
19	BI	75	CYS	N-CA-C	5.75	119.30	109.06
43	mj	106	SER	CA-C-N	-5.75	111.36	122.06
43	mj	106	SER	C-N-CA	-5.75	111.36	122.06
50	sA	427	VAL	CA-CB-CG2	5.75	120.18	110.40
3	A2	463	GLU	CA-C-N	-5.75	112.48	122.37
3	A2	463	GLU	C-N-CA	-5.75	112.48	122.37
19	AI	67	THR	OG1-CB-CG2	5.75	120.80	109.30
61	T6	504	PRO	N-CA-C	5.75	117.72	110.70
53	SE	465	GLU	CA-C-O	-5.75	112.29	120.51
53	sE	465	GLU	CA-C-O	-5.74	112.30	120.51
29	AT	59	DG	O4'-C1'-N9	5.74	112.02	108.00
53	sE	450	GLU	CG-CD-OE1	5.73	131.59	118.40
29	AT	44	DC	O3'-P-O5'	5.73	114.89	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BT	44	DC	O3'-P-O5'	5.73	114.89	104.00
19	BI	92	ARG	CB-CG-CD	-5.73	98.13	111.30
19	BI	92	ARG	CA-CB-CG	5.73	125.55	114.10
19	AI	92	ARG	CA-CB-CG	5.72	125.55	114.10
53	SE	450	GLU	CG-CD-OE1	5.72	131.57	118.40
19	AI	75	CYS	N-CA-C	5.72	119.25	109.06
19	AI	92	ARG	CB-CG-CD	-5.72	98.14	111.30
58	SK	147	LEU	CD1-CG-CD2	5.72	123.38	110.80
61	t6	504	PRO	N-CA-C	5.72	117.67	110.70
24	AN	-63	DA	O5'-C5'-C4'	5.71	113.97	109.40
12	AB	18	PHE	CB-CG-CD1	5.70	130.40	120.70
58	sK	147	LEU	CD1-CG-CD2	5.70	123.34	110.80
29	AT	60	DT	O4'-C1'-C2'	-5.70	101.34	105.90
18	BH	130	ARG	NE-CZ-NH1	5.69	127.19	121.50
12	BB	18	PHE	CB-CG-CD1	5.69	130.37	120.70
19	BI	82	GLU	OE1-CD-OE2	-5.69	109.25	122.90
19	AI	82	GLU	OE1-CD-OE2	-5.69	109.25	122.90
11	BA	464	PRO	CA-C-N	5.68	132.39	121.54
11	BA	464	PRO	C-N-CA	5.68	132.39	121.54
29	BT	60	DT	O4'-C1'-C2'	-5.68	101.36	105.90
60	T3	288	MET	CA-C-N	5.68	130.08	120.88
60	T3	288	MET	C-N-CA	5.68	130.08	120.88
35	mb	49	ARG	N-CA-C	5.67	118.20	111.33
11	AA	464	PRO	CA-C-N	5.67	132.37	121.54
11	AA	464	PRO	C-N-CA	5.67	132.37	121.54
24	BN	-63	DA	O5'-C5'-C4'	5.67	113.94	109.40
18	AH	130	ARG	NE-CZ-NH1	5.66	127.16	121.50
29	AT	61	DA	OP1-P-O3'	-5.66	91.03	108.00
60	t3	288	MET	CA-C-N	5.66	130.05	120.88
60	t3	288	MET	C-N-CA	5.66	130.05	120.88
29	BT	61	DA	OP1-P-O3'	-5.66	91.03	108.00
6	A5	2	ALA	CA-C-N	-5.65	113.58	122.73
6	A5	2	ALA	C-N-CA	-5.65	113.58	122.73
9	SF	360	TYR	CA-C-N	5.64	135.57	121.80
9	SF	360	TYR	C-N-CA	5.64	135.57	121.80
60	E3	678	ASN	CB-CA-C	-5.64	98.72	109.95
61	E6	749	LEU	CA-CB-CG	-5.64	96.56	116.30
24	BN	-43	DA	P-O3'-C3'	-5.64	112.93	119.70
35	Mb	49	ARG	N-CA-C	5.64	118.15	111.33
6	B5	2	ALA	CA-C-N	-5.64	113.59	122.73
6	B5	2	ALA	C-N-CA	-5.64	113.59	122.73
31	BV	12	ARG	CA-C-N	5.64	132.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BV	12	ARG	C-N-CA	5.64	132.31	121.54
24	AN	-43	DA	P-O3'-C3'	-5.63	112.94	119.70
9	sF	360	TYR	CA-C-N	5.63	135.54	121.80
9	sF	360	TYR	C-N-CA	5.63	135.54	121.80
24	AN	-44	DG	P-O3'-C3'	-5.63	112.95	119.70
31	AV	12	ARG	CA-C-N	5.63	132.29	121.54
31	AV	12	ARG	C-N-CA	5.63	132.29	121.54
48	Mo	104	ASP	N-CA-C	-5.63	107.41	114.56
23	BM	234	GLN	CA-CB-CG	5.63	125.36	114.10
24	BN	-44	DG	P-O3'-C3'	-5.62	112.95	119.70
23	AM	234	GLN	CA-CB-CG	5.62	125.34	114.10
48	mo	104	ASP	N-CA-C	-5.61	107.44	114.56
11	AA	683	ILE	CA-C-N	5.59	133.88	121.80
11	AA	683	ILE	C-N-CA	5.59	133.88	121.80
2	A1	229	GLY	N-CA-C	5.59	123.75	112.34
28	AS	197	ALA	CA-C-N	-5.59	111.81	120.31
28	AS	197	ALA	C-N-CA	-5.59	111.81	120.31
43	Mj	107	GLU	N-CA-CB	5.59	119.24	110.46
2	B1	229	GLY	N-CA-C	5.59	123.74	112.34
43	mj	107	GLU	N-CA-CB	5.58	119.22	110.46
28	BS	197	ALA	CA-C-N	-5.57	111.84	120.31
28	BS	197	ALA	C-N-CA	-5.57	111.84	120.31
55	sH	590	GLU	OE1-CD-OE2	-5.57	109.53	122.90
55	SH	590	GLU	OE1-CD-OE2	-5.56	109.55	122.90
19	AI	72	ASP	CB-CA-C	-5.55	100.05	109.38
27	BR	77	LEU	CA-CB-CG	5.55	135.73	116.30
27	AR	77	LEU	CA-CB-CG	5.55	135.73	116.30
29	BT	58	DA	O4'-C1'-N9	5.55	111.89	108.00
55	sH	590	GLU	CB-CG-CD	5.55	122.03	112.60
56	sI	1251	LYS	CG-CD-CE	5.54	124.06	111.30
56	SI	1251	LYS	CG-CD-CE	5.54	124.05	111.30
19	BI	72	ASP	CB-CA-C	-5.54	100.07	109.38
27	BR	96	ARG	CG-CD-NE	5.54	124.18	112.00
55	SH	590	GLU	CB-CG-CD	5.54	122.01	112.60
30	BU	263	LYS	CA-C-N	5.54	132.11	121.54
30	BU	263	LYS	C-N-CA	5.54	132.11	121.54
27	AR	96	ARG	CG-CD-NE	5.53	124.17	112.00
30	AU	263	LYS	CA-C-N	5.53	132.11	121.54
30	AU	263	LYS	C-N-CA	5.53	132.11	121.54
53	SE	544	THR	CA-C-O	-5.53	115.49	122.63
19	AI	8	ARG	CA-C-N	5.53	132.10	121.54
19	AI	8	ARG	C-N-CA	5.53	132.10	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	sB	432	VAL	CA-CB-CG2	5.53	119.80	110.40
23	AM	141	GLU	CA-CB-CG	5.53	125.16	114.10
51	SB	432	VAL	CA-CB-CG2	5.53	119.80	110.40
48	Mo	114	GLY	N-CA-C	5.53	123.61	112.34
63	t2	105	TYR	CB-CA-C	-5.52	101.62	110.79
23	BM	141	GLU	CA-CB-CG	5.52	125.14	114.10
61	E6	160	TYR	N-CA-C	-5.52	100.40	109.40
58	SK	147	LEU	CB-CG-CD2	5.52	127.25	110.70
58	sK	147	LEU	CB-CG-CD2	5.51	127.24	110.70
53	SE	546	LYS	N-CA-CB	5.51	118.50	109.95
19	BI	8	ARG	CA-C-N	5.51	132.06	121.54
19	BI	8	ARG	C-N-CA	5.51	132.06	121.54
53	sE	546	LYS	N-CA-CB	5.51	118.49	109.95
48	mo	114	GLY	N-CA-C	5.50	123.57	112.34
27	BR	228	MET	N-CA-CB	-5.50	101.14	110.50
63	T2	105	TYR	CB-CA-C	-5.50	101.66	110.79
27	AR	228	MET	N-CA-CB	-5.49	101.16	110.50
60	E3	463	ARG	CD-NE-CZ	5.49	132.09	124.40
61	E6	791	PHE	CZ-CE2-CD2	5.49	129.89	120.00
11	AA	683	ILE	CA-C-O	-5.49	113.39	120.03
29	AT	58	DA	O4'-C1'-N9	5.49	111.84	108.00
53	sE	544	THR	CA-C-O	-5.48	115.56	122.63
11	AA	1221	LYS	CA-CB-CG	5.48	125.05	114.10
56	SI	1277	PRO	CA-C-N	5.48	132.00	121.54
56	SI	1277	PRO	C-N-CA	5.48	132.00	121.54
11	BA	683	ILE	CA-C-O	-5.47	113.41	120.03
56	sI	1277	PRO	CA-C-N	5.46	131.98	121.54
56	sI	1277	PRO	C-N-CA	5.46	131.98	121.54
11	BA	1221	LYS	CA-CB-CG	5.46	125.02	114.10
45	t4	1052	GLY	CA-C-N	5.46	131.97	121.54
45	t4	1052	GLY	C-N-CA	5.46	131.97	121.54
64	T5	920	LYS	CA-C-O	-5.46	114.47	119.76
44	mk	87	ILE	CG1-CB-CG2	-5.45	94.34	110.70
44	Mk	87	ILE	CG1-CB-CG2	-5.45	94.34	110.70
45	T4	1052	GLY	CA-C-N	5.45	131.95	121.54
45	T4	1052	GLY	C-N-CA	5.45	131.95	121.54
64	t5	920	LYS	CA-C-O	-5.45	114.48	119.76
16	BF	128	LYS	N-CA-C	5.45	117.28	110.91
16	AF	128	LYS	N-CA-C	5.44	117.28	110.91
43	Mj	87	LEU	CA-C-N	5.44	127.88	120.54
43	Mj	87	LEU	C-N-CA	5.44	127.88	120.54
43	mj	87	LEU	CA-C-N	5.43	127.87	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	mj	87	LEU	C-N-CA	5.43	127.87	120.54
9	sF	398	THR	CA-CB-OG1	5.42	117.73	109.60
53	SE	241	ARG	CG-CD-NE	5.42	123.92	112.00
9	SF	398	THR	CA-CB-OG1	5.42	117.72	109.60
53	sE	241	ARG	CG-CD-NE	5.41	123.91	112.00
64	t5	927	ARG	CB-CG-CD	5.41	123.74	111.30
10	B9	217	GLU	CB-CG-CD	-5.41	103.41	112.60
53	SE	514	GLU	CB-CG-CD	-5.40	103.42	112.60
64	T5	927	ARG	CB-CG-CD	5.40	123.72	111.30
10	A9	217	GLU	CB-CG-CD	-5.39	103.43	112.60
12	AB	18	PHE	CB-CG-CD2	-5.39	111.53	120.70
19	AI	84	VAL	CA-C-O	-5.39	114.77	120.48
12	BB	18	PHE	CB-CG-CD2	-5.38	111.55	120.70
53	sE	514	GLU	CB-CG-CD	-5.38	103.45	112.60
56	sI	1110	VAL	CB-CA-C	5.38	119.64	112.22
56	SI	1110	VAL	CB-CA-C	5.38	119.64	112.22
61	E6	972	MET	CB-CG-SD	-5.37	96.58	112.70
53	sE	562	PHE	CA-C-N	5.37	128.50	120.83
53	sE	562	PHE	C-N-CA	5.37	128.50	120.83
19	BI	84	VAL	CA-C-O	-5.36	114.79	120.48
60	T3	412	ARG	CA-C-N	5.36	127.31	120.56
60	T3	412	ARG	C-N-CA	5.36	127.31	120.56
17	BG	33	GLU	CA-C-N	-5.36	113.81	121.52
17	BG	33	GLU	C-N-CA	-5.36	113.81	121.52
60	t3	412	ARG	CA-C-N	5.36	127.31	120.56
60	t3	412	ARG	C-N-CA	5.36	127.31	120.56
17	AG	33	GLU	CA-C-N	-5.35	113.81	121.52
17	AG	33	GLU	C-N-CA	-5.35	113.81	121.52
56	SI	1110	VAL	CG1-CB-CG2	-5.35	99.03	110.80
11	BA	688	LYS	CD-CE-NZ	-5.35	94.79	111.90
60	T3	860	VAL	N-CA-C	5.35	115.97	110.36
4	A3	49	LEU	CB-CG-CD1	-5.34	94.67	110.70
11	AA	688	LYS	CD-CE-NZ	-5.34	94.80	111.90
53	SE	527	THR	CA-CB-CG2	5.34	119.58	110.50
53	SE	562	PHE	CA-C-N	5.34	128.47	120.83
53	SE	562	PHE	C-N-CA	5.34	128.47	120.83
60	t3	292	ARG	CA-CB-CG	5.34	124.78	114.10
53	sE	503	ILE	CG1-CB-CG2	-5.34	94.69	110.70
4	B3	49	LEU	CB-CG-CD1	-5.33	94.71	110.70
56	sI	1110	VAL	CG1-CB-CG2	-5.33	99.08	110.80
19	BI	108	HIS	CB-CG-ND1	-5.33	114.71	122.70
53	sE	527	THR	CA-CB-CG2	5.33	119.55	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	SE	503	ILE	CG1-CB-CG2	-5.32	94.73	110.70
24	BN	-45	DA	O3'-P-O5'	5.32	114.11	104.00
28	AS	227	PHE	CG-CD1-CE1	5.32	129.74	120.70
29	AT	42	DA	P-O3'-C3'	-5.32	113.32	119.70
11	BA	299	HIS	CA-C-N	-5.32	112.39	121.97
11	BA	299	HIS	C-N-CA	-5.32	112.39	121.97
60	T3	292	ARG	CA-CB-CG	5.31	124.73	114.10
18	AH	145	ARG	CA-C-N	5.31	131.26	121.70
18	AH	145	ARG	C-N-CA	5.31	131.26	121.70
19	AI	108	HIS	CB-CG-ND1	-5.31	114.73	122.70
18	BH	145	ARG	CA-C-N	5.31	131.25	121.70
18	BH	145	ARG	C-N-CA	5.31	131.25	121.70
28	BS	227	PHE	CG-CD1-CE1	5.31	129.73	120.70
60	E3	959	LEU	N-CA-CB	-5.31	101.52	110.49
24	AN	-45	DA	O3'-P-O5'	5.30	114.08	104.00
55	sH	594	LEU	N-CA-CB	-5.30	102.30	110.20
55	SH	594	LEU	N-CA-CB	-5.30	102.31	110.20
29	BT	42	DA	P-O3'-C3'	-5.30	113.34	119.70
50	SA	269	GLN	OE1-CD-NE2	-5.30	117.30	122.60
60	t3	860	VAL	N-CA-C	5.30	115.92	110.36
11	AA	299	HIS	CA-C-N	-5.29	112.45	121.97
11	AA	299	HIS	C-N-CA	-5.29	112.45	121.97
45	t4	1017	PRO	CA-C-N	-5.28	113.68	120.65
45	t4	1017	PRO	C-N-CA	-5.28	113.68	120.65
45	T4	1017	PRO	CA-C-N	-5.28	113.68	120.65
45	T4	1017	PRO	C-N-CA	-5.28	113.68	120.65
46	mm	34	LEU	CA-C-N	5.28	131.47	121.97
46	mm	34	LEU	C-N-CA	5.28	131.47	121.97
19	BI	106	CYS	N-CA-CB	5.27	117.94	110.98
28	BS	253	LEU	CA-C-N	5.27	127.60	120.38
28	BS	253	LEU	C-N-CA	5.27	127.60	120.38
50	sA	269	GLN	OE1-CD-NE2	-5.27	117.33	122.60
11	AA	204	THR	OG1-CB-CG2	-5.27	98.77	109.30
46	Mm	34	LEU	CA-C-N	5.26	131.44	121.97
46	Mm	34	LEU	C-N-CA	5.26	131.44	121.97
55	sH	595	GLU	OE1-CD-OE2	-5.26	110.27	122.90
55	SH	595	GLU	OE1-CD-OE2	-5.26	110.28	122.90
28	AS	253	LEU	CA-C-N	5.26	127.58	120.38
28	AS	253	LEU	C-N-CA	5.26	127.58	120.38
19	AI	106	CYS	N-CA-CB	5.25	117.92	110.98
60	E3	837	TYR	N-CA-C	-5.25	107.04	113.50
11	BA	204	THR	OG1-CB-CG2	-5.25	98.81	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	t3	843	GLY	CA-C-N	5.25	134.60	121.80
60	t3	843	GLY	C-N-CA	5.25	134.60	121.80
41	Mh	112	ARG	CA-C-N	5.24	131.55	121.54
41	Mh	112	ARG	C-N-CA	5.24	131.55	121.54
17	BG	64	THR	CA-C-N	5.24	131.55	121.54
17	BG	64	THR	C-N-CA	5.24	131.55	121.54
60	T3	843	GLY	CA-C-N	5.24	134.58	121.80
60	T3	843	GLY	C-N-CA	5.24	134.58	121.80
17	AG	64	THR	CA-C-N	5.22	131.52	121.54
17	AG	64	THR	C-N-CA	5.22	131.52	121.54
50	sA	304	GLU	CA-C-N	5.22	134.54	121.80
50	sA	304	GLU	C-N-CA	5.22	134.54	121.80
41	mh	112	ARG	CA-C-N	5.22	131.51	121.54
41	mh	112	ARG	C-N-CA	5.22	131.51	121.54
19	BI	77	LYS	N-CA-C	-5.22	107.08	113.50
24	BN	-60	DA	P-O3'-C3'	5.21	125.96	119.70
50	sA	268	TRP	CA-C-N	5.21	128.96	121.71
50	sA	268	TRP	C-N-CA	5.21	128.96	121.71
28	AS	232	ASP	CB-CG-OD2	-5.21	106.42	118.40
53	SE	526	GLN	CB-CG-CD	5.21	121.46	112.60
28	BS	232	ASP	CB-CG-OD2	-5.21	106.42	118.40
4	A3	26	VAL	N-CA-C	-5.21	107.28	111.91
1	A0	619	THR	OG1-CB-CG2	-5.21	98.89	109.30
50	SA	304	GLU	CA-C-N	5.20	134.50	121.80
50	SA	304	GLU	C-N-CA	5.20	134.50	121.80
52	sC	164	LEU	CA-CB-CG	5.20	134.51	116.30
50	SA	268	TRP	CA-C-N	5.20	128.94	121.71
50	SA	268	TRP	C-N-CA	5.20	128.94	121.71
9	SF	534	GLN	CA-C-N	5.20	129.79	122.46
9	SF	534	GLN	C-N-CA	5.20	129.79	122.46
9	SF	756	ASN	CA-C-N	-5.20	115.50	122.42
9	SF	756	ASN	C-N-CA	-5.20	115.50	122.42
19	AI	77	LYS	N-CA-C	-5.20	107.11	113.50
12	BB	473	MET	CA-C-N	5.20	131.47	121.54
12	BB	473	MET	C-N-CA	5.20	131.47	121.54
53	sE	526	GLN	CB-CG-CD	5.20	121.43	112.60
52	SC	164	LEU	CA-CB-CG	5.19	134.48	116.30
1	B0	619	THR	OG1-CB-CG2	-5.19	98.92	109.30
19	AI	111	THR	N-CA-CB	-5.19	102.71	110.60
19	BI	111	THR	N-CA-CB	-5.19	102.71	110.60
12	AB	473	MET	CA-C-N	5.19	131.45	121.54
12	AB	473	MET	C-N-CA	5.19	131.45	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AT	43	DT	O4'-C1'-N1	5.19	111.63	108.00
9	SF	485	LEU	CB-CG-CD1	-5.19	95.14	110.70
9	sF	534	GLN	CA-C-N	5.19	129.77	122.46
9	sF	534	GLN	C-N-CA	5.19	129.77	122.46
24	AN	-60	DA	P-O3'-C3'	5.18	125.92	119.70
28	AS	228	LEU	CB-CG-CD2	5.18	126.25	110.70
11	BA	601	LYS	CA-C-N	5.18	131.44	121.54
11	BA	601	LYS	C-N-CA	5.18	131.44	121.54
12	BB	21	GLU	O-C-N	-5.18	115.70	122.59
12	AB	21	GLU	O-C-N	-5.18	115.70	122.59
9	sF	485	LEU	CB-CG-CD1	-5.18	95.17	110.70
9	sF	756	ASN	CA-C-N	-5.18	115.53	122.42
9	sF	756	ASN	C-N-CA	-5.18	115.53	122.42
56	SI	1248	LEU	CB-CG-CD1	5.17	126.22	110.70
11	AA	601	LYS	CA-C-N	5.17	131.42	121.54
11	AA	601	LYS	C-N-CA	5.17	131.42	121.54
29	AT	43	DT	P-O3'-C3'	-5.17	113.49	119.70
28	BS	228	LEU	CB-CG-CD2	5.17	126.22	110.70
29	BT	43	DT	P-O3'-C3'	-5.17	113.49	119.70
37	Md	255	ASN	CA-C-N	5.17	131.41	121.54
37	Md	255	ASN	C-N-CA	5.17	131.41	121.54
56	sI	1248	LEU	CB-CG-CD1	5.17	126.19	110.70
53	SE	523	VAL	O-C-N	5.16	127.63	121.80
4	B3	26	VAL	N-CA-C	-5.16	107.32	111.91
9	sF	392	MET	CA-CB-CG	5.16	124.41	114.10
29	BT	43	DT	O4'-C1'-N1	5.15	111.61	108.00
9	sF	312	ILE	CA-C-O	-5.15	115.63	121.09
60	t3	859	ASN	CA-C-N	5.15	127.24	120.60
60	t3	859	ASN	C-N-CA	5.15	127.24	120.60
51	SB	453	LEU	CB-CG-CD1	-5.14	95.28	110.70
3	B2	62	LEU	CA-C-N	-5.14	113.08	122.38
3	B2	62	LEU	C-N-CA	-5.14	113.08	122.38
51	sB	453	LEU	CB-CG-CD1	-5.14	95.28	110.70
60	T3	859	ASN	CA-C-N	5.14	127.23	120.60
60	T3	859	ASN	C-N-CA	5.14	127.23	120.60
24	AN	-62	DG	O4'-C4'-C3'	-5.14	102.92	106.00
37	md	255	ASN	CA-C-N	5.13	131.34	121.54
37	md	255	ASN	C-N-CA	5.13	131.34	121.54
9	SF	315	ASP	CB-CG-OD1	5.13	130.20	118.40
9	SF	312	ILE	CA-C-O	-5.13	115.65	121.09
3	A2	62	LEU	CA-C-N	-5.13	113.10	122.38
3	A2	62	LEU	C-N-CA	-5.13	113.10	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SF	392	MET	CA-CB-CG	5.13	124.36	114.10
9	sF	315	ASP	CB-CG-OD1	5.13	130.19	118.40
53	sE	523	VAL	O-C-N	5.12	127.59	121.80
58	SK	195	GLU	CG-CD-OE2	5.12	130.19	118.40
58	sK	195	GLU	CG-CD-OE2	5.12	130.18	118.40
19	AI	36	GLU	CA-C-N	5.12	132.32	122.03
19	AI	36	GLU	C-N-CA	5.12	132.32	122.03
38	Me	57	GLN	CA-CB-CG	5.12	124.33	114.10
60	E3	439	ILE	CA-CB-CG1	5.11	119.09	110.40
3	B2	463	GLU	N-CA-C	5.11	121.69	110.80
3	A2	463	GLU	N-CA-C	5.11	121.68	110.80
38	me	57	GLN	CA-CB-CG	5.11	124.32	114.10
50	sA	308	MET	CG-SD-CE	-5.11	89.66	100.90
19	BI	36	GLU	CA-C-N	5.10	132.29	122.03
19	BI	36	GLU	C-N-CA	5.10	132.29	122.03
50	SA	308	MET	CG-SD-CE	-5.10	89.68	100.90
28	AS	205	ASN	O-C-N	-5.10	116.34	122.15
20	AJ	58	GLU	OE1-CD-OE2	-5.09	110.67	122.90
28	BS	205	ASN	O-C-N	-5.09	116.34	122.15
46	Mm	61	ARG	CA-CB-CG	5.09	124.29	114.10
20	BJ	58	GLU	OE1-CD-OE2	-5.09	110.68	122.90
46	mm	61	ARG	CA-CB-CG	5.09	124.28	114.10
24	BN	-62	DG	O4'-C4'-C3'	-5.09	102.95	106.00
43	Mj	88	GLU	CA-CB-CG	5.08	124.26	114.10
3	A2	66	VAL	CA-CB-CG2	5.08	119.03	110.40
63	t2	105	TYR	CB-CG-CD1	5.08	128.41	120.80
43	mj	88	GLU	CA-CB-CG	5.07	124.25	114.10
61	E6	161	ASN	CB-CG-ND2	-5.07	108.79	116.40
63	T2	105	TYR	CB-CG-CD1	5.07	128.41	120.80
60	E3	413	ILE	CG1-CB-CG2	-5.07	95.48	110.70
9	SF	380	THR	N-CA-C	-5.07	106.93	113.01
11	AA	1160	SER	N-CA-C	5.07	117.82	110.42
56	SI	1194	LEU	CB-CG-CD2	-5.07	95.50	110.70
9	sF	380	THR	N-CA-C	-5.07	106.93	113.01
56	sI	1194	LEU	CB-CG-CD2	-5.07	95.50	110.70
19	AI	86	PHE	CA-C-O	-5.07	116.03	121.45
43	mj	107	GLU	CA-C-N	-5.07	114.18	122.79
43	mj	107	GLU	C-N-CA	-5.07	114.18	122.79
53	sE	511	GLN	CB-CA-C	5.06	120.50	110.42
53	SE	523	VAL	N-CA-CB	5.06	119.93	110.77
3	B2	66	VAL	CA-CB-CG2	5.06	119.00	110.40
53	sE	463	PRO	CA-C-O	-5.06	111.40	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	SE	511	GLN	CB-CA-C	5.06	120.48	110.42
11	BA	1160	SER	N-CA-C	5.05	117.80	110.42
43	Mj	107	GLU	CA-C-N	-5.05	114.21	122.79
43	Mj	107	GLU	C-N-CA	-5.05	114.21	122.79
53	sE	523	VAL	N-CA-CB	5.05	119.91	110.77
19	BI	53	GLY	N-CA-C	5.05	125.14	113.18
53	SE	463	PRO	CA-C-O	-5.04	111.42	120.60
55	SH	592	LEU	CB-CG-CD1	-5.04	95.57	110.70
24	BN	-42	DT	C4-C5-C7	-5.04	114.83	122.40
61	T6	759	VAL	CA-C-N	-5.04	115.99	123.05
61	T6	759	VAL	C-N-CA	-5.04	115.99	123.05
61	E6	159	ILE	N-CA-C	5.04	114.44	106.32
19	BI	86	PHE	CA-C-O	-5.04	116.06	121.45
55	sH	592	LEU	CB-CG-CD1	-5.04	95.58	110.70
60	t3	859	ASN	N-CA-C	5.04	117.50	111.71
28	AS	198	ARG	CB-CG-CD	-5.04	99.71	111.30
28	BS	198	ARG	CB-CG-CD	-5.04	99.72	111.30
3	B2	253	MET	CB-CG-SD	-5.04	97.59	112.70
24	AN	-42	DT	C4-C5-C7	-5.03	114.85	122.40
61	E6	160	TYR	CD1-CG-CD2	-5.03	110.55	118.10
60	T3	289	LYS	CA-C-O	5.03	126.08	120.80
60	T3	859	ASN	N-CA-C	5.03	117.50	111.71
64	t5	919	ARG	NE-CZ-NH2	-5.03	114.67	119.20
61	t6	759	VAL	CA-C-N	-5.03	116.00	123.05
61	t6	759	VAL	C-N-CA	-5.03	116.00	123.05
60	E3	418	LYS	CA-CB-CG	5.03	124.16	114.10
19	AI	53	GLY	N-CA-C	5.03	125.10	113.18
64	T5	919	ARG	NE-CZ-NH2	-5.03	114.67	119.20
53	SE	123	MET	CA-CB-CG	5.03	124.15	114.10
19	AI	65	ASP	CB-CA-C	5.02	115.75	110.17
3	A2	97	MET	CB-CA-C	5.02	118.09	109.80
3	A2	253	MET	CB-CG-SD	-5.02	97.63	112.70
11	AA	330	LYS	N-CA-C	5.02	116.44	110.97
19	BI	65	ASP	CB-CA-C	5.02	115.74	110.17
37	Md	255	ASN	N-CA-C	5.02	119.65	111.37
53	sE	123	MET	CA-CB-CG	5.02	124.14	114.10
3	B2	97	MET	CB-CA-C	5.01	118.07	109.80
8	A7	545	GLN	CG-CD-NE2	5.01	123.92	116.40
37	md	255	ASN	N-CA-C	5.01	119.63	111.37
8	B7	545	GLN	CG-CD-NE2	5.00	123.91	116.40
61	T6	971	GLU	CG-CD-OE1	-5.00	106.90	118.40

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A9	199	GLN	CA
28	AS	206	VAL	CA
50	SA	269	GLN	CA
9	SF	398	THR	CB
10	B9	199	GLN	CA
28	BS	206	VAL	CA
50	sA	269	GLN	CA
9	sF	398	THR	CB
60	T3	836	ILE	CB
64	T5	920	LYS	CA
60	t3	836	ILE	CB
64	t5	920	LYS	CA

All (201) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A0	553	MET	Mainchain
2	A1	193	LYS	Mainchain
3	A2	182	PHE	Peptide
3	A2	257	GLY	Peptide
3	A2	449	ASP	Peptide
3	A2	463	GLU	Sidechain
3	A2	507	ARG	Sidechain
4	A3	64	ARG	Sidechain
4	A3	89	PHE	Sidechain
5	A4	68	ASN	Peptide
6	A5	3	ARG	Sidechain
6	A5	5	ARG	Sidechain
8	A7	231	ARG	Peptide
8	A7	387	PRO	Peptide
8	A7	541	MET	Mainchain
8	A7	584	ASN	Peptide
9	A8	775	TYR	Sidechain
10	A9	199	GLN	Sidechain
10	A9	217	GLU	Sidechain
11	AA	1277	GLU	Peptide,Mainchain
11	AA	1278	ASN	Peptide
11	AA	300	VAL	Peptide
11	AA	464	PRO	Peptide
11	AA	692	ASP	Sidechain
11	AA	71	GLN	Peptide
12	AB	21	GLU	Mainchain
12	AB	22	SER	Mainchain

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Mol	Chain	Res	Type	Group
12	AB	474	SER	Peptide
17	AG	56	ILE	Peptide
18	AH	107	VAL	Peptide
18	AH	108	SER	Peptide
18	AH	130	ARG	Sidechain
19	AI	114	GLN	Sidechain
19	AI	60	GLN	Sidechain,Peptide
19	AI	61	ASP	Sidechain
19	AI	70	ARG	Sidechain
19	AI	72	ASP	Sidechain
19	AI	75	CYS	Mainchain
19	AI	81	ARG	Sidechain
19	AI	82	GLU	Sidechain
19	AI	86	PHE	Sidechain
19	AI	91	ARG	Sidechain
19	AI	92	ARG	Sidechain
19	AI	94	ASP	Sidechain
20	AJ	58	GLU	Sidechain
28	AS	198	ARG	Sidechain
28	AS	210	ASN	Peptide
28	AS	232	ASP	Sidechain
28	AS	236	LEU	Mainchain
31	AV	33	GLU	Peptide
32	AW	144	ARG	Sidechain
1	B0	553	MET	Mainchain
2	B1	193	LYS	Mainchain
3	B2	182	PHE	Peptide
3	B2	257	GLY	Peptide
3	B2	449	ASP	Peptide
3	B2	463	GLU	Sidechain
3	B2	507	ARG	Sidechain
4	B3	64	ARG	Sidechain
4	B3	89	PHE	Sidechain
5	B4	68	ASN	Peptide
6	B5	3	ARG	Sidechain
6	B5	5	ARG	Sidechain
8	B7	231	ARG	Peptide
8	B7	387	PRO	Peptide
8	B7	541	MET	Mainchain
8	B7	584	ASN	Peptide
9	B8	775	TYR	Sidechain
10	B9	199	GLN	Sidechain

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Mol	Chain	Res	Type	Group
10	B9	217	GLU	Sidechain
11	BA	1277	GLU	Peptide,Mainchain
11	BA	1278	ASN	Peptide
11	BA	300	VAL	Peptide
11	BA	464	PRO	Peptide
11	BA	692	ASP	Sidechain
11	BA	71	GLN	Peptide
12	BB	21	GLU	Mainchain
12	BB	22	SER	Mainchain
12	BB	474	SER	Peptide
17	BG	56	ILE	Peptide
18	BH	107	VAL	Peptide
18	BH	108	SER	Peptide
18	BH	130	ARG	Sidechain
19	BI	114	GLN	Sidechain
19	BI	60	GLN	Sidechain,Peptide
19	BI	61	ASP	Sidechain
19	BI	70	ARG	Sidechain
19	BI	72	ASP	Sidechain
19	BI	75	CYS	Mainchain
19	BI	81	ARG	Sidechain
19	BI	82	GLU	Sidechain
19	BI	86	PHE	Sidechain
19	BI	91	ARG	Sidechain
19	BI	92	ARG	Sidechain
19	BI	94	ASP	Sidechain
20	BJ	58	GLU	Sidechain
28	BS	198	ARG	Sidechain
28	BS	210	ASN	Peptide
28	BS	232	ASP	Sidechain
28	BS	236	LEU	Mainchain
31	BV	33	GLU	Peptide
32	BW	144	ARG	Sidechain
60	E3	412	ARG	Sidechain
60	E3	463	ARG	Sidechain
60	E3	914	TYR	Sidechain
60	E3	956	ARG	Sidechain
60	E3	958	SER	Mainchain
60	E3	959	LEU	Mainchain
61	E6	160	TYR	Sidechain
61	E6	161	ASN	Sidechain,Peptide
37	Md	206	ASP	Peptide

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Mol	Chain	Res	Type	Group
38	Me	55	ARG	Sidechain,Peptide
47	Mn	50	VAL	Peptide
50	SA	305	GLU	Peptide
50	SA	425	TYR	Sidechain
51	SB	770	PHE	Sidechain
53	SE	457	ARG	Sidechain
53	SE	465	GLU	Mainchain
53	SE	466	ILE	Mainchain
53	SE	486	ARG	Sidechain
53	SE	489	ARG	Sidechain
53	SE	510	SER	Mainchain
53	SE	515	PHE	Sidechain
53	SE	519	TYR	Sidechain
53	SE	547	ARG	Sidechain
53	SE	560	LYS	Mainchain
9	SF	383	TYR	Mainchain
9	SF	389	ASN	Sidechain
9	SF	393	LYS	Mainchain
9	SF	401	LYS	Mainchain
9	SF	469	ASP	Peptide
9	SF	617	GLY	Peptide
55	SH	590	GLU	Sidechain
55	SH	596	ARG	Mainchain
56	SI	1050	GLU	Peptide
56	SI	1110	VAL	Mainchain
56	SI	866	GLU	Peptide
56	SI	868	ILE	Peptide
58	SK	191	PHE	Mainchain
58	SK	91	TYR	Sidechain
58	SK	98	SER	Mainchain
63	T2	105	TYR	Sidechain
60	T3	288	MET	Mainchain
60	T3	292	ARG	Sidechain
60	T3	406	LYS	Mainchain
60	T3	409	LYS	Mainchain
60	T3	837	TYR	Sidechain
60	T3	912	SER	Peptide
45	T4	1002	HIS	Sidechain
64	T5	923	LYS	Mainchain
64	T5	931	GLN	Sidechain
61	T6	760	ALA	Peptide
37	md	206	ASP	Peptide

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Mol	Chain	Res	Type	Group
38	me	55	ARG	Sidechain,Peptide
47	mn	50	VAL	Peptide
50	sA	305	GLU	Peptide
50	sA	425	TYR	Sidechain
51	sB	770	PHE	Sidechain
53	sE	457	ARG	Sidechain
53	sE	465	GLU	Mainchain
53	sE	466	ILE	Mainchain
53	sE	486	ARG	Sidechain
53	sE	489	ARG	Sidechain
53	sE	510	SER	Mainchain
53	sE	515	PHE	Sidechain
53	sE	519	TYR	Sidechain
53	sE	547	ARG	Sidechain
53	sE	560	LYS	Mainchain
9	sF	383	TYR	Mainchain
9	sF	389	ASN	Sidechain
9	sF	393	LYS	Mainchain
9	sF	401	LYS	Mainchain
9	sF	469	ASP	Peptide
9	sF	617	GLY	Peptide
55	sH	590	GLU	Sidechain
55	sH	596	ARG	Mainchain
56	sI	1050	GLU	Peptide
56	sI	1110	VAL	Mainchain
56	sI	866	GLU	Peptide
56	sI	868	ILE	Peptide
58	sK	191	PHE	Mainchain
58	sK	91	TYR	Sidechain
58	sK	98	SER	Mainchain
63	t2	105	TYR	Sidechain
60	t3	288	MET	Mainchain
60	t3	292	ARG	Sidechain
60	t3	406	LYS	Mainchain
60	t3	409	LYS	Mainchain
60	t3	837	TYR	Sidechain
60	t3	912	SER	Peptide
45	t4	1002	HIS	Sidechain
64	t5	923	LYS	Mainchain
64	t5	931	GLN	Sidechain
61	t6	760	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	6091	0	6155	77	0
1	B0	6091	0	6155	77	0
2	A1	3374	0	3425	26	0
2	B1	3374	0	3425	22	0
3	A2	3597	0	3687	78	0
3	B2	3597	0	3687	74	0
4	A3	1089	0	1069	56	0
4	B3	1089	0	1069	55	0
5	A4	2274	0	2332	21	0
5	B4	2274	0	2332	21	0
6	A5	514	0	541	20	0
6	B5	514	0	541	19	0
7	A6	2946	0	2958	31	0
7	B6	2946	0	2958	31	0
8	A7	4881	0	4868	63	0
8	B7	4881	0	4868	61	0
9	A8	134	0	141	5	0
9	B8	134	0	141	5	0
9	SF	3374	0	3292	76	0
9	sF	3374	0	3292	80	0
10	A9	542	0	537	10	0
10	B9	542	0	537	10	0
11	AA	10996	0	11079	143	0
11	BA	10996	0	11079	145	0
11	MA	575	0	507	6	0
11	mA	575	0	507	5	0
12	AB	9249	0	9247	96	0
12	BB	9249	0	9247	117	0
13	AC	2061	0	2029	15	0
13	BC	2061	0	2029	15	0
14	AD	1253	0	1275	38	0
14	BD	1253	0	1275	38	0
15	AE	1744	0	1772	13	0
15	BE	1744	0	1772	14	0
16	AF	670	0	690	5	0
16	BF	670	0	690	4	0
17	AG	1340	0	1357	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	BG	1340	0	1357	60	0
18	AH	1089	0	1062	37	0
18	BH	1089	0	1062	38	0
19	AI	944	0	901	49	0
19	BI	944	0	901	44	0
20	AJ	569	0	585	10	0
20	BJ	569	0	585	10	0
21	AK	924	0	934	15	0
21	BK	924	0	934	15	0
22	AL	359	0	381	1	0
22	BL	359	0	381	2	0
23	AM	2097	0	2182	88	0
23	BM	2097	0	2182	86	0
24	AN	1413	0	785	14	0
24	BN	1413	0	785	14	0
25	AO	1422	0	1500	7	0
25	BO	1422	0	1500	7	0
26	AQ	1817	0	1843	26	0
26	BQ	1817	0	1843	25	0
27	AR	2173	0	2192	73	0
27	BR	2173	0	2192	71	0
28	AS	1301	0	1294	45	0
28	BS	1301	0	1294	47	0
29	AT	1416	0	782	11	0
29	BT	1416	0	782	11	0
30	AU	843	0	827	11	0
30	BU	843	0	827	11	0
31	AV	815	0	822	13	0
31	BV	815	0	822	12	0
32	AW	1836	0	1854	55	0
32	BW	1836	0	1854	54	0
33	AX	1530	0	1565	6	0
33	BX	1530	0	1565	6	0
34	Ma	1407	0	1385	23	0
34	ma	1407	0	1385	23	0
35	Mb	1295	0	1297	32	0
35	mb	1295	0	1297	32	0
36	Mc	876	0	885	7	0
36	mc	876	0	885	7	0
37	Md	4325	0	4482	22	0
37	md	4325	0	4482	22	0
38	Me	1958	0	1976	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	me	1958	0	1976	18	0
39	Mf	1609	0	1626	6	0
39	mf	1609	0	1626	4	0
40	Mg	847	0	858	10	0
40	mg	847	0	858	10	0
41	Mh	1441	0	1461	7	0
41	mh	1441	0	1461	7	0
42	Mi	1538	0	1576	8	0
42	mi	1538	0	1576	8	0
43	Mj	864	0	870	28	0
43	mj	864	0	870	27	0
44	Mk	1157	0	1142	13	0
44	mk	1157	0	1142	13	0
45	MI	5367	0	5607	57	0
45	T4	1780	0	1765	31	0
45	ml	5367	0	5607	47	0
45	t4	1780	0	1765	39	0
46	Mm	671	0	650	2	0
46	mm	671	0	650	2	0
47	Mn	1124	0	1147	7	0
47	mn	1124	0	1147	8	0
48	Mo	914	0	902	5	0
48	mo	914	0	902	5	0
49	Mp	3330	0	3241	53	0
49	mp	3330	0	3243	36	0
50	SA	3552	0	3509	34	0
50	sA	3552	0	3509	34	0
51	SB	3250	0	3302	45	0
51	SD	3445	0	3505	38	0
51	sB	3250	0	3302	44	0
51	sD	3445	0	3505	40	0
52	SC	1266	0	1264	10	0
52	sC	1266	0	1264	9	0
53	SE	3333	0	3375	76	0
53	sE	3333	0	3375	75	0
54	SG	271	0	131	5	0
54	sG	271	0	131	5	0
55	SH	1958	0	1976	55	0
55	sH	1958	0	1976	54	0
56	SI	4474	0	4633	47	0
56	sI	4474	0	4633	50	0
57	SJ	711	0	695	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	sJ	711	0	695	14	0
58	SK	3453	0	3449	45	0
58	sK	3453	0	3449	42	0
59	SL	3266	0	3264	22	0
59	sL	3266	0	3264	22	0
60	E3	6069	0	6088	99	0
60	T3	6173	0	6169	129	0
60	t3	6173	0	6169	82	0
61	E6	7551	0	7603	135	0
61	T6	7551	0	7605	88	0
61	t6	7551	0	7605	88	0
62	T1	516	0	527	9	0
62	t1	516	0	527	7	0
63	T2	891	0	907	14	0
63	t2	891	0	907	14	0
64	T5	894	0	930	23	0
64	t5	894	0	930	44	0
65	A0	8	0	0	0	0
65	B0	8	0	0	0	0
66	A3	2	0	0	0	0
66	A4	1	0	0	0	0
66	A6	4	0	0	0	0
66	AA	2	0	0	0	0
66	AB	1	0	0	0	0
66	AC	1	0	0	0	0
66	AI	2	0	0	0	0
66	AJ	1	0	0	0	0
66	AL	1	0	0	0	0
66	AM	1	0	0	0	0
66	AS	1	0	0	0	0
66	AW	1	0	0	0	0
66	B3	2	0	0	0	0
66	B4	1	0	0	0	0
66	B6	4	0	0	0	0
66	BA	2	0	0	0	0
66	BB	1	0	0	0	0
66	BC	1	0	0	0	0
66	BI	2	0	0	0	0
66	BJ	1	0	0	0	0
66	BL	1	0	0	0	0
66	BM	1	0	0	0	0
66	BS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	BW	1	0	0	0	0
67	AA	1	0	0	0	0
67	BA	1	0	0	0	0
All	All	319192	0	318855	3855	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (3855) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:T3:837:TYR:CD2	60:T3:837:TYR:CG	1.80	1.68
60:t3:837:TYR:CD2	60:t3:837:TYR:CG	1.80	1.66
19:BI:86:PHE:CD2	19:BI:86:PHE:CG	1.84	1.64
19:AI:86:PHE:CD2	19:AI:86:PHE:CG	1.84	1.64
4:A3:100:ASN:HB3	34:Ma:140:GLY:CA	1.26	1.62
23:BM:302:LEU:HA	27:BR:270:MET:CE	1.19	1.61
61:E6:749:LEU:CG	61:E6:749:LEU:CD1	1.77	1.61
55:SH:592:LEU:CG	55:SH:592:LEU:CD1	1.78	1.61
23:AM:16:PRO:CG	32:AW:151:LEU:HD21	1.17	1.60
4:B3:100:ASN:HB3	34:ma:140:GLY:CA	1.26	1.60
53:SE:523:VAL:CG1	53:SE:523:VAL:CB	1.79	1.59
53:sE:523:VAL:CG1	53:sE:523:VAL:CB	1.79	1.59
23:AM:302:LEU:HA	27:AR:270:MET:CE	1.19	1.57
19:BI:104:LEU:CD2	19:BI:104:LEU:CG	1.82	1.57
19:AI:104:LEU:CG	19:AI:104:LEU:CD2	1.82	1.57
55:sH:592:LEU:CD1	55:sH:592:LEU:CG	1.78	1.56
23:BM:16:PRO:CG	32:BW:151:LEU:HD21	1.17	1.56
55:sH:594:LEU:CD2	55:sH:594:LEU:HB2	1.35	1.56
55:SH:594:LEU:CD2	55:SH:594:LEU:HB2	1.35	1.56
61:E6:749:LEU:CG	61:E6:749:LEU:CD2	1.76	1.56
3:A2:506:LYS:NZ	3:A2:506:LYS:CE	1.68	1.55
23:AM:302:LEU:CA	27:AR:270:MET:HE1	1.10	1.53
3:B2:506:LYS:NZ	3:B2:506:LYS:CE	1.68	1.53
4:A3:49:LEU:HD23	17:AG:164:LYS:CD	1.37	1.51
23:BM:302:LEU:CA	27:BR:270:MET:HE1	1.10	1.50
60:E3:939:THR:CB	60:E3:939:THR:CG2	1.87	1.49
23:AM:302:LEU:C	27:AR:270:MET:CE	1.86	1.49
4:B3:49:LEU:HD23	17:BG:164:LYS:CD	1.37	1.49
23:BM:302:LEU:CA	27:BR:270:MET:CE	1.78	1.49
23:BM:16:PRO:HG3	32:BW:151:LEU:CD2	1.43	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BA:68:GLN:HG3	32:BW:151:LEU:CD1	1.43	1.48
23:AM:16:PRO:HG3	32:AW:151:LEU:CD2	1.43	1.48
60:t3:289:LYS:CB	60:t3:289:LYS:CG	1.88	1.48
60:T3:289:LYS:CG	60:T3:289:LYS:CB	1.88	1.47
11:AA:68:GLN:HG3	32:AW:151:LEU:CD1	1.43	1.47
4:A3:100:ASN:CB	34:Ma:140:GLY:CA	1.93	1.46
4:B3:49:LEU:CD2	17:BG:164:LYS:HD2	1.45	1.44
4:B3:100:ASN:CB	34:ma:140:GLY:CA	1.93	1.44
23:BM:302:LEU:C	27:BR:270:MET:CE	1.87	1.44
55:sH:594:LEU:CD2	55:sH:594:LEU:CG	1.96	1.43
19:AI:75:CYS:SG	19:AI:75:CYS:CB	2.07	1.43
19:BI:75:CYS:CB	19:BI:75:CYS:SG	2.07	1.43
4:A3:49:LEU:CD2	17:AG:164:LYS:HD2	1.45	1.41
55:SH:594:LEU:CD2	55:SH:594:LEU:CG	1.96	1.41
23:BM:302:LEU:C	27:BR:270:MET:HE1	1.45	1.41
49:Mp:548:TYR:CG	61:E6:612:GLU:OE1	1.73	1.41
61:E6:184:LYS:NZ	60:T3:429:PHE:HB2	1.39	1.37
4:A3:100:ASN:ND2	34:Ma:140:GLY:HA3	1.40	1.35
55:sH:594:LEU:CD2	55:sH:594:LEU:CB	2.04	1.35
53:SE:523:VAL:HA	53:SE:547:ARG:NH1	1.38	1.34
53:sE:523:VAL:HA	53:sE:547:ARG:NH1	1.38	1.34
61:E6:749:LEU:CD1	61:E6:749:LEU:CB	2.05	1.34
55:SH:594:LEU:CD2	55:SH:594:LEU:CB	2.04	1.34
4:B3:100:ASN:ND2	34:ma:140:GLY:HA3	1.40	1.34
11:BA:420:ARG:HD3	38:me:60:GLU:CD	1.53	1.33
11:BA:420:ARG:HD3	38:me:60:GLU:OE1	1.21	1.33
23:BM:301:THR:HG23	27:BR:271:ARG:NH2	1.42	1.33
23:AM:14:ARG:NH2	32:AW:126:ILE:HD13	1.43	1.32
11:AA:420:ARG:HD3	38:Me:60:GLU:CD	1.53	1.31
23:AM:303:GLN:HG3	27:AR:270:MET:SD	1.70	1.31
4:B3:100:ASN:CG	34:ma:140:GLY:HA3	1.56	1.30
23:BM:14:ARG:NH2	32:BW:126:ILE:HD13	1.43	1.30
11:AA:420:ARG:HD3	38:Me:60:GLU:OE1	1.21	1.30
23:AM:301:THR:HG23	27:AR:271:ARG:NH2	1.42	1.29
23:BM:303:GLN:HG3	27:BR:270:MET:SD	1.70	1.29
61:E6:159:ILE:O	60:T3:838:SER:HA	1.29	1.29
23:AM:302:LEU:C	27:AR:270:MET:HE1	1.45	1.29
11:AA:420:ARG:CD	38:Me:60:GLU:OE1	1.81	1.28
60:E3:939:THR:HB	60:T3:429:PHE:CZ	1.68	1.28
11:BA:420:ARG:CD	38:me:60:GLU:OE1	1.81	1.27
60:E3:900:THR:HG22	60:T3:431:ASP:OD1	1.21	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:100:ASN:CG	34:Ma:140:GLY:HA3	1.56	1.27
19:BI:86:PHE:CD2	19:BI:86:PHE:CD1	1.98	1.26
55:sH:586:TYR:O	55:sH:590:GLU:N	1.66	1.26
49:mp:157:ASN:ND2	60:E3:495:ASN:HD21	1.30	1.26
55:SH:586:TYR:O	55:SH:590:GLU:N	1.66	1.26
23:AM:303:GLN:CG	27:AR:270:MET:SD	2.24	1.25
60:E3:939:THR:HB	60:T3:429:PHE:CE1	1.71	1.25
19:AI:86:PHE:CD2	19:AI:86:PHE:CD1	1.98	1.25
23:BM:303:GLN:CG	27:BR:270:MET:SD	2.24	1.25
49:Mp:157:ASN:ND2	61:E6:323:PRO:HD2	1.49	1.25
60:t3:837:TYR:CD2	60:t3:837:TYR:CB	2.20	1.24
61:E6:184:LYS:HE2	60:T3:428:LEU:O	1.13	1.24
60:E3:904:ASN:HB2	60:T3:431:ASP:CB	1.68	1.23
60:T3:837:TYR:CD2	60:T3:837:TYR:CB	2.20	1.23
19:BI:104:LEU:CD2	19:BI:104:LEU:CD1	2.17	1.23
10:B9:191:GLU:OE1	9:sF:763:ARG:HA	1.39	1.22
19:AI:104:LEU:CD2	19:AI:104:LEU:CD1	2.17	1.22
23:AM:16:PRO:CG	32:AW:151:LEU:CD2	2.07	1.22
4:A3:100:ASN:CB	34:Ma:140:GLY:HA2	1.54	1.22
4:B3:100:ASN:CB	34:ma:140:GLY:HA2	1.54	1.22
4:B3:49:LEU:HD23	17:BG:164:LYS:CE	1.70	1.21
23:AM:302:LEU:CA	27:AR:270:MET:CE	1.77	1.21
49:Mp:548:TYR:CB	61:E6:612:GLU:OE1	1.87	1.21
4:A3:49:LEU:HD23	17:AG:164:LYS:CE	1.70	1.20
18:AH:128:ASN:HD21	43:Mj:81:ASN:ND2	1.41	1.19
12:BB:15:PRO:CD	64:t5:921:PRO:O	1.90	1.19
60:T3:837:TYR:CD2	60:T3:837:TYR:HB3	1.73	1.19
55:sH:592:LEU:CD1	55:sH:592:LEU:CD2	2.19	1.19
23:AM:301:THR:O	27:AR:271:ARG:NH1	1.76	1.19
55:SH:592:LEU:CD1	55:SH:592:LEU:CD2	2.19	1.19
10:A9:191:GLU:OE1	9:SF:763:ARG:HA	1.40	1.18
18:BH:128:ASN:HD21	43:mj:81:ASN:ND2	1.41	1.18
4:A3:100:ASN:CA	34:Ma:140:GLY:HA2	1.72	1.18
4:B3:100:ASN:CA	34:ma:140:GLY:HA2	1.72	1.18
60:E3:708:GLN:NE2	61:t6:157:TYR:CD2	2.11	1.18
55:SH:585:LEU:O	55:SH:589:HIS:N	1.76	1.17
55:sH:585:LEU:O	55:sH:589:HIS:N	1.76	1.17
23:BM:301:THR:O	27:BR:271:ARG:NH1	1.76	1.16
12:BB:15:PRO:HD3	64:t5:921:PRO:O	1.03	1.16
60:t3:837:TYR:CD2	60:t3:837:TYR:HB3	1.73	1.16
11:AA:678:GLU:OE2	61:T6:761:LYS:NZ	1.76	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BM:16:PRO:CG	32:BW:151:LEU:CD2	2.07	1.15
17:AG:100:GLU:OE2	32:AW:144:ARG:NE	1.80	1.14
17:BG:100:GLU:OE2	32:BW:144:ARG:NE	1.80	1.13
23:AM:302:LEU:C	27:AR:270:MET:HE2	1.71	1.13
23:BM:302:LEU:HA	27:BR:270:MET:HE3	1.22	1.13
9:B8:790:LYS:HB3	9:sF:763:ARG:HH21	1.09	1.13
60:E3:708:GLN:NE2	61:t6:157:TYR:CE2	2.16	1.13
9:A8:790:LYS:HB3	9:SF:763:ARG:HH21	1.09	1.12
60:E3:900:THR:CG2	60:T3:431:ASP:OD1	1.97	1.12
49:Mp:548:TYR:HB3	61:E6:612:GLU:OE1	1.44	1.12
23:AM:16:PRO:CB	32:AW:151:LEU:HD21	1.80	1.12
23:AM:14:ARG:NH2	32:AW:126:ILE:CD1	2.12	1.11
4:B3:49:LEU:CG	17:BG:164:LYS:HB3	1.81	1.11
12:BB:15:PRO:HD3	64:t5:921:PRO:C	1.75	1.11
23:BM:14:ARG:NH2	32:BW:126:ILE:CD1	2.12	1.11
23:BM:16:PRO:CB	32:BW:151:LEU:HD21	1.80	1.11
11:BA:68:GLN:HG3	32:BW:151:LEU:HD11	1.14	1.11
23:AM:245:HIS:HD2	27:AR:264:SER:HB2	1.13	1.10
4:A3:49:LEU:CG	17:AG:164:LYS:HB3	1.81	1.09
55:SH:594:LEU:HB2	55:SH:594:LEU:HD23	1.32	1.09
18:AH:109:LYS:O	43:Mj:83:LEU:HB2	1.52	1.09
60:E3:939:THR:CB	60:T3:429:PHE:CE1	2.36	1.09
11:AA:68:GLN:CG	32:AW:151:LEU:CD1	2.30	1.09
61:E6:184:LYS:CE	60:T3:428:LEU:O	2.00	1.09
18:BH:109:LYS:O	43:mj:83:LEU:HB2	1.52	1.08
11:BA:68:GLN:CG	32:BW:151:LEU:CD1	2.30	1.08
23:AM:302:LEU:HA	27:AR:270:MET:HE3	1.22	1.08
60:E3:904:ASN:HB2	60:T3:431:ASP:HB3	1.19	1.08
11:AA:68:GLN:HG3	32:AW:151:LEU:HD11	1.13	1.07
23:BM:245:HIS:HD2	27:BR:264:SER:HB2	1.13	1.07
23:BM:302:LEU:C	27:BR:270:MET:HE2	1.71	1.07
23:BM:16:PRO:HG2	32:BW:151:LEU:HD21	1.37	1.07
55:sH:584:GLN:O	55:sH:588:ASN:CB	2.03	1.07
45:MI:831:GLN:HG2	45:t4:837:VAL:HB	1.37	1.06
4:B3:100:ASN:HD22	34:ma:140:GLY:CA	1.69	1.06
4:B3:100:ASN:CB	34:ma:140:GLY:HA3	1.67	1.05
23:BM:302:LEU:O	27:BR:270:MET:HE2	1.56	1.05
4:B3:100:ASN:HB3	34:ma:140:GLY:N	1.71	1.05
55:sH:594:LEU:HB2	55:sH:594:LEU:HD23	1.32	1.05
55:SH:584:GLN:O	55:SH:588:ASN:CB	2.03	1.05
4:A3:100:ASN:CB	34:Ma:140:GLY:HA3	1.67	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BB:13:GLU:OE1	64:t5:921:PRO:O	1.75	1.05
4:A3:64:ARG:NH2	17:AG:165:GLU:OE1	1.89	1.04
12:BB:13:GLU:OE1	64:t5:920:LYS:O	1.75	1.04
4:B3:100:ASN:HB3	34:ma:140:GLY:HA2	1.09	1.04
60:E3:939:THR:CG2	60:E3:939:THR:CA	2.35	1.04
4:A3:100:ASN:HB3	34:Ma:140:GLY:N	1.71	1.04
12:AB:868:MET:HE1	23:AM:182:ARG:O	1.57	1.04
4:B3:64:ARG:NH2	17:BG:165:GLU:OE1	1.89	1.04
14:BD:217:LEU:CD2	35:mb:42:GLN:HE22	1.71	1.04
4:A3:100:ASN:HD22	34:Ma:140:GLY:CA	1.69	1.04
55:SH:592:LEU:CD1	55:SH:592:LEU:CB	2.36	1.04
23:AM:302:LEU:O	27:AR:270:MET:HE2	1.55	1.03
53:SE:523:VAL:CG1	53:SE:523:VAL:CG2	2.35	1.03
49:mp:157:ASN:ND2	60:E3:495:ASN:ND2	2.05	1.03
12:BB:868:MET:HE1	23:BM:182:ARG:O	1.57	1.03
53:sE:523:VAL:CG1	53:sE:523:VAL:CG2	2.35	1.03
19:AI:104:LEU:CD2	19:AI:104:LEU:CB	2.37	1.03
23:AM:303:GLN:CD	27:AR:270:MET:SD	2.42	1.03
14:BD:217:LEU:HD21	35:mb:42:GLN:NE2	1.74	1.03
55:sH:585:LEU:HD23	55:sH:589:HIS:CD2	1.94	1.03
23:AM:16:PRO:HG2	32:AW:151:LEU:HD21	1.36	1.03
19:BI:104:LEU:CD2	19:BI:104:LEU:HD13	1.88	1.03
53:sE:523:VAL:HA	53:sE:547:ARG:HH12	1.24	1.02
14:AD:217:LEU:HD21	35:Mb:42:GLN:NE2	1.74	1.02
23:BM:303:GLN:CD	27:BR:270:MET:SD	2.42	1.02
61:E6:184:LYS:HZ1	60:T3:429:PHE:HB2	1.23	1.02
6:A5:7:GLY:HA3	6:A5:41:LEU:HD11	1.42	1.02
55:sH:592:LEU:CD1	55:sH:592:LEU:CB	2.36	1.02
4:A3:100:ASN:ND2	34:Ma:140:GLY:CA	2.23	1.02
19:BI:104:LEU:CD2	19:BI:104:LEU:CB	2.37	1.02
4:A3:49:LEU:HG	17:AG:164:LYS:CB	1.90	1.01
14:AD:217:LEU:CD2	35:Mb:42:GLN:HE22	1.71	1.01
23:BM:301:THR:HG23	27:BR:271:ARG:HH22	0.91	1.01
4:B3:100:ASN:ND2	34:ma:140:GLY:CA	2.23	1.01
45:MI:831:GLN:CG	45:t4:837:VAL:HB	1.90	1.01
60:E3:838:SER:HA	61:T6:157:TYR:CE2	1.95	1.01
4:B3:49:LEU:HG	17:BG:164:LYS:CB	1.90	1.01
60:T3:837:TYR:CD2	60:T3:837:TYR:CD1	2.33	1.01
55:SH:585:LEU:HD23	55:SH:589:HIS:CD2	1.94	1.01
3:B2:506:LYS:NZ	3:B2:506:LYS:CD	2.24	1.00
55:SH:594:LEU:CD2	55:SH:594:LEU:CD1	2.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B5:7:GLY:HA3	6:B5:41:LEU:HD11	1.42	1.00
17:BG:100:GLU:HG3	32:BW:144:ARG:NH2	1.77	1.00
3:A2:506:LYS:NZ	3:A2:506:LYS:CD	2.24	1.00
19:AI:104:LEU:CD2	19:AI:104:LEU:HD13	1.88	1.00
11:AA:420:ARG:CG	38:Me:60:GLU:OE1	2.09	1.00
11:BA:420:ARG:CG	38:me:60:GLU:OE1	2.09	1.00
55:sH:594:LEU:CD2	55:sH:594:LEU:CD1	2.38	1.00
60:E3:904:ASN:CB	60:T3:431:ASP:HB3	1.92	1.00
49:mp:157:ASN:HD22	60:E3:495:ASN:ND2	1.57	0.99
17:AG:100:GLU:HG3	32:AW:144:ARG:NH2	1.77	0.99
19:BI:86:PHE:CD2	19:BI:86:PHE:CB	2.45	0.99
59:sL:430:LEU:HA	59:sL:433:GLN:HE21	1.25	0.99
19:AI:86:PHE:CD2	19:AI:86:PHE:CB	2.45	0.99
23:AM:245:HIS:CD2	27:AR:264:SER:HB2	1.97	0.99
28:BS:274:CYS:HB3	28:BS:302:CYS:SG	2.02	0.99
49:Mp:548:TYR:CD1	61:E6:612:GLU:OE1	2.15	0.99
61:E6:184:LYS:HE2	60:T3:428:LEU:C	1.87	0.98
28:AS:274:CYS:HB3	28:AS:302:CYS:SG	2.03	0.98
59:SL:430:LEU:HA	59:SL:433:GLN:HE21	1.25	0.98
4:B3:49:LEU:HG	17:BG:164:LYS:HB3	0.98	0.98
18:BH:106:GLU:OE2	43:mj:83:LEU:CD1	2.12	0.98
23:BM:245:HIS:CD2	27:BR:264:SER:HB2	1.97	0.98
61:E6:749:LEU:CD1	61:E6:749:LEU:HB2	1.89	0.98
4:A3:49:LEU:HG	17:AG:164:LYS:HB3	0.98	0.97
18:AH:106:GLU:OE2	43:Mj:83:LEU:CD1	2.12	0.97
4:A3:49:LEU:CD2	17:AG:164:LYS:CD	2.20	0.97
23:AM:301:THR:HG23	27:AR:271:ARG:HH22	0.91	0.97
45:ML:831:GLN:HG2	45:t4:837:VAL:CB	1.94	0.97
61:E6:382:SER:OG	60:t3:431:ASP:OD2	1.80	0.97
9:sF:400:GLN:O	9:sF:402:ILE:HG13	1.66	0.96
4:A3:100:ASN:HA	34:Ma:140:GLY:HA2	1.46	0.96
4:B3:100:ASN:HD22	34:ma:140:GLY:HA3	1.19	0.96
4:B3:100:ASN:HA	34:ma:140:GLY:HA2	1.46	0.95
23:BM:14:ARG:HH22	32:BW:126:ILE:HD13	1.14	0.95
11:AA:420:ARG:HD3	38:Me:60:GLU:OE2	1.65	0.95
9:SF:400:GLN:O	9:SF:402:ILE:HG13	1.66	0.95
18:AH:110:ASP:HA	43:Mj:83:LEU:HG	1.49	0.95
61:E6:186:TYR:HE1	60:T3:428:LEU:HD22	1.32	0.95
55:sH:586:TYR:O	55:sH:590:GLU:CA	2.15	0.94
4:A3:49:LEU:HD23	17:AG:164:LYS:HD2	1.01	0.94
9:B8:790:LYS:HB3	9:sF:763:ARG:NH2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:544:TYR:H	2:A1:358:MET:HE1	1.32	0.94
55:SH:586:TYR:O	55:SH:590:GLU:CA	2.15	0.94
11:BA:420:ARG:HG3	38:me:60:GLU:OE1	1.68	0.94
61:E6:184:LYS:NZ	60:T3:429:PHE:CB	2.31	0.94
4:B3:49:LEU:HD23	17:BG:164:LYS:HE2	1.50	0.94
18:BH:110:ASP:HA	43:mj:83:LEU:HG	1.49	0.94
23:BM:301:THR:CG2	27:BR:271:ARG:HH22	1.80	0.94
53:SE:523:VAL:HA	53:SE:547:ARG:HH12	1.24	0.94
11:AA:420:ARG:HG3	38:Me:60:GLU:OE1	1.68	0.94
14:BD:213:GLU:HG2	35:mb:38:MET:SD	2.08	0.94
55:sH:584:GLN:O	55:sH:588:ASN:HB2	1.65	0.94
3:A2:463:GLU:O	9:SF:402:ILE:CG1	2.16	0.93
11:BA:420:ARG:HD3	38:me:60:GLU:OE2	1.65	0.93
53:sE:523:VAL:CA	53:sE:547:ARG:NH1	2.31	0.93
55:SH:584:GLN:O	55:SH:588:ASN:HB2	1.65	0.93
3:B2:463:GLU:O	9:sF:402:ILE:CG1	2.16	0.93
4:A3:100:ASN:HD22	34:Ma:140:GLY:C	1.76	0.93
9:A8:790:LYS:HB3	9:SF:763:ARG:NH2	1.82	0.93
10:A9:191:GLU:OE1	9:SF:763:ARG:CA	2.17	0.93
4:B3:49:LEU:CD2	17:BG:164:LYS:CD	2.20	0.93
61:E6:161:ASN:OD1	60:T3:838:SER:HB3	1.67	0.93
11:BA:420:ARG:CD	38:me:60:GLU:CD	2.38	0.93
14:AD:213:GLU:HG2	35:Mb:38:MET:SD	2.08	0.93
55:SH:584:GLN:O	55:SH:588:ASN:HB3	1.70	0.92
11:AA:420:ARG:CD	38:Me:60:GLU:CD	2.38	0.92
55:SH:594:LEU:CD2	55:SH:594:LEU:HD13	2.00	0.92
4:A3:49:LEU:HD23	17:AG:164:LYS:HE2	1.50	0.92
4:B3:49:LEU:CG	17:BG:164:LYS:HD2	2.00	0.92
18:AH:128:ASN:HD21	43:Mj:81:ASN:HD21	0.97	0.92
10:B9:191:GLU:OE1	9:sF:763:ARG:CA	2.17	0.92
18:BH:128:ASN:HD21	43:mj:81:ASN:HD21	0.97	0.92
60:t3:837:TYR:CD2	60:t3:837:TYR:CD1	2.33	0.92
23:AM:301:THR:CG2	27:AR:271:ARG:HH22	1.80	0.92
55:sH:584:GLN:O	55:sH:588:ASN:HB3	1.70	0.92
4:A3:100:ASN:HB3	34:Ma:140:GLY:HA2	1.10	0.92
4:B3:100:ASN:HD22	34:ma:140:GLY:C	1.76	0.91
49:Mp:157:ASN:ND2	61:E6:323:PRO:CD	2.34	0.91
55:sH:594:LEU:CD2	55:sH:594:LEU:HD13	1.99	0.91
11:AA:68:GLN:HG3	32:AW:151:LEU:HD13	1.52	0.91
49:Mp:183:CYS:SG	61:E6:754:LYS:HE3	2.11	0.91
1:B0:544:TYR:H	2:B1:358:MET:HE1	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:E3:708:GLN:NE2	61:t6:157:TYR:HD2	1.64	0.90
11:BA:110:CYS:HB3	11:BA:167:CYS:SG	2.11	0.90
61:E6:159:ILE:O	60:T3:838:SER:CA	2.17	0.90
4:A3:49:LEU:CG	17:AG:164:LYS:HD2	1.99	0.90
60:E3:708:GLN:HE22	61:t6:157:TYR:HD2	1.19	0.90
53:SE:523:VAL:HA	53:SE:547:ARG:HH11	1.36	0.90
11:BA:68:GLN:HG3	32:BW:151:LEU:HD13	1.52	0.90
11:AA:110:CYS:HB3	11:AA:167:CYS:SG	2.11	0.89
53:sE:523:VAL:HA	53:sE:547:ARG:HH11	1.36	0.89
23:AM:154:TYR:CE1	23:AM:172:MET:HE1	2.07	0.89
55:sH:592:LEU:CD1	55:sH:592:LEU:HD22	2.02	0.89
23:AM:16:PRO:HG3	32:AW:151:LEU:HD21	0.93	0.89
23:AM:14:ARG:HH22	32:AW:126:ILE:HD13	1.14	0.89
24:AN:-62:DG:N2	29:AT:62:DC:O2	2.06	0.89
55:SH:585:LEU:HD23	55:SH:589:HIS:HD2	1.37	0.88
24:BN:-62:DG:N2	29:BT:62:DC:O2	2.06	0.88
61:E6:749:LEU:CD2	61:E6:749:LEU:HG	2.03	0.88
4:A3:100:ASN:HD22	34:Ma:140:GLY:HA3	1.19	0.88
11:BA:420:ARG:HH21	38:me:58:LEU:HD23	1.38	0.88
18:BH:128:ASN:ND2	43:mj:81:ASN:HD21	1.72	0.88
23:BM:154:TYR:CE1	23:BM:172:MET:HE1	2.07	0.88
53:SE:523:VAL:CA	53:SE:547:ARG:NH1	2.31	0.87
12:BB:13:GLU:O	64:t5:922:THR:CB	2.22	0.87
11:AA:420:ARG:HH21	38:Me:58:LEU:HD23	1.38	0.87
23:BM:302:LEU:N	27:BR:270:MET:HE1	1.90	0.87
60:E3:708:GLN:HE21	61:t6:157:TYR:HE2	1.22	0.87
4:A3:17:LYS:HD2	32:AW:173:ASN:OD1	1.75	0.87
23:AM:302:LEU:N	27:AR:270:MET:HE1	1.90	0.86
45:MI:831:GLN:CD	45:t4:837:VAL:HB	1.99	0.86
18:AH:128:ASN:ND2	43:Mj:81:ASN:HD21	1.72	0.86
23:AM:302:LEU:CA	27:AR:270:MET:HE2	1.95	0.86
19:AI:78:CYS:SG	19:AI:106:CYS:HB3	2.16	0.86
23:BM:16:PRO:HG3	32:BW:151:LEU:HD21	0.93	0.86
28:AS:187:ASN:HB2	28:AS:228:LEU:HD21	1.56	0.86
49:Mp:548:TYR:CG	61:E6:612:GLU:CD	2.53	0.86
12:BB:13:GLU:HG3	64:t5:919:ARG:HD2	1.56	0.86
3:A2:261:GLN:HG2	3:A2:263:HIS:H	1.41	0.86
59:SL:333:ILE:HG23	59:SL:409:LEU:HD13	1.57	0.86
4:B3:17:LYS:HD2	32:BW:173:ASN:OD1	1.75	0.85
59:sL:333:ILE:HG23	59:sL:409:LEU:HD13	1.57	0.85
60:E3:904:ASN:CB	60:T3:431:ASP:CB	2.52	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:E3:939:THR:CB	60:T3:429:PHE:CZ	2.56	0.85
49:mp:157:ASN:HD22	60:E3:495:ASN:HD21	0.87	0.85
3:A2:253:MET:HE2	3:A2:258:LEU:HD23	1.58	0.85
49:Mp:157:ASN:HD21	61:E6:323:PRO:HD2	1.40	0.85
9:SF:321:LEU:HD23	55:SH:449:MET:SD	2.16	0.85
3:B2:261:GLN:HG2	3:B2:263:HIS:H	1.41	0.85
3:B2:253:MET:HE2	3:B2:258:LEU:HD23	1.58	0.85
61:E6:749:LEU:HD23	61:E6:749:LEU:HA	1.57	0.85
28:BS:187:ASN:HB2	28:BS:228:LEU:HD21	1.56	0.85
55:SH:592:LEU:CD1	55:SH:592:LEU:HD22	2.02	0.85
28:AS:271:CYS:HB3	28:AS:274:CYS:SG	2.17	0.85
11:BA:1278:ASN:H	11:BA:1279:ILE:HD12	1.42	0.85
28:BS:271:CYS:HB3	28:BS:274:CYS:SG	2.17	0.85
53:sE:533:PHE:HA	53:sE:540:ASP:HA	1.57	0.84
61:E6:749:LEU:CD2	61:E6:749:LEU:CB	2.54	0.84
19:BI:78:CYS:SG	19:BI:106:CYS:HB3	2.16	0.84
61:E6:184:LYS:HZ3	60:T3:429:PHE:HB2	1.05	0.84
17:BG:100:GLU:HG3	32:BW:144:ARG:HH21	1.42	0.84
9:sF:321:LEU:HD23	55:sH:449:MET:SD	2.16	0.84
11:AA:1278:ASN:H	11:AA:1279:ILE:HD12	1.42	0.83
11:AA:68:GLN:CG	32:AW:151:LEU:HD13	2.07	0.83
23:AM:301:THR:CG2	27:AR:271:ARG:NH2	2.37	0.83
31:AV:5:GLY:N	31:AV:121:SER:HG	1.76	0.83
53:SE:533:PHE:HA	53:SE:540:ASP:HA	1.57	0.83
60:E3:904:ASN:HB2	60:T3:431:ASP:CG	2.02	0.83
23:BM:14:ARG:HH21	32:BW:126:ILE:HA	1.43	0.83
23:AM:14:ARG:HH21	32:AW:126:ILE:HA	1.43	0.83
61:E6:749:LEU:HB2	61:E6:749:LEU:HD12	1.60	0.83
28:BS:183:ASN:O	28:BS:228:LEU:HD22	1.78	0.83
14:BD:217:LEU:HD21	35:mb:42:GLN:HE22	1.33	0.82
28:AS:183:ASN:O	28:AS:228:LEU:HD22	1.77	0.82
3:A2:463:GLU:O	9:SF:402:ILE:HG13	1.78	0.82
18:BH:128:ASN:ND2	43:mj:81:ASN:ND2	2.26	0.82
23:BM:301:THR:CG2	27:BR:271:ARG:NH2	2.37	0.82
55:sH:585:LEU:HD23	55:sH:589:HIS:HD2	1.37	0.82
60:E3:708:GLN:NE2	61:t6:157:TYR:HE2	1.75	0.81
3:B2:463:GLU:O	9:sF:402:ILE:HG13	1.78	0.81
61:T6:503:LEU:HG	61:T6:505:PRO:HD2	1.62	0.81
23:BM:302:LEU:CA	27:BR:270:MET:HE2	1.95	0.81
53:sE:468:GLU:HA	53:sE:471:HIS:HD2	1.45	0.81
8:B7:349:ASN:HD22	8:B7:481:GLU:HG2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BV:5:GLY:N	31:BV:121:SER:HG	1.79	0.81
3:B2:454:TYR:HB2	6:B5:9:LEU:HB3	1.64	0.80
4:B3:49:LEU:CG	17:BG:164:LYS:CB	2.56	0.80
1:A0:104:ARG:NH2	1:A0:202:LEU:O	2.14	0.80
18:AH:109:LYS:O	43:Mj:83:LEU:CB	2.30	0.80
53:SE:523:VAL:CA	53:SE:547:ARG:HH12	1.94	0.80
60:E3:900:THR:C	60:T3:431:ASP:OD1	2.02	0.80
28:AS:184:LYS:HD2	28:AS:228:LEU:HD13	1.64	0.80
55:SH:594:LEU:HB2	55:SH:594:LEU:HD22	1.61	0.80
58:SK:237:GLN:HG2	58:SK:307:TYR:HE1	1.45	0.80
1:B0:104:ARG:NH2	1:B0:202:LEU:O	2.14	0.80
53:SE:468:GLU:HA	53:SE:471:HIS:HD2	1.45	0.80
61:t6:503:LEU:HG	61:t6:505:PRO:HD2	1.62	0.80
61:E6:161:ASN:OD1	60:T3:838:SER:CB	2.30	0.79
17:AG:100:GLU:HG3	32:AW:144:ARG:HH21	1.42	0.79
11:BA:68:GLN:CG	32:BW:151:LEU:HD13	2.07	0.79
61:E6:186:TYR:CE1	60:T3:428:LEU:HD22	2.16	0.79
60:E3:939:THR:CG2	60:E3:939:THR:HA	2.11	0.79
12:AB:13:GLU:HB2	64:T5:919:ARG:NH2	1.98	0.79
45:MI:831:GLN:HG2	45:t4:837:VAL:CG2	2.12	0.79
58:sK:237:GLN:HG2	58:sK:307:TYR:HE1	1.45	0.79
3:B2:463:GLU:O	9:sF:402:ILE:HG12	1.83	0.79
8:A7:239:ALA:HA	8:A7:313:VAL:HG21	1.65	0.79
8:A7:349:ASN:HD22	8:A7:481:GLU:HG2	1.46	0.79
14:AD:217:LEU:CD2	35:Mb:42:GLN:NE2	2.38	0.79
24:AN:-75:DT:H3	29:AT:75:DA:H61	1.28	0.78
18:BH:109:LYS:O	43:mj:83:LEU:CB	2.30	0.78
61:E6:923:LEU:HD11	61:E6:972:MET:SD	2.23	0.78
24:BN:-75:DT:H3	29:BT:75:DA:H61	1.28	0.78
61:E6:380:ASP:O	60:t3:429:PHE:HA	1.84	0.78
60:E3:879:ARG:HH22	60:T3:880:LYS:NZ	1.79	0.78
3:A2:454:TYR:HB2	6:A5:9:LEU:HB3	1.64	0.78
12:AB:13:GLU:HB2	64:T5:919:ARG:CZ	2.13	0.78
7:B6:352:CYS:HB3	7:B6:366:CYS:SG	2.24	0.78
55:sH:594:LEU:HB2	55:sH:594:LEU:HD22	1.61	0.78
60:E3:903:ILE:HD13	60:T3:429:PHE:HE1	1.47	0.78
3:A2:463:GLU:O	9:SF:402:ILE:HG12	1.83	0.78
56:sI:865:PRO:O	56:sI:946:ARG:NH2	2.18	0.77
4:A3:49:LEU:CG	17:AG:164:LYS:CB	2.56	0.77
28:AS:184:LYS:HA	28:AS:228:LEU:HD13	1.65	0.77
14:BD:151:PHE:O	14:BD:153:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BS:184:LYS:HD2	28:BS:228:LEU:HD13	1.64	0.77
14:AD:151:PHE:O	14:AD:153:ARG:NH1	2.17	0.77
53:sE:523:VAL:CA	53:sE:547:ARG:HH12	1.94	0.77
28:BS:184:LYS:HA	28:BS:228:LEU:HD13	1.64	0.77
7:A6:352:CYS:HB3	7:A6:366:CYS:SG	2.24	0.77
18:AH:128:ASN:ND2	43:Mj:81:ASN:ND2	2.26	0.77
4:B3:49:LEU:HB3	17:BG:164:LYS:CD	2.15	0.77
8:B7:239:ALA:HA	8:B7:313:VAL:HG21	1.65	0.76
3:B2:506:LYS:NZ	3:B2:506:LYS:HG3	2.00	0.76
3:A2:506:LYS:NZ	3:A2:506:LYS:HG3	2.00	0.76
4:A3:49:LEU:HB3	17:AG:164:LYS:CD	2.15	0.76
56:SI:865:PRO:O	56:SI:946:ARG:NH2	2.18	0.76
1:A0:536:GLY:O	1:A0:537:MET:HE2	1.86	0.76
29:AT:61:DA:H1'	29:AT:62:DC:H5'	1.68	0.76
64:T5:855:LEU:HD22	61:T6:769:ILE:HD11	1.68	0.76
64:t5:855:LEU:HD22	61:t6:769:ILE:HD11	1.68	0.76
49:Mp:183:CYS:SG	61:E6:754:LYS:CE	2.74	0.75
1:B0:536:GLY:O	1:B0:537:MET:HE2	1.86	0.75
23:AM:157:CYS:SG	23:AM:214:LEU:CD2	2.76	0.74
28:AS:211:ASN:HB3	28:AS:238:PRO:HG3	1.69	0.74
23:BM:16:PRO:HG3	32:BW:151:LEU:HD22	1.66	0.74
4:A3:49:LEU:CD2	17:AG:164:LYS:CE	2.59	0.74
7:B6:399:ARG:NH2	7:B6:435:GLU:OE1	2.20	0.74
60:E3:900:THR:OG1	60:T3:428:LEU:C	2.30	0.74
60:t3:837:TYR:HB3	60:t3:837:TYR:HD2	1.50	0.74
7:A6:399:ARG:NH2	7:A6:435:GLU:OE1	2.20	0.74
23:BM:157:CYS:SG	23:BM:214:LEU:CD2	2.76	0.74
58:SK:237:GLN:HG3	58:SK:402:GLU:OE2	1.88	0.73
58:sK:237:GLN:HG3	58:sK:402:GLU:OE2	1.88	0.73
19:AI:5:ARG:NH2	19:AI:36:GLU:OE1	2.21	0.73
55:sH:585:LEU:CD2	55:sH:589:HIS:CD2	2.70	0.73
11:AA:73:GLY:HA3	11:AA:76:GLU:HG2	1.71	0.73
12:BB:13:GLU:O	64:t5:922:THR:HA	1.88	0.73
23:BM:14:ARG:NH2	32:BW:126:ILE:HA	2.03	0.73
23:BM:245:HIS:CD2	27:BR:264:SER:CB	2.72	0.73
61:E6:184:LYS:HZ1	60:T3:429:PHE:CB	1.93	0.73
12:BB:13:GLU:O	64:t5:922:THR:HB	1.89	0.73
28:BS:211:ASN:HB3	28:BS:238:PRO:HG3	1.69	0.73
11:BA:73:GLY:HA3	11:BA:76:GLU:HG2	1.71	0.72
19:BI:5:ARG:NH2	19:BI:36:GLU:OE1	2.21	0.72
29:BT:61:DA:H1'	29:BT:62:DC:H5'	1.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:E3:904:ASN:N	60:T3:431:ASP:OD2	2.21	0.72
4:B3:49:LEU:CD2	17:BG:164:LYS:CE	2.59	0.72
4:A3:49:LEU:HB3	17:AG:164:LYS:HD2	1.71	0.72
4:B3:49:LEU:CB	17:BG:164:LYS:HD2	2.20	0.72
14:AD:209:ARG:NH2	35:Mb:34:ASP:OD2	2.22	0.72
4:B3:49:LEU:HB3	17:BG:164:LYS:HD2	1.71	0.72
23:AM:14:ARG:NH2	32:AW:126:ILE:HA	2.03	0.72
8:B7:224:LYS:HD3	8:B7:338:LEU:O	1.90	0.72
9:SF:309:TYR:HE1	56:SI:653:PRO:HG2	1.55	0.72
9:sF:309:TYR:HE1	56:sI:653:PRO:HG2	1.55	0.72
64:T5:868:ARG:HG2	64:T5:872:ARG:HD2	1.72	0.72
4:A3:49:LEU:HD23	17:AG:164:LYS:CG	2.19	0.72
23:AM:157:CYS:SG	23:AM:214:LEU:HD21	2.30	0.72
6:B5:30:ILE:HD11	6:B5:50:VAL:HG12	1.72	0.72
14:BD:158:GLU:OE1	35:mb:45:HIS:CE1	2.43	0.72
14:BD:217:LEU:CD2	35:mb:42:GLN:NE2	2.38	0.72
19:BI:86:PHE:CD2	19:BI:86:PHE:HB3	2.25	0.72
14:BD:209:ARG:NH2	35:mb:34:ASP:OD2	2.22	0.71
61:E6:749:LEU:CD2	61:E6:749:LEU:HA	2.18	0.71
61:E6:132:MET:HE3	61:E6:152:PHE:HB3	1.72	0.71
11:AA:465:TYR:HE1	21:AK:3:ALA:HA	1.55	0.71
17:AG:100:GLU:CD	32:AW:144:ARG:NE	2.49	0.71
55:SH:585:LEU:CD2	55:SH:589:HIS:CD2	2.70	0.71
60:E3:939:THR:CG2	60:E3:939:THR:OG1	2.38	0.71
4:A3:49:LEU:CB	17:AG:164:LYS:HD2	2.20	0.71
6:A5:30:ILE:HD11	6:A5:50:VAL:HG12	1.72	0.71
14:AD:158:GLU:OE1	35:Mb:45:HIS:CE1	2.43	0.71
49:Mp:183:CYS:SG	61:E6:754:LYS:NZ	2.63	0.71
4:B3:49:LEU:CD2	17:BG:164:LYS:CB	2.68	0.71
60:E3:956:ARG:HH21	60:E3:959:LEU:HD13	1.55	0.71
4:B3:49:LEU:HD23	17:BG:164:LYS:CG	2.19	0.71
4:A3:100:ASN:HB3	34:Ma:140:GLY:HA3	1.35	0.71
23:BM:157:CYS:SG	23:BM:214:LEU:HD21	2.30	0.71
4:A3:49:LEU:CD2	17:AG:164:LYS:CB	2.68	0.71
8:A7:224:LYS:HD3	8:A7:338:LEU:O	1.90	0.71
14:AD:217:LEU:HD21	35:Mb:42:GLN:HE22	1.32	0.71
19:BI:59:VAL:HG13	19:BI:61:ASP:H	1.55	0.71
23:AM:303:GLN:CB	27:AR:270:MET:SD	2.79	0.70
11:BA:465:TYR:HE1	21:BK:3:ALA:HA	1.55	0.70
19:AI:59:VAL:HG13	19:AI:61:ASP:H	1.55	0.70
17:BG:100:GLU:CD	32:BW:144:ARG:NE	2.49	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AR:73:LEU:HD12	27:AR:74:PRO:HD2	1.72	0.70
18:BH:106:GLU:OE2	43:mj:83:LEU:HD13	1.91	0.70
23:AM:245:HIS:CD2	27:AR:264:SER:CB	2.72	0.70
12:BB:13:GLU:O	64:t5:922:THR:CA	2.40	0.70
45:ml:89:GLN:HE21	45:ml:159:PHE:H	1.39	0.70
1:A0:125:LYS:NZ	1:A0:127:THR:OG1	2.21	0.70
60:E3:900:THR:HG23	60:T3:429:PHE:O	1.91	0.70
64:t5:936:ILE:HG23	64:t5:943:LEU:HD11	1.73	0.70
11:BA:72:GLU:HG2	23:BM:20:ILE:HD11	1.74	0.70
23:BM:303:GLN:CB	27:BR:270:MET:SD	2.79	0.70
64:T5:936:ILE:HG23	64:T5:943:LEU:HD11	1.74	0.70
64:t5:868:ARG:HG2	64:t5:872:ARG:HD2	1.71	0.70
12:BB:13:GLU:CG	64:t5:919:ARG:HD2	2.22	0.70
60:E3:415:PHE:CE1	60:E3:439:ILE:HG12	2.26	0.70
60:t3:360:HIS:CD2	60:t3:919:TYR:HE2	2.10	0.70
60:E3:879:ARG:NH2	60:T3:880:LYS:NZ	2.40	0.70
61:E6:917:GLU:O	61:E6:934:ARG:NH2	2.24	0.70
18:AH:106:GLU:OE2	43:Mj:83:LEU:HD13	1.91	0.69
12:AB:705:MET:H	12:AB:710:LEU:HD22	1.57	0.69
12:BB:705:MET:H	12:BB:710:LEU:HD22	1.57	0.69
27:BR:73:LEU:HD12	27:BR:74:PRO:HD2	1.72	0.69
6:A5:5:ARG:NH2	6:A5:33:GLU:OE2	2.26	0.69
50:SA:335:TYR:HD1	51:SB:727:LEU:HD11	1.58	0.69
50:sA:335:TYR:HD1	51:sB:727:LEU:HD11	1.58	0.69
60:T3:360:HIS:CD2	60:T3:919:TYR:HE2	2.10	0.69
45:t4:981:THR:HG1	45:t4:1004:ALA:N	1.90	0.69
11:AA:68:GLN:HG3	32:AW:151:LEU:HD12	1.66	0.69
19:AI:86:PHE:CD2	19:AI:86:PHE:HB3	2.25	0.69
4:B3:49:LEU:CD2	17:BG:164:LYS:HE2	2.21	0.69
61:E6:749:LEU:CD2	61:E6:749:LEU:CA	2.71	0.69
60:T3:360:HIS:HD2	60:T3:919:TYR:HE2	1.41	0.69
61:T6:218:ARG:HH22	61:T6:220:ARG:HB2	1.57	0.69
11:AA:72:GLU:HG2	23:AM:20:ILE:HD11	1.74	0.69
45:MI:89:GLN:HE21	45:MI:159:PHE:H	1.39	0.69
60:E3:553:LYS:HG2	60:t3:834:TYR:OH	1.93	0.69
45:T4:981:THR:HG1	45:T4:1004:ALA:N	1.90	0.69
64:t5:913:ILE:HD11	64:t5:943:LEU:HD13	1.74	0.69
14:BD:213:GLU:CG	35:mb:38:MET:HE1	2.23	0.69
23:AM:16:PRO:HG3	32:AW:151:LEU:HD22	1.66	0.68
3:A2:506:LYS:CD	3:A2:506:LYS:HZ2	2.06	0.68
8:A7:619:ALA:HA	8:A7:622:MET:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:213:GLU:CG	35:Mb:38:MET:HE1	2.23	0.68
53:sE:530:THR:HG22	53:sE:532:ASN:HD21	1.59	0.68
61:E6:175:MET:HE3	61:E6:176:ASN:HB3	1.75	0.68
49:Mp:157:ASN:CG	61:E6:323:PRO:HD2	2.19	0.68
61:t6:218:ARG:HH22	61:t6:220:ARG:HB2	1.57	0.68
1:A0:554:TRP:HA	1:A0:557:MET:SD	2.34	0.68
1:B0:125:LYS:NZ	1:B0:127:THR:OG1	2.21	0.68
23:AM:16:PRO:CB	32:AW:151:LEU:CD2	2.59	0.68
9:SF:503:ASP:OD1	9:SF:506:ARG:NH2	2.27	0.68
23:BM:16:PRO:HB3	32:BW:151:LEU:CD2	2.23	0.68
63:t2:65:ALA:HA	63:t2:68:MET:HE2	1.76	0.68
53:SE:530:THR:HG22	53:SE:532:ASN:HD21	1.59	0.68
6:B5:5:ARG:NH2	6:B5:33:GLU:OE2	2.26	0.68
11:AA:107:CYS:HB3	11:AA:110:CYS:SG	2.34	0.68
4:B3:100:ASN:HB3	34:ma:140:GLY:HA3	1.35	0.68
23:BM:14:ARG:NH2	32:BW:126:ILE:HD12	2.09	0.68
11:BA:107:CYS:HB3	11:BA:110:CYS:SG	2.34	0.68
12:BB:810:GLU:OE1	26:BQ:24:ARG:NH1	2.27	0.68
11:AA:681:GLU:OE1	61:T6:757:GLN:NE2	2.27	0.67
23:AM:16:PRO:HB3	32:AW:151:LEU:CD2	2.23	0.67
61:E6:749:LEU:CB	61:E6:749:LEU:HD13	2.19	0.67
8:B7:619:ALA:HA	8:B7:622:MET:HE2	1.75	0.67
23:AM:16:PRO:HB3	32:AW:151:LEU:HD21	1.76	0.67
55:SH:592:LEU:CD2	55:SH:592:LEU:HD11	2.24	0.67
62:T1:46:MET:HE1	62:T1:66:SER:H	1.59	0.67
63:T2:65:ALA:HA	63:T2:68:MET:HE2	1.76	0.67
64:T5:913:ILE:HD11	64:T5:943:LEU:HD13	1.74	0.67
1:B0:554:TRP:HA	1:B0:557:MET:SD	2.34	0.67
61:E6:746:LEU:HA	61:E6:749:LEU:HD12	1.76	0.67
60:T3:837:TYR:HB3	60:T3:837:TYR:HD2	1.50	0.67
12:AB:810:GLU:OE1	26:AQ:24:ARG:NH1	2.27	0.67
12:BB:21:GLU:O	12:BB:23:ALA:N	2.28	0.67
20:BJ:7:CYS:HA	20:BJ:49:MET:HE2	1.76	0.67
51:sB:688:ARG:HA	51:sB:691:MET:HE2	1.77	0.67
9:sF:503:ASP:OD1	9:sF:506:ARG:NH2	2.27	0.67
12:AB:21:GLU:O	12:AB:23:ALA:N	2.28	0.67
26:AQ:377:SER:OG	27:AR:66:ARG:NH1	2.28	0.67
55:SH:587:LYS:O	55:SH:591:LEU:N	2.24	0.67
7:B6:399:ARG:NH2	7:B6:434:GLN:HA	2.10	0.67
4:A3:31:ASN:HD22	4:A3:63:LEU:HD12	1.60	0.67
8:A7:711:LYS:HA	8:A7:716:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B7:711:LYS:HA	8:B7:716:MET:HE3	1.76	0.67
3:B2:155:LEU:HD12	3:B2:157:LYS:H	1.60	0.67
60:E3:900:THR:HG23	60:T3:429:PHE:C	2.20	0.67
60:t3:360:HIS:HD2	60:t3:919:TYR:HE2	1.41	0.67
51:SD:675:GLU:O	51:SD:679:MET:HE3	1.95	0.67
1:A0:537:MET:HE1	1:A0:619:THR:N	2.10	0.66
51:sD:675:GLU:O	51:sD:679:MET:HE3	1.95	0.66
55:sH:585:LEU:C	55:sH:588:ASN:HB2	2.20	0.66
4:A3:49:LEU:CD2	17:AG:164:LYS:HE2	2.21	0.66
4:A3:54:CYS:HB3	4:A3:59:CYS:SG	2.34	0.66
23:BM:154:TYR:CE1	23:BM:172:MET:CE	2.77	0.66
26:BQ:377:SER:OG	27:BR:66:ARG:NH1	2.28	0.66
61:E6:381:THR:CG2	60:t3:431:ASP:OD1	2.43	0.66
62:t1:46:MET:HE1	62:t1:66:SER:H	1.60	0.66
1:A0:533:THR:HG21	1:A0:537:MET:HE3	1.76	0.66
3:A2:155:LEU:HD12	3:A2:157:LYS:H	1.60	0.66
4:B3:31:ASN:HD22	4:B3:63:LEU:HD12	1.60	0.66
17:BG:100:GLU:CG	32:BW:144:ARG:NH2	2.57	0.66
61:E6:890:LEU:HD11	61:E6:894:ASN:HD22	1.60	0.66
20:AJ:7:CYS:HA	20:AJ:49:MET:HE2	1.76	0.66
1:B0:533:THR:HG21	1:B0:537:MET:HE3	1.76	0.66
61:E6:651:TYR:HA	61:E6:654:ASN:HD21	1.61	0.66
64:T5:874:GLU:OE1	64:T5:874:GLU:N	2.28	0.66
8:A7:719:SER:O	8:A7:722:ARG:N	2.29	0.66
11:AA:420:ARG:CD	38:Me:60:GLU:OE2	2.43	0.66
23:AM:154:TYR:CE1	23:AM:172:MET:CE	2.77	0.66
4:B3:54:CYS:HB3	4:B3:59:CYS:SG	2.34	0.66
17:AG:100:GLU:CG	32:AW:144:ARG:NH2	2.57	0.66
23:AM:14:ARG:NH2	32:AW:126:ILE:HD12	2.09	0.66
23:AM:301:THR:HG23	27:AR:271:ARG:CZ	2.24	0.66
3:B2:480:VAL:HG11	3:B2:497:GLY:HA3	1.78	0.66
1:A0:418:LEU:HD13	1:A0:435:MET:HE1	1.78	0.66
61:E6:113:TRP:HZ3	61:E6:446:MET:HE3	1.61	0.66
7:A6:399:ARG:NH2	7:A6:434:GLN:HA	2.10	0.66
36:Mc:63:THR:HG21	40:Mg:17:LEU:HD12	1.78	0.66
19:BI:104:LEU:CD2	19:BI:104:LEU:HB2	2.25	0.66
45:MI:831:GLN:HE21	45:t4:837:VAL:CG1	2.09	0.66
49:Mp:157:ASN:HD21	61:E6:322:LYS:HA	1.61	0.66
9:sF:391:ARG:NH2	56:sI:701:GLU:OE1	2.29	0.66
60:E3:904:ASN:CG	60:T3:431:ASP:HB3	2.20	0.66
1:B0:537:MET:HE1	1:B0:619:THR:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A9:236:TRP:CE2	10:A9:240:LYS:HE3	2.32	0.65
12:AB:806:THR:H	12:AB:809:MET:HE3	1.62	0.65
11:BA:150:THR:HA	11:BA:166:GLY:HA2	1.78	0.65
49:mp:158:ASN:HD21	60:E3:493:ASN:HB2	1.61	0.65
53:sE:450:GLU:HB2	53:sE:454:LEU:HD23	1.78	0.65
61:E6:205:SER:O	61:E6:558:LYS:NZ	2.28	0.65
4:B3:49:LEU:HD22	17:BG:164:LYS:HD2	1.70	0.65
51:SB:688:ARG:HA	51:SB:691:MET:HE2	1.77	0.65
8:B7:719:SER:O	8:B7:722:ARG:N	2.29	0.65
60:E3:672:TYR:OH	60:E3:688:SER:O	2.10	0.65
4:A3:49:LEU:HB3	17:AG:164:LYS:CG	2.27	0.65
55:SH:585:LEU:C	55:SH:588:ASN:HB2	2.20	0.65
10:B9:236:TRP:CE2	10:B9:240:LYS:HE3	2.32	0.65
12:BB:806:THR:H	12:BB:809:MET:HE3	1.62	0.65
44:mk:122:ARG:HH21	44:mk:123:ASP:HB3	1.62	0.65
18:AH:114:VAL:HG13	18:AH:132:LEU:HD12	1.79	0.65
31:BV:35:SER:HB2	31:BV:39:ARG:HH21	1.62	0.65
60:E3:897:LYS:HA	60:T3:427:ASP:O	1.96	0.65
1:A0:676:TYR:HB3	1:A0:724:MET:HE3	1.79	0.65
19:AI:105:SER:HB2	45:T4:1011:THR:HG21	1.79	0.65
44:Mk:122:ARG:HH21	44:Mk:123:ASP:HB3	1.61	0.65
53:SE:450:GLU:HB2	53:SE:454:LEU:HD23	1.79	0.65
9:SF:381:LEU:HD13	56:SI:689:ILE:HD13	1.79	0.65
9:SF:391:ARG:NH2	56:SI:701:GLU:OE1	2.29	0.65
61:T6:643:GLU:OE1	61:T6:864:ASN:ND2	2.30	0.65
64:t5:874:GLU:OE1	64:t5:874:GLU:N	2.28	0.65
1:B0:676:TYR:HB3	1:B0:724:MET:HE3	1.79	0.65
3:B2:506:LYS:CD	3:B2:506:LYS:HZ2	2.06	0.65
55:sH:592:LEU:CD2	55:sH:592:LEU:HD11	2.24	0.65
3:A2:463:GLU:HB2	9:SF:401:LYS:C	2.23	0.64
1:A0:494:PRO:O	1:A0:495:MET:HE2	1.97	0.64
14:BD:158:GLU:OE1	35:mb:45:HIS:HE1	1.80	0.64
26:BQ:352:MET:HB3	26:BQ:361:TRP:HB2	1.80	0.64
9:sF:381:LEU:HD13	56:sI:689:ILE:HD13	1.79	0.64
8:A7:181:TYR:CZ	8:A7:336:PRO:HB2	2.33	0.64
19:AI:104:LEU:CD2	19:AI:104:LEU:HB2	2.25	0.64
58:SK:262:GLU:O	58:SK:266:GLN:NE2	2.30	0.64
1:B0:418:LEU:HD13	1:B0:435:MET:HE1	1.78	0.64
9:B8:790:LYS:CB	9:sF:763:ARG:HH21	1.98	0.64
14:AD:158:GLU:OE1	35:Mb:45:HIS:HE1	1.80	0.64
8:B7:181:TYR:CZ	8:B7:336:PRO:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:sH:587:LYS:O	55:sH:591:LEU:N	2.24	0.64
58:sK:237:GLN:HG2	58:sK:307:TYR:CE1	2.30	0.64
61:t6:643:GLU:OE1	61:t6:864:ASN:ND2	2.30	0.64
11:AA:10:PRO:HG2	11:AA:12:ARG:HH12	1.63	0.64
31:AV:35:SER:HB2	31:AV:39:ARG:HH21	1.62	0.64
58:SK:237:GLN:HG2	58:SK:307:TYR:CE1	2.30	0.64
60:E3:675:GLU:OE2	60:E3:678:ASN:ND2	2.30	0.64
3:A2:480:VAL:HG11	3:A2:497:GLY:HA3	1.78	0.64
11:AA:978:PRO:HD3	43:Mj:88:GLU:OE2	1.98	0.64
26:AQ:27:MET:N	26:AQ:27:MET:SD	2.67	0.64
53:SE:545:THR:HB	9:SF:754:LEU:HB3	1.80	0.64
1:B0:494:PRO:O	1:B0:495:MET:HE2	1.97	0.64
18:BH:114:VAL:HG13	18:BH:132:LEU:HD12	1.79	0.64
61:T6:651:TYR:HH	61:T6:910:CYS:HG	1.46	0.64
23:BM:301:THR:HG23	27:BR:271:ARG:CZ	2.24	0.64
53:sE:532:ASN:HB2	53:sE:541:GLU:HB2	1.80	0.64
53:sE:545:THR:HB	9:sF:754:LEU:HB3	1.80	0.64
60:E3:769:GLN:OE1	61:E6:338:SER:OG	2.16	0.64
1:A0:550:ILE:HA	1:A0:553:MET:HE3	1.80	0.64
4:A3:49:LEU:HD23	17:AG:164:LYS:CB	2.28	0.64
19:BI:17:ARG:HH21	19:BI:19:ASP:HB2	1.62	0.64
36:mc:63:THR:HG21	40:mg:17:LEU:HD12	1.78	0.64
11:AA:150:THR:HA	11:AA:166:GLY:HA2	1.78	0.63
4:B3:49:LEU:HB3	17:BG:164:LYS:CG	2.27	0.63
11:BA:978:PRO:HD3	43:mj:88:GLU:OE2	1.98	0.63
19:AI:17:ARG:HH21	19:AI:19:ASP:HB2	1.62	0.63
60:E3:879:ARG:HH22	60:T3:880:LYS:HZ1	1.46	0.63
31:AV:36:LEU:HA	31:AV:39:ARG:HG2	1.81	0.63
22:BL:51:CYS:O	23:BM:250:MET:HE3	1.97	0.63
22:AL:51:CYS:O	23:AM:250:MET:HE3	1.97	0.63
53:SE:523:VAL:HG12	53:SE:547:ARG:NH2	2.13	0.63
58:sK:262:GLU:O	58:sK:266:GLN:NE2	2.30	0.63
11:BA:681:GLU:OE2	61:t6:762:PHE:HZ	1.79	0.63
53:sE:464:ASN:OD1	53:sE:465:GLU:N	2.31	0.63
53:sE:523:VAL:HG12	53:sE:547:ARG:NH2	2.13	0.63
12:AB:1106:ARG:NH2	12:AB:1110:PRO:O	2.32	0.63
55:SH:592:LEU:HA	55:SH:595:GLU:HG3	1.80	0.63
55:sH:592:LEU:HA	55:sH:595:GLU:HG3	1.80	0.63
3:B2:463:GLU:HB2	9:sF:401:LYS:C	2.23	0.63
53:sE:531:THR:HA	53:sE:542:THR:HA	1.80	0.63
61:E6:920:ASP:OD2	61:E6:934:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:326:ARG:HG3	11:AA:1406:VAL:HG21	1.81	0.63
26:AQ:144:THR:HA	26:AQ:147:LEU:HD21	1.81	0.63
6:B5:36:ASP:HB2	6:B5:39:HIS:HB2	1.81	0.63
12:AB:486:TYR:HB3	12:AB:1096:ARG:HH22	1.64	0.62
49:Mp:167:TYR:O	49:Mp:171:LEU:HB2	1.99	0.62
18:AH:146:ARG:HG2	18:AH:146:ARG:HH11	1.64	0.62
60:E3:903:ILE:HD13	60:T3:429:PHE:CE1	2.30	0.62
2:A1:209:PHE:O	2:A1:213:ARG:NH2	2.33	0.62
53:SE:464:ASN:OD1	53:SE:465:GLU:N	2.31	0.62
1:B0:507:SER:OG	1:B0:685:ARG:NH2	2.32	0.62
30:BU:50:LYS:O	30:BU:271:ARG:NH1	2.32	0.62
44:mk:122:ARG:HH11	44:mk:147:THR:HG21	1.65	0.62
26:AQ:115:ARG:NH2	26:AQ:345:GLU:OE2	2.32	0.62
53:SE:545:THR:HA	9:SF:756:ASN:HA	1.81	0.62
31:BV:36:LEU:HA	31:BV:39:ARG:HG2	1.81	0.62
61:t6:963:CYS:SG	61:t6:964:ILE:N	2.72	0.62
11:AA:44:THR:OG1	11:AA:47:ARG:NH1	2.32	0.62
53:SE:532:ASN:HB2	53:SE:541:GLU:HB2	1.80	0.62
57:SJ:1:MET:HE2	57:SJ:5:THR:HB	1.82	0.62
12:BB:1106:ARG:NH2	12:BB:1110:PRO:O	2.32	0.62
26:AQ:352:MET:HB3	26:AQ:361:TRP:HB2	1.80	0.62
1:B0:537:MET:HE1	1:B0:619:THR:H	1.64	0.62
11:BA:44:THR:OG1	11:BA:47:ARG:NH1	2.32	0.62
11:BA:68:GLN:HG3	32:BW:151:LEU:HD12	1.66	0.62
61:T6:963:CYS:SG	61:T6:964:ILE:N	2.72	0.62
1:A0:507:SER:OG	1:A0:685:ARG:NH2	2.32	0.62
11:AA:91:PHE:CE1	11:AA:204:THR:HG22	2.35	0.62
1:B0:550:ILE:HA	1:B0:553:MET:HE3	1.80	0.62
2:B1:209:PHE:O	2:B1:213:ARG:NH2	2.33	0.62
3:A2:66:VAL:HG12	5:A4:262:ILE:HA	1.81	0.62
45:MI:831:GLN:NE2	45:t4:837:VAL:CG1	2.63	0.62
9:SF:389:ASN:O	9:SF:392:MET:N	2.33	0.62
23:BM:14:ARG:O	32:BW:126:ILE:HG23	2.00	0.62
62:T1:85:ASP:OD1	63:T2:44:ARG:NH2	2.32	0.62
62:t1:85:ASP:OD1	63:t2:44:ARG:NH2	2.32	0.62
23:AM:14:ARG:O	32:AW:126:ILE:HG23	2.00	0.62
51:SB:766:GLN:HB3	51:SB:770:PHE:HE2	1.64	0.62
18:BH:146:ARG:HG2	18:BH:146:ARG:HH11	1.64	0.62
49:mp:167:TYR:O	49:mp:171:LEU:HB2	1.99	0.62
1:B0:539:VAL:HG12	1:B0:621:LEU:HB2	1.82	0.62
26:BQ:27:MET:N	26:BQ:27:MET:SD	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:sB:436:ASP:C	51:sB:437:MET:HE2	2.24	0.62
53:sE:545:THR:HA	9:sF:756:ASN:HA	1.81	0.62
11:BA:10:PRO:HG2	11:BA:12:ARG:HH12	1.63	0.61
11:BA:326:ARG:HG3	11:BA:1406:VAL:HG21	1.81	0.61
44:Mk:122:ARG:HH11	44:Mk:147:THR:HG21	1.65	0.61
58:SK:429:MET:HG3	59:SL:321:ASP:HB2	1.82	0.61
14:BD:206:GLU:HA	14:BD:209:ARG:HG2	1.82	0.61
58:sK:429:MET:HG3	59:sL:321:ASP:HB2	1.82	0.61
58:SK:36:ILE:HG23	58:SK:54:MET:HE3	1.82	0.61
5:B4:255:ASP:HB3	5:B4:258:LEU:HB2	1.82	0.61
12:BB:13:GLU:OE1	64:t5:921:PRO:C	2.43	0.61
1:A0:537:MET:HE1	1:A0:619:THR:H	1.64	0.61
6:A5:36:ASP:HB2	6:A5:39:HIS:HB2	1.81	0.61
53:SE:531:THR:HA	53:SE:542:THR:HA	1.80	0.61
26:BQ:144:THR:HA	26:BQ:147:LEU:HD21	1.81	0.61
60:E3:943:LYS:HG3	60:T3:429:PHE:CZ	2.36	0.61
1:A0:539:VAL:HG12	1:A0:621:LEU:HB2	1.82	0.61
8:A7:242:LEU:HB2	8:A7:313:VAL:HB	1.82	0.61
3:B2:66:VAL:HG12	5:B4:262:ILE:HA	1.81	0.61
11:BA:420:ARG:CD	38:me:60:GLU:OE2	2.43	0.61
61:E6:397:SER:OG	61:E6:399:GLU:OE1	2.17	0.61
12:AB:13:GLU:CB	64:T5:919:ARG:NH2	2.62	0.61
51:SB:436:ASP:C	51:SB:437:MET:HE2	2.24	0.61
56:sI:1251:LYS:HD2	56:sI:1255:PHE:CZ	2.35	0.61
60:t3:406:LYS:O	60:t3:409:LYS:N	2.29	0.61
3:A2:443:LEU:O	3:A2:447:GLU:HG2	2.00	0.61
45:ML:831:GLN:NE2	45:t4:837:VAL:HG12	2.16	0.61
4:B3:49:LEU:HD23	17:BG:164:LYS:CB	2.28	0.61
51:sB:770:PHE:HE1	51:sD:739:VAL:C	2.08	0.61
5:A4:271:ASP:OD1	5:A4:272:PHE:N	2.34	0.61
12:BB:12:ASP:N	64:t5:923:LYS:HB2	2.16	0.61
14:BD:153:ARG:NH2	14:BD:182:SER:O	2.34	0.61
51:sB:766:GLN:HB3	51:sB:770:PHE:HE2	1.65	0.61
55:sH:586:TYR:O	55:sH:590:GLU:HA	2.01	0.61
61:E6:623:LEU:O	61:E6:627:MET:HG2	2.01	0.61
11:BA:91:PHE:CE1	11:BA:204:THR:HG22	2.35	0.61
14:AD:206:GLU:HA	14:AD:209:ARG:HG2	1.82	0.60
8:B7:242:LEU:HB2	8:B7:313:VAL:HB	1.82	0.60
23:BM:16:PRO:CB	32:BW:151:LEU:CD2	2.59	0.60
27:BR:233:TYR:O	27:BR:234:HIS:ND1	2.34	0.60
55:sH:585:LEU:CD2	55:sH:589:HIS:HD2	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:506:LYS:NZ	3:A2:506:LYS:CG	2.64	0.60
12:AB:21:GLU:OE1	12:AB:22:SER:N	2.33	0.60
18:AH:56:THR:N	18:AH:146:ARG:HH12	1.99	0.60
24:AN:-58:DT:O2	29:AT:59:DG:N2	2.34	0.60
3:B2:443:LEU:O	3:B2:447:GLU:HG2	2.00	0.60
8:B7:742:MET:O	8:B7:742:MET:HE3	2.01	0.60
60:E3:879:ARG:NH2	60:T3:880:LYS:CE	2.64	0.60
61:E6:423:ARG:HB2	61:E6:424:ARG:HH11	1.65	0.60
9:A8:790:LYS:CB	9:SF:763:ARG:HH21	1.99	0.60
55:SH:585:LEU:CD2	55:SH:589:HIS:HD2	2.10	0.60
5:B4:271:ASP:OD1	5:B4:272:PHE:N	2.34	0.60
51:sD:404:ILE:H	9:sF:404:SER:HA	1.67	0.60
61:E6:936:GLY:HA2	61:E6:960:THR:HG22	1.83	0.60
61:t6:503:LEU:HD12	61:t6:504:PRO:HD2	1.84	0.60
8:A7:181:TYR:O	8:A7:184:VAL:HG12	2.01	0.60
14:AD:153:ARG:NH2	14:AD:182:SER:O	2.34	0.60
47:Mn:74:ASN:HA	47:Mn:77:ILE:HD12	1.84	0.60
56:SI:1251:LYS:HD2	56:SI:1255:PHE:CZ	2.35	0.60
4:B3:100:ASN:HA	34:ma:140:GLY:CA	2.25	0.60
61:t6:145:TYR:HB2	61:t6:968:MET:HE3	1.83	0.60
11:AA:465:TYR:CE1	21:AK:4:PRO:HD2	2.37	0.60
49:Mp:548:TYR:CD2	61:E6:612:GLU:CG	2.85	0.60
11:BA:465:TYR:CE1	21:BK:4:PRO:HD2	2.37	0.60
12:BB:15:PRO:HB3	64:t5:921:PRO:HA	1.83	0.60
12:BB:21:GLU:OE1	12:BB:22:SER:N	2.33	0.60
18:BH:56:THR:N	18:BH:146:ARG:HH12	1.99	0.60
27:BR:117:PRO:HA	27:BR:232:ASN:HB2	1.82	0.60
61:E6:695:LEU:O	61:E6:698:SER:OG	2.19	0.60
3:A2:444:TRP:HA	3:A2:448:LEU:HD23	1.84	0.60
4:A3:49:LEU:HD22	17:AG:164:LYS:HD2	1.70	0.60
5:A4:255:ASP:HB3	5:A4:258:LEU:HB2	1.82	0.60
8:A7:243:GLN:HE21	8:A7:244:MET:HE3	1.66	0.60
18:AH:56:THR:OG1	18:AH:146:ARG:NH1	2.34	0.60
12:BB:486:TYR:HB3	12:BB:1096:ARG:HH22	1.64	0.60
57:sJ:1:MET:HE2	57:sJ:5:THR:HB	1.82	0.60
2:A1:510:ASN:ND2	5:A4:264:LYS:O	2.35	0.60
3:A2:172:LEU:HD13	3:A2:188:GLY:HA2	1.84	0.60
8:A7:466:ARG:NH2	8:A7:471:GLN:OE1	2.34	0.60
51:SB:770:PHE:HE1	51:SD:739:VAL:C	2.08	0.60
8:B7:243:GLN:HE21	8:B7:244:MET:HE3	1.66	0.60
17:BG:153:GLN:HB3	17:BG:156:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BQ:115:ARG:NH2	26:BQ:345:GLU:OE2	2.32	0.60
36:mc:2:GLN:NE2	37:md:316:ILE:O	2.33	0.60
45:ml:253:VAL:HG21	45:ml:276:ILE:HG21	1.84	0.60
9:sF:389:ASN:O	9:sF:392:MET:N	2.33	0.60
61:E6:923:LEU:CA	61:E6:934:ARG:HE	2.14	0.60
61:T6:145:TYR:HB2	61:T6:968:MET:HE3	1.83	0.60
3:A2:32:CYS:SG	3:A2:107:SER:OG	2.47	0.60
8:A7:126:ASP:O	8:A7:130:ARG:NH1	2.35	0.60
30:AU:50:LYS:O	30:AU:271:ARG:NH1	2.32	0.60
45:Ml:253:VAL:HG21	45:Ml:276:ILE:HG21	1.84	0.60
51:SB:557:SER:OG	51:SB:559:GLU:OE1	2.20	0.60
51:SD:404:ILE:H	9:SF:404:SER:HA	1.67	0.60
9:SF:599:GLU:HG2	9:SF:603:MET:HE1	1.83	0.60
2:B1:484:LEU:HD13	5:B4:109:ILE:HG21	1.84	0.60
58:sK:201:ILE:HG13	58:sK:202:LYS:HG2	1.83	0.60
17:AG:153:GLN:HB3	17:AG:156:SER:HB2	1.83	0.60
26:AQ:151:LEU:HD23	26:AQ:440:ARG:HH22	1.67	0.60
27:AR:117:PRO:HA	27:AR:232:ASN:HB2	1.82	0.60
27:AR:233:TYR:O	27:AR:234:HIS:ND1	2.34	0.60
3:B2:195:GLU:OE2	3:B2:196:ILE:HG22	2.02	0.60
8:B7:466:ARG:NH2	8:B7:471:GLN:OE1	2.34	0.60
18:BH:56:THR:OG1	18:BH:146:ARG:NH1	2.34	0.60
21:BK:8:GLU:N	21:BK:8:GLU:OE2	2.35	0.60
24:BN:-58:DT:O2	29:BT:59:DG:N2	2.34	0.60
47:mn:74:ASN:HA	47:mn:77:ILE:HD12	1.84	0.60
11:AA:894:GLU:O	11:AA:898:ARG:HB2	2.02	0.60
58:SK:201:ILE:HG13	58:SK:202:LYS:HG2	1.83	0.60
2:A1:484:LEU:HD13	5:A4:109:ILE:HG21	1.84	0.59
12:AB:451:LYS:NZ	23:AM:139:ALA:HA	2.17	0.59
2:B1:510:ASN:ND2	5:B4:264:LYS:O	2.35	0.59
3:B2:506:LYS:NZ	3:B2:506:LYS:CG	2.64	0.59
11:BA:894:GLU:O	11:BA:898:ARG:HB2	2.02	0.59
12:BB:451:LYS:NZ	23:BM:139:ALA:HA	2.17	0.59
42:mi:186:ARG:O	42:mi:190:ARG:NH1	2.35	0.59
1:B0:135:ARG:NH1	1:B0:391:THR:O	2.35	0.59
3:B2:51:VAL:HG21	3:B2:108:LEU:HD22	1.85	0.59
3:B2:51:VAL:O	3:B2:109:ARG:NH2	2.36	0.59
3:B2:172:LEU:HD13	3:B2:188:GLY:HA2	1.84	0.59
11:BA:668:ASP:HA	11:BA:741:ASN:HD21	1.67	0.59
53:sE:543:ILE:HA	9:sF:756:ASN:HB2	1.83	0.59
9:sF:599:GLU:HG2	9:sF:603:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:E6:446:MET:SD	61:E6:446:MET:N	2.74	0.59
1:A0:135:ARG:NH1	1:A0:391:THR:O	2.35	0.59
11:AA:1277:GLU:HB3	11:AA:1312:ASN:HD22	1.67	0.59
24:AN:-60:DA:N6	29:AT:59:DG:O6	2.36	0.59
51:SB:766:GLN:HE22	51:SD:746:LEU:HD12	1.68	0.59
53:SE:542:THR:HB	53:SE:544:THR:HG23	1.84	0.59
3:B2:444:TRP:HA	3:B2:448:LEU:HD23	1.84	0.59
8:B7:181:TYR:O	8:B7:184:VAL:HG12	2.01	0.59
24:BN:-60:DA:N6	29:BT:59:DG:O6	2.36	0.59
51:sB:557:SER:OG	51:sB:559:GLU:OE1	2.20	0.59
55:sH:586:TYR:CD1	55:sH:589:HIS:NE2	2.58	0.59
58:sK:36:ILE:HG23	58:sK:54:MET:HE3	1.82	0.59
61:E6:683:PRO:O	61:E6:687:GLN:NE2	2.35	0.59
8:B7:126:ASP:O	8:B7:130:ARG:NH1	2.35	0.59
11:BA:1277:GLU:HB3	11:BA:1312:ASN:HD22	1.67	0.59
19:BI:104:LEU:CD1	19:BI:104:LEU:HD21	2.28	0.59
42:mi:120:ARG:NH2	47:mn:78:ASP:OD1	2.35	0.59
49:mp:531:ILE:HB	49:mp:538:ILE:HB	1.85	0.59
64:T5:909:VAL:HA	64:T5:912:HIS:HB2	1.84	0.59
49:Mp:548:TYR:CD1	61:E6:612:GLU:CD	2.80	0.59
53:sE:468:GLU:HA	53:sE:471:HIS:CD2	2.34	0.59
53:sE:542:THR:HB	53:sE:544:THR:HG23	1.85	0.59
3:A2:51:VAL:O	3:A2:109:ARG:NH2	2.36	0.59
4:A3:100:ASN:HA	34:Ma:140:GLY:CA	2.25	0.59
23:AM:16:PRO:HG3	32:AW:151:LEU:HD23	1.72	0.59
49:Mp:531:ILE:HB	49:Mp:538:ILE:HB	1.85	0.59
32:BW:191:ASP:O	32:BW:193:ARG:NH2	2.36	0.59
53:sE:523:VAL:HG12	53:sE:547:ARG:HH22	1.68	0.59
9:sF:311:THR:HA	56:sI:657:LYS:H	1.67	0.59
1:A0:464:SER:OG	1:A0:659:MET:HE1	2.02	0.59
8:A7:742:MET:O	8:A7:742:MET:HE3	2.02	0.59
32:AW:191:ASP:O	32:AW:193:ARG:NH2	2.36	0.59
43:Mj:145:ARG:O	43:Mj:149:ARG:NH1	2.36	0.59
58:SK:145:ILE:HD13	58:SK:395:THR:HG21	1.84	0.59
61:T6:127:LEU:HD21	61:T6:182:THR:HG21	1.85	0.59
21:AK:8:GLU:N	21:AK:8:GLU:OE2	2.35	0.59
42:Mi:120:ARG:NH2	47:Mn:78:ASP:OD1	2.35	0.59
42:Mi:186:ARG:O	42:Mi:190:ARG:NH1	2.35	0.59
53:SE:543:ILE:HA	9:SF:756:ASN:HB2	1.83	0.59
1:B0:577:GLN:HE21	2:B1:330:LEU:HD11	1.68	0.59
26:BQ:151:LEU:HD23	26:BQ:440:ARG:HH22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:mj:145:ARG:O	43:mj:149:ARG:NH1	2.36	0.59
3:A2:503:ASP:O	3:A2:506:LYS:HB3	2.03	0.59
11:AA:74:MET:O	12:AB:1116:ARG:NH1	2.30	0.59
19:AI:104:LEU:CD1	19:AI:104:LEU:HD21	2.28	0.59
1:B0:464:SER:OG	1:B0:659:MET:HE1	2.02	0.59
8:B7:134:ILE:HG22	8:B7:141:ILE:HG12	1.85	0.59
51:sB:718:GLN:HE22	52:sC:173:ILE:HD12	1.67	0.59
11:BA:1278:ASN:N	11:BA:1279:ILE:HD12	2.15	0.59
12:BB:15:PRO:CD	64:t5:921:PRO:C	2.58	0.59
1:A0:252:LEU:HB2	1:A0:435:MET:HB3	1.85	0.58
11:AA:30:ILE:HD12	12:AB:1170:THR:HG21	1.84	0.58
51:SB:718:GLN:HE22	52:SC:173:ILE:HD12	1.67	0.58
58:SK:202:LYS:HB3	58:SK:207:MET:CE	2.32	0.58
11:BA:30:ILE:HD12	12:BB:1170:THR:HG21	1.84	0.58
12:BB:919:SER:HB2	12:BB:922:GLU:HB2	1.84	0.58
3:A2:195:GLU:OE2	3:A2:196:ILE:HG22	2.02	0.58
12:AB:919:SER:HB2	12:AB:922:GLU:HB2	1.84	0.58
15:AE:97:VAL:HG13	15:AE:127:ILE:HD11	1.84	0.58
9:SF:311:THR:HA	56:SI:657:LYS:H	1.67	0.58
55:SH:601:ALA:O	55:SH:605:LEU:HB2	2.03	0.58
7:B6:403:CYS:SG	7:B6:437:CYS:HB3	2.43	0.58
15:BE:97:VAL:HG13	15:BE:127:ILE:HD11	1.84	0.58
58:sK:202:LYS:HB3	58:sK:207:MET:CE	2.32	0.58
64:t5:909:VAL:HA	64:t5:912:HIS:HB2	1.84	0.58
3:A2:117:VAL:HG12	3:A2:120:SER:H	1.69	0.58
7:A6:403:CYS:SG	7:A6:437:CYS:HB3	2.43	0.58
45:ml:184:LYS:O	45:ml:188:ASN:ND2	2.36	0.58
61:T6:503:LEU:HD12	61:T6:504:PRO:HD2	1.84	0.58
61:t6:127:LEU:HD21	61:t6:182:THR:HG21	1.85	0.58
11:AA:68:GLN:CG	32:AW:151:LEU:HD11	2.09	0.58
23:AM:302:LEU:C	27:AR:270:MET:SD	2.86	0.58
55:SH:586:TYR:O	55:SH:590:GLU:HA	2.01	0.58
13:BC:148:ARG:HD3	20:BJ:65:PRO:HG3	1.86	0.58
49:Mp:177:GLN:HA	61:E6:668:PHE:CZ	2.39	0.58
3:B2:32:CYS:SG	3:B2:107:SER:OG	2.47	0.58
3:B2:503:ASP:O	3:B2:506:LYS:HB3	2.03	0.58
60:E3:408:VAL:HG22	60:E3:440:ARG:HD3	1.85	0.58
64:T5:923:LYS:O	64:T5:926:GLN:N	2.34	0.58
11:AA:1278:ASN:N	11:AA:1279:ILE:HD12	2.15	0.58
12:AB:294:ASP:OD2	19:AI:13:MET:HG2	2.03	0.58
11:BA:68:GLN:CG	32:BW:151:LEU:HD11	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BA:74:MET:O	12:BB:1116:ARG:NH1	2.30	0.58
55:sH:601:ALA:O	55:sH:605:LEU:HB2	2.03	0.58
58:sK:291:LEU:HD23	58:sK:298:THR:HG22	1.85	0.58
61:E6:184:LYS:HZ3	60:T3:429:PHE:CB	1.96	0.58
11:AA:678:GLU:CD	61:T6:761:LYS:NZ	2.58	0.58
18:AH:106:GLU:OE2	43:Mj:83:LEU:HD11	2.03	0.58
12:BB:63:ILE:HG13	12:BB:95:ILE:HD12	1.86	0.58
12:BB:294:ASP:OD2	19:BI:13:MET:HG2	2.03	0.58
53:sE:545:THR:HG22	9:sF:756:ASN:HB3	1.86	0.58
11:AA:687:LYS:NZ	11:AA:795:GLU:OE2	2.31	0.58
19:AI:58:VAL:HG21	19:AI:109:ILE:HD11	1.86	0.58
31:AV:8:GLU:OE1	31:AV:11:ARG:NH2	2.33	0.58
12:BB:451:LYS:HE3	23:BM:138:ASP:HB3	1.85	0.58
40:mg:16:ILE:HG21	40:mg:72:LEU:HD11	1.85	0.58
53:sE:337:ALA:HB1	53:sE:462:THR:HB	1.86	0.58
3:B2:117:VAL:HG12	3:B2:120:SER:H	1.69	0.58
12:BB:762:ASN:HD21	12:BB:984:HIS:HD2	1.52	0.58
17:BG:100:GLU:OE2	32:BW:144:ARG:CZ	2.52	0.58
62:T1:67:GLN:HA	62:T1:70:GLN:OE1	2.04	0.58
1:A0:577:GLN:HE21	2:A1:330:LEU:HD11	1.67	0.58
11:AA:668:ASP:HA	11:AA:741:ASN:HD21	1.67	0.58
40:Mg:16:ILE:HG21	40:Mg:72:LEU:HD11	1.85	0.58
1:B0:334:PHE:O	1:B0:338:LEU:HD23	2.04	0.58
10:B9:191:GLU:OE1	9:sF:763:ARG:C	2.47	0.58
15:BE:5:ASN:OD1	15:BE:52:ARG:NH2	2.37	0.58
57:sJ:59:ARG:NH1	57:sJ:59:ARG:O	2.37	0.58
9:SF:551:VAL:HG22	9:SF:556:GLN:HG3	1.86	0.57
1:B0:541:PHE:HB2	1:B0:547:MET:HE2	1.86	0.57
11:BA:1140:HIS:HA	11:BA:1275:GLY:HA3	1.86	0.57
19:BI:58:VAL:HG21	19:BI:109:ILE:HD11	1.86	0.57
60:E3:415:PHE:HE1	60:E3:439:ILE:HG12	1.68	0.57
60:E3:900:THR:OG1	60:T3:428:LEU:O	2.22	0.57
11:AA:1158:PRO:HB3	11:AA:1188:GLN:HB2	1.86	0.57
53:SE:337:ALA:HB1	53:SE:462:THR:HB	1.86	0.57
4:B3:64:ARG:HH22	17:BG:165:GLU:CD	2.11	0.57
15:BE:195:VAL:HG22	15:BE:213:ILE:HG22	1.87	0.57
58:sK:145:ILE:HD13	58:sK:395:THR:HG21	1.85	0.57
2:A1:466:ASN:HA	2:A1:469:MET:HE3	1.86	0.57
12:AB:451:LYS:HE3	23:AM:138:ASP:HB3	1.85	0.57
12:AB:957:ASN:HD21	12:AB:961:LEU:HB2	1.69	0.57
15:AE:195:VAL:HG22	15:AE:213:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AH:106:GLU:OE1	18:AH:112:ILE:HG22	2.04	0.57
18:AH:129:TYR:HB2	43:Mj:83:LEU:HD21	1.86	0.57
49:Mp:351:VAL:HA	49:Mp:558:ILE:HD11	1.86	0.57
53:SE:545:THR:HG22	9:SF:756:ASN:HB3	1.86	0.57
57:SJ:59:ARG:NH1	57:SJ:59:ARG:O	2.37	0.57
58:SK:291:LEU:HD23	58:SK:298:THR:HG22	1.85	0.57
18:BH:109:LYS:O	43:mj:83:LEU:HD12	2.05	0.57
64:t5:923:LYS:O	64:t5:926:GLN:N	2.34	0.57
1:A0:541:PHE:HB2	1:A0:547:MET:HE2	1.86	0.57
3:A2:36:TYR:HA	3:A2:39:LEU:HD13	1.86	0.57
45:MI:184:LYS:O	45:MI:188:ASN:ND2	2.37	0.57
28:BS:232:ASP:CG	28:BS:235:ASP:HB2	2.30	0.57
36:mc:72:LEU:O	36:mc:76:ASN:ND2	2.37	0.57
60:E3:415:PHE:HA	60:E3:418:LYS:HG2	1.85	0.57
3:A2:51:VAL:HG21	3:A2:108:LEU:HD22	1.84	0.57
10:A9:191:GLU:OE1	9:SF:763:ARG:C	2.47	0.57
2:B1:466:ASN:HA	2:B1:469:MET:HE3	1.86	0.57
4:B3:85:ARG:HD2	4:B3:89:PHE:CZ	2.40	0.57
27:AR:108:LEU:HD12	27:AR:117:PRO:O	2.05	0.57
28:AS:232:ASP:CG	28:AS:235:ASP:HB2	2.30	0.57
9:sF:551:VAL:HG22	9:sF:556:GLN:HG3	1.85	0.57
64:t5:934:ILE:HG23	64:t5:945:MET:HE1	1.86	0.57
1:A0:334:PHE:O	1:A0:338:LEU:HD23	2.04	0.57
14:AD:213:GLU:CG	35:Mb:38:MET:CE	2.83	0.57
58:SK:202:LYS:HB3	58:SK:207:MET:HE3	1.86	0.57
53:sE:503:ILE:HD12	53:sE:503:ILE:H	1.70	0.57
60:T3:406:LYS:O	60:T3:409:LYS:N	2.29	0.57
7:A6:124:ARG:NH1	7:A6:305:VAL:O	2.38	0.57
12:AB:762:ASN:HD21	12:AB:984:HIS:HD2	1.52	0.57
23:AM:303:GLN:N	27:AR:270:MET:HE1	2.14	0.57
8:B7:227:ILE:O	8:B7:508:HIS:NE2	2.37	0.57
31:BV:8:GLU:OE1	31:BV:11:ARG:NH2	2.33	0.57
8:A7:227:ILE:O	8:A7:508:HIS:NE2	2.37	0.57
11:AA:420:ARG:NH2	38:Me:58:LEU:HD23	2.16	0.57
13:AC:148:ARG:HD3	20:AJ:65:PRO:HG3	1.86	0.57
36:Mc:72:LEU:O	36:Mc:76:ASN:ND2	2.38	0.57
1:B0:252:LEU:HB2	1:B0:435:MET:HB3	1.86	0.57
12:BB:13:GLU:CD	64:t5:920:LYS:O	2.47	0.57
18:BH:106:GLU:OE1	18:BH:112:ILE:HG22	2.04	0.57
58:sK:36:ILE:HG22	58:sK:67:VAL:HG22	1.87	0.57
61:E6:923:LEU:HB3	61:E6:934:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:t4:903:PRO:HG3	45:t4:936:LYS:HB2	1.87	0.57
4:A3:64:ARG:HH22	17:AG:165:GLU:CD	2.11	0.57
6:A5:38:THR:HG23	6:A5:39:HIS:CD2	2.39	0.57
11:AA:1140:HIS:HA	11:AA:1275:GLY:HA3	1.86	0.57
12:AB:13:GLU:CB	64:T5:919:ARG:CZ	2.83	0.57
15:AE:5:ASN:OD1	15:AE:52:ARG:NH2	2.37	0.57
36:Mc:2:GLN:NE2	37:Md:316:ILE:O	2.33	0.57
49:Mp:548:TYR:CD2	61:E6:612:GLU:HG2	2.40	0.57
5:B4:196:ILE:HG22	5:B4:197:MET:HE2	1.87	0.57
32:BW:119:PRO:O	32:BW:133:GLN:NE2	2.25	0.57
62:t1:67:GLN:HA	62:t1:70:GLN:OE1	2.04	0.57
4:A3:85:ARG:HD2	4:A3:89:PHE:CZ	2.40	0.56
12:AB:63:ILE:HG13	12:AB:95:ILE:HD12	1.86	0.56
17:AG:46:LEU:HB2	17:AG:77:VAL:HG23	1.87	0.56
24:AN:-44:DG:H2"	24:AN:-43:DA:C8	2.40	0.56
28:AS:283:GLN:HB3	28:AS:293:LEU:HD13	1.87	0.56
30:AU:25:PHE:HE1	31:AV:36:LEU:HD11	1.70	0.56
32:AW:101:LYS:HA	32:AW:104:GLN:HG3	1.87	0.56
1:B0:603:ARG:NH2	1:B0:657:ASP:OD2	2.38	0.56
6:B5:38:THR:HG23	6:B5:39:HIS:CD2	2.39	0.56
11:BA:465:TYR:CE1	21:BK:3:ALA:HA	2.38	0.56
60:E3:306:TRP:CH2	60:E3:372:LYS:HE2	2.39	0.56
63:t2:71:TYR:HA	63:t2:74:ILE:HG12	1.87	0.56
8:A7:134:ILE:HG22	8:A7:141:ILE:HG12	1.85	0.56
27:AR:63:ARG:NH2	27:AR:65:ASN:O	2.37	0.56
31:AV:87:VAL:O	31:AV:103:GLN:N	2.38	0.56
32:AW:119:PRO:O	32:AW:133:GLN:NE2	2.25	0.56
53:SE:523:VAL:HG12	53:SE:547:ARG:HH22	1.68	0.56
7:B6:124:ARG:NH1	7:B6:305:VAL:O	2.38	0.56
7:B6:234:ILE:HG23	7:B6:263:VAL:HG23	1.87	0.56
14:BD:213:GLU:CG	35:mb:38:MET:CE	2.83	0.56
18:BH:129:TYR:HB2	43:mj:83:LEU:HD21	1.86	0.56
24:BN:-44:DG:H2"	24:BN:-43:DA:C8	2.40	0.56
27:BR:63:ARG:NH2	27:BR:65:ASN:O	2.37	0.56
49:mp:351:VAL:HA	49:mp:558:ILE:HD11	1.86	0.56
1:A0:509:ARG:NH1	1:A0:511:GLU:OE2	2.39	0.56
3:A2:454:TYR:HD2	6:A5:9:LEU:HD23	1.70	0.56
36:Mc:33:ILE:HG23	36:Mc:44:VAL:HG12	1.87	0.56
1:B0:167:VAL:CG2	1:B0:199:MET:HE1	2.36	0.56
11:BA:1158:PRO:HB3	11:BA:1188:GLN:HB2	1.86	0.56
51:sB:766:GLN:HE22	51:sD:746:LEU:HD12	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:sK:202:LYS:HB3	58:sK:207:MET:HE3	1.86	0.56
4:A3:114:GLU:HA	4:A3:117:ILE:HG22	1.88	0.56
28:AS:265:VAL:HG12	28:AS:280:SER:HB3	1.88	0.56
12:BB:957:ASN:HD21	12:BB:961:LEU:HB2	1.69	0.56
13:BC:86:CYS:SG	13:BC:87:PHE:N	2.79	0.56
27:BR:108:LEU:HD12	27:BR:117:PRO:O	2.05	0.56
60:E3:934:PHE:CE2	61:E6:183:ARG:HG2	2.39	0.56
45:T4:903:PRO:HG3	45:T4:936:LYS:HB2	1.87	0.56
64:T5:934:ILE:HG23	64:T5:945:MET:HE1	1.86	0.56
63:t2:36:ALA:O	63:t2:40:ILE:HG12	2.05	0.56
1:A0:642:MET:HE1	1:A0:646:TYR:CD2	2.41	0.56
7:A6:352:CYS:CB	7:A6:366:CYS:SG	2.84	0.56
45:MI:490:GLN:HG2	45:MI:502:GLN:HE21	1.70	0.56
51:SB:329:GLU:HB3	9:SF:537:LEU:HD23	1.88	0.56
9:sF:662:ARG:HA	9:sF:665:LYS:HE2	1.88	0.56
13:AC:145:CYS:SG	13:AC:146:LYS:N	2.79	0.56
15:AE:116:ILE:HG13	15:AE:121:MET:CE	2.36	0.56
11:BA:1221:LYS:HD2	11:BA:1222:ASN:H	1.70	0.56
44:mk:12:GLN:OE1	45:ml:152:ARG:NH2	2.39	0.56
11:AA:465:TYR:CE1	21:AK:3:ALA:HA	2.38	0.56
3:B2:36:TYR:HA	3:B2:39:LEU:HD13	1.86	0.56
11:BA:687:LYS:NZ	11:BA:795:GLU:OE2	2.31	0.56
15:BE:116:ILE:HG13	15:BE:121:MET:CE	2.36	0.56
61:E6:471:GLU:OE2	61:E6:493:SER:OG	2.23	0.56
44:Mk:12:GLN:OE1	45:MI:152:ARG:NH2	2.39	0.56
45:MI:831:GLN:HG2	45:t4:837:VAL:HG21	1.87	0.56
17:BG:46:LEU:HB2	17:BG:77:VAL:HG23	1.87	0.56
23:BM:303:GLN:N	27:BR:270:MET:HE1	2.14	0.56
31:BV:87:VAL:O	31:BV:103:GLN:N	2.38	0.56
38:me:1:MET:N	39:mf:102:GLU:OE2	2.38	0.56
45:ml:490:GLN:HG2	45:ml:502:GLN:HE21	1.70	0.56
4:A3:84:ILE:HG23	4:A3:120:LEU:HD23	1.88	0.56
5:A4:196:ILE:HG22	5:A4:197:MET:HE2	1.87	0.56
49:Mp:180:GLN:O	61:E6:664:ARG:HD3	2.05	0.56
53:SE:468:GLU:HA	53:SE:471:HIS:CD2	2.34	0.56
1:B0:544:TYR:N	2:B1:358:MET:HE1	2.14	0.56
3:B2:405:HIS:HD1	3:B2:407:GLN:H	1.54	0.56
4:B3:114:GLU:HA	4:B3:117:ILE:HG22	1.88	0.56
11:BA:66:LYS:HA	11:BA:72:GLU:HG3	1.87	0.56
23:BM:302:LEU:C	27:BR:270:MET:SD	2.86	0.56
28:BS:226:GLU:O	28:BS:230:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BS:227:PHE:HA	28:BS:230:THR:HG23	1.88	0.56
60:E3:838:SER:CA	61:T6:157:TYR:CE2	2.82	0.56
61:E6:159:ILE:HG13	60:T3:838:SER:HA	1.88	0.56
60:t3:888:LEU:HD21	61:t6:274:ARG:HD3	1.88	0.56
1:A0:167:VAL:CG2	1:A0:199:MET:HE1	2.36	0.56
11:AA:1221:LYS:HD2	11:AA:1222:ASN:H	1.70	0.56
18:AH:109:LYS:O	43:Mj:83:LEU:HD12	2.05	0.56
23:AM:301:THR:C	27:AR:270:MET:HE1	2.31	0.56
28:AS:227:PHE:C	28:AS:230:THR:H	2.14	0.56
3:B2:138:TYR:HE2	3:B2:260:PHE:CD1	2.24	0.56
3:B2:463:GLU:HA	9:sF:400:GLN:O	2.06	0.56
18:BH:109:LYS:O	43:mj:83:LEU:CG	2.54	0.56
30:BU:25:PHE:HE1	31:BV:36:LEU:HD11	1.70	0.56
41:mh:192:MET:HE3	48:mo:20:PRO:HB3	1.88	0.56
60:T3:301:ASN:ND2	60:T3:974:LEU:O	2.38	0.56
3:B2:372:ASN:HB3	3:B2:373:MET:HE2	1.88	0.55
12:BB:560:GLU:HG3	12:BB:561:TRP:HD1	1.71	0.55
12:BB:1187:ASN:HD21	12:BB:1190:ASP:HB3	1.71	0.55
32:BW:101:LYS:HA	32:BW:104:GLN:HG3	1.87	0.55
3:A2:22:GLN:HE21	3:A2:26:TYR:HE1	1.54	0.55
51:SB:315:ASN:HB3	51:SB:318:LYS:HD2	1.87	0.55
1:B0:509:ARG:NH1	1:B0:511:GLU:OE2	2.39	0.55
1:B0:642:MET:HE1	1:B0:646:TYR:CD2	2.41	0.55
49:mp:166:LYS:NZ	49:mp:230:GLU:OE2	2.39	0.55
60:E3:306:TRP:CZ3	60:E3:372:LYS:HE2	2.42	0.55
60:E3:879:ARG:NH1	60:T3:892:GLU:OE1	2.40	0.55
61:E6:253:GLN:NE2	61:E6:254:PHE:O	2.39	0.55
60:T3:289:LYS:CB	60:T3:289:LYS:CD	2.67	0.55
60:t3:541:VAL:HG11	60:t3:581:PHE:HB2	1.87	0.55
7:A6:322:MET:HE1	7:A6:369:MET:HG3	1.88	0.55
23:AM:301:THR:HA	27:AR:271:ARG:CZ	2.36	0.55
49:Mp:166:LYS:NZ	49:Mp:230:GLU:OE2	2.39	0.55
8:B7:641:GLN:NE2	8:B7:645:TYR:HE2	2.04	0.55
11:BA:313:GLN:NE2	11:BA:314:ALA:O	2.37	0.55
27:BR:73:LEU:HD11	27:BR:77:LEU:HB2	1.89	0.55
51:sB:329:GLU:HB3	9:sF:537:LEU:HD23	1.88	0.55
63:T2:36:ALA:O	63:T2:40:ILE:HG12	2.05	0.55
60:T3:769:GLN:NE2	61:T6:338:SER:O	2.39	0.55
7:A6:234:ILE:HG23	7:A6:263:VAL:HG23	1.87	0.55
8:A7:462:ASN:ND2	8:A7:465:ASN:OD1	2.34	0.55
12:AB:496:ARG:NH2	12:AB:540:SER:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Mp:261:ASN:ND2	49:Mp:325:ILE:O	2.39	0.55
58:SK:108:MET:HE1	58:SK:138:ILE:HD12	1.88	0.55
58:SK:237:GLN:CD	58:SK:303:LEU:HD11	2.31	0.55
3:B2:454:TYR:HD2	6:B5:9:LEU:HD23	1.70	0.55
13:BC:145:CYS:SG	13:BC:146:LYS:N	2.79	0.55
17:BG:116:PRO:HD3	17:BG:164:LYS:HA	1.89	0.55
28:BS:227:PHE:C	28:BS:230:THR:H	2.14	0.55
28:BS:283:GLN:HB3	28:BS:293:LEU:HD13	1.87	0.55
63:T2:71:TYR:HA	63:T2:74:ILE:HG12	1.88	0.55
28:AS:227:PHE:HA	28:AS:230:THR:HG23	1.88	0.55
38:Me:1:MET:N	39:Mf:102:GLU:OE2	2.38	0.55
55:SH:447:ASP:O	55:SH:448:MET:HE2	2.07	0.55
12:BB:496:ARG:NH2	12:BB:540:SER:O	2.39	0.55
51:sB:705:GLU:HA	51:sB:708:MET:HG2	1.89	0.55
60:E3:301:ASN:ND2	60:E3:974:LEU:O	2.39	0.55
60:T3:541:VAL:HG11	60:T3:581:PHE:HB2	1.87	0.55
60:T3:888:LEU:HD21	61:T6:274:ARG:HD3	1.88	0.55
4:A3:49:LEU:HB3	17:AG:164:LYS:HG2	1.88	0.55
13:AC:86:CYS:SG	13:AC:87:PHE:N	2.79	0.55
17:AG:116:PRO:HD3	17:AG:164:LYS:HA	1.89	0.55
12:BB:15:PRO:CD	64:t5:922:THR:HB	2.37	0.55
9:sF:536:ARG:NH2	9:sF:540:ASP:OD1	2.40	0.55
58:sK:237:GLN:CD	58:sK:303:LEU:HD11	2.31	0.55
61:E6:186:TYR:HE1	60:T3:428:LEU:CD2	2.14	0.55
3:A2:463:GLU:HA	9:SF:400:GLN:O	2.06	0.55
18:AH:109:LYS:O	43:Mj:83:LEU:CG	2.54	0.55
28:AS:226:GLU:O	28:AS:230:THR:N	2.39	0.55
51:SD:676:GLU:HA	51:SD:679:MET:HG2	1.89	0.55
14:BD:213:GLU:HG3	35:mb:38:MET:HE1	1.88	0.55
32:BW:24:SER:HA	32:BW:27:LEU:HD12	1.88	0.55
51:sD:676:GLU:HA	51:sD:679:MET:HG2	1.89	0.55
58:sK:108:MET:HE1	58:sK:138:ILE:HD12	1.88	0.55
45:t4:835:GLN:HG2	45:t4:886:THR:HG21	1.89	0.55
8:A7:641:GLN:NE2	8:A7:645:TYR:HE2	2.04	0.55
12:AB:868:MET:SD	23:AM:182:ARG:NH1	2.80	0.55
27:AR:132:GLU:O	27:AR:217:THR:OG1	2.25	0.55
9:SF:662:ARG:HA	9:SF:665:LYS:HE2	1.88	0.55
5:B4:221:SER:OG	5:B4:224:LEU:HD23	2.07	0.55
23:BM:191:GLU:OE2	27:BR:268:MET:CA	2.55	0.55
26:BQ:141:ARG:NH1	26:BQ:348:TYR:O	2.40	0.55
36:mc:33:ILE:HG23	36:mc:44:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:md:503:LEU:HB3	37:md:507:MET:HE1	1.89	0.55
51:sB:315:ASN:HB3	51:sB:318:LYS:HD2	1.87	0.55
45:T4:835:GLN:HG2	45:T4:886:THR:HG21	1.89	0.55
5:A4:221:SER:OG	5:A4:224:LEU:HD23	2.07	0.55
27:AR:73:LEU:HD11	27:AR:77:LEU:HB2	1.89	0.55
41:Mh:192:MET:HE3	48:Mo:20:PRO:HB3	1.88	0.55
45:Ml:161:VAL:O	45:Ml:165:LEU:HB2	2.07	0.55
53:SE:503:ILE:H	53:SE:503:ILE:HD12	1.70	0.55
4:B3:84:ILE:HG23	4:B3:120:LEU:HD23	1.88	0.55
7:B6:322:MET:HE1	7:B6:369:MET:HG3	1.88	0.55
23:BM:301:THR:C	27:BR:270:MET:HE1	2.31	0.55
61:T6:618:ILE:O	61:T6:653:LYS:NZ	2.39	0.55
11:AA:66:LYS:HA	11:AA:72:GLU:HG3	1.88	0.55
14:AD:213:GLU:HG3	35:Mb:38:MET:HE1	1.88	0.55
23:AM:191:GLU:OE2	27:AR:268:MET:CA	2.55	0.55
4:B3:49:LEU:HB3	17:BG:164:LYS:HG2	1.88	0.55
8:B7:154:GLN:O	8:B7:158:VAL:HG23	2.07	0.55
28:BS:227:PHE:CD1	28:BS:230:THR:HG21	2.41	0.55
28:BS:230:THR:C	28:BS:232:ASP:H	2.15	0.55
35:mb:156:THR:HG21	40:mg:32:ASP:HA	1.89	0.55
45:T4:971:TYR:HB2	45:T4:980:ILE:HB	1.89	0.55
45:T4:1000:HIS:O	45:T4:1002:HIS:HD2	1.90	0.55
60:t3:416:THR:O	60:t3:420:ASP:HB2	2.06	0.55
45:t4:1000:HIS:O	45:t4:1002:HIS:HD2	1.90	0.55
12:AB:560:GLU:HG3	12:AB:561:TRP:HD1	1.71	0.54
28:AS:227:PHE:CD1	28:AS:230:THR:HG21	2.41	0.54
35:Mb:156:THR:HG21	40:Mg:32:ASP:HA	1.89	0.54
58:SK:36:ILE:HG22	58:SK:67:VAL:HG22	1.87	0.54
14:BD:157:GLN:HA	14:BD:160:VAL:HG22	1.89	0.54
23:BM:301:THR:HA	27:BR:271:ARG:CZ	2.36	0.54
60:T3:416:THR:O	60:T3:420:ASP:HB2	2.06	0.54
61:T6:429:ARG:NH1	61:T6:430:HIS:O	2.40	0.54
3:A2:138:TYR:HE2	3:A2:260:PHE:CD1	2.24	0.54
8:A7:154:GLN:O	8:A7:158:VAL:HG23	2.07	0.54
32:AW:227:MET:N	32:AW:227:MET:SD	2.79	0.54
56:SI:1288:ASN:HD22	56:SI:1291:VAL:HG13	1.71	0.54
1:B0:493:LEU:HG	1:B0:495:MET:HE3	1.88	0.54
2:B1:498:LYS:O	2:B1:502:ARG:NE	2.40	0.54
60:E3:400:LEU:HB3	60:E3:461:TYR:CE2	2.43	0.54
1:A0:550:ILE:HD13	1:A0:553:MET:HE1	1.89	0.54
45:Ml:629:LEU:HD11	45:Ml:692:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BF:118:LEU:HG	16:BF:122:MET:HE2	1.90	0.54
53:sE:540:ASP:O	9:sF:759:THR:OG1	2.25	0.54
28:AS:248:ILE:HG13	28:AS:252:ASN:HD21	1.73	0.54
45:Ml:803:VAL:HG12	45:Ml:806:GLU:H	1.72	0.54
53:SE:504:PRO:HG2	53:SE:507:LEU:HD11	1.89	0.54
28:BS:265:VAL:HG12	28:BS:280:SER:HB3	1.88	0.54
32:BW:227:MET:N	32:BW:227:MET:SD	2.79	0.54
57:sJ:28:ASP:HA	57:sJ:61:LYS:HZ2	1.72	0.54
60:t3:769:GLN:NE2	61:t6:338:SER:O	2.39	0.54
3:A2:372:ASN:HB3	3:A2:373:MET:HE2	1.88	0.54
12:AB:1187:ASN:HD21	12:AB:1190:ASP:HB3	1.71	0.54
13:AC:5:GLY:O	13:AC:7:GLN:NE2	2.41	0.54
53:SE:523:VAL:HG12	53:SE:547:ARG:CZ	2.38	0.54
8:B7:626:PHE:HE2	8:B7:628:TYR:HE1	1.54	0.54
12:BB:868:MET:SD	23:BM:182:ARG:NH1	2.80	0.54
40:mg:46:SER:HB2	40:mg:49:ALA:HB3	1.89	0.54
56:sI:1288:ASN:HD22	56:sI:1291:VAL:HG13	1.71	0.54
3:A2:405:HIS:HD1	3:A2:407:GLN:H	1.54	0.54
7:A6:129:THR:HG22	7:A6:174:MET:HE1	1.90	0.54
51:SB:705:GLU:HA	51:SB:708:MET:HG2	1.89	0.54
3:B2:506:LYS:HZ2	3:B2:506:LYS:HD2	1.73	0.54
26:BQ:108:LYS:HA	26:BQ:111:LEU:HD13	1.89	0.54
9:sF:505:THR:O	9:sF:509:HIS:ND1	2.41	0.54
61:E6:161:ASN:CG	60:T3:838:SER:HB3	2.31	0.54
60:T3:1126:MET:HA	60:T3:1129:THR:HG22	1.90	0.54
11:AA:66:LYS:HB3	23:AM:18:LEU:HD22	1.90	0.54
12:AB:882:THR:OG1	12:AB:885:MET:SD	2.66	0.54
37:Md:120:ASN:HB2	37:Md:123:GLU:HG2	1.89	0.54
51:SB:715:LEU:HD13	51:SD:718:GLN:HE21	1.73	0.54
5:B4:303:ASN:ND2	5:B4:314:GLU:OE2	2.38	0.54
6:B5:31:VAL:HG22	6:B5:42:VAL:HG12	1.89	0.54
11:BA:590:ARG:NH2	11:BA:618:GLU:OE2	2.41	0.54
14:BD:213:GLU:HG2	35:mb:38:MET:CE	2.38	0.54
14:BD:213:GLU:OE2	35:mb:38:MET:CE	2.56	0.54
18:BH:106:GLU:OE2	43:mj:83:LEU:HD11	2.03	0.54
27:BR:132:GLU:O	27:BR:217:THR:OG1	2.25	0.54
55:sH:447:ASP:O	55:sH:448:MET:HE2	2.07	0.54
58:sK:140:ILE:HG22	58:sK:142:PRO:HD2	1.90	0.54
6:A5:16:ILE:HA	6:A5:19:LEU:HD12	1.90	0.54
11:AA:590:ARG:NH2	11:AA:618:GLU:OE2	2.41	0.54
11:AA:1279:ILE:HG23	11:AA:1308:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AM:303:GLN:OE1	27:AR:270:MET:HG2	2.08	0.54
37:Md:503:LEU:HB3	37:Md:507:MET:HE1	1.89	0.54
53:SE:523:VAL:CG1	53:SE:523:VAL:HG21	2.35	0.54
1:B0:550:ILE:HD13	1:B0:553:MET:HE1	1.89	0.54
12:BB:661:LEU:HD11	12:BB:684:LEU:HD11	1.88	0.54
45:ml:629:LEU:HD11	45:ml:692:GLN:HG3	1.89	0.54
56:sI:1190:PRO:HG3	56:sI:1251:LYS:HG3	1.89	0.54
60:E3:943:LYS:HG3	60:T3:429:PHE:HZ	1.72	0.54
61:E6:381:THR:HG23	60:t3:431:ASP:OD1	2.06	0.54
60:t3:1126:MET:HA	60:t3:1129:THR:HG22	1.90	0.54
64:t5:922:THR:OG1	64:t5:923:LYS:N	2.41	0.54
61:t6:429:ARG:NH1	61:t6:430:HIS:O	2.40	0.54
14:AD:24:ALA:N	14:AD:28:GLN:O	2.40	0.54
26:AQ:141:ARG:NH1	26:AQ:348:TYR:O	2.40	0.54
9:SF:536:ARG:NH2	9:SF:540:ASP:OD1	2.40	0.54
30:BU:247:LEU:HB3	31:BV:118:SER:HB3	1.90	0.54
37:md:120:ASN:HB2	37:md:123:GLU:HG2	1.89	0.54
45:t4:971:TYR:HB2	45:t4:980:ILE:HB	1.89	0.54
6:A5:31:VAL:HG22	6:A5:42:VAL:HG12	1.89	0.54
51:SB:327:LEU:HD13	51:SB:330:PHE:HD2	1.73	0.54
5:B4:299:ILE:HD12	5:B4:300:PRO:HD2	1.90	0.54
45:ml:161:VAL:O	45:ml:165:LEU:HB2	2.07	0.54
49:mp:297:PRO:HG2	49:mp:300:ILE:HD12	1.90	0.54
9:sF:539:GLY:HA3	9:sF:566:SER:HB3	1.90	0.54
60:E3:436:SER:HB3	60:E3:463:ARG:NE	2.23	0.54
61:t6:381:THR:HG22	61:t6:383:LYS:H	1.72	0.54
1:A0:676:TYR:HB3	1:A0:724:MET:CE	2.37	0.53
5:A4:299:ILE:HD12	5:A4:300:PRO:HD2	1.90	0.53
8:A7:626:PHE:HE2	8:A7:628:TYR:HE1	1.54	0.53
11:AA:381:THR:HG23	11:AA:383:TYR:H	1.74	0.53
44:Mk:60:LEU:HD23	45:ML:104:MET:HE2	1.90	0.53
11:BA:68:GLN:HE21	32:BW:151:LEU:HD13	1.74	0.53
15:BE:116:ILE:HD12	15:BE:121:MET:HB3	1.90	0.53
23:BM:303:GLN:OE1	27:BR:270:MET:HG2	2.08	0.53
45:ml:803:VAL:HG12	45:ml:806:GLU:H	1.72	0.53
53:sE:523:VAL:CG1	53:sE:523:VAL:HG21	2.35	0.53
54:sG:54:UNK:HA	54:sG:59:UNK:HA	1.91	0.53
61:E6:173:LYS:NZ	61:E6:175:MET:HB2	2.23	0.53
61:T6:381:THR:HG22	61:T6:383:LYS:H	1.72	0.53
61:t6:23:SER:O	61:t6:179:ARG:NH2	2.41	0.53
12:AB:248:SER:H	12:AB:418:LYS:HE3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:661:LEU:HD11	12:AB:684:LEU:HD11	1.88	0.53
16:AF:118:LEU:HG	16:AF:122:MET:HE2	1.90	0.53
28:AS:230:THR:C	28:AS:232:ASP:H	2.15	0.53
32:AW:24:SER:HA	32:AW:27:LEU:HD12	1.88	0.53
49:Mp:177:GLN:OE1	61:E6:668:PHE:CZ	2.60	0.53
11:BA:381:THR:HG23	11:BA:383:TYR:H	1.74	0.53
14:BD:24:ALA:N	14:BD:28:GLN:O	2.40	0.53
30:BU:25:PHE:O	30:BU:29:GLY:N	2.42	0.53
1:A0:493:LEU:HG	1:A0:495:MET:HE3	1.88	0.53
1:A0:603:ARG:NH2	1:A0:657:ASP:OD2	2.38	0.53
6:A5:46:LYS:O	6:A5:50:VAL:HG13	2.08	0.53
12:AB:342:GLY:O	12:AB:348:ARG:NH1	2.41	0.53
12:AB:583:ASN:HD21	12:AB:628:THR:H	1.56	0.53
14:AD:213:GLU:HG2	35:Mb:38:MET:CE	2.38	0.53
20:AJ:65:PRO:HD2	20:AJ:68:LYS:HE2	1.91	0.53
24:AN:-43:DA:H2"	24:AN:-42:DT:C7	2.38	0.53
45:MI:438:LEU:HG	45:MI:460:ILE:HG13	1.91	0.53
45:MI:461:VAL:HG13	45:MI:463:ASN:H	1.73	0.53
11:BA:1279:ILE:HG23	11:BA:1308:THR:HG23	1.90	0.53
18:BH:113:ALA:HB2	18:BH:126:GLU:HG3	1.91	0.53
53:sE:129:LEU:HD23	53:sE:185:TYR:HB3	1.91	0.53
53:sE:523:VAL:HG12	53:sE:547:ARG:CZ	2.38	0.53
53:sE:527:THR:OG1	53:sE:546:LYS:HA	2.08	0.53
55:sH:443:ILE:HD11	56:sI:662:ARG:HD2	1.91	0.53
45:t4:879:ASP:O	45:t4:902:ASN:ND2	2.39	0.53
11:AA:68:GLN:HE21	32:AW:151:LEU:HD13	1.74	0.53
19:AI:117:LYS:HG2	61:T6:801:LYS:CE	2.38	0.53
26:AQ:108:LYS:HA	26:AQ:111:LEU:HD13	1.89	0.53
50:SA:484:ASP:OD1	51:SD:693:LYS:NZ	2.42	0.53
51:SD:370:ASN:ND2	9:SF:739:MET:HE2	2.24	0.53
53:SE:529:VAL:HA	53:SE:544:THR:HG22	1.90	0.53
8:B7:122:ARG:NH1	8:B7:123:LEU:O	2.42	0.53
11:BA:172:PRO:HB3	11:BA:185:TRP:HD1	1.73	0.53
45:ml:461:VAL:HG13	45:ml:463:ASN:H	1.73	0.53
53:sE:504:PRO:HG2	53:sE:507:LEU:HD11	1.89	0.53
53:sE:527:THR:OG1	53:sE:545:THR:O	2.22	0.53
1:A0:210:TYR:OH	1:A0:235:ASP:O	2.27	0.53
1:A0:544:TYR:N	2:A1:358:MET:HE1	2.14	0.53
1:A0:577:GLN:NE2	2:A1:330:LEU:HD11	2.23	0.53
11:AA:1280:GLU:OE1	11:AA:1309:ASP:HB2	2.08	0.53
12:AB:309:GLN:O	12:AB:313:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:420:LEU:HD13	12:AB:453:ILE:HA	1.90	0.53
14:AD:213:GLU:OE2	35:Mb:38:MET:CE	2.56	0.53
42:Mi:11:SER:OG	42:Mi:12:LEU:N	2.41	0.53
53:SE:526:GLN:HB3	53:SE:547:ARG:CD	2.39	0.53
53:SE:540:ASP:O	9:SF:759:THR:OG1	2.25	0.53
56:SI:1297:ASN:HA	56:SI:1300:GLN:HE21	1.73	0.53
59:SL:98:ASN:HB3	59:SL:101:ALA:HB2	1.90	0.53
1:B0:676:TYR:HB3	1:B0:724:MET:CE	2.37	0.53
12:BB:342:GLY:O	12:BB:348:ARG:NH1	2.41	0.53
28:BS:184:LYS:HD2	28:BS:228:LEU:CD1	2.37	0.53
53:sE:529:VAL:HA	53:sE:544:THR:HG22	1.90	0.53
58:sK:235:MET:HE1	58:sK:290:PHE:HB2	1.90	0.53
60:t3:301:ASN:ND2	60:t3:974:LEU:O	2.38	0.53
61:t6:651:TYR:OH	61:t6:910:CYS:SG	2.61	0.53
5:A4:303:ASN:ND2	5:A4:314:GLU:OE2	2.38	0.53
25:AO:107:ARG:NH1	30:AU:286:VAL:OXT	2.42	0.53
33:AX:234:ARG:NH1	33:AX:239:LYS:O	2.35	0.53
56:SI:1190:PRO:HG3	56:SI:1251:LYS:HG3	1.89	0.53
57:SJ:59:ARG:HH22	58:SK:134:PRO:HG3	1.74	0.53
1:B0:577:GLN:NE2	2:B1:330:LEU:HD11	2.23	0.53
6:B5:16:ILE:HA	6:B5:19:LEU:HD12	1.90	0.53
6:B5:46:LYS:O	6:B5:50:VAL:HG13	2.08	0.53
18:BH:10:PHE:HB3	18:BH:28:ALA:HB1	1.90	0.53
45:ml:438:LEU:HG	45:ml:460:ILE:HG13	1.91	0.53
9:sF:506:ARG:HG3	9:sF:510:ILE:HD11	1.90	0.53
19:Al:117:LYS:HG2	61:T6:801:LYS:HE2	1.89	0.53
40:Mg:46:SER:HB2	40:Mg:49:ALA:HB3	1.89	0.53
9:SF:539:GLY:HA3	9:SF:566:SER:HB3	1.90	0.53
11:BA:818:MET:HA	12:BB:514:LEU:HD21	1.91	0.53
12:BB:309:GLN:O	12:BB:313:MET:HG3	2.08	0.53
13:BC:5:GLY:O	13:BC:7:GLN:NE2	2.41	0.53
24:BN:-43:DA:H2"	24:BN:-42:DT:C7	2.38	0.53
25:BO:107:ARG:NH1	30:BU:286:VAL:OXT	2.42	0.53
28:BS:248:ILE:HG13	28:BS:252:ASN:HD21	1.73	0.53
50:sA:484:ASP:OD1	51:sD:693:LYS:NZ	2.42	0.53
58:sK:196:ARG:HD3	58:sK:197:LEU:HB2	1.91	0.53
61:T6:679:GLN:O	61:T6:682:ASN:ND2	2.42	0.53
30:AU:247:LEU:HB3	31:AV:118:SER:HB3	1.90	0.53
49:Mp:297:PRO:HG2	49:Mp:300:ILE:HD12	1.90	0.53
9:SF:544:ILE:HG22	9:SF:629:MET:HE1	1.91	0.53
14:BD:63:LEU:HB3	14:BD:130:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:sF:544:ILE:HG22	9:sF:629:MET:HE1	1.91	0.53
61:T6:23:SER:O	61:T6:179:ARG:NH2	2.41	0.53
8:A7:122:ARG:NH1	8:A7:123:LEU:O	2.42	0.53
9:SF:505:THR:O	9:SF:509:HIS:ND1	2.41	0.53
58:SK:235:MET:HE1	58:SK:290:PHE:HB2	1.90	0.53
50:sA:303:PRO:HB3	50:sA:450:LEU:HB2	1.91	0.53
51:sB:327:LEU:HD13	51:sB:330:PHE:HD2	1.73	0.53
51:sB:715:LEU:HD13	51:sD:718:GLN:HE21	1.73	0.53
61:E6:146:GLU:OE1	61:E6:146:GLU:N	2.42	0.53
61:E6:173:LYS:HZ2	61:E6:175:MET:HB2	1.74	0.53
61:T6:361:LYS:HB3	61:T6:370:PRO:HA	1.91	0.53
61:t6:618:ILE:O	61:t6:653:LYS:NZ	2.39	0.53
7:A6:322:MET:HE1	7:A6:369:MET:HB3	1.91	0.53
7:A6:325:PRO:HG3	7:A6:359:LEU:HD21	1.90	0.53
11:AA:313:GLN:NE2	11:AA:314:ALA:O	2.37	0.53
14:AD:157:GLN:HA	14:AD:160:VAL:HG22	1.90	0.53
17:AG:100:GLU:OE2	32:AW:144:ARG:CZ	2.52	0.53
23:AM:241:ARG:O	23:AM:245:HIS:ND1	2.39	0.53
51:SD:744:LEU:HD23	51:SD:771:LYS:HD3	1.92	0.53
58:SK:140:ILE:HG22	58:SK:142:PRO:HD2	1.90	0.53
3:B2:22:GLN:HG3	3:B2:26:TYR:CZ	2.44	0.53
50:SA:303:PRO:HB3	50:SA:450:LEU:HB2	1.91	0.52
58:SK:390:THR:O	58:SK:422:THR:OG1	2.26	0.52
2:B1:587:LYS:HA	2:B1:590:ILE:HG22	1.91	0.52
11:BA:1280:GLU:OE1	11:BA:1309:ASP:HB2	2.08	0.52
12:BB:248:SER:H	12:BB:418:LYS:HE3	1.73	0.52
16:BF:112:GLU:N	16:BF:112:GLU:OE1	2.42	0.52
44:mk:60:LEU:HD23	45:ml:104:MET:HE2	1.91	0.52
53:sE:526:GLN:HB3	53:sE:547:ARG:CD	2.39	0.52
59:sL:322:ASP:HB3	59:sL:325:LYS:HG2	1.91	0.52
61:E6:292:ASP:O	61:E6:294:CYS:N	2.41	0.52
61:t6:361:LYS:HB3	61:t6:370:PRO:HA	1.91	0.52
11:AA:28:ARG:NH2	11:AA:238:CYS:SG	2.82	0.52
11:AA:172:PRO:HB3	11:AA:185:TRP:HD1	1.73	0.52
11:AA:818:MET:HA	12:AB:514:LEU:HD21	1.91	0.52
14:AD:158:GLU:HG3	35:Mb:49:ARG:HE	1.74	0.52
19:AI:104:LEU:HD13	19:AI:104:LEU:HD22	1.87	0.52
53:SE:129:LEU:HD23	53:SE:185:TYR:HB3	1.91	0.52
53:SE:504:PRO:HG3	53:SE:518:LYS:HE3	1.91	0.52
12:BB:583:ASN:HD21	12:BB:628:THR:H	1.56	0.52
23:BM:182:ARG:NH1	23:BM:225:ILE:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:22:GLN:HG3	3:A2:26:TYR:CZ	2.44	0.52
8:A7:598:HIS:CD2	8:A7:605:ILE:HD11	2.44	0.52
11:AA:66:LYS:HG2	11:AA:72:GLU:HG3	1.92	0.52
56:SI:712:MET:HA	56:SI:712:MET:HE3	1.91	0.52
7:B6:129:THR:HG22	7:B6:174:MET:HE1	1.90	0.52
9:B8:775:TYR:HA	10:B9:187:THR:HG22	1.91	0.52
37:md:446:LYS:NZ	37:md:462:GLU:O	2.42	0.52
49:mp:261:ASN:ND2	49:mp:325:ILE:O	2.39	0.52
51:sB:557:SER:HB3	51:sB:560:GLN:HG3	1.91	0.52
53:sE:530:THR:HB	53:sE:543:ILE:HB	1.91	0.52
55:sH:587:LYS:O	55:sH:591:LEU:CB	2.57	0.52
11:AA:532:ARG:HE	11:AA:749:ALA:HB2	1.74	0.52
16:AF:112:GLU:OE1	16:AF:112:GLU:N	2.42	0.52
17:AG:100:GLU:CG	32:AW:144:ARG:HH21	2.18	0.52
18:AH:113:ALA:HB2	18:AH:126:GLU:HG3	1.91	0.52
30:AU:25:PHE:O	30:AU:29:GLY:N	2.42	0.52
50:SA:181:PHE:HB3	50:SA:444:VAL:HG21	1.92	0.52
53:SE:527:THR:OG1	53:SE:546:LYS:HA	2.08	0.52
9:SF:506:ARG:HG3	9:SF:510:ILE:HD11	1.90	0.52
9:SF:600:GLN:HA	9:SF:603:MET:SD	2.50	0.52
55:SH:587:LYS:O	55:SH:591:LEU:CB	2.57	0.52
1:B0:625:ILE:HD12	1:B0:627:PHE:CE1	2.45	0.52
2:B1:363:ASP:OD1	2:B1:367:ASN:N	2.40	0.52
11:BA:66:LYS:HG2	11:BA:72:GLU:HG3	1.92	0.52
12:BB:420:LEU:HD13	12:BB:453:ILE:HA	1.90	0.52
20:BJ:65:PRO:HD2	20:BJ:68:LYS:HE2	1.90	0.52
28:BS:188:CYS:HB2	28:BS:195:TYR:HB2	1.91	0.52
45:ml:414:ARG:NH1	45:ml:415:TYR:O	2.42	0.52
59:sL:98:ASN:HB3	59:sL:101:ALA:HB2	1.90	0.52
64:T5:922:THR:OG1	64:T5:923:LYS:N	2.41	0.52
1:A0:625:ILE:HD12	1:A0:627:PHE:CE1	2.44	0.52
3:A2:62:LEU:HA	3:A2:65:TRP:HD1	1.75	0.52
4:A3:49:LEU:CG	17:AG:164:LYS:CD	2.77	0.52
51:SD:420:ARG:NH2	51:SD:425:PHE:O	2.43	0.52
1:B0:132:LYS:O	1:B0:136:MET:HE3	2.09	0.52
7:B6:325:PRO:HG3	7:B6:359:LEU:HD21	1.90	0.52
61:t6:679:GLN:O	61:t6:682:ASN:ND2	2.42	0.52
1:A0:132:LYS:O	1:A0:136:MET:HE3	2.10	0.52
2:A1:363:ASP:OD1	2:A1:367:ASN:N	2.40	0.52
18:AH:10:PHE:HB3	18:AH:28:ALA:HB1	1.90	0.52
26:AQ:386:MET:HE1	27:AR:92:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:MI:414:ARG:NH1	45:MI:415:TYR:O	2.42	0.52
53:SE:532:ASN:HD22	53:SE:543:ILE:HD12	1.74	0.52
54:SG:54:UNK:HA	54:SG:59:UNK:HA	1.91	0.52
11:BA:420:ARG:CG	38:me:60:GLU:CD	2.78	0.52
53:sE:456:GLU:HA	53:sE:459:LYS:HE2	1.92	0.52
57:sJ:59:ARG:HH22	58:sK:134:PRO:HG3	1.74	0.52
60:E3:848:GLU:OE1	60:E3:848:GLU:N	2.42	0.52
2:A1:587:LYS:HA	2:A1:590:ILE:HG22	1.91	0.52
15:AE:116:ILE:HD12	15:AE:121:MET:HB3	1.90	0.52
3:B2:62:LEU:HA	3:B2:65:TRP:HD1	1.75	0.52
51:sD:370:ASN:ND2	9:sF:739:MET:HE2	2.24	0.52
53:sE:504:PRO:HG3	53:sE:518:LYS:HE3	1.92	0.52
45:t4:896:VAL:O	45:t4:908:GLN:NE2	2.38	0.52
61:t6:683:PRO:O	61:t6:687:GLN:NE2	2.43	0.52
11:AA:186:LYS:NZ	11:AA:187:LYS:O	2.43	0.52
11:AA:455:MET:HE1	12:AB:1134:GLU:HA	1.92	0.52
11:AA:503:GLN:OE1	16:AF:90:ARG:NH1	2.41	0.52
12:AB:1174:LYS:HB3	12:AB:1177:HIS:HD2	1.75	0.52
8:B7:400:ALA:HA	8:B7:403:ILE:HG22	1.92	0.52
8:B7:462:ASN:ND2	8:B7:465:ASN:OD1	2.34	0.52
8:B7:598:HIS:CD2	8:B7:605:ILE:HD11	2.44	0.52
11:BA:66:LYS:HB3	23:BM:18:LEU:HD22	1.90	0.52
11:BA:543:LEU:HA	11:BA:546:VAL:HG22	1.91	0.52
50:sA:181:PHE:HB3	50:sA:444:VAL:HG21	1.91	0.52
52:sC:121:LEU:HD21	51:sD:664:LEU:HD11	1.92	0.52
51:sD:420:ARG:NH2	51:sD:425:PHE:O	2.43	0.52
56:sI:1297:ASN:HA	56:sI:1300:GLN:HE21	1.73	0.52
61:T6:445:GLU:OE1	61:T6:448:ASP:HB2	2.10	0.52
61:t6:220:ARG:NH1	61:t6:221:ALA:O	2.43	0.52
7:A6:214:LEU:CD1	7:A6:250:THR:HG21	2.40	0.52
8:A7:400:ALA:HA	8:A7:403:ILE:HG22	1.92	0.52
37:Md:614:ARG:NH1	37:Md:636:GLU:OE2	2.43	0.52
41:Mh:57:VAL:HG23	43:Mj:87:LEU:HD23	1.92	0.52
45:MI:267:ASN:HD21	47:Mn:139:SER:HA	1.75	0.52
55:SH:443:ILE:HD11	56:SI:662:ARG:HD2	1.91	0.52
2:B1:357:THR:O	2:B1:358:MET:HE2	2.10	0.52
3:B2:488:LYS:HD2	3:B2:490:LYS:HE3	1.91	0.52
4:B3:100:ASN:CA	34:ma:140:GLY:CA	2.56	0.52
7:B6:322:MET:HE1	7:B6:369:MET:HB3	1.91	0.52
11:BA:806:ARG:NH2	12:BB:727:LYS:O	2.43	0.52
12:BB:777:ALA:O	12:BB:1096:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:T3:360:HIS:CD2	60:T3:919:TYR:CE2	2.95	0.52
61:T6:696:ILE:HG13	61:T6:773:SER:HB3	1.92	0.52
11:AA:1300:LYS:HE2	28:AS:302:CYS:HA	1.91	0.52
28:AS:184:LYS:HD2	28:AS:228:LEU:CD1	2.37	0.52
51:SB:557:SER:HB3	51:SB:560:GLN:HG3	1.91	0.52
58:SK:196:ARG:HD3	58:SK:197:LEU:HB2	1.91	0.52
59:SL:322:ASP:HB3	59:SL:325:LYS:HG2	1.92	0.52
11:BA:28:ARG:NH2	11:BA:238:CYS:SG	2.82	0.52
13:BC:6:PRO:O	21:BK:104:ASN:ND2	2.38	0.52
28:BS:170:SER:HA	28:BS:173:HIS:CE1	2.45	0.52
45:T4:1021:GLN:OE1	45:T4:1025:GLN:NE2	2.43	0.52
45:t4:881:THR:HB	45:t4:897:GLN:HB2	1.92	0.52
11:AA:881:GLN:NE2	11:AA:957:PRO:O	2.43	0.51
23:AM:218:SER:OG	23:AM:226:ASP:OD1	2.27	0.51
28:AS:251:GLN:O	28:AS:255:ASN:ND2	2.43	0.51
38:Me:178:ARG:HE	38:Me:179:SER:H	1.57	0.51
50:SA:61:ILE:HG13	50:SA:72:LEU:HD12	1.92	0.51
55:SH:586:TYR:CD1	55:SH:589:HIS:NE2	2.58	0.51
11:BA:261:ASP:OD2	11:BA:320:ARG:NH1	2.33	0.51
11:BA:455:MET:HE1	12:BB:1134:GLU:HA	1.92	0.51
11:BA:503:GLN:OE1	16:BF:90:ARG:NH1	2.41	0.51
23:BM:16:PRO:HG3	32:BW:151:LEU:HD23	1.72	0.51
24:BN:-66:DA:H2'	24:BN:-65:DT:H71	1.92	0.51
29:BT:62:DC:H2''	29:BT:63:DT:C6	2.45	0.51
9:sF:600:GLN:HA	9:sF:603:MET:SD	2.50	0.51
56:sI:712:MET:HA	56:sI:712:MET:HE3	1.91	0.51
61:E6:923:LEU:HA	61:E6:934:ARG:HE	1.74	0.51
45:T4:881:THR:HB	45:T4:897:GLN:HB2	1.92	0.51
11:AA:543:LEU:HA	11:AA:546:VAL:HG22	1.91	0.51
12:AB:230:ALA:O	12:AB:261:ARG:NH1	2.44	0.51
5:B4:176:LEU:HB2	5:B4:210:ILE:HG22	1.92	0.51
11:BA:5:GLN:O	12:BB:1159:ARG:NH1	2.43	0.51
11:BA:420:ARG:NH2	38:me:58:LEU:HD23	2.16	0.51
11:BA:956:LEU:HD13	11:BA:1021:LEU:HD22	1.92	0.51
51:sB:453:LEU:HD11	51:sD:441:LYS:NZ	2.25	0.51
51:sD:624:GLN:O	51:sD:632:GLN:NE2	2.44	0.51
55:sH:594:LEU:CB	55:sH:594:LEU:HD22	2.23	0.51
58:sK:390:THR:O	58:sK:422:THR:OG1	2.26	0.51
61:E6:380:ASP:O	60:t3:428:LEU:O	2.29	0.51
61:T6:220:ARG:NH1	61:T6:221:ALA:O	2.43	0.51
45:t4:1021:GLN:OE1	45:t4:1025:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:t6:445:GLU:OE1	61:t6:448:ASP:HB2	2.10	0.51
61:t6:696:ILE:HG13	61:t6:773:SER:HB3	1.92	0.51
10:A9:209:MET:HE3	10:A9:227:LEU:CD2	2.40	0.51
14:AD:160:VAL:HA	14:AD:163:VAL:HG12	1.93	0.51
23:AM:182:ARG:NH1	23:AM:225:ILE:O	2.42	0.51
23:AM:302:LEU:O	27:AR:270:MET:CE	2.26	0.51
50:SA:127:ILE:HD12	50:SA:442:ILE:HD12	1.91	0.51
51:SB:453:LEU:HD11	51:SD:441:LYS:NZ	2.25	0.51
53:SE:456:GLU:HA	53:SE:459:LYS:HE2	1.92	0.51
53:SE:530:THR:HB	53:SE:543:ILE:HB	1.91	0.51
56:SI:1255:PHE:O	56:SI:1259:LEU:HB2	2.11	0.51
1:B0:141:ALA:HB1	1:B0:153:VAL:HG21	1.92	0.51
11:BA:186:LYS:NZ	11:BA:187:LYS:O	2.43	0.51
11:BA:760:GLN:HE22	11:BA:765:VAL:HA	1.75	0.51
28:BS:251:GLN:O	28:BS:255:ASN:ND2	2.43	0.51
37:md:397:ILE:HD11	37:md:404:ILE:HG23	1.93	0.51
50:sA:61:ILE:HG13	50:sA:72:LEU:HD12	1.92	0.51
60:E3:956:ARG:NH2	60:E3:959:LEU:HD13	2.24	0.51
61:T6:557:VAL:HG22	61:T6:603:PHE:CE1	2.46	0.51
60:t3:981:GLU:OE1	60:t3:985:GLN:NE2	2.43	0.51
45:t4:918:TYR:HA	45:t4:921:ILE:HD12	1.93	0.51
61:t6:557:VAL:HG22	61:t6:603:PHE:CE1	2.46	0.51
3:A2:488:LYS:HD2	3:A2:490:LYS:HE3	1.91	0.51
11:AA:956:LEU:HD13	11:AA:1021:LEU:HD22	1.92	0.51
12:AB:559:SER:HA	12:AB:563:MET:HE3	1.93	0.51
24:AN:-66:DA:H2'	24:AN:-65:DT:H71	1.92	0.51
30:AU:32:GLU:HA	30:AU:35:LEU:HD12	1.93	0.51
37:Md:355:ALA:HA	37:Md:370:PRO:HA	1.93	0.51
49:Mp:157:ASN:HD21	61:E6:323:PRO:CD	2.13	0.51
51:SB:770:PHE:CZ	51:SD:743:CYS:HB2	2.45	0.51
1:B0:210:TYR:OH	1:B0:235:ASP:O	2.27	0.51
10:B9:209:MET:HE3	10:B9:227:LEU:CD2	2.40	0.51
12:BB:1174:LYS:HB3	12:BB:1177:HIS:HD2	1.75	0.51
19:BI:57:GLY:C	19:BI:59:VAL:N	2.68	0.51
23:BM:303:GLN:HB2	27:BR:270:MET:SD	2.51	0.51
41:mh:57:VAL:HG23	43:mj:87:LEU:HD23	1.92	0.51
61:E6:159:ILE:HD11	60:T3:837:TYR:HA	1.92	0.51
61:T6:369:SER:O	61:T6:390:ARG:NH1	2.44	0.51
12:AB:199:MET:SD	12:AB:199:MET:N	2.83	0.51
17:AG:95:SER:HB2	32:AW:144:ARG:CG	2.40	0.51
34:Ma:168:LYS:HA	34:Ma:171:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:384:GLN:HE22	51:SB:731:GLN:HA	1.75	0.51
45:ml:252:THR:HG21	45:ml:290:THR:HG21	1.93	0.51
49:mp:298:PRO:HA	49:mp:301:ASP:HB2	1.92	0.51
50:sA:127:ILE:HD12	50:sA:442:ILE:HD12	1.91	0.51
51:sB:770:PHE:CZ	51:sD:743:CYS:HB2	2.45	0.51
60:E3:436:SER:HB3	60:E3:463:ARG:HE	1.75	0.51
61:T6:683:PRO:O	61:T6:687:GLN:NE2	2.43	0.51
60:t3:782:ASP:OD1	60:t3:783:ILE:N	2.44	0.51
64:t5:857:ASP:OD2	64:t5:954:ARG:NH2	2.43	0.51
64:t5:871:HIS:HA	64:t5:874:GLU:OE2	2.11	0.51
61:t6:328:ASP:N	61:t6:328:ASP:OD1	2.44	0.51
7:A6:129:THR:HG23	7:A6:172:ILE:HG23	1.93	0.51
14:AD:63:LEU:HB3	14:AD:130:LEU:HD22	1.91	0.51
19:AI:57:GLY:C	19:AI:59:VAL:N	2.68	0.51
28:AS:188:CYS:HB2	28:AS:195:TYR:HB2	1.91	0.51
12:BB:21:GLU:CD	12:BB:22:SER:H	2.19	0.51
12:BB:763:GLN:HG2	12:BB:765:PRO:HD2	1.93	0.51
60:t3:438:ASP:OD1	60:t3:441:HIS:ND1	2.44	0.51
11:AA:5:GLN:O	12:AB:1159:ARG:NH1	2.43	0.51
12:AB:709:ASP:HB3	12:AB:710:LEU:HD12	1.93	0.51
14:AD:202:ILE:HG23	14:AD:207:LEU:HD21	1.93	0.51
28:AS:170:SER:HA	28:AS:173:HIS:CE1	2.45	0.51
35:Mb:145:ILE:HB	37:Md:270:ILE:HD11	1.93	0.51
37:Md:446:LYS:NZ	37:Md:462:GLU:O	2.42	0.51
45:Ml:505:THR:HA	45:Ml:560:LYS:HE2	1.93	0.51
49:Mp:298:PRO:HA	49:Mp:301:ASP:HB2	1.92	0.51
51:SD:624:GLN:O	51:SD:632:GLN:NE2	2.44	0.51
1:B0:102:ASP:OD1	1:B0:173:LYS:HE2	2.10	0.51
3:B2:138:TYR:CE2	3:B2:260:PHE:CD1	2.99	0.51
8:B7:519:ARG:HG2	8:B7:520:GLU:H	1.76	0.51
14:BD:158:GLU:HG3	35:mb:49:ARG:HE	1.74	0.51
14:BD:160:VAL:HA	14:BD:163:VAL:HG12	1.93	0.51
21:BK:7:PHE:HB2	21:BK:11:LEU:HD12	1.93	0.51
37:md:355:ALA:HA	37:md:370:PRO:HA	1.92	0.51
37:md:614:ARG:NH1	37:md:636:GLU:OE2	2.43	0.51
54:sG:118:ARG:NH1	54:sG:118:ARG:O	2.43	0.51
55:sH:475:ALA:O	56:sI:670:ARG:NH1	2.44	0.51
59:sL:189:MET:HE3	59:sL:305:LEU:HD12	1.93	0.51
61:T6:218:ARG:HH12	61:T6:220:ARG:HB2	1.76	0.51
61:t6:369:SER:O	61:t6:390:ARG:NH1	2.43	0.51
2:A1:336:ILE:HG23	2:A1:337:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A4:289:CYS:HB3	5:A4:292:CYS:SG	2.51	0.51
17:AG:95:SER:OG	17:AG:96:GLN:N	2.43	0.51
52:SC:121:LEU:HD21	51:SD:664:LEU:HD11	1.92	0.51
56:SI:1099:ASN:HB3	56:SI:1100:ASN:HD21	1.76	0.51
58:SK:224:ALA:HA	58:SK:228:ILE:HD13	1.92	0.51
1:B0:399:LEU:HD13	1:B0:402:ILE:HD11	1.92	0.51
8:B7:553:GLN:NE2	8:B7:554:CYS:O	2.43	0.51
11:BA:532:ARG:HE	11:BA:749:ALA:HB2	1.74	0.51
11:BA:635:ARG:NH2	11:BA:876:ALA:O	2.38	0.51
11:BA:1300:LYS:HE2	28:BS:302:CYS:HA	1.91	0.51
14:BD:217:LEU:HD23	35:mb:42:GLN:HE22	1.71	0.51
17:BG:95:SER:OG	17:BG:96:GLN:N	2.43	0.51
18:BH:83:GLN:HA	21:BK:54:ARG:HH21	1.76	0.51
23:BM:218:SER:OG	23:BM:226:ASP:OD1	2.27	0.51
35:mb:145:ILE:HB	37:md:270:ILE:HD11	1.93	0.51
51:sD:744:LEU:HD23	51:sD:771:LYS:HD3	1.92	0.51
60:E3:880:LYS:NZ	60:T3:879:ARG:HE	2.09	0.51
45:T4:879:ASP:O	45:T4:902:ASN:ND2	2.39	0.51
61:t6:218:ARG:HH12	61:t6:220:ARG:HB2	1.76	0.51
8:A7:553:GLN:NE2	8:A7:554:CYS:O	2.43	0.51
11:AA:261:ASP:OD2	11:AA:320:ARG:NH1	2.33	0.51
29:AT:62:DC:H2''	29:AT:63:DT:C6	2.45	0.51
45:MI:115:VAL:HA	46:Mm:141:VAL:HG11	1.93	0.51
53:SE:449:TYR:O	53:SE:450:GLU:N	2.44	0.51
53:SE:539:THR:HB	9:SF:760:TYR:HD1	1.76	0.51
7:B6:214:LEU:CD1	7:B6:250:THR:HG21	2.40	0.51
12:BB:230:ALA:O	12:BB:261:ARG:NH1	2.44	0.51
17:BG:95:SER:HB2	32:BW:144:ARG:CG	2.40	0.51
24:BN:-57:DT:H2''	24:BN:-56:DT:H5''	1.92	0.51
51:sD:566:LEU:HD11	51:sD:615:VAL:HG11	1.93	0.51
53:sE:532:ASN:HD22	53:sE:543:ILE:HD12	1.74	0.51
64:T5:857:ASP:OD2	64:T5:954:ARG:NH2	2.43	0.51
11:AA:1221:LYS:HD2	11:AA:1222:ASN:HB2	1.93	0.51
53:SE:527:THR:OG1	53:SE:545:THR:O	2.22	0.51
1:B0:198:ARG:C	1:B0:199:MET:HE2	2.36	0.51
11:BA:881:GLN:NE2	11:BA:957:PRO:O	2.43	0.51
14:BD:202:ILE:HG23	14:BD:207:LEU:HD21	1.93	0.51
45:ml:428:THR:OG1	45:ml:443:ASP:OD2	2.27	0.51
58:sK:224:ALA:HA	58:sK:228:ILE:HD13	1.92	0.51
60:t3:289:LYS:CB	60:t3:289:LYS:CD	2.67	0.51
61:t6:877:GLN:NE2	61:t6:882:GLY:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:t6:914:SER:OG	61:t6:917:GLU:OE1	2.29	0.51
1:A0:141:ALA:HB1	1:A0:153:VAL:HG21	1.92	0.50
1:A0:198:ARG:C	1:A0:199:MET:HE2	2.36	0.50
8:A7:224:LYS:HG2	8:A7:337:VAL:HG23	1.92	0.50
8:A7:519:ARG:HG2	8:A7:520:GLU:H	1.76	0.50
11:AA:635:ARG:NH2	11:AA:876:ALA:O	2.38	0.50
11:AA:806:ARG:NH2	12:AB:727:LYS:O	2.43	0.50
15:AE:116:ILE:HG13	15:AE:121:MET:HE3	1.93	0.50
19:AI:71:SER:HB3	19:AI:85:PHE:CE1	2.47	0.50
19:AI:117:LYS:HG3	61:T6:834:PHE:CE1	2.46	0.50
21:AK:7:PHE:HB2	21:AK:11:LEU:HD12	1.93	0.50
45:MI:252:THR:HG21	45:MI:290:THR:HG21	1.93	0.50
50:SA:556:ASN:ND2	55:SH:553:GLU:OE1	2.41	0.50
3:B2:124:VAL:HG22	3:B2:126:GLU:H	1.77	0.50
11:BA:681:GLU:OE2	61:t6:762:PHE:CZ	2.62	0.50
33:BX:234:ARG:NH1	33:BX:239:LYS:O	2.35	0.50
42:mi:11:SER:OG	42:mi:12:LEU:N	2.41	0.50
45:ml:115:VAL:HA	46:mm:141:VAL:HG11	1.93	0.50
64:T5:871:HIS:HA	64:T5:874:GLU:OE2	2.11	0.50
61:T6:914:SER:OG	61:T6:917:GLU:OE1	2.29	0.50
2:A1:357:THR:O	2:A1:358:MET:HE2	2.10	0.50
4:A3:49:LEU:CG	17:AG:164:LYS:CG	2.89	0.50
9:A8:775:TYR:HA	10:A9:187:THR:HG22	1.91	0.50
11:AA:760:GLN:HE22	11:AA:765:VAL:HA	1.75	0.50
12:AB:777:ALA:O	12:AB:1096:ARG:NH2	2.43	0.50
15:AE:119:SER:HA	15:AE:122:LYS:HE3	1.94	0.50
18:AH:82:PRO:O	21:AK:54:ARG:NH2	2.45	0.50
18:AH:83:GLN:HA	21:AK:54:ARG:HH21	1.76	0.50
26:AQ:377:SER:HA	27:AR:68:VAL:HG22	1.93	0.50
50:SA:310:TYR:OH	50:SA:324:THR:O	2.30	0.50
3:B2:368:ALA:HA	8:B7:113:PHE:CE1	2.46	0.50
4:B3:49:LEU:CG	17:BG:164:LYS:CG	2.89	0.50
5:B4:289:CYS:HB3	5:B4:292:CYS:SG	2.51	0.50
8:B7:224:LYS:HG2	8:B7:337:VAL:HG23	1.92	0.50
12:BB:882:THR:OG1	12:BB:885:MET:SD	2.66	0.50
15:BE:4:GLU:OE1	15:BE:7:ARG:NH1	2.45	0.50
18:BH:82:PRO:O	21:BK:54:ARG:NH2	2.45	0.50
19:BI:4:PHE:CD2	19:BI:13:MET:HE1	2.46	0.50
50:sA:310:TYR:OH	50:sA:324:THR:O	2.30	0.50
50:sA:384:GLN:HE22	51:sB:731:GLN:HA	1.75	0.50
3:A2:138:TYR:CE2	3:A2:260:PHE:CD1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:354:PRO:HA	3:A2:357:ILE:HB	1.94	0.50
13:AC:6:PRO:HA	13:AC:24:ASN:HB3	1.93	0.50
13:AC:211:ASP:N	13:AC:211:ASP:OD1	2.44	0.50
23:AM:154:TYR:CD1	23:AM:172:MET:HE1	2.46	0.50
53:SE:538:ASN:HB3	9:SF:762:SER:HA	1.93	0.50
8:B7:224:LYS:HE3	8:B7:340:GLU:O	2.11	0.50
13:BC:211:ASP:OD1	13:BC:211:ASP:N	2.44	0.50
19:BI:71:SER:HB3	19:BI:85:PHE:CE1	2.46	0.50
19:BI:108:HIS:HE1	19:BI:110:PHE:HB3	1.76	0.50
26:BQ:377:SER:HA	27:BR:68:VAL:HG22	1.93	0.50
28:BS:271:CYS:CB	28:BS:274:CYS:SG	2.90	0.50
45:ml:480:ARG:NH1	45:ml:496:SER:O	2.45	0.50
9:sF:312:ILE:H	56:sI:657:LYS:H	1.60	0.50
56:sI:1255:PHE:O	56:sI:1259:LEU:HB2	2.11	0.50
60:T3:405:GLU:O	60:T3:406:LYS:C	2.53	0.50
60:T3:981:GLU:OE1	60:T3:985:GLN:NE2	2.43	0.50
5:A4:176:LEU:HB2	5:A4:210:ILE:HG22	1.92	0.50
6:A5:17:LYS:HG3	6:A5:40:LEU:HD21	1.94	0.50
19:AI:4:PHE:CD2	19:AI:13:MET:HE1	2.46	0.50
19:AI:108:HIS:HE1	19:AI:110:PHE:HB3	1.76	0.50
38:Me:237:GLN:NE2	38:Me:239:GLU:OE2	2.45	0.50
51:SB:767:ILE:HA	51:SB:770:PHE:HD2	1.76	0.50
11:BA:1195:LEU:HB2	11:BA:1238:ILE:HB	1.94	0.50
12:BB:322:PHE:HB2	26:BQ:420:VAL:HG11	1.94	0.50
12:BB:559:SER:HA	12:BB:563:MET:HE3	1.93	0.50
26:BQ:386:MET:O	26:BQ:387:ILE:HD13	2.11	0.50
38:me:178:ARG:HE	38:me:179:SER:H	1.57	0.50
45:ml:508:VAL:HG22	45:ml:681:GLU:HB2	1.93	0.50
60:T3:782:ASP:OD1	60:T3:783:ILE:N	2.44	0.50
12:AB:763:GLN:HG2	12:AB:765:PRO:HD2	1.93	0.50
2:B1:336:ILE:HG23	2:B1:337:ILE:HG23	1.93	0.50
3:B2:22:GLN:HE21	3:B2:26:TYR:HE1	1.54	0.50
12:BB:15:PRO:HD2	64:t5:922:THR:HB	1.94	0.50
15:BE:116:ILE:HG13	15:BE:121:MET:HE3	1.93	0.50
45:ml:263:PRO:HD2	45:ml:266:LEU:HD12	1.93	0.50
45:ml:267:ASN:HD21	47:mn:139:SER:HA	1.75	0.50
53:sE:40:ARG:HH21	55:sH:517:LEU:HD13	1.76	0.50
60:E3:907:TRP:CH2	60:E3:950:PRO:HD2	2.47	0.50
60:E3:982:GLU:OE2	60:E3:1084:LYS:NZ	2.44	0.50
61:E6:890:LEU:HD12	61:E6:891:PRO:HD2	1.92	0.50
60:t3:360:HIS:HD2	60:t3:919:TYR:CE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A7:224:LYS:HE3	8:A7:340:GLU:O	2.11	0.50
8:A7:331:GLN:HG3	8:A7:529:PHE:HA	1.94	0.50
11:AA:1195:LEU:HB2	11:AA:1238:ILE:HB	1.94	0.50
14:AD:216:ASN:OD1	35:Mb:39:ARG:NH1	2.44	0.50
51:SD:705:GLU:HA	51:SD:708:MET:HE1	1.94	0.50
54:SG:118:ARG:NH1	54:SG:118:ARG:O	2.43	0.50
3:B2:354:PRO:HA	3:B2:357:ILE:HB	1.94	0.50
6:B5:17:LYS:HG3	6:B5:40:LEU:HD21	1.94	0.50
34:ma:168:LYS:HA	34:ma:171:GLN:HG2	1.93	0.50
42:mi:207:GLN:HG3	43:mj:148:GLN:HG3	1.94	0.50
45:ml:505:THR:HA	45:ml:560:LYS:HE2	1.93	0.50
47:mn:84:ASP:N	47:mn:84:ASP:OD1	2.44	0.50
53:sE:150:ILE:HG12	53:sE:158:VAL:HG21	1.93	0.50
59:sL:54:HIS:CD2	59:sL:56:THR:O	2.65	0.50
61:E6:423:ARG:C	61:E6:424:ARG:HD2	2.37	0.50
45:T4:918:TYR:HA	45:T4:921:ILE:HD12	1.93	0.50
61:T6:888:ASP:O	61:T6:895:ARG:NH2	2.45	0.50
1:A0:399:LEU:HD13	1:A0:402:ILE:HD11	1.92	0.50
7:A6:147:ALA:HA	7:A6:200:ARG:HH12	1.77	0.50
23:AM:303:GLN:HB2	27:AR:270:MET:SD	2.51	0.50
28:AS:175:ALA:HA	28:AS:178:ILE:HG12	1.94	0.50
9:SF:312:ILE:H	56:SI:657:LYS:H	1.60	0.50
59:SL:189:MET:HE3	59:SL:305:LEU:HD12	1.93	0.50
12:BB:709:ASP:HB3	12:BB:710:LEU:HD12	1.93	0.50
23:BM:241:ARG:O	23:BM:245:HIS:ND1	2.39	0.50
37:md:424:ASP:O	37:md:428:GLN:NE2	2.42	0.50
50:sA:335:TYR:HA	51:sB:727:LEU:HD21	1.92	0.50
60:t3:869:ARG:HH21	60:t3:882:LEU:HD23	1.76	0.50
1:A0:102:ASP:OD1	1:A0:173:LYS:HE2	2.11	0.50
1:A0:220:GLU:O	1:A0:224:ASN:ND2	2.45	0.50
7:A6:322:MET:HE2	7:A6:322:MET:HA	1.93	0.50
24:AN:-57:DT:H2"	24:AN:-56:DT:H5"	1.92	0.50
28:AS:181:GLU:HG3	28:AS:182:MET:HE2	1.94	0.50
37:Md:539:ILE:O	37:Md:543:ARG:NH2	2.44	0.50
44:Mk:64:ASN:OD1	44:Mk:68:ASN:ND2	2.45	0.50
53:SE:150:ILE:HG12	53:SE:158:VAL:HG21	1.93	0.50
53:SE:529:VAL:O	53:SE:531:THR:N	2.45	0.50
15:BE:118:PRO:HA	15:BE:121:MET:SD	2.52	0.50
26:BQ:386:MET:HE1	27:BR:92:LEU:HD23	1.91	0.50
52:sC:200:GLN:NE2	52:sC:203:GLY:O	2.45	0.50
51:sD:705:GLU:HA	51:sD:708:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:E6:161:ASN:OD1	61:E6:161:ASN:N	2.44	0.50
45:T4:994:ARG:HH12	45:T4:996:LYS:HG2	1.77	0.50
61:T6:328:ASP:N	61:T6:328:ASP:OD1	2.44	0.50
52:SC:90:LEU:HD13	52:SC:93:ILE:HG21	1.94	0.50
52:SC:106:ASN:O	52:SC:110:ASN:ND2	2.45	0.50
57:SJ:89:ARG:NH2	57:SJ:93:LYS:HD2	2.27	0.50
11:BA:110:CYS:CB	11:BA:167:CYS:SG	2.88	0.50
12:BB:771:SER:O	12:BB:775:LYS:NZ	2.44	0.50
28:BS:175:ALA:HA	28:BS:178:ILE:HG12	1.94	0.50
28:BS:181:GLU:HG3	28:BS:182:MET:HE2	1.94	0.50
37:md:86:LEU:HD13	45:ml:209:LEU:HD21	1.94	0.50
50:sA:68:LEU:HD23	50:sA:69:ILE:HG13	1.94	0.50
53:sE:449:TYR:O	53:sE:450:GLU:N	2.44	0.50
61:E6:578:LEU:HD23	61:E6:879:LEU:HD13	1.93	0.50
61:T6:218:ARG:NH2	61:T6:220:ARG:HB2	2.26	0.50
61:T6:877:GLN:NE2	61:T6:882:GLY:O	2.44	0.50
60:t3:289:LYS:CG	60:t3:289:LYS:CA	2.88	0.50
3:A2:204:LEU:O	3:A2:208:LEU:HD23	2.12	0.49
15:AE:4:GLU:OE1	15:AE:7:ARG:NH1	2.45	0.49
15:AE:118:PRO:HA	15:AE:121:MET:SD	2.52	0.49
19:AI:45:ARG:NH2	19:AI:47:GLU:OE1	2.41	0.49
19:AI:108:HIS:CE1	19:AI:110:PHE:HB3	2.47	0.49
56:SI:1107:ASN:OD1	56:SI:1193:TRP:NE1	2.37	0.49
59:SL:54:HIS:CD2	59:SL:56:THR:O	2.65	0.49
1:B0:220:GLU:O	1:B0:224:ASN:ND2	2.45	0.49
30:BU:32:GLU:HA	30:BU:35:LEU:HD12	1.93	0.49
44:mk:64:ASN:OD1	44:mk:68:ASN:ND2	2.45	0.49
45:ml:158:ASN:ND2	46:mm:38:TYR:O	2.45	0.49
51:sB:767:ILE:HA	51:sB:770:PHE:HD2	1.76	0.49
52:sC:106:ASN:O	52:sC:110:ASN:ND2	2.45	0.49
56:sI:1107:ASN:OD1	56:sI:1193:TRP:NE1	2.37	0.49
3:A2:506:LYS:HZ2	3:A2:506:LYS:HD2	1.72	0.49
12:AB:451:LYS:HZ2	23:AM:139:ALA:HA	1.77	0.49
17:AG:119:LEU:HD21	17:AG:130:TYR:HB3	1.93	0.49
35:Mb:33:LEU:HD13	37:Md:228:LEU:HD22	1.94	0.49
45:ML:158:ASN:ND2	46:Mm:38:TYR:O	2.45	0.49
45:ML:831:GLN:NE2	45:t4:837:VAL:HB	2.27	0.49
49:Mp:62:VAL:HB	49:Mp:80:VAL:HB	1.94	0.49
9:SF:473:LEU:HD21	9:SF:499:TYR:HE2	1.77	0.49
7:B6:322:MET:HA	7:B6:322:MET:HE2	1.93	0.49
17:BG:119:LEU:HD21	17:BG:130:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:sI:1099:ASN:HB3	56:sI:1100:ASN:HD21	1.75	0.49
61:E6:186:TYR:OH	60:T3:428:LEU:HD13	2.11	0.49
4:A3:85:ARG:HE	4:A3:117:ILE:HD13	1.77	0.49
10:A9:236:TRP:CZ2	10:A9:240:LYS:HE3	2.47	0.49
11:AA:551:TYR:OH	21:AK:72:LYS:NZ	2.37	0.49
12:AB:21:GLU:CD	12:AB:22:SER:H	2.19	0.49
12:AB:771:SER:O	12:AB:775:LYS:NZ	2.44	0.49
37:Md:397:ILE:HD11	37:Md:404:ILE:HG23	1.93	0.49
50:SA:335:TYR:HA	51:SB:727:LEU:HD21	1.92	0.49
56:SI:707:LEU:HA	56:SI:710:LEU:HD12	1.94	0.49
3:B2:204:LEU:O	3:B2:208:LEU:HD23	2.12	0.49
7:B6:147:ALA:HA	7:B6:200:ARG:HH12	1.77	0.49
12:BB:199:MET:N	12:BB:199:MET:SD	2.83	0.49
12:BB:797:TYR:HE1	12:BB:854:LEU:HG	1.77	0.49
49:mp:62:VAL:HB	49:mp:80:VAL:HB	1.94	0.49
50:sA:556:ASN:ND2	55:sH:553:GLU:OE1	2.41	0.49
60:E3:415:PHE:CZ	60:E3:439:ILE:HG12	2.47	0.49
63:T2:28:LYS:HA	63:T2:31:LYS:HE2	1.94	0.49
60:T3:289:LYS:CG	60:T3:289:LYS:CA	2.88	0.49
63:t2:28:LYS:HA	63:t2:31:LYS:HE2	1.94	0.49
60:t3:405:GLU:O	60:t3:406:LYS:C	2.53	0.49
45:t4:909:PRO:O	45:t4:913:ASN:ND2	2.45	0.49
3:A2:368:ALA:HA	8:A7:113:PHE:CE1	2.46	0.49
11:AA:451:HIS:HD2	11:AA:453:MET:HE2	1.78	0.49
11:AA:506:ALA:O	11:AA:510:GLN:NE2	2.46	0.49
20:AJ:48:ARG:NH1	20:AJ:49:MET:SD	2.85	0.49
51:SD:320:HIS:HD2	51:SD:322:ILE:HG12	1.76	0.49
51:SD:566:LEU:HD11	51:SD:615:VAL:HG11	1.93	0.49
55:SH:475:ALA:O	56:SI:670:ARG:NH1	2.44	0.49
7:B6:129:THR:HG23	7:B6:172:ILE:HG23	1.93	0.49
8:B7:349:ASN:O	8:B7:405:LYS:NZ	2.40	0.49
11:BA:506:ALA:O	11:BA:510:GLN:NE2	2.46	0.49
30:BU:270:ASN:O	30:BU:272:ASN:ND2	2.46	0.49
51:sB:440:LEU:HA	51:sB:443:MET:HE2	1.94	0.49
53:sE:529:VAL:O	53:sE:531:THR:N	2.45	0.49
57:sJ:89:ARG:NH2	57:sJ:93:LYS:HD2	2.27	0.49
61:t6:266:GLN:NE2	61:t6:276:LYS:O	2.46	0.49
61:t6:888:ASP:O	61:t6:895:ARG:NH2	2.45	0.49
3:A2:124:VAL:HG22	3:A2:126:GLU:H	1.77	0.49
32:AW:60:ARG:NH2	33:AX:264:GLU:OE2	2.44	0.49
4:B3:85:ARG:HE	4:B3:117:ILE:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B9:236:TRP:CZ2	10:B9:240:LYS:HE3	2.47	0.49
12:BB:467:GLY:HA2	12:BB:473:MET:SD	2.52	0.49
53:sE:538:ASN:HB3	9:sF:762:SER:HA	1.93	0.49
60:t3:360:HIS:CD2	60:t3:919:TYR:CE2	2.95	0.49
45:t4:994:ARG:HH12	45:t4:996:LYS:HG2	1.77	0.49
12:AB:797:TYR:HE1	12:AB:854:LEU:HG	1.77	0.49
18:AH:146:ARG:HG2	18:AH:146:ARG:NH1	2.28	0.49
42:Mi:207:GLN:HG3	43:Mj:148:GLN:HG3	1.94	0.49
45:Ml:263:PRO:HD2	45:Ml:266:LEU:HD12	1.93	0.49
45:Ml:480:ARG:NH1	45:Ml:496:SER:O	2.45	0.49
45:Ml:508:VAL:HG22	45:Ml:681:GLU:HB2	1.93	0.49
50:SA:268:TRP:HD1	50:SA:271:ASP:CG	2.20	0.49
56:SI:758:ASN:O	56:SI:762:ASN:ND2	2.43	0.49
20:BJ:48:ARG:NH1	20:BJ:49:MET:SD	2.86	0.49
51:sD:320:HIS:HD2	51:sD:322:ILE:HG12	1.76	0.49
53:sE:539:THR:HB	9:sF:760:TYR:HD1	1.76	0.49
63:T2:60:GLU:O	63:T2:67:ARG:NH2	2.46	0.49
6:A5:7:GLY:HA3	6:A5:41:LEU:CD1	2.30	0.49
35:Mb:98:LEU:HD12	37:Md:253:SER:HA	1.95	0.49
37:Md:424:ASP:O	37:Md:428:GLN:NE2	2.42	0.49
53:SE:40:ARG:HH21	55:SH:517:LEU:HD13	1.76	0.49
7:B6:352:CYS:CB	7:B6:366:CYS:SG	2.84	0.49
12:BB:954:VAL:HG12	12:BB:964:VAL:HG12	1.95	0.49
26:BQ:110:ASP:O	26:BQ:114:MET:HG2	2.13	0.49
32:BW:60:ARG:NH2	33:BX:264:GLU:OE2	2.44	0.49
36:mc:92:GLY:O	36:mc:95:THR:OG1	2.30	0.49
52:sC:90:LEU:HD13	52:sC:93:ILE:HG21	1.94	0.49
56:sI:1149:VAL:O	56:sI:1153:LYS:HB2	2.13	0.49
8:A7:341:TYR:CZ	8:A7:343:PHE:HB2	2.47	0.49
11:AA:1280:GLU:OE1	11:AA:1281:ARG:HB2	2.12	0.49
11:BA:1221:LYS:HD2	11:BA:1222:ASN:HB2	1.94	0.49
15:BE:119:SER:HA	15:BE:122:LYS:HE3	1.94	0.49
38:me:237:GLN:NE2	38:me:239:GLU:OE2	2.45	0.49
9:sF:400:GLN:HB2	9:sF:402:ILE:CD1	2.43	0.49
57:sJ:89:ARG:CZ	57:sJ:93:LYS:HB3	2.43	0.49
60:E3:879:ARG:NH2	60:T3:880:LYS:HZ3	2.11	0.49
61:t6:934:ARG:HG2	61:t6:937:ASN:HD21	1.78	0.49
1:A0:570:LEU:HB2	1:A0:598:LEU:HD23	1.95	0.49
1:A0:711:ASP:OD1	1:A0:711:ASP:N	2.45	0.49
12:AB:467:GLY:HA2	12:AB:473:MET:SD	2.52	0.49
26:AQ:110:ASP:O	26:AQ:114:MET:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Mb:97:PRO:HA	37:Md:254:LEU:HD23	1.95	0.49
50:SA:68:LEU:HD23	50:SA:69:ILE:HG13	1.94	0.49
8:B7:349:ASN:HD22	8:B7:481:GLU:CG	2.22	0.49
11:BA:11:LEU:C	11:BA:12:ARG:HD3	2.38	0.49
19:BI:108:HIS:CE1	19:BI:110:PHE:HB3	2.47	0.49
23:BM:154:TYR:CD1	23:BM:172:MET:HE1	2.46	0.49
31:BV:5:GLY:N	31:BV:121:SER:OG	2.44	0.49
51:sD:567:GLN:O	51:sD:629:ARG:NH2	2.46	0.49
60:E3:553:LYS:CG	60:t3:834:TYR:OH	2.60	0.49
60:t3:301:ASN:HD22	60:t3:974:LEU:HB3	1.78	0.49
2:A1:498:LYS:O	2:A1:502:ARG:NE	2.41	0.49
11:AA:420:ARG:CG	38:Me:60:GLU:CD	2.78	0.49
51:SB:440:LEU:HA	51:SB:443:MET:HE2	1.94	0.49
52:SC:200:GLN:NE2	52:SC:203:GLY:O	2.45	0.49
59:SL:327:LYS:HZ2	59:SL:405:THR:H	1.60	0.49
1:B0:570:LEU:HB2	1:B0:598:LEU:HD23	1.95	0.49
11:BA:1221:LYS:HD2	11:BA:1222:ASN:N	2.27	0.49
62:t1:92:SER:HA	63:t2:37:ARG:HH22	1.78	0.49
1:A0:108:LEU:HB2	1:A0:208:TYR:HB3	1.95	0.48
11:AA:849:MET:HE3	11:AA:1061:GLY:HA2	1.95	0.48
24:AN:-58:DT:H1'	24:AN:-57:DT:H5'	1.95	0.48
30:AU:270:ASN:O	30:AU:272:ASN:ND2	2.46	0.48
47:Mn:84:ASP:N	47:Mn:84:ASP:OD1	2.44	0.48
50:SA:300:LYS:NZ	50:SA:301:SER:O	2.46	0.48
9:SF:400:GLN:HB2	9:SF:402:ILE:CD1	2.43	0.48
56:SI:1149:VAL:O	56:SI:1153:LYS:HB2	2.13	0.48
8:B7:331:GLN:HG3	8:B7:529:PHE:HA	1.94	0.48
11:BA:901:LEU:HD22	11:BA:919:ILE:HG13	1.94	0.48
11:BA:1280:GLU:OE1	11:BA:1281:ARG:HB2	2.12	0.48
12:BB:15:PRO:HG3	64:t5:921:PRO:CA	2.42	0.48
24:BN:-94:DA:H2'	24:BN:-93:DA:C8	2.48	0.48
30:BU:10:TYR:HB2	30:BU:54:PHE:HE1	1.78	0.48
55:sH:593:LYS:HE2	56:sI:1050:GLU:HB3	1.95	0.48
63:t2:60:GLU:O	63:t2:67:ARG:NH2	2.46	0.48
45:t4:1070:HIS:O	45:t4:1074:LYS:N	2.46	0.48
11:AA:1221:LYS:HD2	11:AA:1222:ASN:N	2.28	0.48
12:AB:21:GLU:OE2	12:AB:656:GLY:N	2.34	0.48
14:AD:213:GLU:OE2	35:Mb:38:MET:HE2	2.14	0.48
21:AK:1:MET:HB2	21:AK:1:MET:HE2	1.54	0.48
26:AQ:386:MET:O	26:AQ:387:ILE:HD13	2.12	0.48
32:AW:16:VAL:O	32:AW:20:PHE:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Mc:94:ASP:N	36:Mc:94:ASP:OD1	2.46	0.48
44:Mk:32:LEU:HD12	44:Mk:52:ASN:HB3	1.95	0.48
45:Ml:641:SER:HB2	45:Ml:652:GLU:HB2	1.95	0.48
9:SF:473:LEU:HD21	9:SF:499:TYR:CE2	2.49	0.48
3:B2:463:GLU:HB3	9:sF:401:LYS:HB2	1.94	0.48
13:BC:6:PRO:HA	13:BC:24:ASN:HB3	1.94	0.48
23:BM:14:ARG:O	32:BW:126:ILE:CG2	2.61	0.48
35:mb:33:LEU:HD13	37:md:228:LEU:HD22	1.94	0.48
37:md:650:SER:HA	37:md:658:VAL:HA	1.95	0.48
55:sH:629:PHE:O	55:sH:633:LEU:HD23	2.13	0.48
56:sI:707:LEU:HA	56:sI:710:LEU:HD12	1.94	0.48
57:sJ:7:ILE:HG13	57:sJ:8:THR:HG23	1.96	0.48
60:E3:495:ASN:OD1	60:E3:496:SER:N	2.46	0.48
45:T4:1070:HIS:O	45:T4:1074:LYS:N	2.46	0.48
11:AA:465:TYR:HA	21:AK:2:ASN:OD1	2.14	0.48
11:MA:1581:SER:HB2	35:Mb:115:ARG:HH22	1.78	0.48
51:SB:716:GLU:OE2	56:SI:1306:LYS:NZ	2.44	0.48
55:SH:468:LEU:O	55:SH:472:SER:HB3	2.14	0.48
57:SJ:89:ARG:CZ	57:SJ:93:LYS:HB3	2.43	0.48
8:B7:121:LEU:HD13	8:B7:204:PRO:HG2	1.96	0.48
35:mb:98:LEU:HD12	37:md:253:SER:HA	1.95	0.48
45:ml:734:GLN:O	45:ml:770:ARG:NH1	2.44	0.48
49:mp:78:LYS:NZ	49:mp:79:LEU:O	2.44	0.48
50:sA:268:TRP:HD1	50:sA:271:ASP:CG	2.20	0.48
60:E3:900:THR:HG1	60:T3:428:LEU:C	2.21	0.48
61:T6:934:ARG:HG2	61:T6:937:ASN:HD21	1.78	0.48
61:t6:342:ASP:OD2	61:t6:387:LYS:NZ	2.46	0.48
3:A2:463:GLU:HB3	9:SF:401:LYS:HB2	1.94	0.48
30:AU:10:TYR:HB2	30:AU:54:PHE:HE1	1.78	0.48
31:AV:5:GLY:N	31:AV:121:SER:OG	2.44	0.48
53:SE:523:VAL:N	53:SE:547:ARG:HH12	2.12	0.48
57:SJ:28:ASP:C	57:SJ:61:LYS:HG3	2.39	0.48
8:B7:341:TYR:CZ	8:B7:343:PHE:HB2	2.47	0.48
26:BQ:122:GLN:NE2	26:BQ:395:PHE:O	2.47	0.48
30:BU:45:LYS:HE3	31:BV:21:ASP:HB3	1.95	0.48
51:sD:397:SER:HB3	53:sE:551:PRO:HG2	1.95	0.48
9:sF:461:ARG:NH2	9:sF:728:ARG:O	2.46	0.48
9:sF:473:LEU:HD21	9:sF:499:TYR:HE2	1.77	0.48
56:sI:1220:LYS:HA	56:sI:1225:GLN:HG2	1.95	0.48
60:T3:1095:ARG:O	60:T3:1099:ASN:ND2	2.46	0.48
61:T6:266:GLN:NE2	61:T6:276:LYS:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:T6:342:ASP:OD2	61:T6:387:LYS:NZ	2.46	0.48
60:t3:698:ASP:HA	60:t3:702:ASN:HD22	1.79	0.48
5:A4:206:MET:HA	5:A4:206:MET:HE3	1.96	0.48
21:AK:29:ASN:ND2	21:AK:78:THR:O	2.47	0.48
27:AR:73:LEU:HD11	27:AR:77:LEU:CB	2.44	0.48
1:B0:550:ILE:HA	1:B0:553:MET:CE	2.44	0.48
3:B2:50:MET:HG3	3:B2:100:LEU:HD13	1.95	0.48
11:BA:465:TYR:HA	21:BK:2:ASN:OD1	2.13	0.48
12:BB:15:PRO:HG3	64:t5:921:PRO:HB3	1.96	0.48
14:BD:190:GLU:HG2	14:BD:194:LEU:HD23	1.95	0.48
26:BQ:373:TYR:OH	27:BR:72:ARG:NH2	2.44	0.48
51:sB:716:GLU:OE2	56:sI:1306:LYS:NZ	2.44	0.48
9:sF:525:GLN:HE22	9:sF:609:ALA:HB3	1.78	0.48
60:T3:869:ARG:HH21	60:T3:882:LEU:HD23	1.76	0.48
8:A7:493:VAL:O	8:A7:495:ALA:N	2.46	0.48
49:Mp:549:ASP:OD1	49:Mp:554:TRP:NE1	2.46	0.48
55:SH:593:LYS:HE2	56:SI:1050:GLU:HB3	1.95	0.48
1:B0:27:ASP:OD2	1:B0:483:TYR:OH	2.30	0.48
27:BR:104:ILE:HG13	27:BR:122:LEU:HB3	1.96	0.48
32:BW:16:VAL:O	32:BW:20:PHE:HB2	2.13	0.48
57:sJ:27:TYR:CE2	57:sJ:61:LYS:HD2	2.49	0.48
62:T1:92:SER:HA	63:T2:37:ARG:HH22	1.78	0.48
61:T6:55:LEU:O	61:T6:164:MET:HE1	2.14	0.48
61:t6:467:ASP:OD1	61:t6:467:ASP:N	2.46	0.48
1:A0:244:CYS:SG	1:A0:245:ILE:N	2.87	0.48
3:A2:43:ALA:O	3:A2:47:ILE:HG12	2.14	0.48
12:AB:322:PHE:HB2	26:AQ:420:VAL:HG11	1.93	0.48
12:AB:957:ASN:OD1	12:AB:961:LEU:N	2.45	0.48
21:AK:12:LEU:HD23	21:AK:13:GLY:O	2.14	0.48
24:AN:-94:DA:H2'	24:AN:-93:DA:C8	2.48	0.48
49:Mp:78:LYS:NZ	49:Mp:79:LEU:O	2.44	0.48
50:SA:544:ASN:ND2	51:SB:578:ASP:O	2.40	0.48
1:B0:711:ASP:N	1:B0:711:ASP:OD1	2.45	0.48
8:B7:566:TYR:HA	8:B7:569:TYR:HB3	1.96	0.48
11:BA:1444:MET:CE	17:BG:58:ARG:HD2	2.44	0.48
18:BH:146:ARG:HG2	18:BH:146:ARG:NH1	2.28	0.48
44:mk:32:LEU:HD12	44:mk:52:ASN:HB3	1.95	0.48
61:E6:508:GLU:N	61:E6:508:GLU:OE1	2.46	0.48
8:A7:121:LEU:HD13	8:A7:204:PRO:HG2	1.96	0.48
11:AA:1191:TRP:HZ3	19:AI:43:VAL:HG21	1.79	0.48
14:AD:190:GLU:HG2	14:AD:194:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Md:650:SER:HA	37:Md:658:VAL:HA	1.95	0.48
51:SD:338:LYS:NZ	9:SF:455:GLU:OE2	2.47	0.48
9:SF:465:ASP:HB3	9:SF:468:ARG:HD3	1.96	0.48
9:SF:525:GLN:HE22	9:SF:609:ALA:HB3	1.78	0.48
55:SH:587:LYS:C	55:SH:588:ASN:CA	2.62	0.48
1:B0:108:LEU:HB2	1:B0:208:TYR:HB3	1.95	0.48
8:B7:720:THR:HA	8:B7:723:GLN:NE2	2.29	0.48
11:BA:122:MET:HE3	11:BA:141:LEU:HD21	1.96	0.48
11:BA:1191:TRP:HZ3	19:BI:43:VAL:HG21	1.79	0.48
12:BB:106:ASP:N	23:BM:241:ARG:NH2	2.62	0.48
14:BD:213:GLU:OE2	35:mb:38:MET:HE2	2.14	0.48
21:BK:1:MET:HE2	21:BK:1:MET:HB2	1.54	0.48
26:BQ:113:ASN:O	26:BQ:114:MET:HE2	2.13	0.48
11:mA:1581:SER:HB2	35:mb:115:ARG:HH22	1.78	0.48
56:sI:1084:LEU:O	56:sI:1088:LEU:HD23	2.14	0.48
58:sK:207:MET:N	58:sK:207:MET:HE2	2.29	0.48
60:T3:698:ASP:HA	60:T3:702:ASN:HD22	1.79	0.48
45:T4:981:THR:OG1	45:T4:1004:ALA:N	2.46	0.48
60:t3:1095:ARG:O	60:t3:1099:ASN:ND2	2.46	0.48
60:t3:1114:GLU:HA	60:t3:1117:ILE:HG22	1.95	0.48
61:t6:218:ARG:NH2	61:t6:220:ARG:HB2	2.26	0.48
1:A0:1:MET:SD	1:A0:15:PRO:HA	2.54	0.48
3:A2:423:ASP:N	3:A2:423:ASP:OD1	2.47	0.48
23:AM:14:ARG:CZ	32:AW:126:ILE:CD1	2.90	0.48
26:AQ:122:GLN:NE2	26:AQ:395:PHE:O	2.47	0.48
11:MA:1648:SER:HB2	11:MA:1651:SER:HB3	1.96	0.48
53:SE:290:ILE:HG21	9:SF:745:VAL:HG21	1.96	0.48
53:SE:487:LYS:O	53:SE:490:THR:OG1	2.30	0.48
9:SF:461:ARG:NH2	9:SF:728:ARG:O	2.46	0.48
9:SF:496:LEU:HD12	9:SF:510:ILE:HD13	1.96	0.48
58:SK:243:LEU:O	58:SK:247:GLU:HB2	2.14	0.48
3:B2:506:LYS:NZ	3:B2:506:LYS:HD2	2.19	0.48
28:BS:230:THR:C	28:BS:232:ASP:N	2.72	0.48
49:mp:549:ASP:OD1	49:mp:554:TRP:NE1	2.46	0.48
60:E3:412:ARG:HG3	60:E3:413:ILE:N	2.28	0.48
61:E6:749:LEU:CD2	61:E6:791:PHE:HE2	2.26	0.48
60:T3:1087:SER:OG	60:T3:1088:PHE:N	2.47	0.48
8:A7:720:THR:HA	8:A7:723:GLN:NE2	2.29	0.48
11:AA:122:MET:HE3	11:AA:141:LEU:HD21	1.96	0.48
11:AA:901:LEU:HD22	11:AA:919:ILE:HG13	1.94	0.48
11:AA:1444:MET:CE	17:AG:58:ARG:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:108:VAL:CA	23:AM:241:ARG:HH11	1.81	0.48
14:AD:213:GLU:CG	35:Mb:38:MET:SD	2.94	0.48
27:AR:104:ILE:HG13	27:AR:122:LEU:HB3	1.96	0.48
33:AX:284:LYS:HD3	33:AX:285:PRO:HD2	1.96	0.48
45:MI:734:GLN:O	45:MI:770:ARG:NH1	2.44	0.48
49:MP:180:GLN:C	61:E6:664:ARG:HD3	2.39	0.48
51:SD:567:GLN:O	51:SD:629:ARG:NH2	2.46	0.48
56:SI:1084:LEU:O	56:SI:1088:LEU:HD23	2.14	0.48
2:B1:472:GLN:HE22	5:B4:37:TRP:HB3	1.79	0.48
8:B7:626:PHE:HE2	8:B7:628:TYR:CE1	2.31	0.48
14:BD:216:ASN:OD1	35:mb:39:ARG:NH1	2.44	0.48
18:BH:110:ASP:HA	43:mj:83:LEU:CG	2.33	0.48
36:mc:94:ASP:N	36:mc:94:ASP:OD1	2.46	0.48
45:ml:413:VAL:HB	45:ml:427:ILE:HB	1.95	0.48
50:sA:544:ASN:ND2	51:sB:578:ASP:O	2.40	0.48
9:sF:473:LEU:HD21	9:sF:499:TYR:CE2	2.49	0.48
9:sF:496:LEU:HD12	9:sF:510:ILE:HD13	1.96	0.48
56:sI:1224:LEU:HD13	56:sI:1230:SER:HB2	1.95	0.48
57:sJ:28:ASP:C	57:sJ:61:LYS:HG3	2.38	0.48
45:T4:909:PRO:O	45:T4:913:ASN:ND2	2.46	0.48
60:t3:518:SER:O	60:t3:524:GLN:NE2	2.47	0.48
61:t6:203:ILE:HA	61:t6:223:GLN:HA	1.96	0.48
4:A3:49:LEU:CD2	17:AG:164:LYS:HB2	2.44	0.47
11:AA:11:LEU:C	11:AA:12:ARG:HD3	2.38	0.47
12:AB:954:VAL:HG12	12:AB:964:VAL:HG12	1.95	0.47
19:AI:54:GLU:HG3	19:AI:55:THR:O	2.14	0.47
44:Mk:21:GLN:OE1	44:Mk:66:ARG:NH2	2.39	0.47
49:MP:53:ARG:NH1	49:MP:66:ASP:OD1	2.47	0.47
50:SA:126:ARG:HD2	50:SA:165:LEU:HD21	1.96	0.47
58:SK:91:TYR:CE2	58:SK:99:PRO:HD3	2.49	0.47
6:B5:30:ILE:HG23	6:B5:31:VAL:HG23	1.96	0.47
12:BB:21:GLU:OE2	12:BB:656:GLY:N	2.34	0.47
12:BB:106:ASP:CA	23:BM:241:ARG:NH2	2.45	0.47
12:BB:957:ASN:OD1	12:BB:961:LEU:N	2.45	0.47
19:BI:54:GLU:HG3	19:BI:55:THR:O	2.14	0.47
35:mb:97:PRO:HA	37:md:254:LEU:HD23	1.95	0.47
45:ml:641:SER:HB2	45:ml:652:GLU:HB2	1.95	0.47
53:sE:523:VAL:N	53:sE:547:ARG:HH12	2.12	0.47
60:T3:438:ASP:OD1	60:T3:441:HIS:ND1	2.44	0.47
60:T3:1114:GLU:HA	60:T3:1117:ILE:HG22	1.95	0.47
60:t3:483:ASN:OD1	60:t3:487:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:t6:609:ALA:HB1	61:t6:613:ILE:HD12	1.96	0.47
13:AC:36:VAL:HG21	13:AC:251:LEU:HD13	1.97	0.47
26:AQ:113:ASN:O	26:AQ:114:MET:HE2	2.13	0.47
30:AU:45:LYS:HE3	31:AV:21:ASP:HB3	1.95	0.47
33:AX:135:ILE:HD11	33:AX:147:LEU:HD11	1.96	0.47
37:Md:86:LEU:HD13	45:MI:209:LEU:HD21	1.94	0.47
55:SH:629:PHE:O	55:SH:633:LEU:HD23	2.13	0.47
57:SJ:7:ILE:HG13	57:SJ:8:THR:HG23	1.96	0.47
11:BA:1148:ILE:HD12	11:BA:1196:GLU:HG3	1.97	0.47
27:BR:73:LEU:HD11	27:BR:77:LEU:CB	2.44	0.47
27:BR:106:LEU:C	27:BR:107:LEU:HD12	2.39	0.47
27:BR:228:MET:HE2	27:BR:228:MET:HA	1.97	0.47
27:BR:309:GLU:OE2	27:BR:321:ARG:NH1	2.40	0.47
33:BX:135:ILE:HD11	33:BX:147:LEU:HD11	1.96	0.47
48:mo:46:GLN:O	48:mo:50:LYS:HB3	2.14	0.47
49:mp:53:ARG:HH12	49:mp:64:ASP:HB3	1.79	0.47
60:T3:539:GLU:OE1	60:T3:542:LYS:NZ	2.47	0.47
60:t3:539:GLU:OE1	60:t3:542:LYS:NZ	2.47	0.47
60:t3:830:SER:HB2	60:t3:841:ALA:HB1	1.96	0.47
1:A0:550:ILE:HA	1:A0:553:MET:CE	2.44	0.47
3:A2:50:MET:HG3	3:A2:100:LEU:HD13	1.95	0.47
51:SD:397:SER:HB3	53:SE:551:PRO:HG2	1.95	0.47
9:SF:511:ASP:N	9:SF:511:ASP:OD1	2.46	0.47
56:SI:1220:LYS:HA	56:SI:1225:GLN:HG2	1.95	0.47
56:SI:1224:LEU:HD13	56:SI:1230:SER:HB2	1.95	0.47
3:B2:43:ALA:O	3:B2:47:ILE:HG12	2.14	0.47
5:B4:206:MET:HA	5:B4:206:MET:HE3	1.96	0.47
8:B7:493:VAL:O	8:B7:495:ALA:N	2.46	0.47
11:BA:849:MET:HE3	11:BA:1061:GLY:HA2	1.95	0.47
45:ml:246:LEU:HD21	45:ml:274:GLY:H	1.79	0.47
53:sE:308:ILE:HG21	53:sE:492:LYS:HB3	1.96	0.47
53:sE:449:TYR:HB2	54:sG:65:UNK:HA	1.95	0.47
9:sF:465:ASP:HB3	9:sF:468:ARG:HD3	1.96	0.47
1:A0:27:ASP:OD2	1:A0:483:TYR:OH	2.30	0.47
1:A0:104:ARG:NE	1:A0:203:CYS:HA	2.29	0.47
6:A5:30:ILE:HG23	6:A5:31:VAL:HG23	1.96	0.47
19:AI:114:GLN:H	19:AI:115:LYS:HZ3	1.62	0.47
27:AR:106:LEU:C	27:AR:107:LEU:HD12	2.39	0.47
49:Mp:548:TYR:CD2	61:E6:612:GLU:CD	2.92	0.47
52:SC:146:MET:HA	52:SC:146:MET:HE3	1.96	0.47
53:SE:73:TYR:OH	53:SE:194:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SJ:27:TYR:CE2	57:SJ:61:LYS:HD2	2.49	0.47
1:B0:244:CYS:SG	1:B0:245:ILE:N	2.87	0.47
5:B4:146:ARG:NH1	7:B6:457:LYS:O	2.48	0.47
21:BK:29:ASN:ND2	21:BK:78:THR:O	2.47	0.47
27:BR:138:GLN:N	27:BR:211:LYS:O	2.44	0.47
11:mA:1648:SER:HB2	11:mA:1651:SER:HB3	1.96	0.47
42:mi:128:LEU:HD21	44:mk:136:LEU:HD13	1.97	0.47
49:mp:53:ARG:NH1	49:mp:66:ASP:OD1	2.47	0.47
55:sH:468:LEU:O	55:sH:472:SER:HB3	2.14	0.47
56:sI:758:ASN:O	56:sI:762:ASN:ND2	2.43	0.47
61:t6:55:LEU:O	61:t6:164:MET:HE1	2.14	0.47
61:t6:297:ILE:HB	61:t6:310:TYR:HB2	1.96	0.47
61:t6:779:LEU:O	61:t6:783:GLU:HB2	2.14	0.47
1:A0:251:ASP:OD1	1:A0:436:ARG:HG3	2.14	0.47
3:A2:368:ALA:HB3	3:A2:375:LEU:HD21	1.97	0.47
3:A2:493:ILE:HD13	3:A2:501:VAL:HG21	1.96	0.47
8:A7:438:PHE:HZ	8:A7:470:SER:HB3	1.79	0.47
8:A7:605:ILE:HG12	8:A7:669:CYS:HB3	1.97	0.47
32:AW:116:ASN:O	32:AW:118:GLU:N	2.47	0.47
45:Ml:722:MET:HE2	45:Ml:727:LYS:HB3	1.96	0.47
49:Mp:548:TYR:CD2	61:E6:612:GLU:HB2	2.49	0.47
50:SA:270:TYR:O	50:SA:275:PRO:HB3	2.14	0.47
50:SA:308:MET:HE3	50:SA:308:MET:HB3	1.71	0.47
53:SE:526:GLN:HB3	53:SE:547:ARG:HD2	1.96	0.47
55:SH:594:LEU:CB	55:SH:594:LEU:HD22	2.23	0.47
4:B3:49:LEU:CD2	17:BG:164:LYS:HB2	2.44	0.47
17:BG:46:LEU:HD11	17:BG:79:PHE:HB2	1.96	0.47
23:BM:283:TYR:HA	23:BM:286:ILE:HG22	1.96	0.47
60:T3:371:ARG:O	60:T3:375:ILE:HG12	2.14	0.47
5:A4:146:ARG:NH1	7:A6:457:LYS:O	2.48	0.47
12:AB:21:GLU:CD	12:AB:22:SER:N	2.73	0.47
23:AM:14:ARG:O	32:AW:126:ILE:CG2	2.61	0.47
25:AO:185:TYR:HB2	25:AO:193:LEU:HD13	1.96	0.47
28:AS:163:GLU:HG2	28:AS:215:LYS:CE	2.44	0.47
45:Ml:246:LEU:HD21	45:Ml:274:GLY:H	1.79	0.47
49:Mp:53:ARG:HH12	49:Mp:64:ASP:HB3	1.79	0.47
50:SA:376:VAL:HG13	50:SA:402:LYS:HD3	1.96	0.47
11:BA:208:LEU:HD13	11:BA:235:ILE:HG21	1.96	0.47
12:BB:100:PRO:HA	12:BB:126:SER:HB3	1.97	0.47
19:BI:80:SER:O	19:BI:81:ARG:HG3	2.15	0.47
50:sA:126:ARG:HD2	50:sA:165:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:sB:344:MET:HA	51:sB:347:ARG:HG2	1.96	0.47
51:sD:338:LYS:NZ	9:sF:455:GLU:OE2	2.47	0.47
60:E3:596:ASP:OD1	60:E3:597:LEU:N	2.47	0.47
61:E6:877:GLN:NE2	61:E6:882:GLY:O	2.48	0.47
61:E6:898:LYS:HA	61:E6:972:MET:CE	2.44	0.47
60:T3:360:HIS:HD2	60:T3:919:TYR:CE2	2.26	0.47
45:T4:896:VAL:O	45:T4:908:GLN:NE2	2.38	0.47
61:T6:297:ILE:HB	61:T6:310:TYR:HB2	1.96	0.47
61:t6:627:MET:SD	61:t6:649:ILE:HD11	2.54	0.47
1:A0:136:MET:HB3	1:A0:136:MET:HE2	1.80	0.47
2:A1:472:GLN:HE22	5:A4:37:TRP:HB3	1.79	0.47
8:A7:349:ASN:HD22	8:A7:481:GLU:CG	2.22	0.47
8:A7:566:TYR:HA	8:A7:569:TYR:HB3	1.96	0.47
11:AA:208:LEU:HD13	11:AA:235:ILE:HG21	1.96	0.47
17:AG:86:VAL:HA	17:AG:146:LYS:HA	1.97	0.47
26:AQ:377:SER:O	26:AQ:385:THR:N	2.48	0.47
27:AR:98:ASN:OD1	27:AR:103:LYS:HB3	2.15	0.47
28:AS:239:ALA:O	28:AS:242:LYS:N	2.48	0.47
32:AW:132:THR:OG1	32:AW:135:GLU:OE1	2.31	0.47
56:SI:1091:LEU:O	56:SI:1095:ASN:ND2	2.48	0.47
3:B2:62:LEU:O	3:B2:65:TRP:HB2	2.15	0.47
3:B2:423:ASP:OD1	3:B2:423:ASP:N	2.47	0.47
8:B7:438:PHE:HZ	8:B7:470:SER:HB3	1.80	0.47
11:BA:148:CYS:HB3	11:BA:169:ASN:H	1.79	0.47
21:BK:13:GLY:N	21:BK:16:GLU:OE2	2.48	0.47
23:BM:14:ARG:CZ	32:BW:126:ILE:CD1	2.90	0.47
50:sA:270:TYR:O	50:sA:275:PRO:HB3	2.14	0.47
50:sA:300:LYS:NZ	50:sA:301:SER:O	2.47	0.47
50:sA:376:VAL:HG13	50:sA:402:LYS:HD3	1.96	0.47
56:sI:1020:SER:OG	56:sI:1021:GLU:N	2.48	0.47
61:E6:355:ASN:OD1	61:E6:356:LEU:N	2.48	0.47
64:T5:849:ARG:O	64:T5:853:LEU:HD23	2.15	0.47
61:T6:467:ASP:N	61:T6:467:ASP:OD1	2.46	0.47
61:T6:609:ALA:HB1	61:T6:613:ILE:HD12	1.96	0.47
60:t3:371:ARG:O	60:t3:375:ILE:HG12	2.14	0.47
3:A2:123:VAL:HG13	3:A2:238:LYS:HB3	1.96	0.47
21:AK:13:GLY:N	21:AK:16:GLU:OE2	2.48	0.47
23:AM:191:GLU:OE1	27:AR:269:SER:O	2.33	0.47
26:AQ:373:TYR:OH	27:AR:72:ARG:NH2	2.44	0.47
56:SI:951:LEU:HD23	56:SI:975:LEU:HD11	1.97	0.47
1:B0:68:LYS:HD2	1:B0:204:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:302:MET:N	2:B1:302:MET:SD	2.88	0.47
2:B1:484:LEU:HD13	5:B4:109:ILE:CG2	2.44	0.47
17:BG:12:THR:HA	17:BG:69:GLU:HA	1.97	0.47
19:BI:56:ALA:O	19:BI:57:GLY:C	2.58	0.47
28:BS:184:LYS:HA	28:BS:228:LEU:CD1	2.42	0.47
33:BX:284:LYS:HD3	33:BX:285:PRO:HD2	1.96	0.47
58:sK:91:TYR:CE2	58:sK:99:PRO:HD3	2.49	0.47
58:sK:243:LEU:O	58:sK:247:GLU:HB2	2.14	0.47
61:T6:559:SER:OG	61:T6:566:ALA:HB2	2.14	0.47
12:AB:106:ASP:N	23:AM:241:ARG:NH2	2.62	0.47
12:AB:1156:ASP:N	12:AB:1156:ASP:OD1	2.48	0.47
20:AJ:69:ARG:HA	20:AJ:69:ARG:HE	1.80	0.47
28:AS:227:PHE:HD1	28:AS:230:THR:HG21	1.80	0.47
28:AS:230:THR:C	28:AS:232:ASP:N	2.72	0.47
51:SB:344:MET:HA	51:SB:347:ARG:HG2	1.96	0.47
59:SL:54:HIS:NE2	59:SL:57:ASN:HA	2.30	0.47
1:B0:1:MET:SD	1:B0:15:PRO:HA	2.54	0.47
12:BB:21:GLU:CD	12:BB:22:SER:N	2.73	0.47
12:BB:1163:CYS:HB2	12:BB:1187:ASN:HD22	1.80	0.47
19:BI:45:ARG:NH2	19:BI:47:GLU:OE1	2.41	0.47
26:BQ:377:SER:O	26:BQ:385:THR:N	2.48	0.47
28:BS:239:ALA:O	28:BS:242:LYS:N	2.48	0.47
32:BW:132:THR:OG1	32:BW:135:GLU:OE1	2.31	0.47
61:E6:920:ASP:CG	61:E6:934:ARG:HH12	2.23	0.47
60:T3:301:ASN:HD22	60:T3:974:LEU:HB3	1.78	0.47
45:T4:1001:ILE:HG23	45:T4:1055:VAL:HB	1.97	0.47
61:T6:393:PRO:HA	61:T6:425:TYR:HA	1.97	0.47
60:t3:1103:LEU:HD22	60:t3:1113:ASN:HD22	1.80	0.47
45:t4:902:ASN:O	45:t4:905:HIS:ND1	2.44	0.47
61:t6:559:SER:OG	61:t6:566:ALA:HB2	2.14	0.47
6:A5:6:LYS:HB3	6:A5:44:PRO:HG2	1.97	0.47
8:A7:622:MET:HE1	8:A7:653:PHE:CG	2.50	0.47
19:AI:56:ALA:O	19:AI:57:GLY:C	2.58	0.47
19:AI:80:SER:O	19:AI:81:ARG:HG3	2.15	0.47
42:Mi:128:LEU:HD21	44:Mk:136:LEU:HD13	1.97	0.47
45:MI:113:THR:O	45:MI:117:THR:OG1	2.30	0.47
45:MI:413:VAL:HB	45:MI:427:ILE:HB	1.95	0.47
9:SF:318:GLU:O	9:SF:320:LYS:N	2.48	0.47
3:B2:123:VAL:HG13	3:B2:238:LYS:HB3	1.96	0.47
8:B7:130:ARG:HD3	8:B7:202:LYS:HA	1.97	0.47
13:BC:36:VAL:HG21	13:BC:251:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BD:141:LEU:O	14:BD:145:MET:HE3	2.15	0.47
23:BM:191:GLU:OE2	27:BR:268:MET:HA	2.15	0.47
24:BN:-58:DT:H1'	24:BN:-57:DT:H5'	1.96	0.47
25:BO:185:TYR:HB2	25:BO:193:LEU:HD13	1.96	0.47
37:md:403:TYR:HE2	37:md:473:LYS:HE3	1.80	0.47
45:ml:722:MET:HE2	45:ml:727:LYS:HB3	1.96	0.47
9:sF:318:GLU:O	9:sF:320:LYS:N	2.48	0.47
61:T6:203:ILE:HA	61:T6:223:GLN:HA	1.96	0.47
61:T6:627:MET:SD	61:T6:649:ILE:HD11	2.54	0.47
60:t3:920:LEU:O	60:t3:924:ILE:HG12	2.14	0.47
45:t4:981:THR:OG1	45:t4:1004:ALA:N	2.46	0.47
1:A0:277:VAL:HG23	1:A0:278:ASP:OD1	2.15	0.46
5:A4:180:THR:OG1	5:A4:181:CYS:N	2.48	0.46
14:AD:141:LEU:O	14:AD:145:MET:HE3	2.15	0.46
49:Mp:105:LEU:O	49:Mp:109:THR:OG1	2.32	0.46
51:SB:399:LEU:HD11	53:SE:483:GLN:HE21	1.79	0.46
53:SE:449:TYR:HB2	54:SG:65:UNK:HA	1.95	0.46
1:B0:251:ASP:OD1	1:B0:436:ARG:HG3	2.14	0.46
1:B0:277:VAL:HG23	1:B0:278:ASP:OD1	2.15	0.46
3:B2:368:ALA:HB3	3:B2:375:LEU:HD21	1.97	0.46
8:B7:622:MET:HE1	8:B7:653:PHE:CG	2.50	0.46
11:BA:1144:LYS:HZ3	11:BA:1268:LEU:HB3	1.80	0.46
21:BK:12:LEU:HD23	21:BK:13:GLY:O	2.14	0.46
23:BM:169:GLU:OE2	23:BM:169:GLU:N	2.45	0.46
23:BM:191:GLU:OE1	27:BR:269:SER:O	2.33	0.46
28:BS:163:GLU:HG2	28:BS:215:LYS:CE	2.44	0.46
29:BT:43:DT:H2''	29:BT:44:DC:C6	2.50	0.46
52:sC:146:MET:HA	52:sC:146:MET:HE3	1.96	0.46
51:sD:722:LEU:HB2	51:sD:726:ARG:HH21	1.80	0.46
53:sE:526:GLN:HB3	53:sE:547:ARG:HD2	1.96	0.46
56:sI:1091:LEU:O	56:sI:1095:ASN:ND2	2.48	0.46
57:sJ:89:ARG:HH21	57:sJ:93:LYS:HD2	1.80	0.46
60:T3:783:ILE:O	60:T3:787:ILE:HG12	2.15	0.46
45:T4:917:ASP:HB3	45:T4:920:PHE:HD2	1.81	0.46
61:T6:411:ASP:OD1	61:T6:411:ASP:N	2.48	0.46
61:T6:779:LEU:O	61:T6:783:GLU:HB2	2.14	0.46
60:t3:289:LYS:HB3	60:t3:290:LEU:HD22	1.98	0.46
6:A5:41:LEU:HA	6:A5:41:LEU:HD12	1.54	0.46
12:AB:1163:CYS:HB2	12:AB:1187:ASN:HD22	1.80	0.46
17:AG:46:LEU:HD11	17:AG:79:PHE:HB2	1.96	0.46
27:AR:320:GLU:O	27:AR:323:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Mg:35:ASP:N	40:Mg:35:ASP:OD1	2.48	0.46
45:MI:273:ASN:O	45:MI:275:ARG:NH1	2.48	0.46
48:MO:46:GLN:O	48:MO:50:LYS:HB3	2.14	0.46
51:SD:722:LEU:HB2	51:SD:726:ARG:HH21	1.80	0.46
55:SH:593:LYS:HA	55:SH:593:LYS:HD3	1.58	0.46
6:B5:6:LYS:HB3	6:B5:44:PRO:HG2	1.97	0.46
28:BS:163:GLU:HG2	28:BS:215:LYS:CD	2.45	0.46
53:sE:290:ILE:HG21	9:sF:745:VAL:HG21	1.96	0.46
61:E6:699:LEU:HD22	61:E6:777:LEU:HD21	1.96	0.46
64:T5:896:ASP:N	64:T5:896:ASP:OD1	2.48	0.46
45:t4:1001:ILE:HG23	45:t4:1055:VAL:HB	1.97	0.46
64:t5:896:ASP:N	64:t5:896:ASP:OD1	2.48	0.46
61:t6:170:ASP:N	61:t6:170:ASP:OD1	2.48	0.46
3:A2:62:LEU:O	3:A2:65:TRP:HB2	2.15	0.46
11:AA:148:CYS:HB3	11:AA:169:ASN:H	1.79	0.46
23:AM:283:TYR:HA	23:AM:286:ILE:HG22	1.96	0.46
29:AT:43:DT:H2"	29:AT:44:DC:C6	2.50	0.46
9:SF:624:ASP:O	9:SF:627:SER:OG	2.31	0.46
58:SK:107:THR:HG22	58:SK:139:VAL:HB	1.97	0.46
3:B2:493:ILE:HD13	3:B2:501:VAL:HG21	1.96	0.46
12:BB:182:SER:OG	12:BB:183:GLU:OE1	2.33	0.46
14:BD:141:LEU:C	14:BD:145:MET:HE3	2.40	0.46
17:BG:86:VAL:HA	17:BG:146:LYS:HA	1.97	0.46
17:BG:100:GLU:CG	32:BW:144:ARG:HH21	2.18	0.46
51:sB:399:LEU:HD11	53:sE:483:GLN:HE21	1.79	0.46
54:sG:55:UNK:N	54:sG:58:ARG:O	2.48	0.46
58:sK:149:MET:HA	58:sK:149:MET:HE3	1.97	0.46
61:E6:382:SER:N	60:t3:431:ASP:OD2	2.48	0.46
61:E6:923:LEU:CB	61:E6:934:ARG:HE	2.27	0.46
60:T3:920:LEU:O	60:T3:924:ILE:HG12	2.14	0.46
61:T6:651:TYR:OH	61:T6:910:CYS:SG	2.61	0.46
61:t6:670:ILE:HA	61:t6:673:ILE:HD12	1.97	0.46
2:A1:484:LEU:HD13	5:A4:109:ILE:CG2	2.45	0.46
11:AA:99:ILE:HA	11:AA:102:VAL:HG12	1.96	0.46
11:AA:1143:LEU:HD11	11:AA:1216:ILE:HD11	1.98	0.46
11:AA:1148:ILE:HD12	11:AA:1196:GLU:HG3	1.97	0.46
14:AD:141:LEU:C	14:AD:145:MET:HE3	2.40	0.46
17:AG:100:GLU:CD	32:AW:144:ARG:CZ	2.88	0.46
23:AM:301:THR:C	27:AR:271:ARG:NH1	2.66	0.46
25:AO:202:ILE:HD11	25:AO:222:GLU:HG2	1.98	0.46
35:Mb:153:ARG:O	35:Mb:157:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:1020:SER:OG	56:SI:1021:GLU:N	2.48	0.46
1:B0:104:ARG:NE	1:B0:203:CYS:HA	2.29	0.46
3:B2:39:LEU:O	3:B2:44:LYS:NZ	2.48	0.46
11:BA:99:ILE:HA	11:BA:102:VAL:HG12	1.96	0.46
37:md:539:ILE:O	37:md:543:ARG:NH2	2.44	0.46
53:sE:101:GLY:O	53:sE:189:ARG:NH1	2.47	0.46
58:sK:239:SER:HB3	58:sK:307:TYR:CZ	2.51	0.46
60:T3:306:TRP:HD1	60:T3:580:SER:HA	1.80	0.46
60:T3:541:VAL:HG22	60:T3:578:ILE:HD13	1.98	0.46
2:A1:205:PRO:HA	2:A1:206:PRO:HD3	1.82	0.46
28:AS:163:GLU:HG2	28:AS:215:LYS:HD3	1.98	0.46
28:AS:271:CYS:CB	28:AS:274:CYS:SG	2.90	0.46
53:SE:308:ILE:HG21	53:SE:492:LYS:HB3	1.96	0.46
59:SL:457:LYS:HB2	59:SL:461:ALA:HB2	1.98	0.46
5:B4:180:THR:OG1	5:B4:181:CYS:N	2.48	0.46
6:B5:53:GLU:HB2	6:B5:56:ARG:CZ	2.46	0.46
45:ml:354:GLU:OE1	45:ml:358:LYS:NZ	2.48	0.46
9:sF:460:ILE:HB	9:sF:477:LEU:HB2	1.98	0.46
56:sI:951:LEU:HD23	56:sI:975:LEU:HD11	1.97	0.46
59:sL:54:HIS:NE2	59:sL:57:ASN:HA	2.30	0.46
60:E3:879:ARG:HH21	60:T3:880:LYS:CE	2.28	0.46
60:E3:938:LYS:O	60:E3:941:GLU:HG3	2.15	0.46
60:E3:939:THR:HA	60:E3:939:THR:HG22	1.94	0.46
63:T2:77:LYS:HA	63:T2:80:GLN:NE2	2.30	0.46
60:T3:483:ASN:OD1	60:T3:487:ILE:N	2.47	0.46
61:T6:670:ILE:HA	61:T6:673:ILE:HD12	1.97	0.46
60:t3:541:VAL:HG22	60:t3:578:ILE:HD13	1.98	0.46
45:t4:917:ASP:HB3	45:t4:920:PHE:HD2	1.81	0.46
45:t4:1010:THR:O	45:t4:1013:SER:OG	2.27	0.46
61:t6:411:ASP:OD1	61:t6:411:ASP:N	2.48	0.46
1:A0:523:GLY:O	1:A0:527:VAL:HG23	2.16	0.46
11:AA:68:GLN:NE2	32:AW:151:LEU:HD13	2.31	0.46
13:AC:6:PRO:O	21:AK:104:ASN:ND2	2.38	0.46
17:AG:95:SER:HB2	32:AW:144:ARG:HG3	1.98	0.46
45:MI:92:LEU:HD21	45:MI:148:VAL:HG22	1.98	0.46
9:SF:485:LEU:N	9:SF:485:LEU:HD12	2.30	0.46
58:SK:207:MET:HE2	58:SK:207:MET:N	2.29	0.46
11:BA:451:HIS:HD2	11:BA:453:MET:HE2	1.78	0.46
12:BB:451:LYS:HZ2	23:BM:139:ALA:HA	1.79	0.46
27:BR:95:ILE:HD13	27:BR:106:LEU:HD13	1.98	0.46
32:BW:190:ASP:OD1	32:BW:190:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:ml:140:GLN:HA	45:ml:143:LYS:HD2	1.98	0.46
9:sF:511:ASP:N	9:sF:511:ASP:OD1	2.46	0.46
58:sK:107:THR:HG22	58:sK:139:VAL:HB	1.97	0.46
61:E6:311:LYS:HB2	61:E6:336:ILE:HD11	1.97	0.46
60:T3:830:SER:HB2	60:T3:841:ALA:HB1	1.96	0.46
60:t3:869:ARG:NH2	60:t3:882:LEU:HD23	2.31	0.46
2:A1:302:MET:N	2:A1:302:MET:SD	2.88	0.46
11:AA:20:GLY:O	12:AB:1213:THR:OG1	2.27	0.46
12:AB:182:SER:OG	12:AB:183:GLU:OE1	2.33	0.46
12:AB:879:ARG:HA	12:AB:885:MET:HE1	1.98	0.46
19:AI:105:SER:HB2	45:T4:1011:THR:CG2	2.43	0.46
23:AM:294:THR:HG23	23:AM:297:LYS:H	1.80	0.46
27:AR:256:ASP:OD1	27:AR:256:ASP:N	2.47	0.46
36:Mc:92:GLY:O	36:Mc:95:THR:OG1	2.30	0.46
45:MI:140:GLN:HA	45:MI:143:LYS:HD2	1.98	0.46
49:Mp:45:GLU:HB3	49:Mp:53:ARG:HB2	1.98	0.46
50:SA:557:ILE:HG21	51:SB:563:LEU:HD21	1.97	0.46
19:BI:103:CYS:HB2	19:BI:106:CYS:SG	2.56	0.46
27:BR:320:GLU:O	27:BR:323:ARG:NH1	2.48	0.46
53:sE:508:LYS:N	53:sE:511:GLN:OE1	2.49	0.46
58:sK:386:SER:O	58:sK:390:THR:OG1	2.31	0.46
60:E3:869:ARG:NH2	60:E3:872:ASN:O	2.48	0.46
61:T6:408:LEU:O	61:T6:412:ARG:NH2	2.48	0.46
60:t3:364:SER:HB2	60:t3:366:LEU:HD13	1.97	0.46
45:t4:1023:ARG:NH1	45:t4:1027:PHE:O	2.48	0.46
1:A0:68:LYS:HD2	1:A0:204:ASN:HA	1.97	0.46
8:A7:592:GLN:NE2	8:A7:747:ASN:O	2.47	0.46
8:A7:612:VAL:HG11	8:A7:628:TYR:CZ	2.51	0.46
12:AB:510:LYS:HD2	12:AB:510:LYS:HA	1.83	0.46
28:AS:163:GLU:HG2	28:AS:215:LYS:CD	2.45	0.46
37:Md:403:TYR:HE2	37:Md:473:LYS:HE3	1.80	0.46
43:Mj:90:LEU:H	43:Mj:90:LEU:HG	1.50	0.46
53:SE:101:GLY:O	53:SE:189:ARG:NH1	2.47	0.46
58:SK:149:MET:HA	58:SK:149:MET:HE3	1.97	0.46
3:B2:338:SER:HB2	3:B2:405:HIS:HB2	1.98	0.46
6:B5:7:GLY:HA3	6:B5:41:LEU:CD1	2.30	0.46
17:BG:100:GLU:CD	32:BW:144:ARG:CZ	2.88	0.46
23:BM:294:THR:HG23	23:BM:297:LYS:H	1.80	0.46
9:sF:485:LEU:HD12	9:sF:485:LEU:N	2.30	0.46
59:sL:457:LYS:HB2	59:sL:461:ALA:HB2	1.98	0.46
61:E6:890:LEU:HD23	61:E6:895:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:t6:662:VAL:HB	61:t6:695:LEU:HD21	1.98	0.46
3:A2:506:LYS:NZ	3:A2:506:LYS:HD2	2.20	0.46
8:A7:164:ILE:HD11	8:A7:174:LYS:HE3	1.98	0.46
11:AA:900:ASP:OD1	11:AA:900:ASP:N	2.49	0.46
17:AG:12:THR:HA	17:AG:69:GLU:HA	1.97	0.46
29:AT:42:DA:H2"	29:AT:43:DT:C6	2.51	0.46
56:SI:1194:LEU:HD23	56:SI:1194:LEU:HA	1.72	0.46
3:B2:455:GLU:C	3:B2:495:LYS:HG3	2.41	0.46
28:BS:248:ILE:HD12	28:BS:248:ILE:HA	1.79	0.46
35:mb:153:ARG:O	35:mb:157:ASN:ND2	2.48	0.46
45:ml:273:ASN:O	45:ml:275:ARG:NH1	2.48	0.46
55:sH:534:TYR:O	55:sH:538:LEU:HB2	2.16	0.46
60:E3:734:GLU:OE2	61:E6:424:ARG:NH2	2.43	0.46
60:T3:518:SER:O	60:T3:524:GLN:NE2	2.47	0.46
60:t3:789:ASN:OD1	60:t3:846:ASN:ND2	2.47	0.46
61:t6:393:PRO:HA	61:t6:425:TYR:HA	1.97	0.46
3:A2:338:SER:HB2	3:A2:405:HIS:HB2	1.98	0.46
23:AM:14:ARG:HH21	32:AW:126:ILE:CD1	2.19	0.46
23:AM:169:GLU:OE2	23:AM:169:GLU:N	2.45	0.46
27:AR:95:ILE:HD13	27:AR:106:LEU:HD13	1.98	0.46
49:Mp:273:PHE:HB3	49:Mp:278:ILE:HD12	1.97	0.46
51:SD:359:ASN:HA	51:SD:395:VAL:HA	1.98	0.46
55:SH:518:ASN:O	55:SH:526:ARG:NH2	2.49	0.46
58:SK:386:SER:O	58:SK:390:THR:OG1	2.31	0.46
20:BJ:45:CYS:SG	20:BJ:46:CYS:N	2.89	0.46
20:BJ:69:ARG:HE	20:BJ:69:ARG:HA	1.80	0.46
24:BN:-43:DA:H2"	24:BN:-42:DT:C6	2.51	0.46
11:mA:1675:TYR:HD2	45:ml:170:ARG:HD2	1.81	0.46
49:mp:273:PHE:HB3	49:mp:278:ILE:HD12	1.97	0.46
60:E3:903:ILE:CD1	60:T3:429:PHE:HE1	2.25	0.46
61:E6:154:ASP:HA	61:E6:159:ILE:HG22	1.98	0.46
61:E6:446:MET:HE2	61:E6:446:MET:HB2	1.81	0.46
60:T3:1103:LEU:HD22	60:T3:1113:ASN:HD22	1.80	0.46
45:T4:1023:ARG:NH1	45:T4:1027:PHE:O	2.48	0.46
64:t5:849:ARG:O	64:t5:853:LEU:HD23	2.15	0.46
64:t5:950:ASN:HB3	64:t5:954:ARG:HD2	1.98	0.46
8:A7:130:ARG:HD3	8:A7:202:LYS:HA	1.97	0.45
11:AA:1423:GLY:O	11:AA:1427:ASN:ND2	2.48	0.45
12:AB:576:ASP:OD1	12:AB:576:ASP:N	2.46	0.45
14:AD:140:ASP:N	14:AD:140:ASP:OD1	2.49	0.45
20:AJ:45:CYS:SG	20:AJ:46:CYS:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AM:191:GLU:OE2	27:AR:268:MET:HA	2.15	0.45
27:AR:66:ARG:HG3	27:AR:68:VAL:HG23	1.98	0.45
28:AS:201:ILE:O	28:AS:205:ASN:ND2	2.49	0.45
28:AS:248:ILE:HA	28:AS:248:ILE:HD12	1.79	0.45
45:ML:212:PRO:HG3	48:MO:76:PRO:HB2	1.99	0.45
9:SF:460:ILE:HB	9:SF:477:LEU:HB2	1.98	0.45
54:SG:55:UNK:N	54:SG:58:ARG:O	2.48	0.45
56:SI:1255:PHE:O	56:SI:1259:LEU:CB	2.64	0.45
58:SK:239:SER:HB3	58:SK:307:TYR:CZ	2.51	0.45
11:BA:900:ASP:N	11:BA:900:ASP:OD1	2.49	0.45
11:BA:1143:LEU:HD11	11:BA:1216:ILE:HD11	1.98	0.45
17:BG:118:ASP:OD1	17:BG:118:ASP:N	2.50	0.45
18:BH:130:ARG:HA	18:BH:130:ARG:HD2	1.39	0.45
23:BM:301:THR:C	27:BR:271:ARG:NH1	2.66	0.45
43:mj:67:PRO:HA	43:mj:70:PHE:HB3	1.98	0.45
45:ml:92:LEU:HD21	45:ml:148:VAL:HG22	1.98	0.45
49:mp:45:GLU:O	49:mp:53:ARG:N	2.44	0.45
49:mp:105:LEU:O	49:mp:109:THR:OG1	2.32	0.45
53:sE:306:GLN:NE2	9:sF:739:MET:O	2.44	0.45
56:sI:934:ASN:HB3	56:sI:938:MET:HE2	1.97	0.45
58:sK:380:SER:HA	58:sK:381:PRO:HD3	1.87	0.45
45:T4:1058:ASP:OD1	45:T4:1061:GLU:HG2	2.17	0.45
61:T6:506:SER:OG	61:T6:523:GLN:OE1	2.31	0.45
60:t3:783:ILE:O	60:t3:787:ILE:HG12	2.15	0.45
61:t6:322:LYS:HA	61:t6:322:LYS:HD3	1.74	0.45
3:A2:56:GLU:OE2	3:A2:99:ASN:HB2	2.16	0.45
7:A6:358:SER:C	7:A6:359:LEU:HD12	2.41	0.45
12:AB:21:GLU:O	12:AB:22:SER:C	2.59	0.45
12:AB:650:GLU:OE2	12:AB:654:ARG:NH2	2.49	0.45
19:AI:103:CYS:HB2	19:AI:106:CYS:SG	2.56	0.45
23:AM:301:THR:O	27:AR:270:MET:CE	2.65	0.45
27:AR:228:MET:HE2	27:AR:228:MET:HA	1.97	0.45
11:MA:1675:TYR:HD2	45:ML:170:ARG:HD2	1.81	0.45
50:SA:186:VAL:HG22	50:SA:267:LYS:HG3	1.98	0.45
51:SD:432:VAL:HA	51:SD:437:MET:HE3	1.98	0.45
55:SH:534:TYR:O	55:SH:538:LEU:HB2	2.16	0.45
56:SI:1276:PHE:HB3	56:SI:1306:LYS:HD2	1.98	0.45
2:B1:270:TYR:OH	2:B1:280:GLU:OE1	2.31	0.45
7:B6:452:PRO:O	7:B6:456:SER:OG	2.29	0.45
8:B7:605:ILE:HG12	8:B7:669:CYS:HB3	1.97	0.45
8:B7:676:HIS:O	8:B7:722:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BA:7:SER:OG	12:BB:1193:GLN:OE1	2.34	0.45
17:BG:95:SER:HB2	32:BW:144:ARG:HG3	1.98	0.45
19:BI:114:GLN:H	19:BI:115:LYS:HZ3	1.63	0.45
27:BR:98:ASN:OD1	27:BR:103:LYS:HB3	2.15	0.45
53:sE:73:TYR:OH	53:sE:194:GLU:OE1	2.32	0.45
9:sF:524:PHE:CE1	9:sF:602:HIS:CD2	3.04	0.45
55:sH:562:ASN:HD21	56:sI:905:ARG:HA	1.81	0.45
57:sJ:1:MET:HB2	57:sJ:1:MET:HE3	1.81	0.45
60:E3:907:TRP:CE3	60:E3:950:PRO:HB2	2.50	0.45
61:E6:920:ASP:OD1	61:E6:934:ARG:NH1	2.49	0.45
64:T5:937:SER:O	64:T5:943:LEU:HD12	2.17	0.45
64:T5:950:ASN:HB3	64:T5:954:ARG:HD2	1.98	0.45
63:t2:77:LYS:HA	63:t2:80:GLN:NE2	2.30	0.45
2:A1:483:LYS:HA	2:A1:483:LYS:HD3	1.81	0.45
3:A2:134:LEU:HD12	3:A2:134:LEU:HA	1.68	0.45
8:A7:626:PHE:HE2	8:A7:628:TYR:CE1	2.31	0.45
12:AB:108:VAL:HA	23:AM:241:ARG:HH11	1.74	0.45
14:AD:158:GLU:HG3	35:Mb:49:ARG:NE	2.32	0.45
18:AH:40:LEU:HD13	18:AH:123:MET:HG3	1.99	0.45
53:SE:306:GLN:NE2	9:SF:739:MET:O	2.44	0.45
1:B0:86:LEU:O	1:B0:90:MET:HG2	2.16	0.45
11:BA:362:ASP:OD1	11:BA:362:ASP:N	2.48	0.45
12:BB:108:VAL:HA	23:BM:241:ARG:HH11	1.74	0.45
13:BC:217:ASP:N	13:BC:217:ASP:OD1	2.49	0.45
14:BD:158:GLU:HG3	35:mb:49:ARG:NE	2.31	0.45
24:BN:-74:DT:H2"	24:BN:-73:DT:C5	2.52	0.45
27:BR:63:ARG:HE	27:BR:66:ARG:HB2	1.81	0.45
50:sA:186:VAL:HG22	50:sA:267:LYS:HG3	1.98	0.45
50:sA:557:ILE:HG21	51:sB:563:LEU:HD21	1.97	0.45
51:sD:359:ASN:HA	51:sD:395:VAL:HA	1.98	0.45
61:E6:596:LEU:HD23	61:E6:599:LEU:HD12	1.98	0.45
60:T3:869:ARG:NH2	60:T3:882:LEU:HD23	2.31	0.45
60:t3:1087:SER:OG	60:t3:1088:PHE:N	2.47	0.45
45:t4:1058:ASP:OD1	45:t4:1061:GLU:HG2	2.17	0.45
1:A0:199:MET:HE2	1:A0:199:MET:N	2.31	0.45
6:A5:53:GLU:HB2	6:A5:56:ARG:CZ	2.46	0.45
7:A6:246:ASP:OD1	7:A6:246:ASP:N	2.49	0.45
12:AB:100:PRO:HA	12:AB:126:SER:HB3	1.97	0.45
38:Me:231:GLU:OE1	38:Me:233:GLN:NE2	2.47	0.45
53:SE:511:GLN:HA	53:SE:514:GLU:OE2	2.16	0.45
1:B0:523:GLY:O	1:B0:527:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B0:553:MET:HB3	1:B0:557:MET:HE1	1.98	0.45
3:B2:197:ASN:OD1	3:B2:198:SER:N	2.50	0.45
7:B6:358:SER:C	7:B6:359:LEU:HD12	2.41	0.45
7:B6:429:CYS:HB3	7:B6:432:CYS:SG	2.56	0.45
11:BA:68:GLN:NE2	32:BW:151:LEU:HD13	2.31	0.45
11:BA:219:PHE:HA	11:BA:222:LEU:HB2	1.98	0.45
18:BH:108:SER:OG	18:BH:111:LEU:N	2.50	0.45
27:BR:73:LEU:HG	27:BR:74:PRO:O	2.17	0.45
28:BS:209:LYS:HA	28:BS:210:ASN:HA	1.84	0.45
29:BT:42:DA:H2"	29:BT:43:DT:C6	2.51	0.45
55:sH:518:ASN:O	55:sH:526:ARG:NH2	2.49	0.45
60:T3:364:SER:HB2	60:T3:366:LEU:HD13	1.98	0.45
61:T6:322:LYS:HD3	61:T6:322:LYS:HA	1.74	0.45
60:t3:775:LYS:HB2	60:t3:826:PHE:HE1	1.81	0.45
3:A2:174:GLU:HG3	3:A2:183:LYS:HB3	1.99	0.45
4:A3:9:ASN:HB2	4:A3:12:MET:HE3	1.98	0.45
17:AG:137:ILE:HG12	17:AG:170:ALA:HB2	1.99	0.45
27:AR:63:ARG:HE	27:AR:66:ARG:HB2	1.81	0.45
28:AS:227:PHE:HA	28:AS:230:THR:CG2	2.47	0.45
28:AS:227:PHE:HD1	28:AS:230:THR:CG2	2.29	0.45
56:SI:934:ASN:HB3	56:SI:938:MET:HE2	1.97	0.45
19:BI:104:LEU:HD13	19:BI:104:LEU:HD22	1.87	0.45
40:mg:35:ASP:N	40:mg:35:ASP:OD1	2.48	0.45
49:mp:45:GLU:HB3	49:mp:53:ARG:HB2	1.98	0.45
53:sE:511:GLN:HA	53:sE:514:GLU:OE2	2.16	0.45
55:sH:593:LYS:HD3	55:sH:593:LYS:HA	1.58	0.45
58:sK:238:VAL:HG21	58:sK:404:MET:SD	2.56	0.45
60:E3:444:ILE:O	60:E3:448:ILE:HG12	2.15	0.45
60:T3:289:LYS:HB3	60:T3:290:LEU:HD22	1.97	0.45
60:t3:306:TRP:HD1	60:t3:580:SER:HA	1.80	0.45
3:A2:197:ASN:OD1	3:A2:198:SER:N	2.50	0.45
11:AA:890:ASP:OD1	11:AA:940:ARG:NH2	2.50	0.45
11:AA:1144:LYS:HZ3	11:AA:1268:LEU:HB3	1.80	0.45
13:AC:217:ASP:N	13:AC:217:ASP:OD1	2.49	0.45
27:AR:73:LEU:HG	27:AR:74:PRO:O	2.17	0.45
29:AT:60:DT:H2"	29:AT:61:DA:H8	1.81	0.45
45:MI:563:HIS:O	45:MI:567:THR:OG1	2.30	0.45
50:SA:335:TYR:CD1	51:SB:727:LEU:HD11	2.46	0.45
1:B0:25:MET:HE1	1:B0:51:SER:O	2.17	0.45
1:B0:465:PRO:HG2	1:B0:468:MET:HB2	1.99	0.45
4:B3:9:ASN:HB2	4:B3:12:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B7:162:GLU:N	8:B7:174:LYS:O	2.49	0.45
12:BB:21:GLU:O	12:BB:22:SER:C	2.59	0.45
12:BB:650:GLU:OE2	12:BB:654:ARG:NH2	2.49	0.45
14:BD:140:ASP:OD1	14:BD:140:ASP:N	2.49	0.45
23:BM:301:THR:O	27:BR:270:MET:CE	2.65	0.45
50:sA:377:SER:HB2	50:sA:403:LEU:HD22	1.99	0.45
56:sI:1255:PHE:O	56:sI:1259:LEU:CB	2.64	0.45
60:E3:439:ILE:HD12	60:E3:439:ILE:HG23	1.69	0.45
61:E6:113:TRP:CZ3	61:E6:446:MET:HE3	2.45	0.45
60:t3:288:MET:HG2	60:t3:292:ARG:NH1	2.32	0.45
11:AA:7:SER:OG	12:AB:1193:GLN:OE1	2.34	0.45
11:AA:219:PHE:HA	11:AA:222:LEU:HB2	1.98	0.45
49:Mp:61:ILE:HD12	49:Mp:128:ASP:HB2	1.99	0.45
9:SF:524:PHE:CE1	9:SF:602:HIS:CD2	3.04	0.45
54:SG:128:TYR:HB2	56:SI:940:ARG:HH21	1.82	0.45
57:SJ:89:ARG:HH21	57:SJ:93:LYS:HD2	1.80	0.45
8:B7:181:TYR:OH	8:B7:336:PRO:O	2.33	0.45
11:BA:20:GLY:O	12:BB:1213:THR:OG1	2.27	0.45
12:BB:879:ARG:HA	12:BB:885:MET:HE1	1.98	0.45
17:BG:89:GLY:HA3	17:BG:103:VAL:HG22	1.99	0.45
25:BO:202:ILE:HD11	25:BO:222:GLU:HG2	1.98	0.45
28:BS:163:GLU:HG2	28:BS:215:LYS:HD3	1.98	0.45
28:BS:244:LYS:HA	28:BS:247:GLU:HG2	1.99	0.45
41:mh:186:ASP:N	41:mh:186:ASP:OD1	2.50	0.45
9:sF:624:ASP:O	9:sF:627:SER:OG	2.32	0.45
63:T2:48:ASN:O	63:T2:52:GLN:NE2	2.50	0.45
61:t6:739:LYS:HZ3	61:t6:799:ASN:CG	2.25	0.45
2:A1:582:LEU:O	2:A1:586:LEU:HD23	2.16	0.45
3:A2:261:GLN:HG2	3:A2:263:HIS:N	2.22	0.45
8:A7:351:ASP:OD1	8:A7:405:LYS:NZ	2.50	0.45
12:AB:227:LYS:H	12:AB:395:GLN:HE21	1.65	0.45
24:AN:-43:DA:H2"	24:AN:-42:DT:C6	2.51	0.45
26:AQ:105:ALA:H	27:AR:89:GLY:HA2	1.80	0.45
34:Ma:195:GLN:OE1	34:Ma:198:GLN:NE2	2.41	0.45
45:MI:354:GLU:OE1	45:MI:358:LYS:NZ	2.48	0.45
50:SA:536:ASN:HB3	50:SA:539:MET:HG2	1.98	0.45
9:SF:311:THR:HA	56:SI:657:LYS:N	2.32	0.45
58:SK:404:MET:HA	58:SK:404:MET:HE3	1.98	0.45
2:B1:582:LEU:O	2:B1:586:LEU:HD23	2.16	0.45
3:B2:213:THR:O	3:B2:216:MET:N	2.50	0.45
7:B6:246:ASP:N	7:B6:246:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BH:40:LEU:HD13	18:BH:123:MET:HG3	1.99	0.45
23:BM:273:SER:O	23:BM:276:THR:OG1	2.35	0.45
28:BS:227:PHE:HD1	28:BS:230:THR:CG2	2.29	0.45
32:BW:116:ASN:O	32:BW:118:GLU:N	2.47	0.45
44:mk:21:GLN:OE1	44:mk:66:ARG:NH2	2.39	0.45
45:ml:771:ILE:HG23	45:ml:778:ILE:HG22	1.99	0.45
50:sA:536:ASN:HB3	50:sA:539:MET:HG2	1.98	0.45
64:T5:922:THR:HG23	64:T5:925:ALA:H	1.82	0.45
4:A3:133:LEU:HD12	4:A3:134:ARG:HG3	1.99	0.45
45:Ml:771:ILE:HG23	45:Ml:778:ILE:HG22	1.99	0.45
53:SE:508:LYS:N	53:SE:511:GLN:OE1	2.49	0.45
56:SI:712:MET:HE3	56:SI:712:MET:CA	2.47	0.45
11:BA:1196:GLU:OE1	11:BA:1235:LYS:NZ	2.41	0.45
26:BQ:105:ALA:H	27:BR:89:GLY:HA2	1.80	0.45
49:mp:61:ILE:HD12	49:mp:128:ASP:HB2	1.99	0.45
53:sE:463:PRO:O	53:sE:466:ILE:HG12	2.17	0.45
56:sI:1276:PHE:HB3	56:sI:1306:LYS:HD2	1.98	0.45
59:sL:283:THR:HG22	59:sL:293:LYS:HB3	1.98	0.45
61:T6:176:ASN:OD1	61:T6:176:ASN:N	2.49	0.45
61:T6:825:PRO:HA	61:T6:826:PRO:HD3	1.85	0.45
61:t6:187:ASN:HB3	61:t6:245:ASN:HB3	1.99	0.45
3:A2:90:ASN:OD1	3:A2:97:MET:HB2	2.17	0.45
3:A2:213:THR:O	3:A2:216:MET:N	2.50	0.45
12:AB:474:SER:O	12:AB:476:ARG:N	2.50	0.45
28:AS:244:LYS:HA	28:AS:247:GLU:HG2	1.99	0.45
58:SK:238:VAL:HG21	58:SK:404:MET:SD	2.56	0.45
58:SK:389:LEU:HG	58:SK:421:LEU:HB3	1.99	0.45
59:SL:283:THR:HG22	59:SL:293:LYS:HB3	1.98	0.45
3:B2:253:MET:HE3	3:B2:256:TYR:HB2	1.99	0.45
23:BM:303:GLN:HE21	27:BR:271:ARG:HA	0.69	0.45
37:md:23:PRO:HB2	37:md:86:LEU:HD11	1.99	0.45
45:ml:423:SER:HG	45:ml:444:ASN:HD21	1.60	0.45
51:sD:432:VAL:HA	51:sD:437:MET:HE3	1.98	0.45
53:sE:487:LYS:O	53:sE:490:THR:OG1	2.30	0.45
60:E3:959:LEU:HD12	60:E3:960:ASP:N	2.32	0.45
61:T6:181:GLN:HB2	61:T6:183:ARG:HH11	1.82	0.45
1:A0:25:MET:HE1	1:A0:51:SER:O	2.17	0.44
3:A2:455:GLU:C	3:A2:495:LYS:HG3	2.41	0.44
32:AW:42:ASP:OD2	32:AW:217:TYR:OH	2.34	0.44
8:B7:351:ASP:OD1	8:B7:405:LYS:NZ	2.50	0.44
23:BM:191:GLU:OE2	27:BR:268:MET:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BQ:105:ALA:HB2	26:BQ:386:MET:HE3	2.00	0.44
32:BW:42:ASP:OD2	32:BW:217:TYR:OH	2.34	0.44
45:ml:212:PRO:HG3	48:mo:76:PRO:HB2	1.99	0.44
51:sD:771:LYS:HA	51:sD:774:LEU:HG	2.00	0.44
53:sE:302:ILE:HD12	9:sF:657:ALA:HB2	1.98	0.44
9:sF:311:THR:HA	56:sI:657:LYS:N	2.32	0.44
60:T3:288:MET:HG2	60:T3:292:ARG:NH1	2.32	0.44
60:T3:775:LYS:HB2	60:T3:826:PHE:HE1	1.81	0.44
61:T6:187:ASN:HB3	61:T6:245:ASN:HB3	1.99	0.44
63:t2:77:LYS:HA	63:t2:80:GLN:CD	2.42	0.44
60:t3:532:VAL:HB	60:t3:537:GLN:HE21	1.82	0.44
61:t6:506:SER:OG	61:t6:523:GLN:OE1	2.31	0.44
2:A1:167:ASP:OD1	2:A1:167:ASP:N	2.50	0.44
12:AB:107:GLY:O	23:AM:241:ARG:CD	2.61	0.44
12:AB:451:LYS:HE2	12:AB:451:LYS:HB2	1.71	0.44
18:AH:108:SER:OG	18:AH:111:LEU:N	2.50	0.44
18:AH:110:ASP:HA	43:Mj:83:LEU:CG	2.33	0.44
23:AM:273:SER:O	23:AM:276:THR:OG1	2.35	0.44
45:MI:89:GLN:HB3	45:MI:90:VAL:H	1.67	0.44
50:SA:377:SER:HB2	50:SA:403:LEU:HD22	1.99	0.44
51:SB:377:ALA:HA	51:SB:380:ARG:HH21	1.82	0.44
53:SE:99:LYS:NZ	53:SE:209:ASP:O	2.45	0.44
55:SH:623:LYS:O	55:SH:627:LEU:HD23	2.18	0.44
1:B0:195:ILE:O	1:B0:199:MET:HE3	2.18	0.44
3:B2:56:GLU:OE2	3:B2:99:ASN:HB2	2.16	0.44
5:B4:126:VAL:HA	5:B4:129:ILE:HG22	2.00	0.44
8:B7:612:VAL:HG11	8:B7:628:TYR:CZ	2.51	0.44
11:BA:880:LYS:HA	11:BA:955:PRO:HA	2.00	0.44
12:BB:15:PRO:HD3	64:t5:922:THR:HB	1.99	0.44
28:BS:201:ILE:O	28:BS:205:ASN:ND2	2.49	0.44
28:BS:227:PHE:HD1	28:BS:230:THR:HG21	1.80	0.44
29:BT:60:DT:H2"	29:BT:61:DA:H8	1.81	0.44
38:me:231:GLU:OE1	38:me:233:GLN:NE2	2.47	0.44
49:mp:276:ASP:HB2	49:mp:320:THR:HG22	1.99	0.44
51:sD:410:SER:OG	51:sD:411:GLN:N	2.51	0.44
9:sF:313:GLN:HG2	56:sI:660:ILE:HG23	1.99	0.44
55:sH:439:LYS:O	56:sI:661:VAL:N	2.50	0.44
57:sJ:88:ASP:OD2	57:sJ:90:ARG:NH2	2.50	0.44
45:T4:1003:PHE:CZ	45:T4:1019:MET:HG3	2.52	0.44
12:AB:1121:GLY:O	12:AB:1126:GLY:N	2.48	0.44
12:AB:1165:ILE:HD12	12:AB:1185:CYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AU:247:LEU:HD23	31:AV:118:SER:HA	2.00	0.44
50:SA:490:VAL:HG13	51:SD:682:LEU:HD12	1.99	0.44
51:SB:776:LYS:NZ	51:SB:777:PRO:O	2.46	0.44
9:SF:470:ARG:O	9:SF:470:ARG:NH1	2.44	0.44
11:BA:1120:LEU:HD11	11:BA:1306:LEU:HG	1.99	0.44
12:BB:130:VAL:HB	12:BB:167:ILE:HD11	1.99	0.44
17:BG:137:ILE:HG12	17:BG:170:ALA:HB2	1.99	0.44
27:BR:63:ARG:NE	27:BR:66:ARG:HB2	2.32	0.44
51:sB:377:ALA:HA	51:sB:380:ARG:HH21	1.82	0.44
55:sH:623:LYS:O	55:sH:627:LEU:HD23	2.18	0.44
58:sK:404:MET:HA	58:sK:404:MET:HE3	1.98	0.44
61:E6:51:LEU:HD22	61:E6:131:THR:HG21	1.99	0.44
60:t3:731:LEU:HD23	60:t3:731:LEU:HA	1.86	0.44
64:t5:922:THR:HG23	64:t5:925:ALA:H	1.82	0.44
1:A0:195:ILE:O	1:A0:199:MET:HE3	2.18	0.44
2:A1:270:TYR:OH	2:A1:280:GLU:OE1	2.31	0.44
8:A7:228:LYS:HG3	8:A7:233:PHE:H	1.81	0.44
8:A7:373:MET:HE1	8:A7:511:LEU:HD11	2.00	0.44
8:A7:410:LEU:HD11	8:A7:485:ILE:HD11	1.98	0.44
12:AB:102:VAL:HG21	12:AB:122:LEU:HD13	1.99	0.44
49:Mp:74:ILE:HG22	49:Mp:108:LEU:HD22	1.99	0.44
51:SD:606:PRO:O	51:SD:610:THR:OG1	2.35	0.44
53:SE:302:ILE:HD12	9:SF:657:ALA:HB2	1.98	0.44
53:SE:532:ASN:ND2	53:SE:543:ILE:HD12	2.32	0.44
53:SE:543:ILE:HG23	9:SF:756:ASN:HD22	1.83	0.44
55:SH:439:LYS:O	56:SI:661:VAL:N	2.50	0.44
57:SJ:88:ASP:OD2	57:SJ:90:ARG:NH2	2.50	0.44
8:B7:121:LEU:HD13	8:B7:204:PRO:HD2	2.00	0.44
8:B7:410:LEU:HD11	8:B7:485:ILE:HD11	1.98	0.44
12:BB:1156:ASP:OD1	12:BB:1156:ASP:N	2.48	0.44
18:BH:106:GLU:OE2	43:mj:83:LEU:HD12	2.10	0.44
19:BI:76:PRO:HB2	19:BI:77:LYS:HZ3	1.82	0.44
20:BJ:31:ASP:OD1	20:BJ:31:ASP:N	2.50	0.44
23:BM:301:THR:O	27:BR:270:MET:HE1	2.18	0.44
45:ml:728:LEU:HB2	45:ml:733:ILE:HD11	1.99	0.44
50:sA:402:LYS:HD2	50:sA:403:LEU:HD23	2.00	0.44
59:sL:327:LYS:HZ2	59:sL:405:THR:H	1.65	0.44
61:E6:890:LEU:HD11	61:E6:894:ASN:ND2	2.31	0.44
45:T4:985:GLU:OE1	45:T4:1002:HIS:NE2	2.50	0.44
63:t2:48:ASN:O	63:t2:52:GLN:NE2	2.50	0.44
60:t3:578:ILE:O	60:t3:581:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:t6:176:ASN:OD1	61:t6:176:ASN:N	2.49	0.44
1:A0:553:MET:HB3	1:A0:557:MET:HE1	1.98	0.44
4:A3:119:LYS:O	4:A3:123:GLY:N	2.51	0.44
7:A6:429:CYS:HB3	7:A6:432:CYS:SG	2.56	0.44
12:AB:185:THR:OG1	12:AB:186:GLU:N	2.51	0.44
23:AM:191:GLU:OE2	27:AR:268:MET:C	2.60	0.44
24:AN:-74:DT:H2"	24:AN:-73:DT:C5	2.52	0.44
28:AS:267:ASP:N	28:AS:267:ASP:OD1	2.50	0.44
44:Mk:19:GLN:HA	44:Mk:22:VAL:HG12	2.00	0.44
49:Mp:276:ASP:HB2	49:Mp:320:THR:HG22	1.99	0.44
51:SD:383:LYS:HD3	51:SD:383:LYS:HA	1.79	0.44
55:SH:562:ASN:HD21	56:SI:905:ARG:HA	1.81	0.44
59:SL:286:ASP:OD1	59:SL:290:ASN:N	2.44	0.44
3:B2:174:GLU:HG3	3:B2:183:LYS:HB3	1.99	0.44
4:B3:133:LEU:HD12	4:B3:134:ARG:HG3	1.99	0.44
5:B4:36:LEU:O	5:B4:39:THR:OG1	2.33	0.44
12:BB:13:GLU:O	64:t5:922:THR:OG1	2.36	0.44
12:BB:16:TYR:HB3	12:BB:17:GLY:H	1.69	0.44
38:me:266:ASP:N	38:me:266:ASP:OD1	2.49	0.44
44:mk:19:GLN:HA	44:mk:22:VAL:HG12	2.00	0.44
49:mp:74:ILE:HG22	49:mp:108:LEU:HD22	1.99	0.44
3:A2:253:MET:HE3	3:A2:256:TYR:HB2	1.98	0.44
13:AC:4:GLU:HG3	13:AC:7:GLN:HE22	1.83	0.44
15:AE:58:MET:HE2	15:AE:58:MET:HA	2.00	0.44
17:AG:118:ASP:OD1	17:AG:118:ASP:N	2.50	0.44
18:AH:106:GLU:OE2	43:Mj:83:LEU:HD12	2.10	0.44
26:AQ:105:ALA:HB2	26:AQ:386:MET:HE3	2.00	0.44
26:AQ:440:ARG:NH1	27:AR:199:ASP:OD1	2.51	0.44
27:AR:63:ARG:NE	27:AR:66:ARG:HB2	2.32	0.44
35:Mb:80:THR:HG21	40:Mg:52:THR:HG21	2.00	0.44
42:Mi:161:LEU:HD12	42:Mi:161:LEU:HA	1.83	0.44
44:Mk:128:LYS:HG3	47:Mn:67:ILE:HG13	2.00	0.44
45:MI:564:VAL:HG12	45:MI:568:MET:HE2	2.00	0.44
50:SA:402:LYS:HD2	50:SA:403:LEU:HD23	2.00	0.44
51:SB:559:GLU:O	51:SB:563:LEU:HD23	2.18	0.44
3:B2:408:MET:HG3	3:B2:409:ARG:HD3	1.99	0.44
11:BA:212:LYS:HB2	11:BA:212:LYS:HE3	1.84	0.44
11:BA:1444:MET:HE2	17:BG:58:ARG:HD2	2.00	0.44
12:BB:474:SER:O	12:BB:476:ARG:N	2.50	0.44
14:BD:213:GLU:CG	35:mb:38:MET:SD	2.94	0.44
25:BO:214:LEU:HB3	25:BO:223:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BS:227:PHE:HA	28:BS:230:THR:CG2	2.47	0.44
28:BS:267:ASP:OD1	28:BS:267:ASP:N	2.50	0.44
29:BT:57:DA:H2''	29:BT:58:DA:H2'	1.99	0.44
43:mj:108:ASN:OD1	43:mj:112:LYS:NZ	2.51	0.44
50:sA:490:VAL:HG13	51:sD:682:LEU:HD12	1.99	0.44
56:sI:1207:LEU:HA	56:sI:1210:ILE:HG12	2.00	0.44
60:T3:532:VAL:HB	60:T3:537:GLN:HE21	1.82	0.44
64:t5:937:SER:O	64:t5:943:LEU:HD12	2.17	0.44
1:A0:86:LEU:O	1:A0:90:MET:HG2	2.16	0.44
5:A4:126:VAL:HA	5:A4:129:ILE:HG22	2.00	0.44
11:AA:1267:MET:HA	11:AA:1271:ILE:HG12	1.99	0.44
45:MI:728:LEU:HB2	45:MI:733:ILE:HD11	1.99	0.44
52:SC:96:ASP:OD2	56:SI:884:TYR:OH	2.34	0.44
51:SD:626:MET:HA	51:SD:626:MET:HE2	2.00	0.44
12:BB:1048:THR:HG22	12:BB:1050:ILE:HG12	2.00	0.44
12:BB:1121:GLY:O	12:BB:1126:GLY:N	2.48	0.44
13:BC:23:SER:OG	13:BC:24:ASN:N	2.51	0.44
13:BC:33:LEU:O	13:BC:37:MET:HG3	2.17	0.44
11:mA:1606:SER:HA	11:mA:1607:PRO:HD3	1.88	0.44
49:mp:101:SER:OG	49:mp:106:ASN:ND2	2.51	0.44
51:sB:559:GLU:O	51:sB:563:LEU:HD23	2.18	0.44
60:E3:675:GLU:OE2	60:E3:678:ASN:HB2	2.17	0.44
60:E3:956:ARG:HH21	60:E3:959:LEU:CD1	2.27	0.44
61:E6:575:THR:HG22	61:E6:883:LEU:HD23	1.99	0.44
63:T2:34:ASN:N	63:T2:34:ASN:OD1	2.46	0.44
63:T2:77:LYS:HA	63:T2:80:GLN:CD	2.42	0.44
61:T6:662:VAL:HB	61:T6:695:LEU:HD21	1.98	0.44
61:T6:739:LYS:HZ3	61:T6:799:ASN:CG	2.26	0.44
60:t3:359:TYR:HE2	60:t3:913:THR:HB	1.83	0.44
45:t4:1003:PHE:CZ	45:t4:1019:MET:HG3	2.52	0.44
61:t6:138:ARG:HD3	61:t6:138:ARG:HA	1.79	0.44
11:AA:880:LYS:HA	11:AA:955:PRO:HA	2.00	0.44
11:AA:1196:GLU:OE1	11:AA:1235:LYS:NZ	2.40	0.44
17:AG:163:ILE:HA	17:AG:168:LEU:HD23	1.99	0.44
19:AI:51:ASN:OD1	19:AI:52:ILE:N	2.41	0.44
23:AM:154:TYR:HE1	23:AM:172:MET:CE	2.27	0.44
23:AM:301:THR:O	27:AR:270:MET:HE1	2.18	0.44
31:AV:26:LEU:HB3	31:AV:32:ILE:HG21	1.99	0.44
37:Md:23:PRO:HB2	37:Md:86:LEU:HD11	1.99	0.44
45:MI:428:THR:OG1	45:MI:443:ASP:OD2	2.27	0.44
49:Mp:339:SER:HA	49:Mp:342:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:676:GLU:O	51:SB:680:ASN:ND2	2.51	0.44
53:SE:463:PRO:O	53:SE:466:ILE:HG12	2.17	0.44
56:SI:1251:LYS:HA	56:SI:1251:LYS:HD3	1.78	0.44
2:B1:167:ASP:N	2:B1:167:ASP:OD1	2.50	0.44
11:BA:67:CYS:O	11:BA:70:CYS:N	2.42	0.44
23:BM:293:ILE:HG23	23:BM:297:LYS:HD3	2.00	0.44
27:BR:66:ARG:HG3	27:BR:68:VAL:HG23	1.98	0.44
34:ma:124:ASP:N	34:ma:124:ASP:OD1	2.51	0.44
34:ma:195:GLN:OE1	34:ma:198:GLN:NE2	2.41	0.44
39:mf:25:SER:HA	39:mf:28:ILE:HD12	1.99	0.44
53:sE:543:ILE:HG23	9:sF:756:ASN:HD22	1.83	0.44
54:sG:128:TYR:HB2	56:sI:940:ARG:HH21	1.82	0.44
60:E3:939:THR:O	60:T3:429:PHE:CZ	2.71	0.44
60:T3:731:LEU:HD23	60:T3:731:LEU:HA	1.86	0.44
45:T4:902:ASN:O	45:T4:905:HIS:ND1	2.44	0.44
3:A2:125:VAL:HG22	3:A2:238:LYS:HB2	2.00	0.44
3:A2:368:ALA:O	3:A2:375:LEU:HD23	2.18	0.44
11:AA:663:SER:OG	11:AA:664:THR:N	2.51	0.44
12:AB:177:LYS:HE3	27:AR:251:ARG:HH21	1.83	0.44
12:AB:293:PRO:HG2	12:AB:296:GLU:HB2	1.99	0.44
14:AD:71:LYS:HA	14:AD:74:GLN:HG2	2.00	0.44
51:SB:712:ARG:HA	51:SB:715:LEU:HD12	2.00	0.44
3:B2:90:ASN:OD1	3:B2:97:MET:HB2	2.17	0.44
4:B3:49:LEU:CB	17:BG:164:LYS:CG	2.95	0.44
11:BA:663:SER:OG	11:BA:664:THR:N	2.51	0.44
11:BA:739:ASP:OD2	18:BH:19:ARG:NH2	2.51	0.44
11:BA:1172:LEU:HA	28:BS:203:TYR:HE2	1.83	0.44
19:BI:113:ASP:HB3	19:BI:114:GLN:H	1.75	0.44
21:BK:102:LYS:O	21:BK:105:PHE:N	2.49	0.44
28:BS:236:LEU:HB2	28:BS:237:ALA:H	1.65	0.44
30:BU:247:LEU:HD23	31:BV:118:SER:HA	2.00	0.44
35:mb:80:THR:HG21	40:mg:52:THR:HG21	2.00	0.44
36:mc:3:PRO:HA	36:mc:4:PRO:HD3	1.92	0.44
37:md:276:ASN:HD22	40:mg:50:VAL:HG22	1.83	0.44
44:mk:128:LYS:HG3	47:mn:67:ILE:HG13	2.00	0.44
61:E6:682:ASN:OD1	61:E6:684:LYS:N	2.51	0.44
61:T6:222:GLN:NE2	61:T6:223:GLN:O	2.51	0.44
3:A2:434:PRO:HA	3:A2:435:PRO:HD3	1.94	0.43
8:A7:121:LEU:HD13	8:A7:204:PRO:HD2	2.00	0.43
11:AA:1444:MET:HE2	17:AG:58:ARG:HD2	2.00	0.43
28:AS:184:LYS:HA	28:AS:228:LEU:CD1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:MA:1668:TYR:OH	11:MA:1672:SER:O	2.34	0.43
39:Mf:144:SER:OG	39:Mf:145:SER:N	2.51	0.43
41:Mh:206:ILE:HD12	41:Mh:207:PRO:HD2	2.00	0.43
43:Mj:108:ASN:OD1	43:Mj:112:LYS:NZ	2.51	0.43
49:Mp:45:GLU:O	49:Mp:53:ARG:N	2.44	0.43
57:SJ:28:ASP:HA	57:SJ:61:LYS:HZ2	1.83	0.43
7:B6:214:LEU:HD13	7:B6:250:THR:HG21	2.00	0.43
8:B7:164:ILE:HD11	8:B7:174:LYS:HE3	1.98	0.43
8:B7:228:LYS:HG3	8:B7:233:PHE:H	1.81	0.43
8:B7:688:GLY:HA2	8:B7:691:LEU:HG	2.00	0.43
11:BA:122:MET:HA	11:BA:125:ALA:HB3	2.00	0.43
49:mp:157:ASN:HD21	60:E3:495:ASN:ND2	2.06	0.43
51:sB:776:LYS:NZ	51:sB:777:PRO:O	2.46	0.43
51:sD:626:MET:HA	51:sD:626:MET:HE2	2.00	0.43
53:sE:312:LEU:HD12	53:sE:312:LEU:HA	1.83	0.43
60:T3:578:ILE:O	60:T3:581:PHE:N	2.50	0.43
62:t1:31:LYS:HA	62:t1:34:VAL:HG12	2.00	0.43
45:t4:985:GLU:OE1	45:t4:1002:HIS:NE2	2.50	0.43
61:t6:181:GLN:HB2	61:t6:183:ARG:HH11	1.82	0.43
61:t6:222:GLN:NE2	61:t6:223:GLN:O	2.51	0.43
7:A6:130:LEU:HB2	7:A6:173:ILE:HG22	2.00	0.43
8:A7:162:GLU:N	8:A7:174:LYS:O	2.49	0.43
11:AA:74:MET:HE2	11:AA:74:MET:N	2.34	0.43
11:AA:408:ASP:OD1	11:AA:408:ASP:N	2.51	0.43
17:AG:91:VAL:HB	17:AG:139:ILE:HA	2.00	0.43
18:AH:130:ARG:HA	18:AH:130:ARG:HD2	1.39	0.43
19:AI:76:PRO:HB2	19:AI:77:LYS:HZ1	1.83	0.43
38:Me:266:ASP:N	38:Me:266:ASP:OD1	2.49	0.43
9:SF:313:GLN:HG2	56:SI:660:ILE:HG23	1.99	0.43
1:B0:199:MET:HE2	1:B0:199:MET:N	2.32	0.43
1:B0:695:LYS:HA	1:B0:698:ALA:HB3	2.01	0.43
8:B7:477:LEU:HA	8:B7:482:TRP:HE1	1.83	0.43
12:BB:177:LYS:HE3	27:BR:251:ARG:HH21	1.83	0.43
12:BB:1165:ILE:HD12	12:BB:1185:CYS:HB3	1.99	0.43
13:BC:54:ASN:ND2	13:BC:60:ASP:OD1	2.47	0.43
19:BI:117:LYS:HB2	19:BI:117:LYS:HE2	1.65	0.43
26:BQ:440:ARG:NH1	27:BR:199:ASP:OD1	2.51	0.43
41:mh:97:LEU:HA	41:mh:100:ILE:HG22	2.00	0.43
51:sB:308:PRO:HG2	51:sB:389:GLY:HA3	2.00	0.43
51:sB:676:GLU:O	51:sB:680:ASN:ND2	2.51	0.43
55:sH:473:ASP:OD1	55:sH:473:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:260:ALA:HB2	1:A0:398:ALA:HB3	2.00	0.43
1:A0:564:TRP:HE1	2:A1:232:ASN:HB2	1.83	0.43
3:A2:30:ALA:O	3:A2:33:LEU:HG	2.18	0.43
8:A7:711:LYS:HA	8:A7:716:MET:CE	2.46	0.43
11:AA:252:PHE:CE2	11:AA:256:GLN:HG3	2.53	0.43
25:AO:214:LEU:HB3	25:AO:223:ILE:HD11	1.99	0.43
28:AS:176:LYS:O	28:AS:179:GLU:HG3	2.18	0.43
41:Mh:97:LEU:HA	41:Mh:100:ILE:HG22	2.00	0.43
41:Mh:186:ASP:OD1	41:Mh:186:ASP:N	2.50	0.43
50:SA:314:LEU:HB3	50:SA:388:LEU:HD11	2.01	0.43
3:B2:229:GLY:O	3:B2:279:THR:OG1	2.27	0.43
7:B6:130:LEU:HB2	7:B6:173:ILE:HG22	2.00	0.43
11:BA:1267:MET:HA	11:BA:1271:ILE:HG12	1.99	0.43
12:BB:185:THR:OG1	12:BB:186:GLU:N	2.51	0.43
17:BG:94:CYS:HB3	17:BG:128:PRO:HB2	2.00	0.43
51:sB:779:THR:OG1	51:sB:780:LEU:N	2.51	0.43
62:T1:40:LEU:HA	62:T1:40:LEU:HD13	1.69	0.43
61:T6:350:VAL:HG23	61:T6:379:CYS:HB3	1.99	0.43
45:t4:840:THR:HA	45:t4:843:VAL:HG12	2.00	0.43
3:A2:408:MET:HG3	3:A2:409:ARG:HD3	1.99	0.43
3:A2:463:GLU:HA	9:SF:400:GLN:C	2.44	0.43
11:AA:894:GLU:OE1	11:AA:906:HIS:NE2	2.51	0.43
18:AH:109:LYS:HD2	18:AH:109:LYS:HA	1.68	0.43
20:AJ:31:ASP:OD1	20:AJ:31:ASP:N	2.50	0.43
32:AW:111:ASP:HA	32:AW:114:ASP:HB2	2.01	0.43
55:SH:592:LEU:CD1	55:SH:592:LEU:HB2	2.41	0.43
56:SI:1207:LEU:HA	56:SI:1210:ILE:HG12	1.99	0.43
58:SK:206:ASP:C	58:SK:207:MET:HE2	2.43	0.43
12:BB:102:VAL:HG21	12:BB:122:LEU:HD13	1.99	0.43
17:BG:91:VAL:HB	17:BG:139:ILE:HA	2.00	0.43
18:BH:109:LYS:HD2	18:BH:109:LYS:HA	1.68	0.43
23:BM:154:TYR:HE1	23:BM:172:MET:CE	2.27	0.43
58:sK:226:THR:HG23	58:sK:227:TRP:HD1	1.83	0.43
63:T2:104:GLU:HA	63:T2:107:LYS:HG2	2.00	0.43
60:T3:789:ASN:OD1	60:T3:846:ASN:ND2	2.47	0.43
61:t6:843:VAL:HG22	61:t6:844:ILE:H	1.83	0.43
1:A0:280:GLN:HA	1:A0:283:GLN:HB3	2.01	0.43
3:A2:39:LEU:O	3:A2:44:LYS:NZ	2.48	0.43
3:A2:101:ASN:HD21	3:A2:104:PHE:HB3	1.83	0.43
12:AB:130:VAL:HB	12:AB:167:ILE:HD11	1.99	0.43
12:AB:215:GLN:HG3	12:AB:476:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:205:ASP:OD1	14:AD:205:ASP:N	2.52	0.43
14:AD:213:GLU:OE2	35:Mb:38:MET:HE1	2.18	0.43
14:AD:217:LEU:HD23	35:Mb:42:GLN:HE22	1.72	0.43
23:AM:293:ILE:HG23	23:AM:297:LYS:HD3	2.00	0.43
32:AW:190:ASP:OD1	32:AW:190:ASP:N	2.49	0.43
34:Ma:124:ASP:OD1	34:Ma:124:ASP:N	2.51	0.43
43:Mj:67:PRO:HA	43:Mj:70:PHE:HB3	1.98	0.43
49:Mp:76:ASP:OD1	49:Mp:76:ASP:N	2.51	0.43
51:SD:410:SER:OG	51:SD:411:GLN:N	2.51	0.43
53:SE:518:LYS:HD3	53:SE:522:ASP:OD2	2.19	0.43
1:B0:106:LEU:O	1:B0:206:ILE:HD12	2.19	0.43
3:B2:368:ALA:O	3:B2:375:LEU:HD23	2.18	0.43
4:B3:119:LYS:O	4:B3:123:GLY:N	2.51	0.43
11:BA:1444:MET:HB3	16:BF:133:VAL:HG13	2.01	0.43
13:BC:4:GLU:HG3	13:BC:7:GLN:HE22	1.83	0.43
14:BD:212:LYS:O	14:BD:216:ASN:ND2	2.51	0.43
43:mj:78:LYS:O	49:mp:147:LYS:NZ	2.45	0.43
45:ml:220:LYS:HE2	45:ml:220:LYS:HB2	1.89	0.43
45:ml:563:HIS:O	45:ml:567:THR:OG1	2.30	0.43
50:sA:480:ILE:HG23	51:sD:693:LYS:HZ2	1.83	0.43
51:sB:432:VAL:HG12	53:sE:568:TYR:OH	2.19	0.43
61:E6:249:ASP:OD1	61:E6:250:PHE:N	2.49	0.43
60:T3:658:ILE:O	60:T3:662:ILE:HG12	2.18	0.43
60:T3:732:SER:O	60:T3:734:GLU:N	2.51	0.43
60:T3:833:ASN:HB2	60:T3:834:TYR:H	1.70	0.43
61:t6:350:VAL:HG23	61:t6:379:CYS:HB3	1.99	0.43
1:A0:233:ILE:HG22	1:A0:457:ILE:HB	2.01	0.43
1:A0:493:LEU:HB3	1:A0:678:VAL:HG12	2.00	0.43
8:A7:688:GLY:HA2	8:A7:691:LEU:HG	2.00	0.43
11:AA:532:ARG:HH22	11:AA:745:GLN:HB3	1.84	0.43
13:AC:23:SER:OG	13:AC:24:ASN:N	2.51	0.43
17:AG:89:GLY:HA3	17:AG:103:VAL:HG22	1.99	0.43
17:AG:94:CYS:HB3	17:AG:128:PRO:HB2	2.00	0.43
27:AR:138:GLN:N	27:AR:211:LYS:O	2.44	0.43
51:SB:432:VAL:HG12	53:SE:568:TYR:OH	2.19	0.43
53:SE:460:GLN:O	53:SE:463:PRO:HG3	2.18	0.43
55:SH:610:LYS:HA	55:SH:613:ILE:HG12	2.00	0.43
56:SI:708:HIS:O	56:SI:712:MET:HG2	2.19	0.43
3:B2:125:VAL:HG22	3:B2:238:LYS:HB2	2.00	0.43
11:BA:532:ARG:HH22	11:BA:745:GLN:HB3	1.84	0.43
11:BA:978:PRO:CD	43:mj:88:GLU:OE2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BB:227:LYS:H	12:BB:395:GLN:HE21	1.65	0.43
14:BD:205:ASP:OD1	14:BD:205:ASP:N	2.52	0.43
18:BH:133:ASN:OD1	18:BH:134:ASN:ND2	2.52	0.43
19:BI:29:CYS:O	26:BQ:426:LYS:NZ	2.50	0.43
44:mk:22:VAL:HA	44:mk:25:ILE:HG12	2.01	0.43
53:sE:518:LYS:HD3	53:sE:522:ASP:OD2	2.19	0.43
57:sJ:28:ASP:O	57:sJ:61:LYS:HG3	2.19	0.43
60:T3:869:ARG:HG2	60:T3:876:ASP:OD2	2.19	0.43
45:T4:1003:PHE:CE1	45:T4:1019:MET:HE2	2.54	0.43
61:T6:138:ARG:HD3	61:T6:138:ARG:HA	1.79	0.43
61:t6:408:LEU:O	61:t6:412:ARG:NH2	2.48	0.43
1:A0:695:LYS:HA	1:A0:698:ALA:HB3	2.01	0.43
11:AA:67:CYS:O	11:AA:70:CYS:N	2.42	0.43
13:AC:33:LEU:O	13:AC:37:MET:HG3	2.17	0.43
19:AI:78:CYS:C	19:AI:79:HIS:CG	2.96	0.43
24:AN:-44:DG:H2"	24:AN:-43:DA:H8	1.83	0.43
51:SB:524:ASP:OD1	51:SB:524:ASP:N	2.51	0.43
51:SD:769:HIS:CD2	51:SD:773:MET:HE1	2.54	0.43
9:SF:490:ASP:OD2	9:SF:490:ASP:N	2.52	0.43
56:SI:658:ARG:HH22	56:SI:662:ARG:HG2	1.84	0.43
3:B2:463:GLU:CA	9:sF:400:GLN:O	2.67	0.43
6:B5:30:ILE:HG21	6:B5:30:ILE:HD13	1.79	0.43
7:B6:148:MET:HE2	7:B6:148:MET:HB2	1.83	0.43
12:BB:639:ILE:HD11	12:BB:691:GLU:HG3	2.01	0.43
12:BB:760:ASP:OD1	12:BB:760:ASP:N	2.52	0.43
12:BB:1152:MET:HE1	12:BB:1197:PRO:HD3	2.00	0.43
45:ml:113:THR:O	45:ml:117:THR:OG1	2.30	0.43
58:sK:389:LEU:HG	58:sK:421:LEU:HB3	1.99	0.43
60:T3:378:THR:HG22	60:T3:379:LYS:HD3	2.01	0.43
60:t3:869:ARG:HG2	60:t3:876:ASP:OD2	2.19	0.43
60:t3:887:PHE:HE1	60:t3:919:TYR:HD1	1.67	0.43
60:t3:909:LEU:HG	60:t3:967:TYR:HE2	1.84	0.43
45:t4:1000:HIS:ND1	45:t4:1002:HIS:CD2	2.87	0.43
61:t6:739:LYS:HZ3	61:t6:799:ASN:ND2	2.17	0.43
1:A0:106:LEU:O	1:A0:206:ILE:HD12	2.19	0.43
1:A0:465:PRO:HG2	1:A0:468:MET:HB2	1.99	0.43
1:A0:495:MET:N	1:A0:679:MET:O	2.51	0.43
11:AA:91:PHE:CZ	11:AA:204:THR:HG22	2.54	0.43
11:AA:1172:LEU:HA	28:AS:203:TYR:HE2	1.83	0.43
12:AB:1048:THR:HG22	12:AB:1050:ILE:HG12	2.00	0.43
45:Ml:161:VAL:O	45:Ml:165:LEU:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Mp:134:GLU:H	49:Mp:161:LYS:HG3	1.84	0.43
53:SE:480:THR:OG1	53:SE:481:GLY:N	2.52	0.43
9:SF:448:GLN:HE22	9:SF:483:ASP:HA	1.83	0.43
58:SK:262:GLU:C	58:SK:266:GLN:HE22	2.27	0.43
1:B0:280:GLN:HA	1:B0:283:GLN:HB3	2.01	0.43
5:B4:146:ARG:HD3	7:B6:458:PRO:HA	2.01	0.43
12:BB:293:PRO:HG2	12:BB:296:GLU:HB2	1.99	0.43
14:BD:213:GLU:OE2	35:mb:38:MET:HE1	2.18	0.43
15:BE:43:LYS:O	15:BE:47:CYS:HB2	2.18	0.43
17:BG:163:ILE:HA	17:BG:168:LEU:HD23	1.99	0.43
19:BI:77:LYS:H	19:BI:77:LYS:HG2	1.77	0.43
25:BO:202:ILE:HD13	25:BO:223:ILE:HD12	2.01	0.43
28:BS:176:LYS:O	28:BS:179:GLU:HG3	2.18	0.43
28:BS:287:ARG:CG	28:BS:291:GLU:HG3	2.49	0.43
50:sA:526:LEU:HD23	51:sB:597:HIS:HB3	2.01	0.43
51:sB:712:ARG:HA	51:sB:715:LEU:HD12	2.00	0.43
9:sF:448:GLN:HE22	9:sF:483:ASP:HA	1.83	0.43
9:sF:470:ARG:O	9:sF:470:ARG:NH1	2.44	0.43
56:sI:952:LEU:HD21	56:sI:1000:LEU:HD22	2.01	0.43
45:t4:1003:PHE:CE1	45:t4:1019:MET:HE2	2.53	0.43
8:A7:477:LEU:HA	8:A7:482:TRP:HE1	1.83	0.43
11:AA:212:LYS:HB2	11:AA:212:LYS:HE3	1.84	0.43
11:AA:1120:LEU:HD11	11:AA:1306:LEU:HG	2.00	0.43
12:AB:409:ALA:O	12:AB:413:LEU:HD13	2.19	0.43
12:AB:1152:MET:HE1	12:AB:1197:PRO:HD3	2.00	0.43
23:AM:303:GLN:HE21	27:AR:271:ARG:HA	0.69	0.43
25:AO:202:ILE:HD13	25:AO:223:ILE:HD12	2.01	0.43
27:AR:73:LEU:HD21	27:AR:78:ALA:HA	2.01	0.43
37:Md:276:ASN:HD22	40:Mg:50:VAL:HG22	1.83	0.43
59:SL:327:LYS:NZ	59:SL:405:THR:H	2.17	0.43
1:B0:533:THR:HG21	1:B0:537:MET:CE	2.47	0.43
6:B5:41:LEU:HA	6:B5:41:LEU:HD12	1.54	0.43
11:BA:74:MET:HE2	11:BA:74:MET:N	2.33	0.43
11:BA:408:ASP:OD1	11:BA:408:ASP:N	2.51	0.43
12:BB:868:MET:CE	23:BM:182:ARG:O	2.47	0.43
31:BV:26:LEU:HB3	31:BV:32:ILE:HG21	1.99	0.43
58:sK:262:GLU:C	58:sK:266:GLN:HE22	2.27	0.43
60:T3:888:LEU:HA	61:T6:278:LEU:HD21	2.00	0.43
45:T4:1000:HIS:ND1	45:T4:1002:HIS:CD2	2.87	0.43
61:T6:119:ASP:OD1	61:T6:119:ASP:N	2.52	0.43
60:t3:883:GLY:HA2	61:t6:275:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:t3:888:LEU:HA	61:t6:278:LEU:HD21	2.00	0.43
61:t6:127:LEU:HD13	61:t6:186:TYR:CE2	2.54	0.43
3:A2:229:GLY:O	3:A2:279:THR:OG1	2.27	0.43
3:A2:463:GLU:CA	9:SF:400:GLN:O	2.67	0.43
13:AC:29:MET:HE2	13:AC:29:MET:HB3	1.96	0.43
14:AD:212:LYS:O	14:AD:216:ASN:ND2	2.51	0.43
17:AG:21:ARG:HH21	17:AG:24:GLN:HG3	1.84	0.43
17:AG:91:VAL:HG22	17:AG:101:VAL:HG12	2.01	0.43
41:Mh:82:GLU:HA	41:Mh:85:LYS:HE2	2.00	0.43
44:Mk:22:VAL:HA	44:Mk:25:ILE:HG12	2.01	0.43
50:SA:131:ASN:ND2	50:SA:427:VAL:HG23	2.34	0.43
59:SL:363:GLU:HA	59:SL:366:LYS:HG2	2.01	0.43
3:B2:184:ILE:HG22	3:B2:185:THR:O	2.19	0.43
3:B2:463:GLU:HA	9:sF:400:GLN:C	2.44	0.43
11:BA:894:GLU:OE1	11:BA:906:HIS:NE2	2.51	0.43
14:BD:71:LYS:HA	14:BD:74:GLN:HG2	2.00	0.43
49:mp:76:ASP:OD1	49:mp:76:ASP:N	2.51	0.43
53:sE:532:ASN:ND2	53:sE:543:ILE:HD12	2.32	0.43
55:sH:423:LYS:H	55:sH:423:LYS:HG2	1.64	0.43
58:sK:206:ASP:C	58:sK:207:MET:HE2	2.43	0.43
60:E3:956:ARG:CB	60:E3:959:LEU:HD11	2.49	0.43
61:T6:111:ASN:HD21	61:T6:119:ASP:H	1.67	0.43
61:t6:597:LYS:HG3	61:t6:816:PHE:HE2	1.84	0.43
4:A3:49:LEU:CB	17:AG:164:LYS:CG	2.95	0.42
6:A5:37:ASP:OD1	6:A5:37:ASP:N	2.52	0.42
8:A7:676:HIS:O	8:A7:722:ARG:NH2	2.48	0.42
11:AA:75:ASN:HB3	23:AM:55:LYS:HE3	2.01	0.42
28:AS:287:ARG:CG	28:AS:291:GLU:HG3	2.49	0.42
43:Mj:136:LYS:HE3	47:Mn:137:LYS:HA	2.01	0.42
51:SB:589:LEU:HG	51:SB:592:LEU:HB2	2.01	0.42
57:SJ:28:ASP:O	57:SJ:61:LYS:HG3	2.19	0.42
58:SK:380:SER:HA	58:SK:381:PRO:HD3	1.87	0.42
3:B2:30:ALA:O	3:B2:33:LEU:HG	2.18	0.42
3:B2:101:ASN:HD21	3:B2:104:PHE:HB3	1.83	0.42
8:B7:580:LEU:HD23	8:B7:580:LEU:HA	1.87	0.42
11:BA:115:LEU:HG	11:BA:122:MET:HE2	2.01	0.42
18:BH:108:SER:OG	18:BH:109:LYS:N	2.51	0.42
19:BI:51:ASN:OD1	19:BI:52:ILE:N	2.41	0.42
19:BI:59:VAL:HG22	19:BI:60:GLN:H	1.85	0.42
19:BI:73:ARG:HE	19:BI:73:ARG:HB3	1.52	0.42
28:BS:234:LYS:O	28:BS:235:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:mh:206:ILE:HD12	41:mh:207:PRO:HD2	2.00	0.42
49:mp:113:ASP:OD1	49:mp:113:ASP:N	2.52	0.42
50:sA:314:LEU:HB3	50:sA:388:LEU:HD11	2.01	0.42
51:sD:769:HIS:CD2	51:sD:773:MET:HE1	2.54	0.42
53:sE:161:THR:HG1	53:sE:183:PHE:H	1.65	0.42
55:sH:587:LYS:C	55:sH:588:ASN:CA	2.62	0.42
60:E3:309:SER:OG	60:E3:580:SER:O	2.36	0.42
61:E6:8:MET:HE3	61:E6:520:ILE:HD11	2.01	0.42
60:T3:480:PHE:HB3	60:T3:488:GLN:HB3	2.01	0.42
45:T4:1003:PHE:CE2	45:T4:1019:MET:HG3	2.54	0.42
61:T6:102:PHE:HD1	61:T6:177:ILE:HG22	1.84	0.42
61:T6:739:LYS:HZ3	61:T6:799:ASN:ND2	2.17	0.42
63:t2:34:ASN:N	63:t2:34:ASN:OD1	2.46	0.42
60:t3:658:ILE:O	60:t3:662:ILE:HG12	2.18	0.42
1:A0:4:TYR:CZ	1:A0:9:PRO:HB3	2.54	0.42
3:A2:184:ILE:HG22	3:A2:185:THR:O	2.19	0.42
7:A6:148:MET:HE2	7:A6:148:MET:HB2	1.83	0.42
12:AB:639:ILE:HD11	12:AB:691:GLU:HG3	2.01	0.42
29:AT:57:DA:H2''	29:AT:58:DA:H2'	1.99	0.42
39:Mf:25:SER:HA	39:Mf:28:ILE:HD12	1.99	0.42
51:SD:771:LYS:HA	51:SD:774:LEU:HG	2.00	0.42
9:SF:579:MET:HE3	9:SF:579:MET:HB2	1.87	0.42
1:B0:549:SER:O	1:B0:553:MET:HG3	2.19	0.42
3:B2:134:LEU:HA	3:B2:134:LEU:HD12	1.68	0.42
6:B5:37:ASP:OD1	6:B5:37:ASP:N	2.52	0.42
11:BA:252:PHE:CE2	11:BA:256:GLN:HG3	2.53	0.42
12:BB:409:ALA:O	12:BB:413:LEU:HD13	2.19	0.42
15:BE:58:MET:HE2	15:BE:58:MET:HA	2.00	0.42
34:ma:27:VAL:HG13	34:ma:28:LEU:HD12	2.01	0.42
50:sA:138:TRP:NE1	50:sA:429:VAL:O	2.41	0.42
51:sB:589:LEU:HG	51:sB:592:LEU:HB2	2.01	0.42
51:sD:705:GLU:HA	51:sD:708:MET:CE	2.48	0.42
53:sE:460:GLN:O	53:sE:463:PRO:HG3	2.17	0.42
59:sL:189:MET:HE3	59:sL:305:LEU:CD1	2.48	0.42
61:E6:745:ILE:HA	61:E6:748:ILE:HD12	2.01	0.42
61:E6:788:PHE:HA	61:E6:791:PHE:HB3	2.01	0.42
60:T3:359:TYR:HE2	60:T3:913:THR:HB	1.83	0.42
61:T6:597:LYS:HG3	61:T6:816:PHE:HE2	1.84	0.42
61:t6:102:PHE:HD1	61:t6:177:ILE:HG22	1.84	0.42
61:t6:621:ARG:O	61:t6:625:LYS:NZ	2.52	0.42
8:A7:457:TYR:OH	8:A7:488:ASP:O	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:115:LEU:HG	11:AA:122:MET:HE2	2.01	0.42
11:AA:1039:LYS:HB2	11:AA:1039:LYS:HE3	1.86	0.42
19:AI:74:GLU:HB2	19:AI:81:ARG:HH21	1.85	0.42
49:Mp:101:SER:OG	49:Mp:106:ASN:ND2	2.51	0.42
50:SA:158:MET:HE3	50:SA:158:MET:HB3	1.70	0.42
1:B0:4:TYR:CZ	1:B0:9:PRO:HB3	2.55	0.42
8:B7:373:MET:HE1	8:B7:511:LEU:HD11	2.00	0.42
11:BA:75:ASN:HB3	23:BM:55:LYS:HE3	2.01	0.42
11:BA:1267:MET:HB3	11:BA:1267:MET:HE3	1.86	0.42
12:BB:15:PRO:HG3	64:t5:921:PRO:CB	2.49	0.42
18:BH:92:ASP:OD1	18:BH:92:ASP:N	2.44	0.42
19:BI:27:PHE:N	19:BI:36:GLU:O	2.49	0.42
35:mb:49:ARG:HH11	35:mb:49:ARG:HD3	1.44	0.42
42:mi:161:LEU:HD12	42:mi:161:LEU:HA	1.83	0.42
49:mp:339:SER:HA	49:mp:342:LEU:HD12	1.99	0.42
50:sA:131:ASN:ND2	50:sA:427:VAL:HG23	2.34	0.42
56:sI:658:ARG:HH22	56:sI:662:ARG:HG2	1.84	0.42
59:sL:7:ASP:OD1	59:sL:7:ASP:N	2.52	0.42
60:T3:958:SER:O	60:T3:962:GLU:HB2	2.20	0.42
62:t1:95:SER:OG	63:t2:37:ARG:NH2	2.53	0.42
60:t3:867:ASP:HB3	60:t3:870:ILE:HG12	2.00	0.42
61:t6:119:ASP:OD1	61:t6:119:ASP:N	2.52	0.42
61:t6:625:LYS:H	61:t6:625:LYS:HG2	1.66	0.42
1:A0:179:GLU:HA	1:A0:182:LEU:HG	2.01	0.42
11:AA:739:ASP:OD2	18:AH:19:ARG:NH2	2.51	0.42
15:AE:43:LYS:O	15:AE:47:CYS:HB2	2.19	0.42
17:AG:96:GLN:HE21	17:AG:97:HIS:HD2	1.67	0.42
18:AH:109:LYS:C	43:Mj:83:LEU:HD12	2.45	0.42
28:AS:178:ILE:O	28:AS:182:MET:HB2	2.20	0.42
36:Mc:3:PRO:HA	36:Mc:4:PRO:HD3	1.92	0.42
51:SB:397:SER:O	51:SB:398:LYS:HG2	2.19	0.42
55:SH:505:LEU:HD21	55:SH:539:LEU:HD21	2.01	0.42
58:SK:38:ARG:HB3	58:SK:65:ASP:HB3	2.02	0.42
11:BA:746:MET:HE2	12:BB:1015:HIS:CD2	2.55	0.42
11:BA:1301:GLU:HA	11:BA:1302:PRO:HD3	1.83	0.42
12:BB:15:PRO:CG	64:t5:921:PRO:C	2.92	0.42
15:BE:55:ARG:HA	15:BE:58:MET:HG2	2.01	0.42
41:mh:82:GLU:HA	41:mh:85:LYS:HE2	2.00	0.42
45:ml:161:VAL:O	45:ml:165:LEU:CB	2.67	0.42
45:ml:564:VAL:HG12	45:ml:568:MET:HE2	2.00	0.42
51:sD:728:ASN:O	51:sD:732:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:sE:463:PRO:HB2	53:sE:466:ILE:HD11	2.01	0.42
53:sE:480:THR:OG1	53:sE:481:GLY:N	2.52	0.42
60:E3:409:LYS:HG2	60:E3:412:ARG:HH21	1.84	0.42
61:T6:621:ARG:O	61:T6:625:LYS:NZ	2.52	0.42
1:A0:533:THR:HG21	1:A0:537:MET:CE	2.47	0.42
1:A0:681:LEU:HD12	1:A0:686:PHE:CE2	2.55	0.42
3:A2:63:ASP:HB3	9:A8:780:ILE:CG1	2.49	0.42
5:A4:146:ARG:HD3	7:A6:458:PRO:HA	2.01	0.42
8:A7:181:TYR:OH	8:A7:336:PRO:O	2.33	0.42
8:A7:349:ASN:O	8:A7:405:LYS:NZ	2.40	0.42
12:AB:1043:ASP:OD1	12:AB:1043:ASP:N	2.45	0.42
13:AC:54:ASN:ND2	13:AC:60:ASP:OD1	2.47	0.42
53:SE:463:PRO:HB2	53:SE:466:ILE:HD11	2.01	0.42
55:SH:605:LEU:HD21	58:SK:152:SER:HB2	2.02	0.42
56:SI:1293:ILE:HD12	56:SI:1293:ILE:HG23	1.86	0.42
58:SK:243:LEU:HD11	58:SK:307:TYR:HB3	2.02	0.42
59:SL:189:MET:HE3	59:SL:305:LEU:CD1	2.48	0.42
3:B2:63:ASP:HB3	9:B8:780:ILE:CG1	2.50	0.42
11:BA:91:PHE:CZ	11:BA:204:THR:HG22	2.54	0.42
11:BA:968:GLN:HA	11:BA:973:ILE:HD13	2.01	0.42
17:BG:91:VAL:HG22	17:BG:101:VAL:HG12	2.01	0.42
56:sI:708:HIS:O	56:sI:712:MET:HG2	2.19	0.42
59:sL:111:LEU:HB2	59:sL:137:ILE:HG21	2.02	0.42
59:sL:363:GLU:HA	59:sL:366:LYS:HG2	2.01	0.42
61:E6:464:ASN:OD1	61:E6:465:GLN:N	2.53	0.42
60:T3:482:ARG:HH22	60:T3:517:ASP:HA	1.85	0.42
60:T3:867:ASP:HB3	60:T3:870:ILE:HG12	2.00	0.42
60:T3:887:PHE:HE1	60:T3:919:TYR:HD1	1.67	0.42
63:t2:104:GLU:HA	63:t2:107:LYS:HG2	2.00	0.42
60:t3:378:THR:HG22	60:t3:379:LYS:HD3	2.01	0.42
60:t3:913:THR:OG1	60:t3:914:TYR:N	2.44	0.42
60:t3:976:ASP:OD2	60:t3:1123:TYR:OH	2.38	0.42
45:t4:859:ALA:HB3	45:t4:866:SER:HB2	2.02	0.42
64:t5:880:PRO:HA	64:t5:883:LEU:HG	2.01	0.42
61:t6:111:ASN:HD21	61:t6:119:ASP:H	1.67	0.42
3:A2:30:ALA:HA	3:A2:33:LEU:HD21	2.02	0.42
3:A2:468:TYR:OH	3:A2:490:LYS:O	2.31	0.42
4:A3:49:LEU:CD2	17:AG:164:LYS:CG	2.90	0.42
11:AA:122:MET:HA	11:AA:125:ALA:HB3	2.00	0.42
14:AD:127:ASP:HB3	14:AD:142:LYS:HE3	2.02	0.42
19:AI:59:VAL:HG22	19:AI:60:GLN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AJ:5:VAL:HG12	20:AJ:6:ARG:HG2	2.01	0.42
23:AM:303:GLN:CD	27:AR:270:MET:CG	2.92	0.42
35:Mb:35:ALA:HA	35:Mb:38:MET:HE3	2.01	0.42
35:Mb:100:LYS:HE2	35:Mb:100:LYS:HB3	1.81	0.42
41:Mh:49:TYR:HD2	43:Mj:98:LEU:HD21	1.85	0.42
51:SB:308:PRO:HG2	51:SB:389:GLY:HA3	2.01	0.42
51:SB:335:ILE:HG21	51:SB:338:LYS:HD3	2.01	0.42
51:SB:626:MET:HG2	51:SD:626:MET:SD	2.59	0.42
51:SD:705:GLU:HA	51:SD:708:MET:CE	2.48	0.42
55:SH:633:LEU:HD11	59:SL:438:GLN:HG2	2.02	0.42
59:SL:205:TRP:HZ3	59:SL:213:LEU:HD22	1.84	0.42
11:BA:1116:LEU:HB3	11:BA:1308:THR:HB	2.01	0.42
12:BB:215:GLN:HG3	12:BB:476:ARG:NH2	2.34	0.42
12:BB:841:MET:HG2	12:BB:846:ILE:HD11	2.02	0.42
14:BD:39:ASN:OD1	14:BD:43:GLU:N	2.48	0.42
17:BG:96:GLN:HE21	17:BG:97:HIS:HD2	1.67	0.42
20:BJ:5:VAL:HG12	20:BJ:6:ARG:HG2	2.01	0.42
27:BR:108:LEU:HD11	27:BR:120:TYR:HE2	1.85	0.42
39:mf:144:SER:OG	39:mf:145:SER:N	2.51	0.42
45:ml:195:LEU:HA	45:ml:196:PRO:HD3	1.92	0.42
53:sE:322:ARG:HA	53:sE:322:ARG:HD3	1.85	0.42
53:sE:518:LYS:HA	53:sE:521:LYS:HB2	2.02	0.42
59:sL:276:ASN:OD1	59:sL:282:ASN:ND2	2.38	0.42
59:sL:286:ASP:OD1	59:sL:290:ASN:N	2.44	0.42
61:E6:161:ASN:OD1	60:T3:838:SER:HB2	2.13	0.42
62:T1:31:LYS:HA	62:T1:34:VAL:HG12	2.00	0.42
60:t3:534:PRO:HA	60:t3:537:GLN:HG3	2.02	0.42
60:t3:732:SER:O	60:t3:734:GLU:N	2.51	0.42
45:t4:914:SER:HB2	45:t4:916:MET:HE2	2.01	0.42
1:A0:5:ILE:HG22	1:A0:6:ASP:H	1.85	0.42
3:A2:106:ILE:HD13	3:A2:106:ILE:HA	1.89	0.42
8:A7:194:ILE:HD11	8:A7:213:ILE:HG21	2.01	0.42
12:AB:276:ILE:HG22	12:AB:278:GLN:H	1.85	0.42
18:AH:133:ASN:OD1	18:AH:134:ASN:ND2	2.52	0.42
28:AS:234:LYS:O	28:AS:235:ASP:C	2.62	0.42
49:Mp:180:GLN:C	61:E6:664:ARG:CD	2.93	0.42
50:SA:526:LEU:HD23	51:SB:597:HIS:HB3	2.01	0.42
50:SA:557:ILE:HA	50:SA:560:ILE:HG22	2.02	0.42
58:SK:192:GLN:O	58:SK:196:ARG:HB2	2.20	0.42
58:SK:226:THR:HG23	58:SK:227:TRP:HD1	1.83	0.42
1:B0:260:ALA:HB2	1:B0:398:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B3:49:LEU:CG	17:BG:164:LYS:CD	2.77	0.42
8:B7:194:ILE:HD11	8:B7:213:ILE:HG21	2.01	0.42
19:BI:78:CYS:C	19:BI:79:HIS:CG	2.96	0.42
33:BX:193:LEU:HA	33:BX:196:LEU:HD12	2.01	0.42
35:mb:35:ALA:HA	35:mb:38:MET:HE3	2.01	0.42
45:ml:424:LYS:O	45:ml:444:ASN:ND2	2.49	0.42
51:sB:443:MET:C	51:sB:444:MET:HE2	2.45	0.42
56:sI:1251:LYS:HD3	56:sI:1251:LYS:HA	1.78	0.42
59:sL:205:TRP:HZ3	59:sL:213:LEU:HD22	1.84	0.42
60:E3:296:ASN:OD1	60:E3:297:ILE:N	2.52	0.42
60:T3:838:SER:O	60:T3:839:SER:C	2.62	0.42
60:T3:883:GLY:HA2	61:T6:275:PHE:HE1	1.84	0.42
45:T4:914:SER:HB2	45:T4:916:MET:HE2	2.01	0.42
8:A7:318:ILE:HD12	8:A7:322:SER:HB3	2.02	0.42
11:AA:618:GLU:HG2	11:AA:620:LYS:H	1.84	0.42
11:AA:968:GLN:HA	11:AA:973:ILE:HD13	2.01	0.42
11:AA:978:PRO:CD	43:Mj:88:GLU:OE2	2.66	0.42
14:AD:39:ASN:OD1	14:AD:43:GLU:N	2.48	0.42
15:AE:117:THR:O	15:AE:120:ALA:N	2.53	0.42
30:AU:244:MET:HB2	30:AU:267:VAL:HG23	2.02	0.42
35:Mb:59:LEU:HA	35:Mb:60:PRO:HD3	1.88	0.42
51:SB:377:ALA:HA	51:SB:380:ARG:HE	1.85	0.42
51:SB:443:MET:C	51:SB:444:MET:HE2	2.45	0.42
52:SC:169:TYR:HD2	51:SD:719:GLN:HG2	1.85	0.42
1:B0:681:LEU:HD12	1:B0:686:PHE:CE2	2.55	0.42
3:B2:30:ALA:HA	3:B2:33:LEU:HD21	2.02	0.42
3:B2:249:MET:HE2	3:B2:249:MET:HB2	1.97	0.42
7:B6:297:LEU:HG	7:B6:301:PHE:HE2	1.85	0.42
8:B7:318:ILE:HD12	8:B7:322:SER:HB3	2.02	0.42
12:BB:276:ILE:HG22	12:BB:278:GLN:H	1.85	0.42
19:BI:57:GLY:O	19:BI:59:VAL:N	2.53	0.42
28:BS:178:ILE:O	28:BS:182:MET:HB2	2.20	0.42
40:mg:71:ASP:N	40:mg:71:ASP:OD1	2.52	0.42
45:ml:769:LEU:HB3	45:ml:780:LEU:HD12	2.02	0.42
51:sB:626:MET:HG2	51:sD:626:MET:SD	2.59	0.42
51:sD:439:LYS:NZ	51:sD:579:GLY:O	2.45	0.42
55:sH:610:LYS:HA	55:sH:613:ILE:HG12	2.01	0.42
58:sK:38:ARG:HB3	58:sK:65:ASP:HB3	2.02	0.42
60:E3:673:TYR:O	60:E3:675:GLU:N	2.53	0.42
61:E6:275:PHE:HA	61:E6:278:LEU:HD23	2.02	0.42
45:T4:840:THR:HA	45:T4:843:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:T6:127:LEU:HD13	61:T6:186:TYR:CE2	2.54	0.42
61:T6:218:ARG:HH12	61:T6:220:ARG:CB	2.33	0.42
61:T6:628:LEU:HD23	61:T6:631:LEU:HD12	2.01	0.42
60:t3:509:SER:O	60:t3:513:SER:OG	2.38	0.42
60:t3:838:SER:O	60:t3:839:SER:C	2.62	0.42
64:t5:869:PHE:O	64:t5:873:GLN:HG3	2.20	0.42
61:t6:739:LYS:HZ3	61:t6:799:ASN:HD21	1.67	0.42
1:A0:521:ASN:O	1:A0:525:MET:HG2	2.20	0.42
1:A0:571:VAL:HG12	1:A0:599:LEU:HB2	2.02	0.42
5:A4:36:LEU:O	5:A4:39:THR:OG1	2.33	0.42
7:A6:214:LEU:HD13	7:A6:250:THR:HG21	2.00	0.42
7:A6:452:PRO:O	7:A6:456:SER:OG	2.29	0.42
8:A7:677:TYR:O	8:A7:722:ARG:NH2	2.52	0.42
11:AA:110:CYS:CB	11:AA:167:CYS:SG	2.88	0.42
11:AA:174:ILE:HG22	11:AA:183:GLY:HA2	2.02	0.42
14:AD:164:ILE:O	14:AD:168:LYS:HB3	2.20	0.42
19:AI:27:PHE:N	19:AI:36:GLU:O	2.50	0.42
45:MI:423:SER:HG	45:MI:444:ASN:HD21	1.61	0.42
51:SD:361:TYR:OH	9:SF:435:ARG:NH1	2.53	0.42
51:SD:628:GLN:O	51:SD:640:GLN:NE2	2.45	0.42
56:SI:952:LEU:HD21	56:SI:1000:LEU:HD22	2.01	0.42
1:B0:521:ASN:O	1:B0:525:MET:HG2	2.20	0.42
3:B2:261:GLN:HG2	3:B2:263:HIS:N	2.22	0.42
7:B6:291:LEU:HD13	7:B6:297:LEU:HD12	2.02	0.42
8:B7:711:LYS:HA	8:B7:716:MET:CE	2.46	0.42
11:BA:1032:LEU:HD23	11:BA:1032:LEU:HA	1.92	0.42
12:BB:914:LYS:HE2	12:BB:914:LYS:HB3	1.84	0.42
19:BI:74:GLU:HB2	19:BI:81:ARG:HH21	1.85	0.42
28:BS:242:LYS:HA	28:BS:245:ILE:HG12	2.02	0.42
32:BW:111:ASP:HA	32:BW:114:ASP:HB2	2.00	0.42
41:mh:49:TYR:HD2	43:mj:98:LEU:HD21	1.85	0.42
50:sA:557:ILE:HA	50:sA:560:ILE:HG22	2.02	0.42
59:sL:327:LYS:NZ	59:sL:405:THR:H	2.17	0.42
61:T6:196:LEU:HD23	61:T6:196:LEU:HA	1.92	0.42
45:t4:1003:PHE:CE2	45:t4:1019:MET:HG3	2.54	0.42
1:A0:533:THR:HA	1:A0:534:PRO:HD3	1.96	0.42
1:A0:642:MET:HE2	1:A0:642:MET:HA	2.02	0.42
2:A1:297:ARG:NE	2:A1:299:GLU:OE2	2.51	0.42
5:A4:264:LYS:HA	5:A4:265:PRO:HD3	1.93	0.42
7:A6:297:LEU:HG	7:A6:301:PHE:HE2	1.85	0.42
11:AA:106:VAL:HG23	11:AA:113:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1301:GLU:HA	11:AA:1302:PRO:HD3	1.83	0.42
11:AA:1444:MET:HB3	16:AF:133:VAL:HG13	2.01	0.42
12:AB:550:ASP:HA	12:AB:551:PRO:HD3	1.92	0.42
21:AK:102:LYS:O	21:AK:105:PHE:N	2.49	0.42
31:AV:36:LEU:HA	31:AV:36:LEU:HD13	1.88	0.42
51:SD:728:ASN:O	51:SD:732:ASN:ND2	2.53	0.42
59:SL:276:ASN:OD1	59:SL:282:ASN:ND2	2.38	0.42
7:B6:154:ILE:HD11	7:B6:196:LEU:HD22	2.01	0.42
11:BA:618:GLU:HG2	11:BA:620:LYS:H	1.84	0.42
11:BA:890:ASP:OD1	11:BA:940:ARG:NH2	2.50	0.42
12:BB:806:THR:N	12:BB:809:MET:HE3	2.33	0.42
13:BC:14:SER:HB2	13:BC:17:ASN:HB2	2.01	0.42
14:BD:127:ASP:HB3	14:BD:142:LYS:HE3	2.02	0.42
15:BE:117:THR:O	15:BE:120:ALA:N	2.53	0.42
17:BG:21:ARG:HH21	17:BG:24:GLN:HG3	1.84	0.42
18:BH:116:TYR:HB2	18:BH:123:MET:HE2	2.01	0.42
32:BW:124:CYS:HB3	32:BW:127:CYS:SG	2.60	0.42
42:mi:175:ILE:O	42:mi:179:GLU:HG3	2.20	0.42
49:mp:95:ASP:OD1	49:mp:189:ARG:NH1	2.52	0.42
51:sB:328:PRO:HD2	9:sF:537:LEU:HD21	2.02	0.42
53:sE:333:LEU:HD23	53:sE:333:LEU:HA	1.88	0.42
56:sI:712:MET:HE3	56:sI:712:MET:CA	2.47	0.42
61:E6:334:GLN:N	61:E6:334:GLN:OE1	2.53	0.42
61:E6:610:PRO:HD2	61:E6:613:ILE:HD12	2.02	0.42
64:T5:880:PRO:HA	64:T5:883:LEU:HG	2.01	0.42
60:t3:768:GLU:OE1	60:t3:819:LEU:HD23	2.20	0.42
61:t6:628:LEU:HD23	61:t6:631:LEU:HD12	2.01	0.42
61:t6:643:GLU:H	61:t6:643:GLU:HG2	1.52	0.42
7:A6:291:LEU:HD13	7:A6:297:LEU:HD12	2.02	0.41
11:AA:368:LYS:HE3	11:AA:368:LYS:HB2	1.92	0.41
11:AA:746:MET:HE2	12:AB:1015:HIS:CD2	2.55	0.41
12:AB:760:ASP:OD1	12:AB:760:ASP:N	2.52	0.41
45:Ml:769:LEU:HB3	45:Ml:780:LEU:HD12	2.02	0.41
49:Mp:548:TYR:HB2	61:E6:612:GLU:HB2	2.01	0.41
53:SE:32:LYS:HA	53:SE:35:ILE:HD12	2.01	0.41
59:SL:111:LEU:HB2	59:SL:137:ILE:HG21	2.02	0.41
59:SL:369:ARG:NH2	59:SL:372:GLU:HB3	2.35	0.41
1:B0:233:ILE:HG22	1:B0:457:ILE:HB	2.01	0.41
1:B0:493:LEU:HB3	1:B0:678:VAL:HG12	2.00	0.41
1:B0:564:TRP:HE1	2:B1:232:ASN:HB2	1.83	0.41
8:B7:677:TYR:O	8:B7:722:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BB:451:LYS:HB2	12:BB:451:LYS:HE2	1.71	0.41
25:BO:85:VAL:HG12	25:BO:146:ILE:HD13	2.01	0.41
49:mp:134:GLU:H	49:mp:161:LYS:HG3	1.84	0.41
55:sH:505:LEU:HD21	55:sH:539:LEU:HD21	2.01	0.41
58:sK:394:ILE:HG21	58:sK:394:ILE:HD13	1.86	0.41
60:E3:386:LEU:HD12	60:E3:450:LEU:HD13	2.02	0.41
60:T3:909:LEU:HG	60:T3:967:TYR:HE2	1.84	0.41
61:T6:653:LYS:HE2	61:T6:653:LYS:HB2	1.81	0.41
60:t3:666:PRO:HA	60:t3:765:TYR:HB3	2.02	0.41
61:t6:623:LEU:HD11	61:t6:653:LYS:HE3	2.02	0.41
61:t6:760:ALA:O	61:t6:761:LYS:HG3	2.20	0.41
61:t6:769:ILE:HG21	61:t6:769:ILE:HD13	1.89	0.41
1:A0:241:ASP:N	1:A0:241:ASP:OD1	2.53	0.41
1:A0:538:VAL:HG12	1:A0:598:LEU:HD12	2.03	0.41
12:AB:915:THR:HA	12:AB:936:ASP:HA	2.02	0.41
13:AC:14:SER:HB2	13:AC:17:ASN:HB2	2.01	0.41
32:AW:124:CYS:HB3	32:AW:127:CYS:SG	2.60	0.41
33:AX:164:LYS:HG2	33:AX:171:PHE:CG	2.56	0.41
42:Mi:175:ILE:O	42:Mi:179:GLU:HG3	2.20	0.41
45:Ml:708:LEU:HB3	45:Ml:713:ILE:HB	2.02	0.41
49:Mp:23:PRO:HG2	49:Mp:115:LYS:HA	2.03	0.41
49:Mp:95:ASP:OD1	49:Mp:189:ARG:NH1	2.52	0.41
49:Mp:177:GLN:CA	61:E6:668:PHE:CZ	2.70	0.41
50:SA:566:MET:SD	53:SE:566:TYR:OH	2.69	0.41
9:SF:318:GLU:HG3	55:SH:449:MET:HG2	2.02	0.41
58:SK:321:ASP:OD1	58:SK:321:ASP:N	2.53	0.41
58:SK:446:LEU:HA	58:SK:447:PRO:HD3	1.85	0.41
1:B0:495:MET:N	1:B0:679:MET:O	2.51	0.41
11:BA:106:VAL:HG23	11:BA:113:LEU:HA	2.02	0.41
11:BA:1423:GLY:O	11:BA:1427:ASN:ND2	2.48	0.41
12:BB:778:MET:HE2	12:BB:794:ASN:HD22	1.86	0.41
18:BH:109:LYS:O	43:mj:83:LEU:CD1	2.68	0.41
20:BJ:65:PRO:HB2	20:BJ:68:LYS:HG2	2.03	0.41
23:BM:303:GLN:CD	27:BR:270:MET:CG	2.92	0.41
50:sA:477:LYS:HA	50:sA:480:ILE:HD13	2.02	0.41
51:sB:377:ALA:HA	51:sB:380:ARG:HE	1.85	0.41
9:sF:556:GLN:N	9:sF:653:LEU:O	2.47	0.41
9:sF:633:ILE:HD12	9:sF:633:ILE:HG23	1.84	0.41
56:sI:1293:ILE:HD12	56:sI:1293:ILE:HG23	1.85	0.41
58:sK:243:LEU:HD11	58:sK:307:TYR:HB3	2.02	0.41
64:T5:869:PHE:O	64:T5:873:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:T5:913:ILE:HG21	64:T5:938:ILE:HB	2.02	0.41
61:T6:623:LEU:HD11	61:T6:653:LYS:HE3	2.02	0.41
61:T6:739:LYS:HZ3	61:T6:799:ASN:HD21	1.66	0.41
45:t4:1023:ARG:HA	45:t4:1027:PHE:HB2	2.02	0.41
1:A0:549:SER:O	1:A0:553:MET:HG3	2.19	0.41
10:A9:209:MET:HE3	10:A9:227:LEU:HD22	2.02	0.41
11:AA:549:MET:HE1	11:AA:656:TRP:HD1	1.84	0.41
11:AA:958:VAL:HG11	11:AA:1052:GLN:HB3	2.03	0.41
11:AA:1116:LEU:HB3	11:AA:1308:THR:HB	2.01	0.41
27:AR:108:LEU:HD11	27:AR:120:TYR:HE2	1.85	0.41
35:Mb:122:VAL:HG12	35:Mb:126:MET:HE2	2.02	0.41
45:Ml:220:LYS:HE2	45:Ml:220:LYS:HB2	1.89	0.41
45:Ml:424:LYS:O	45:Ml:444:ASN:ND2	2.49	0.41
9:SF:365:ILE:HD12	9:SF:365:ILE:HA	1.93	0.41
3:B2:394:ASP:HA	3:B2:397:ILE:HG12	2.03	0.41
11:BA:174:ILE:HG22	11:BA:183:GLY:HA2	2.02	0.41
11:BA:549:MET:HE1	11:BA:656:TRP:HD1	1.84	0.41
11:BA:1025:ARG:HA	11:BA:1025:ARG:HD3	1.87	0.41
17:BG:119:LEU:HB2	17:BG:132:SER:HB3	2.02	0.41
18:BH:109:LYS:C	43:mj:83:LEU:HD12	2.45	0.41
43:mj:136:LYS:HE3	47:mn:137:LYS:HA	2.01	0.41
50:sA:341:LEU:HD22	50:sA:380:LYS:HB2	2.03	0.41
51:sB:335:ILE:HG21	51:sB:338:LYS:HD3	2.01	0.41
52:sC:169:TYR:HD2	51:sD:719:GLN:HG2	1.85	0.41
58:sK:192:GLN:O	58:sK:196:ARG:HB2	2.20	0.41
59:sL:369:ARG:NH2	59:sL:372:GLU:HB3	2.35	0.41
63:T2:31:LYS:HA	63:T2:34:ASN:HD21	1.85	0.41
60:T3:534:PRO:HA	60:T3:537:GLN:HG3	2.02	0.41
45:T4:859:ALA:HB3	45:T4:866:SER:HB2	2.02	0.41
61:T6:625:LYS:H	61:T6:625:LYS:HG2	1.66	0.41
61:T6:843:VAL:HG22	61:T6:844:ILE:H	1.83	0.41
61:t6:8:MET:HE3	61:t6:8:MET:HB3	1.91	0.41
3:A2:117:VAL:HG12	3:A2:120:SER:N	2.35	0.41
11:AA:55:ASP:OD1	11:AA:58:LEU:HG	2.20	0.41
45:Ml:195:LEU:HD12	45:Ml:195:LEU:HA	1.90	0.41
51:SB:520:LEU:HD13	51:SB:529:LYS:HE2	2.02	0.41
53:SE:518:LYS:HA	53:SE:521:LYS:HB2	2.02	0.41
10:B9:201:VAL:HG21	10:B9:222:ILE:HD12	2.01	0.41
11:BA:1151:GLU:OE2	19:BI:45:ARG:NH1	2.53	0.41
17:BG:5:LYS:HD2	17:BG:5:LYS:HA	1.94	0.41
19:BI:90:GLN:O	19:BI:92:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BQ:21:PHE:C	26:BQ:22:ILE:HG13	2.44	0.41
27:BR:73:LEU:HD21	27:BR:78:ALA:HA	2.01	0.41
33:BX:164:LYS:HG2	33:BX:171:PHE:CG	2.55	0.41
44:mk:123:ASP:OD1	44:mk:124:SER:N	2.53	0.41
48:mo:55:LYS:HE2	48:mo:89:MET:SD	2.61	0.41
49:mp:190:THR:HG22	49:mp:198:ILE:HG23	2.02	0.41
60:E3:412:ARG:HH11	60:E3:412:ARG:HD2	1.71	0.41
61:E6:764:GLU:N	61:E6:771:ASN:OD1	2.54	0.41
7:A6:227:HIS:CD2	7:A6:318:THR:HG21	2.56	0.41
17:AG:119:LEU:HB2	17:AG:132:SER:HB3	2.02	0.41
19:AI:29:CYS:O	26:AQ:426:LYS:NZ	2.50	0.41
27:AR:309:GLU:OE2	27:AR:321:ARG:NH1	2.40	0.41
34:Ma:171:GLN:O	34:Ma:175:MET:HG2	2.21	0.41
37:Md:276:ASN:OD1	40:Mg:33:ARG:NH2	2.54	0.41
53:SE:28:PHE:O	53:SE:116:THR:OG1	2.38	0.41
53:SE:147:ASP:OD1	53:SE:184:LYS:NZ	2.54	0.41
9:SF:545:ARG:HD2	9:SF:560:GLN:HE21	1.85	0.41
56:SI:1110:VAL:HG11	56:SI:1193:TRP:CZ2	2.56	0.41
56:SI:1212:LEU:O	56:SI:1216:ASN:ND2	2.53	0.41
58:SK:303:LEU:HA	58:SK:303:LEU:HD12	1.82	0.41
59:SL:161:ILE:HG22	59:SL:334:ILE:HB	2.02	0.41
1:B0:136:MET:HB3	1:B0:136:MET:HE2	1.80	0.41
8:B7:354:ILE:HG22	8:B7:430:LEU:HB2	2.02	0.41
8:B7:592:GLN:NE2	8:B7:747:ASN:O	2.47	0.41
10:B9:209:MET:HE3	10:B9:227:LEU:HD22	2.02	0.41
11:BA:898:ARG:HD2	11:BA:898:ARG:HA	1.89	0.41
22:BL:26:THR:OG1	22:BL:27:LEU:N	2.53	0.41
50:sA:311:SER:OG	50:sA:414:HIS:ND1	2.49	0.41
60:E3:507:LEU:HD13	60:E3:510:ILE:HD12	2.03	0.41
62:T1:95:SER:OG	63:T2:37:ARG:NH2	2.53	0.41
60:T3:683:ASP:OD1	60:T3:683:ASP:N	2.53	0.41
60:T3:768:GLU:OE1	60:T3:819:LEU:HD23	2.20	0.41
61:T6:170:ASP:OD1	61:T6:170:ASP:N	2.48	0.41
61:T6:480:GLN:NE2	61:T6:486:ASN:OD1	2.41	0.41
62:t1:40:LEU:HA	62:t1:40:LEU:HD13	1.69	0.41
60:t3:958:SER:O	60:t3:962:GLU:HB2	2.20	0.41
7:A6:154:ILE:HD11	7:A6:196:LEU:HD22	2.02	0.41
8:A7:188:LEU:HD23	8:A7:188:LEU:HA	1.94	0.41
12:AB:841:MET:HG2	12:AB:846:ILE:HD11	2.02	0.41
19:AI:57:GLY:O	19:AI:59:VAL:N	2.53	0.41
19:AI:90:GLN:O	19:AI:92:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AS:242:LYS:HA	28:AS:245:ILE:HG12	2.02	0.41
32:AW:72:GLN:NE2	32:AW:86:TYR:OH	2.54	0.41
33:AX:193:LEU:HA	33:AX:196:LEU:HD12	2.01	0.41
11:MA:1638:PRO:HG3	48:Mo:115:PRO:HB3	2.02	0.41
34:Ma:27:VAL:HG13	34:Ma:28:LEU:HD12	2.01	0.41
34:Ma:111:ASP:HB3	34:Ma:134:THR:HA	2.03	0.41
42:Mi:175:ILE:HD12	42:Mi:175:ILE:HA	1.96	0.41
50:SA:341:LEU:HD22	50:SA:380:LYS:HB2	2.03	0.41
51:SB:385:LEU:HD23	51:SB:385:LEU:HA	1.91	0.41
53:SE:522:ASP:C	53:SE:547:ARG:NH1	2.79	0.41
1:B0:488:ALA:O	1:B0:489:LYS:HE2	2.21	0.41
7:B6:227:HIS:CD2	7:B6:318:THR:HG21	2.56	0.41
39:mf:45:SER:HB2	39:mf:117:MET:HE1	2.03	0.41
49:mp:92:ASN:HD21	49:mp:194:ASP:HA	1.86	0.41
51:sB:520:LEU:HD13	51:sB:529:LYS:HE2	2.02	0.41
51:sD:403:ASN:HD21	9:sF:410:ASN:HD21	1.68	0.41
53:sE:32:LYS:HA	53:sE:35:ILE:HD12	2.01	0.41
9:sF:545:ARG:HD2	9:sF:560:GLN:HE21	1.85	0.41
56:sI:1194:LEU:HA	56:sI:1194:LEU:HD23	1.72	0.41
61:E6:446:MET:CE	61:E6:446:MET:H	2.33	0.41
45:T4:1023:ARG:HA	45:T4:1027:PHE:HB2	2.02	0.41
60:t3:824:ARG:NH1	60:t3:870:ILE:O	2.42	0.41
8:A7:354:ILE:HG22	8:A7:430:LEU:HB2	2.03	0.41
11:AA:1197:LEU:HD12	11:AA:1209:MET:HE1	2.03	0.41
19:AI:117:LYS:HB2	19:AI:117:LYS:HE2	1.65	0.41
27:AR:223:GLN:NE2	27:AR:224:VAL:O	2.53	0.41
51:SB:578:ASP:OD1	51:SB:578:ASP:N	2.47	0.41
51:SD:736:ILE:HA	51:SD:739:VAL:HG22	2.03	0.41
1:B0:179:GLU:HA	1:B0:182:LEU:HG	2.01	0.41
1:B0:241:ASP:OD1	1:B0:241:ASP:N	2.53	0.41
2:B1:214:ILE:HG22	2:B1:218:ARG:HH11	1.86	0.41
2:B1:371:THR:HA	2:B1:374:ILE:HG12	2.03	0.41
7:B6:148:MET:N	7:B6:148:MET:SD	2.94	0.41
11:BA:55:ASP:OD1	11:BA:58:LEU:HG	2.20	0.41
11:BA:419:LYS:HD2	11:BA:419:LYS:HA	1.89	0.41
11:BA:958:VAL:HG11	11:BA:1052:GLN:HB3	2.02	0.41
12:BB:921:ASP:OD1	12:BB:921:ASP:N	2.54	0.41
21:BK:54:ARG:HA	21:BK:54:ARG:HD2	1.83	0.41
24:BN:-85:DT:H2'	24:BN:-84:DA:C8	2.56	0.41
32:BW:72:GLN:NE2	32:BW:86:TYR:OH	2.54	0.41
34:ma:171:GLN:O	34:ma:175:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:md:115:LYS:HD3	37:md:115:LYS:HA	1.95	0.41
51:sB:524:ASP:N	51:sB:524:ASP:OD1	2.51	0.41
9:sF:490:ASP:OD2	9:sF:490:ASP:N	2.52	0.41
55:sH:592:LEU:HB3	55:sH:593:LYS:HZ2	1.85	0.41
55:sH:633:LEU:HD11	59:sL:438:GLN:HG2	2.02	0.41
61:E6:791:PHE:HA	61:E6:794:PHE:CZ	2.55	0.41
60:T3:666:PRO:HA	60:T3:765:TYR:HB3	2.02	0.41
4:A3:97:ASP:N	4:A3:97:ASP:OD1	2.53	0.41
7:A6:148:MET:N	7:A6:148:MET:SD	2.94	0.41
11:AA:420:ARG:HE	11:AA:420:ARG:HB2	1.64	0.41
12:AB:707:PRO:O	12:AB:711:GLU:HB2	2.21	0.41
18:AH:109:LYS:O	43:Mj:83:LEU:CD1	2.68	0.41
34:Ma:107:LEU:HD23	34:Ma:107:LEU:HA	1.95	0.41
37:Md:257:ASP:OD1	37:Md:258:LYS:N	2.51	0.41
39:Mf:88:PRO:HA	39:Mf:89:PRO:HD3	1.88	0.41
9:SF:599:GLU:HG2	9:SF:603:MET:CE	2.51	0.41
57:SJ:59:ARG:HH22	58:SK:134:PRO:CG	2.34	0.41
58:SK:247:GLU:OE1	58:SK:248:ARG:NH2	2.54	0.41
3:B2:463:GLU:O	9:sF:400:GLN:O	2.39	0.41
5:B4:234:VAL:HB	5:B4:252:MET:HE1	2.02	0.41
11:BA:1204:ASP:OD1	11:BA:1204:ASP:N	2.53	0.41
12:BB:578:THR:HG22	12:BB:622:LYS:HB3	2.03	0.41
26:BQ:27:MET:HA	26:BQ:30:ASN:HB3	2.02	0.41
27:BR:223:GLN:NE2	27:BR:224:VAL:O	2.53	0.41
28:BS:245:ILE:O	28:BS:248:ILE:HG22	2.21	0.41
51:sB:397:SER:O	51:sB:398:LYS:HG2	2.19	0.41
52:sC:162:LYS:HE2	52:sC:162:LYS:HB2	1.81	0.41
51:sD:317:GLU:HA	51:sD:344:MET:HE2	2.03	0.41
9:sF:506:ARG:O	9:sF:510:ILE:HG12	2.21	0.41
60:E3:475:THR:HG22	60:E3:476:ARG:NH1	2.36	0.41
60:T3:509:SER:O	60:T3:513:SER:OG	2.38	0.41
61:t6:825:PRO:HA	61:t6:826:PRO:HD3	1.85	0.41
3:A2:463:GLU:O	9:SF:400:GLN:O	2.39	0.41
10:A9:201:VAL:HG21	10:A9:222:ILE:HD12	2.01	0.41
10:A9:236:TRP:NE1	10:A9:240:LYS:HE3	2.35	0.41
11:AA:108:MET:SD	11:AA:108:MET:N	2.82	0.41
11:AA:261:ASP:CG	11:AA:320:ARG:HH22	2.28	0.41
11:AA:579:SER:HA	11:AA:582:ILE:HG12	2.03	0.41
11:AA:1151:GLU:OE2	19:AI:45:ARG:NH1	2.53	0.41
12:AB:578:THR:HG22	12:AB:622:LYS:HB3	2.03	0.41
15:AE:55:ARG:HA	15:AE:58:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AF:101:ILE:HD13	16:AF:101:ILE:HA	1.95	0.41
18:AH:92:ASP:OD1	18:AH:92:ASP:N	2.44	0.41
18:AH:108:SER:OG	18:AH:109:LYS:N	2.51	0.41
18:AH:116:TYR:HB2	18:AH:123:MET:HE2	2.01	0.41
18:AH:124:ARG:NH1	18:AH:126:GLU:OE2	2.54	0.41
20:AJ:65:PRO:HB2	20:AJ:68:LYS:HG2	2.03	0.41
25:AO:85:VAL:HG12	25:AO:146:ILE:HD13	2.01	0.41
26:AQ:27:MET:HA	26:AQ:30:ASN:HB3	2.02	0.41
28:AS:197:ALA:O	28:AS:201:ILE:HG13	2.21	0.41
31:AV:44:PHE:HA	31:AV:47:VAL:HG22	2.03	0.41
37:Md:232:VAL:HG12	37:Md:233:LYS:HG3	2.02	0.41
39:Mf:45:SER:HB2	39:Mf:117:MET:HE1	2.03	0.41
39:Mf:67:ARG:HA	39:Mf:67:ARG:HD3	1.94	0.41
50:SA:477:LYS:HA	50:SA:480:ILE:HD13	2.02	0.41
53:SE:516:LYS:O	53:SE:519:TYR:HB2	2.21	0.41
9:SF:506:ARG:O	9:SF:510:ILE:HG12	2.21	0.41
57:SJ:9:LYS:HA	57:SJ:9:LYS:HD2	1.99	0.41
58:SK:197:LEU:HD12	58:SK:197:LEU:HA	1.82	0.41
1:B0:5:ILE:HG22	1:B0:6:ASP:H	1.85	0.41
1:B0:605:LYS:HE3	1:B0:605:LYS:HB2	1.89	0.41
1:B0:642:MET:HE2	1:B0:642:MET:HA	2.02	0.41
11:BA:946:VAL:HA	15:BE:201:LYS:HD3	2.02	0.41
12:BB:13:GLU:CD	64:t5:919:ARG:HD2	2.45	0.41
12:BB:344:LYS:HB2	12:BB:347:LYS:HB2	2.02	0.41
20:BJ:44:TYR:HA	20:BJ:47:ARG:HD3	2.02	0.41
23:BM:191:GLU:OE2	27:BR:268:MET:HB3	2.21	0.41
24:BN:-43:DA:H2"	24:BN:-42:DT:C5	2.56	0.41
25:BO:104:MET:SD	25:BO:104:MET:N	2.94	0.41
27:BR:96:ARG:NH2	27:BR:107:LEU:HD22	2.36	0.41
30:BU:244:MET:HB2	30:BU:267:VAL:HG23	2.02	0.41
31:BV:36:LEU:HA	31:BV:36:LEU:HD13	1.88	0.41
11:mA:1638:PRO:HG3	48:mo:115:PRO:HB3	2.02	0.41
35:mb:122:VAL:HG12	35:mb:126:MET:HE2	2.02	0.41
40:mg:49:ALA:HA	40:mg:52:THR:HG22	2.02	0.41
42:mi:172:GLU:HA	42:mi:175:ILE:HG22	2.03	0.41
47:mN:85:VAL:HG11	47:mN:90:GLN:HE21	1.86	0.41
49:mp:23:PRO:HG2	49:mp:115:LYS:HA	2.03	0.41
9:sF:318:GLU:HG3	55:sH:449:MET:HG2	2.02	0.41
9:sF:343:ILE:HG21	9:sF:343:ILE:HD13	1.88	0.41
9:sF:599:GLU:HG2	9:sF:603:MET:CE	2.51	0.41
56:sI:1212:LEU:O	56:sI:1216:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:sL:161:ILE:HG22	59:sL:334:ILE:HB	2.02	0.41
60:E3:419:ASP:OD1	60:E3:435:THR:N	2.54	0.41
61:E6:920:ASP:OD1	61:E6:934:ARG:NH2	2.54	0.41
60:T3:1082:ILE:HD11	61:T6:380:ASP:HB3	2.03	0.41
45:T4:1010:THR:O	45:T4:1013:SER:OG	2.27	0.41
61:T6:760:ALA:O	61:T6:761:LYS:HG3	2.20	0.41
63:t2:31:LYS:HA	63:t2:34:ASN:HD21	1.85	0.41
60:t3:356:ASN:O	60:t3:360:HIS:ND1	2.52	0.41
60:t3:579:LEU:HD23	60:t3:579:LEU:HA	1.93	0.41
60:t3:1082:ILE:HD11	61:t6:380:ASP:HB3	2.03	0.41
60:t3:1126:MET:HE3	60:t3:1126:MET:HB2	1.95	0.41
64:t5:913:ILE:HG21	64:t5:938:ILE:HB	2.02	0.41
2:A1:562:LYS:HD3	7:A6:365:CYS:HA	2.03	0.41
6:A5:30:ILE:HD13	6:A5:30:ILE:HG21	1.79	0.41
6:A5:51:LYS:O	6:A5:54:LEU:HG	2.21	0.41
7:A6:138:GLU:N	7:A6:138:GLU:OE1	2.54	0.41
17:AG:19:GLY:O	17:AG:22:MET:HG3	2.21	0.41
20:AJ:44:TYR:HA	20:AJ:47:ARG:HD3	2.02	0.41
23:AM:191:GLU:OE2	27:AR:268:MET:HB3	2.21	0.41
38:Me:228:LEU:HD21	38:Me:278:LEU:HD12	2.03	0.41
40:Mg:101:GLU:HA	40:Mg:104:ILE:HD12	2.03	0.41
51:SB:328:PRO:HD2	9:SF:537:LEU:HD21	2.02	0.41
53:SE:523:VAL:CG1	53:SE:523:VAL:CA	2.84	0.41
55:SH:423:LYS:H	55:SH:423:LYS:HG2	1.64	0.41
5:B4:31:GLU:HA	5:B4:32:ILE:HD12	2.03	0.41
11:BA:368:LYS:HE3	11:BA:368:LYS:HB2	1.92	0.41
12:BB:915:THR:HA	12:BB:936:ASP:HA	2.02	0.41
17:BG:19:GLY:O	17:BG:22:MET:HG3	2.21	0.41
18:BH:124:ARG:NH1	18:BH:126:GLU:OE2	2.54	0.41
45:ml:769:LEU:HA	45:ml:781:TYR:H	1.86	0.41
50:sA:308:MET:HE3	50:sA:308:MET:HB3	1.71	0.41
51:sD:329:GLU:OE1	51:sD:380:ARG:NH1	2.54	0.41
51:sD:361:TYR:OH	9:sF:435:ARG:NH1	2.53	0.41
51:sD:736:ILE:HA	51:sD:739:VAL:HG22	2.03	0.41
61:E6:729:TYR:O	61:E6:732:VAL:HG12	2.21	0.41
8:A7:622:MET:HE1	8:A7:653:PHE:CD1	2.57	0.40
11:AA:353:ILE:HG22	11:AA:468:PHE:HB2	2.04	0.40
12:AB:344:LYS:HB2	12:AB:347:LYS:HB2	2.02	0.40
19:AI:73:ARG:HE	19:AI:73:ARG:HB3	1.52	0.40
19:AI:76:PRO:HB2	19:AI:77:LYS:NZ	2.36	0.40
27:AR:96:ARG:NH2	27:AR:107:LEU:HD22	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AT:58:DA:H4'	29:AT:59:DG:H5'	2.03	0.40
48:Mo:55:LYS:HE2	48:Mo:89:MET:SD	2.61	0.40
56:SI:725:ALA:O	56:SI:729:LEU:HD23	2.21	0.40
18:BH:104:PHE:CE2	18:BH:136:LYS:HA	2.57	0.40
23:BM:227:THR:OG1	23:BM:229:ASN:OD1	2.37	0.40
45:ml:708:LEU:HB3	45:ml:713:ILE:HB	2.02	0.40
50:sA:186:VAL:HB	50:sA:296:SER:HB2	2.04	0.40
9:sF:315:ASP:O	9:sF:317:PRO:HD3	2.21	0.40
61:E6:381:THR:HG22	60:t3:431:ASP:OD1	2.19	0.40
61:E6:610:PRO:O	61:E6:614:MET:N	2.54	0.40
60:t3:480:PHE:HB3	60:t3:488:GLN:HB3	2.01	0.40
60:t3:482:ARG:HH22	60:t3:517:ASP:HA	1.85	0.40
2:A1:587:LYS:O	2:A1:590:ILE:HG22	2.21	0.40
3:A2:448:LEU:HD13	3:A2:448:LEU:HA	1.89	0.40
11:AA:122:MET:SD	11:AA:122:MET:N	2.92	0.40
11:AA:481:ASP:OD1	11:AA:481:ASP:N	2.53	0.40
11:AA:847:ASP:OD1	11:AA:847:ASP:N	2.51	0.40
12:AB:921:ASP:OD1	12:AB:921:ASP:N	2.54	0.40
19:AI:113:ASP:HB3	19:AI:114:GLN:H	1.75	0.40
25:AO:104:MET:N	25:AO:104:MET:SD	2.94	0.40
26:AQ:420:VAL:HA	26:AQ:421:PRO:HD3	1.97	0.40
40:Mg:49:ALA:HA	40:Mg:52:THR:HG22	2.02	0.40
44:Mk:64:ASN:OD1	45:MI:97:ARG:NH1	2.54	0.40
44:Mk:123:ASP:OD1	44:Mk:124:SER:N	2.53	0.40
52:SC:184:LYS:HA	52:SC:184:LYS:HD2	1.92	0.40
55:SH:595:GLU:HA	55:SH:598:LYS:HB2	2.03	0.40
58:SK:189:LEU:O	58:SK:193:VAL:HG12	2.21	0.40
4:B3:97:ASP:OD1	4:B3:97:ASP:N	2.53	0.40
6:B5:51:LYS:O	6:B5:54:LEU:HG	2.21	0.40
12:BB:707:PRO:O	12:BB:711:GLU:HB2	2.21	0.40
12:BB:782:LEU:HD23	12:BB:782:LEU:HA	1.92	0.40
14:BD:164:ILE:O	14:BD:168:LYS:HB3	2.20	0.40
27:BR:274:ASN:OD1	27:BR:274:ASN:N	2.54	0.40
37:md:232:VAL:HG12	37:md:233:LYS:HG3	2.02	0.40
53:sE:147:ASP:OD1	53:sE:184:LYS:NZ	2.54	0.40
9:sF:335:ASP:OD1	9:sF:336:THR:N	2.54	0.40
9:sF:510:ILE:HD12	9:sF:510:ILE:HG23	1.86	0.40
56:sI:685:ILE:O	56:sI:689:ILE:HG12	2.21	0.40
57:sJ:59:ARG:HH22	58:sK:134:PRO:CG	2.34	0.40
58:sK:202:LYS:HB3	58:sK:207:MET:HE1	2.04	0.40
58:sK:247:GLU:OE1	58:sK:248:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:E6:8:MET:SD	61:E6:9:SER:N	2.95	0.40
61:E6:202:VAL:HG12	61:E6:225:PRO:HB3	2.02	0.40
61:T6:574:LYS:HA	61:T6:577:ILE:HG22	2.04	0.40
61:t6:218:ARG:HH12	61:t6:220:ARG:CB	2.33	0.40
2:A1:214:ILE:HG22	2:A1:218:ARG:HH11	1.86	0.40
3:A2:394:ASP:HA	3:A2:397:ILE:HG12	2.03	0.40
12:AB:778:MET:HE2	12:AB:794:ASN:HD22	1.86	0.40
27:AR:51:LYS:HA	27:AR:51:LYS:HD2	1.92	0.40
28:AS:245:ILE:O	28:AS:248:ILE:HG22	2.21	0.40
37:Md:396:LYS:HG2	37:Md:403:TYR:CE1	2.57	0.40
43:Mj:87:LEU:HG	43:Mj:91:THR:HG23	2.03	0.40
50:SA:186:VAL:HB	50:SA:296:SER:HB2	2.03	0.40
53:SE:489:ARG:HH22	53:SE:493:TRP:HE1	1.70	0.40
9:SF:604:TYR:O	9:SF:608:LEU:HD23	2.22	0.40
55:SH:594:LEU:O	55:SH:597:LYS:HG2	2.22	0.40
59:SL:313:VAL:HA	59:SL:316:THR:HG22	2.04	0.40
7:B6:399:ARG:HH21	7:B6:434:GLN:HA	1.82	0.40
8:B7:670:LEU:HB2	8:B7:690:ILE:HG21	2.04	0.40
11:BA:88:LYS:HA	11:BA:88:LYS:HD3	1.96	0.40
12:BB:896:ASP:N	12:BB:896:ASP:OD1	2.50	0.40
35:mb:59:LEU:HA	35:mb:60:PRO:HD3	1.88	0.40
37:md:276:ASN:OD1	40:mg:33:ARG:NH2	2.54	0.40
38:me:105:THR:HA	38:me:108:ILE:HD12	2.04	0.40
47:mn:6:THR:O	47:mn:10:ILE:HG13	2.22	0.40
51:sD:628:GLN:O	51:sD:640:GLN:NE2	2.45	0.40
53:sE:516:LYS:O	53:sE:519:TYR:HB2	2.21	0.40
55:sH:594:LEU:HD13	55:sH:594:LEU:HD22	1.92	0.40
56:sI:725:ALA:O	56:sI:729:LEU:HD23	2.21	0.40
56:sI:882:THR:HA	56:sI:883:PRO:HD3	1.96	0.40
56:sI:1110:VAL:HG11	56:sI:1193:TRP:CZ2	2.56	0.40
61:E6:749:LEU:HD22	61:E6:791:PHE:HE2	1.87	0.40
61:E6:920:ASP:CG	61:E6:934:ARG:NH1	2.79	0.40
62:T1:47:MET:O	62:T1:51:GLN:N	2.55	0.40
60:T3:976:ASP:OD2	60:T3:1123:TYR:OH	2.38	0.40
60:T3:1126:MET:HE3	60:T3:1126:MET:HB2	1.95	0.40
61:t6:144:THR:OG1	61:t6:146:GLU:OE2	2.19	0.40
6:A5:53:GLU:HB2	6:A5:56:ARG:NH2	2.36	0.40
8:A7:662:ILE:HG13	8:A7:689:ARG:HH12	1.87	0.40
11:AA:1204:ASP:OD1	11:AA:1204:ASP:N	2.53	0.40
26:AQ:27:MET:HE3	26:AQ:27:MET:HB3	1.91	0.40
26:AQ:411:LYS:HA	26:AQ:411:LYS:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:MA:1606:SER:HA	11:MA:1607:PRO:HD3	1.88	0.40
47:Mn:85:VAL:HG11	47:Mn:90:GLN:HE21	1.86	0.40
49:Mp:190:THR:HG22	49:Mp:198:ILE:HG23	2.03	0.40
52:SC:108:LEU:HA	52:SC:108:LEU:HD23	1.84	0.40
51:SD:400:LEU:HA	51:SD:401:PRO:HD3	1.98	0.40
7:B6:138:GLU:OE1	7:B6:138:GLU:N	2.54	0.40
11:BA:353:ILE:HG22	11:BA:468:PHE:HB2	2.03	0.40
11:BA:579:SER:HA	11:BA:582:ILE:HG12	2.03	0.40
11:BA:1197:LEU:HD12	11:BA:1209:MET:HE1	2.03	0.40
11:BA:1221:LYS:CD	11:BA:1222:ASN:H	2.33	0.40
13:BC:222:LYS:HB2	13:BC:222:LYS:HE2	1.92	0.40
17:BG:80:LYS:HA	17:BG:81:PRO:HD3	1.95	0.40
26:BQ:383:SER:OG	26:BQ:384:PHE:N	2.55	0.40
44:mk:64:ASN:OD1	45:ml:97:ARG:NH1	2.54	0.40
51:sB:327:LEU:HD21	51:sB:343:TYR:OH	2.22	0.40
53:sE:28:PHE:O	53:sE:116:THR:OG1	2.38	0.40
53:sE:522:ASP:C	53:sE:547:ARG:NH1	2.79	0.40
58:sK:321:ASP:N	58:sK:321:ASP:OD1	2.53	0.40
60:E3:879:ARG:HH22	60:T3:880:LYS:HZ3	1.65	0.40
60:E3:932:PHE:O	60:E3:936:VAL:HG23	2.21	0.40
62:T1:31:LYS:HZ3	62:T1:83:ILE:HD12	1.86	0.40
60:T3:824:ARG:NH1	60:T3:870:ILE:O	2.42	0.40
61:T6:568:ASP:N	61:T6:568:ASP:OD1	2.54	0.40
61:t6:15:ILE:HD11	61:t6:145:TYR:HB3	2.03	0.40
1:A0:488:ALA:O	1:A0:489:LYS:HE2	2.21	0.40
5:A4:234:VAL:HB	5:A4:252:MET:HE1	2.02	0.40
8:A7:675:SER:OG	8:A7:676:HIS:N	2.52	0.40
11:AA:1002:GLY:O	11:AA:1008:GLN:NE2	2.55	0.40
12:AB:228:LYS:O	12:AB:261:ARG:NH1	2.49	0.40
24:AN:-43:DA:H2"	24:AN:-42:DT:C5	2.56	0.40
49:Mp:113:ASP:OD1	49:Mp:113:ASP:N	2.52	0.40
53:SE:546:LYS:HB2	9:SF:755:ARG:HG3	2.04	0.40
1:B0:538:VAL:HG12	1:B0:598:LEU:HB2	2.03	0.40
1:B0:571:VAL:HG12	1:B0:599:LEU:HB2	2.02	0.40
8:B7:457:TYR:OH	8:B7:488:ASP:O	2.32	0.40
10:B9:236:TRP:NE1	10:B9:240:LYS:HE3	2.35	0.40
11:BA:75:ASN:OD1	11:BA:75:ASN:N	2.54	0.40
11:BA:219:PHE:HB2	11:BA:224:PHE:HD2	1.86	0.40
11:BA:705:LYS:HB2	11:BA:708:MET:HE2	2.04	0.40
28:BS:197:ALA:O	28:BS:201:ILE:HG13	2.21	0.40
29:BT:73:DA:H2"	29:BT:74:DA:C5	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BW:207:ILE:HA	32:BW:208:PRO:HD3	1.96	0.40
34:ma:111:ASP:HB3	34:ma:134:THR:HA	2.03	0.40
37:md:257:ASP:OD1	37:md:258:LYS:N	2.51	0.40
38:me:228:LEU:HD21	38:me:278:LEU:HD12	2.04	0.40
49:mp:130:TYR:OH	49:mp:251:GLY:O	2.36	0.40
52:sC:108:LEU:HD23	52:sC:108:LEU:HA	1.84	0.40
9:sF:313:GLN:HG3	56:sI:659:SER:H	1.87	0.40
56:sI:679:ILE:HD12	56:sI:679:ILE:HG23	1.90	0.40
60:T3:413:ILE:O	60:T3:417:GLU:HG3	2.22	0.40
61:T6:521:VAL:HB	61:T6:530:GLN:HE21	1.87	0.40
61:t6:232:PRO:HD2	61:t6:235:ILE:HD12	2.04	0.40
61:t6:521:VAL:HB	61:t6:530:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
1	B0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
2	A1	406/642 (63%)	389 (96%)	17 (4%)	0	100	100
2	B1	406/642 (63%)	389 (96%)	17 (4%)	0	100	100
3	A2	435/513 (85%)	418 (96%)	13 (3%)	4 (1%)	14	41
3	B2	435/513 (85%)	418 (96%)	13 (3%)	4 (1%)	14	41
4	A3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
4	B3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
5	A4	287/338 (85%)	281 (98%)	6 (2%)	0	100	100
5	B4	287/338 (85%)	281 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A5	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
6	B5	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
7	A6	368/461 (80%)	354 (96%)	14 (4%)	0	100	100
7	B6	368/461 (80%)	354 (96%)	14 (4%)	0	100	100
8	A7	605/843 (72%)	572 (94%)	32 (5%)	1 (0%)	43	72
8	B7	605/843 (72%)	572 (94%)	32 (5%)	1 (0%)	43	72
9	A8	15/905 (2%)	12 (80%)	3 (20%)	0	100	100
9	B8	15/905 (2%)	12 (80%)	3 (20%)	0	100	100
9	SF	407/905 (45%)	366 (90%)	36 (9%)	5 (1%)	10	34
9	sF	407/905 (45%)	366 (90%)	36 (9%)	5 (1%)	10	34
10	A9	66/244 (27%)	65 (98%)	1 (2%)	0	100	100
10	B9	66/244 (27%)	65 (98%)	1 (2%)	0	100	100
11	AA	1386/1733 (80%)	1315 (95%)	69 (5%)	2 (0%)	48	77
11	BA	1386/1733 (80%)	1316 (95%)	68 (5%)	2 (0%)	48	77
11	MA	73/1733 (4%)	64 (88%)	7 (10%)	2 (3%)	4	15
11	mA	73/1733 (4%)	64 (88%)	7 (10%)	2 (3%)	4	15
12	AB	1147/1224 (94%)	1103 (96%)	42 (4%)	2 (0%)	43	72
12	BB	1147/1224 (94%)	1102 (96%)	43 (4%)	2 (0%)	43	72
13	AC	260/318 (82%)	251 (96%)	9 (4%)	0	100	100
13	BC	260/318 (82%)	252 (97%)	8 (3%)	0	100	100
14	AD	153/221 (69%)	148 (97%)	5 (3%)	0	100	100
14	BD	153/221 (69%)	148 (97%)	5 (3%)	0	100	100
15	AE	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
15	BE	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
16	AF	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
16	BF	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
17	AG	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
17	BG	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
18	AH	132/146 (90%)	122 (92%)	10 (8%)	0	100	100
18	BH	132/146 (90%)	122 (92%)	10 (8%)	0	100	100
19	AI	114/122 (93%)	88 (77%)	18 (16%)	8 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	BI	114/122 (93%)	88 (77%)	18 (16%)	8 (7%)	1	2
20	AJ	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
20	BJ	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
21	AK	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
21	BK	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
22	AL	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
22	BL	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
23	AM	267/345 (77%)	255 (96%)	12 (4%)	0	100	100
23	BM	267/345 (77%)	255 (96%)	12 (4%)	0	100	100
25	AO	179/240 (75%)	166 (93%)	12 (7%)	1 (1%)	21	51
25	BO	179/240 (75%)	166 (93%)	12 (7%)	1 (1%)	21	51
26	AQ	208/735 (28%)	199 (96%)	9 (4%)	0	100	100
26	BQ	208/735 (28%)	200 (96%)	8 (4%)	0	100	100
27	AR	251/400 (63%)	241 (96%)	10 (4%)	0	100	100
27	BR	251/400 (63%)	241 (96%)	10 (4%)	0	100	100
28	AS	162/309 (52%)	139 (86%)	19 (12%)	4 (2%)	4	16
28	BS	162/309 (52%)	139 (86%)	19 (12%)	4 (2%)	4	16
30	AU	98/286 (34%)	91 (93%)	6 (6%)	1 (1%)	12	38
30	BU	98/286 (34%)	91 (93%)	6 (6%)	1 (1%)	12	38
31	AV	100/122 (82%)	93 (93%)	6 (6%)	1 (1%)	12	38
31	BV	100/122 (82%)	93 (93%)	6 (6%)	1 (1%)	12	38
32	AW	222/482 (46%)	212 (96%)	9 (4%)	1 (0%)	24	55
32	BW	222/482 (46%)	212 (96%)	9 (4%)	1 (0%)	24	55
33	AX	189/328 (58%)	180 (95%)	9 (5%)	0	100	100
33	BX	189/328 (58%)	180 (95%)	9 (5%)	0	100	100
34	Ma	163/295 (55%)	153 (94%)	10 (6%)	0	100	100
34	ma	163/295 (55%)	153 (94%)	10 (6%)	0	100	100
35	Mb	151/223 (68%)	145 (96%)	5 (3%)	1 (1%)	18	47
35	mb	151/223 (68%)	145 (96%)	5 (3%)	1 (1%)	18	47
36	Mc	104/115 (90%)	99 (95%)	4 (4%)	1 (1%)	12	38
36	mc	104/115 (90%)	99 (95%)	4 (4%)	1 (1%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Md	525/687 (76%)	511 (97%)	13 (2%)	1 (0%)	43	72
37	md	525/687 (76%)	511 (97%)	13 (2%)	1 (0%)	43	72
38	Me	244/307 (80%)	234 (96%)	10 (4%)	0	100	100
38	me	244/307 (80%)	234 (96%)	10 (4%)	0	100	100
39	Mf	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
39	mf	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
40	Mg	102/121 (84%)	89 (87%)	13 (13%)	0	100	100
40	mg	102/121 (84%)	89 (87%)	13 (13%)	0	100	100
41	Mh	175/284 (62%)	164 (94%)	10 (6%)	1 (1%)	21	51
41	mh	175/284 (62%)	164 (94%)	10 (6%)	1 (1%)	21	51
42	Mi	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
42	mi	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
43	Mj	99/149 (66%)	91 (92%)	7 (7%)	1 (1%)	12	38
43	mj	99/149 (66%)	91 (92%)	7 (7%)	1 (1%)	12	38
44	Mk	140/157 (89%)	139 (99%)	1 (1%)	0	100	100
44	mk	140/157 (89%)	139 (99%)	1 (1%)	0	100	100
45	MI	640/1082 (59%)	607 (95%)	32 (5%)	1 (0%)	43	72
45	T4	214/1082 (20%)	203 (95%)	10 (5%)	1 (0%)	24	55
45	ml	640/1082 (59%)	607 (95%)	32 (5%)	1 (0%)	43	72
45	t4	214/1082 (20%)	203 (95%)	10 (5%)	1 (0%)	24	55
46	Mm	79/220 (36%)	69 (87%)	8 (10%)	2 (2%)	4	16
46	mm	79/220 (36%)	69 (87%)	8 (10%)	2 (2%)	4	16
47	Mn	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
47	mn	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
48	Mo	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
48	mo	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
49	Mp	405/566 (72%)	385 (95%)	20 (5%)	0	100	100
49	mp	405/566 (72%)	385 (95%)	20 (5%)	0	100	100
50	SA	438/566 (77%)	413 (94%)	23 (5%)	2 (0%)	24	55
50	sA	438/566 (77%)	413 (94%)	23 (5%)	2 (0%)	24	55
51	SB	385/825 (47%)	370 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	SD	413/825 (50%)	391 (95%)	22 (5%)	0	100	100
51	sB	385/825 (47%)	370 (96%)	15 (4%)	0	100	100
51	sD	413/825 (50%)	391 (95%)	22 (5%)	0	100	100
52	SC	146/332 (44%)	141 (97%)	5 (3%)	0	100	100
52	sC	146/332 (44%)	141 (97%)	5 (3%)	0	100	100
53	SE	401/623 (64%)	359 (90%)	37 (9%)	5 (1%)	10	34
53	sE	401/623 (64%)	359 (90%)	37 (9%)	5 (1%)	10	34
54	SG	13/47 (28%)	11 (85%)	1 (8%)	1 (8%)	1	2
54	sG	13/47 (28%)	11 (85%)	1 (8%)	1 (8%)	1	2
55	SH	237/1703 (14%)	228 (96%)	8 (3%)	1 (0%)	30	60
55	sH	237/1703 (14%)	228 (96%)	8 (3%)	1 (0%)	30	60
56	SI	536/1314 (41%)	517 (96%)	17 (3%)	2 (0%)	30	60
56	sI	536/1314 (41%)	517 (96%)	17 (3%)	2 (0%)	30	60
57	SJ	78/157 (50%)	72 (92%)	6 (8%)	0	100	100
57	sJ	78/157 (50%)	72 (92%)	6 (8%)	0	100	100
58	SK	427/477 (90%)	403 (94%)	24 (6%)	0	100	100
58	sK	427/477 (90%)	403 (94%)	24 (6%)	0	100	100
59	SL	400/467 (86%)	386 (96%)	12 (3%)	2 (0%)	24	55
59	sL	400/467 (86%)	386 (96%)	12 (3%)	2 (0%)	24	55
60	E3	743/1132 (66%)	684 (92%)	55 (7%)	4 (0%)	24	55
60	T3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55
60	t3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55
61	E6	928/974 (95%)	874 (94%)	53 (6%)	1 (0%)	48	77
61	T6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
61	t6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
62	T1	61/431 (14%)	61 (100%)	0	0	100	100
62	t1	61/431 (14%)	61 (100%)	0	0	100	100
63	T2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
63	t2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
64	T5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23
64	t5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	38187/67916 (56%)	36248 (95%)	1808 (5%)	131 (0%)	37 66

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	22	SER
12	AB	474	SER
19	AI	76	PRO
19	AI	113	ASP
28	AS	238	PRO
31	AV	13	SER
35	Mb	56	LYS
36	Mc	77	VAL
41	Mh	40	VAL
53	SE	328	SER
53	SE	467	LYS
9	SF	320	LYS
9	SF	322	PRO
9	SF	334	THR
9	SF	361	ASP
12	BB	22	SER
12	BB	474	SER
19	BI	76	PRO
19	BI	113	ASP
28	BS	238	PRO
31	BV	13	SER
35	mb	56	LYS
36	mc	77	VAL
41	mh	40	VAL
53	sE	328	SER
53	sE	467	LYS
9	sF	320	LYS
9	sF	322	PRO
9	sF	334	THR
9	sF	361	ASP
60	T3	844	ASP
45	T4	1053	ASN
61	T6	761	LYS
60	t3	844	ASP
45	t4	1053	ASN
61	t6	761	LYS
3	A2	68	SER

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Mol	Chain	Res	Type
3	A2	173	MET
3	A2	463	GLU
8	A7	313	VAL
19	AI	57	GLY
19	AI	91	ARG
30	AU	255	LYS
37	Md	256	SER
43	Mj	64	GLU
45	MI	646	LYS
50	SA	302	SER
59	SL	304	ASN
3	B2	68	SER
3	B2	173	MET
3	B2	463	GLU
8	B7	313	VAL
19	BI	57	GLY
19	BI	91	ARG
30	BU	255	LYS
37	md	256	SER
43	mj	64	GLU
45	ml	646	LYS
50	sA	302	SER
59	sL	304	ASN
60	E3	674	LEU
60	E3	679	VAL
60	T3	839	SER
61	T6	156	VAL
60	t3	839	SER
61	t6	156	VAL
3	A2	235	LYS
28	AS	239	ALA
9	SF	357	THR
55	SH	592	LEU
56	SI	1051	LYS
3	B2	235	LYS
28	BS	239	ALA
9	sF	357	THR
55	sH	592	LEU
56	sI	1051	LYS
60	E3	949	VAL
64	T5	906	PRO
64	t5	906	PRO

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Mol	Chain	Res	Type
11	AA	569	LYS
19	AI	47	GLU
19	AI	79	HIS
25	AO	128	SER
28	AS	235	ASP
11	MA	1574	SER
11	BA	569	LYS
19	BI	47	GLU
19	BI	79	HIS
25	BO	128	SER
28	BS	235	ASP
11	mA	1574	SER
60	T3	362	ALA
61	T6	844	ILE
60	t3	362	ALA
61	t6	844	ILE
19	AI	56	ALA
28	AS	206	VAL
32	AW	120	ASN
53	SE	336	LYS
53	SE	511	GLN
54	SG	90	LEU
59	SL	57	ASN
19	BI	56	ALA
28	BS	206	VAL
32	BW	120	ASN
53	sE	336	LYS
53	sE	511	GLN
54	sG	90	LEU
59	sL	57	ASN
60	E3	288	MET
61	E6	490	SER
64	T5	921	PRO
64	t5	921	PRO
19	AI	58	VAL
11	MA	1584	TYR
46	Mm	19	PRO
53	SE	504	PRO
11	mA	1584	TYR
46	mm	19	PRO
53	sE	504	PRO
19	BI	58	VAL

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Mol	Chain	Res	Type
46	Mm	35	ILE
46	mm	35	ILE
11	AA	464	PRO
11	BA	464	PRO
50	SA	62	PRO
56	SI	867	PRO
50	sA	62	PRO
56	sI	867	PRO
60	T3	928	THR
60	t3	928	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	684/707 (97%)	684 (100%)	0	100	100
1	B0	684/707 (97%)	684 (100%)	0	100	100
2	A1	388/589 (66%)	388 (100%)	0	100	100
2	B1	388/589 (66%)	388 (100%)	0	100	100
3	A2	408/468 (87%)	406 (100%)	2 (0%)	81	93
3	B2	408/468 (87%)	406 (100%)	2 (0%)	81	93
4	A3	125/303 (41%)	123 (98%)	2 (2%)	55	83
4	B3	125/303 (41%)	123 (98%)	2 (2%)	55	83
5	A4	260/300 (87%)	260 (100%)	0	100	100
5	B4	260/300 (87%)	260 (100%)	0	100	100
6	A5	59/66 (89%)	59 (100%)	0	100	100
6	B5	59/66 (89%)	59 (100%)	0	100	100
7	A6	338/418 (81%)	338 (100%)	0	100	100
7	B6	338/418 (81%)	338 (100%)	0	100	100
8	A7	539/737 (73%)	539 (100%)	0	100	100
8	B7	539/737 (73%)	539 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	A8	16/823 (2%)	16 (100%)	0	100	100
9	B8	16/823 (2%)	16 (100%)	0	100	100
9	SF	379/823 (46%)	377 (100%)	2 (0%)	81	93
9	sF	379/823 (46%)	377 (100%)	2 (0%)	81	93
10	A9	63/219 (29%)	62 (98%)	1 (2%)	55	83
10	B9	63/219 (29%)	63 (100%)	0	100	100
11	AA	1221/1520 (80%)	1218 (100%)	3 (0%)	87	96
11	BA	1221/1520 (80%)	1218 (100%)	3 (0%)	87	96
11	MA	79/1520 (5%)	79 (100%)	0	100	100
11	mA	79/1520 (5%)	79 (100%)	0	100	100
12	AB	1007/1061 (95%)	1006 (100%)	1 (0%)	88	97
12	BB	1007/1061 (95%)	1006 (100%)	1 (0%)	88	97
13	AC	230/274 (84%)	230 (100%)	0	100	100
13	BC	230/274 (84%)	230 (100%)	0	100	100
14	AD	139/200 (70%)	139 (100%)	0	100	100
14	BD	139/200 (70%)	139 (100%)	0	100	100
15	AE	195/197 (99%)	195 (100%)	0	100	100
15	BE	195/197 (99%)	195 (100%)	0	100	100
16	AF	73/137 (53%)	73 (100%)	0	100	100
16	BF	73/137 (53%)	73 (100%)	0	100	100
17	AG	152/152 (100%)	152 (100%)	0	100	100
17	BG	152/152 (100%)	152 (100%)	0	100	100
18	AH	119/128 (93%)	117 (98%)	2 (2%)	53	83
18	BH	119/128 (93%)	117 (98%)	2 (2%)	53	83
19	AI	110/116 (95%)	101 (92%)	9 (8%)	10	33
19	BI	110/116 (95%)	101 (92%)	9 (8%)	10	33
20	AJ	64/65 (98%)	64 (100%)	0	100	100
20	BJ	64/65 (98%)	64 (100%)	0	100	100
21	AK	99/102 (97%)	99 (100%)	0	100	100
21	BK	99/102 (97%)	99 (100%)	0	100	100
22	AL	40/57 (70%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	BL	40/57 (70%)	40 (100%)	0	100	100
23	AM	234/299 (78%)	234 (100%)	0	100	100
23	BM	234/299 (78%)	234 (100%)	0	100	100
25	AO	153/205 (75%)	153 (100%)	0	100	100
25	BO	153/205 (75%)	153 (100%)	0	100	100
26	AQ	198/641 (31%)	198 (100%)	0	100	100
26	BQ	198/641 (31%)	198 (100%)	0	100	100
27	AR	247/363 (68%)	247 (100%)	0	100	100
27	BR	247/363 (68%)	247 (100%)	0	100	100
28	AS	143/274 (52%)	140 (98%)	3 (2%)	47	79
28	BS	143/274 (52%)	140 (98%)	3 (2%)	47	79
30	AU	94/260 (36%)	94 (100%)	0	100	100
30	BU	94/260 (36%)	94 (100%)	0	100	100
31	AV	94/108 (87%)	94 (100%)	0	100	100
31	BV	94/108 (87%)	94 (100%)	0	100	100
32	AW	207/429 (48%)	207 (100%)	0	100	100
32	BW	207/429 (48%)	207 (100%)	0	100	100
33	AX	171/295 (58%)	171 (100%)	0	100	100
33	BX	171/295 (58%)	171 (100%)	0	100	100
34	Ma	158/259 (61%)	158 (100%)	0	100	100
34	ma	158/259 (61%)	158 (100%)	0	100	100
35	Mb	148/207 (72%)	148 (100%)	0	100	100
35	mb	148/207 (72%)	148 (100%)	0	100	100
36	Mc	101/108 (94%)	101 (100%)	0	100	100
36	mc	101/108 (94%)	101 (100%)	0	100	100
37	Md	499/642 (78%)	499 (100%)	0	100	100
37	md	499/642 (78%)	499 (100%)	0	100	100
38	Me	224/280 (80%)	224 (100%)	0	100	100
38	me	224/280 (80%)	224 (100%)	0	100	100
39	Mf	178/178 (100%)	178 (100%)	0	100	100
39	mf	178/178 (100%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Mg	98/113 (87%)	98 (100%)	0	100	100
40	mg	98/113 (87%)	98 (100%)	0	100	100
41	Mh	164/258 (64%)	164 (100%)	0	100	100
41	mh	164/258 (64%)	164 (100%)	0	100	100
42	Mi	175/208 (84%)	175 (100%)	0	100	100
42	mi	175/208 (84%)	175 (100%)	0	100	100
43	Mj	101/144 (70%)	101 (100%)	0	100	100
43	mj	101/144 (70%)	101 (100%)	0	100	100
44	Mk	132/145 (91%)	132 (100%)	0	100	100
44	mk	132/145 (91%)	132 (100%)	0	100	100
45	MI	618/1001 (62%)	618 (100%)	0	100	100
45	T4	205/1001 (20%)	205 (100%)	0	100	100
45	ml	618/1001 (62%)	618 (100%)	0	100	100
45	t4	205/1001 (20%)	205 (100%)	0	100	100
46	Mm	77/195 (40%)	77 (100%)	0	100	100
46	mm	77/195 (40%)	77 (100%)	0	100	100
47	Mn	132/132 (100%)	132 (100%)	0	100	100
47	mn	132/132 (100%)	132 (100%)	0	100	100
48	Mo	102/117 (87%)	102 (100%)	0	100	100
48	mo	102/117 (87%)	102 (100%)	0	100	100
49	Mp	390/528 (74%)	390 (100%)	0	100	100
49	mp	390/528 (74%)	390 (100%)	0	100	100
50	SA	408/517 (79%)	406 (100%)	2 (0%)	81	93
50	sA	408/517 (79%)	407 (100%)	1 (0%)	87	96
51	SB	368/751 (49%)	368 (100%)	0	100	100
51	SD	392/751 (52%)	392 (100%)	0	100	100
51	sB	368/751 (49%)	368 (100%)	0	100	100
51	sD	392/751 (52%)	392 (100%)	0	100	100
52	SC	141/288 (49%)	141 (100%)	0	100	100
52	sC	141/288 (49%)	141 (100%)	0	100	100
53	SE	368/558 (66%)	368 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	sE	368/558 (66%)	368 (100%)	0	100	100
54	SG	7/13 (54%)	7 (100%)	0	100	100
54	sG	7/13 (54%)	7 (100%)	0	100	100
55	SH	221/1520 (14%)	221 (100%)	0	100	100
55	sH	221/1520 (14%)	221 (100%)	0	100	100
56	SI	528/1218 (43%)	528 (100%)	0	100	100
56	sI	528/1218 (43%)	528 (100%)	0	100	100
57	SJ	80/140 (57%)	80 (100%)	0	100	100
57	sJ	80/140 (57%)	80 (100%)	0	100	100
58	SK	381/420 (91%)	381 (100%)	0	100	100
58	sK	381/420 (91%)	381 (100%)	0	100	100
59	SL	370/423 (88%)	370 (100%)	0	100	100
59	sL	370/423 (88%)	370 (100%)	0	100	100
60	E3	701/1053 (67%)	698 (100%)	3 (0%)	84	94
60	T3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
60	t3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
61	E6	861/897 (96%)	861 (100%)	0	100	100
61	T6	861/897 (96%)	860 (100%)	1 (0%)	88	97
61	t6	861/897 (96%)	860 (100%)	1 (0%)	88	97
62	T1	60/389 (15%)	60 (100%)	0	100	100
62	t1	60/389 (15%)	60 (100%)	0	100	100
63	T2	100/339 (30%)	100 (100%)	0	100	100
63	t2	100/339 (30%)	100 (100%)	0	100	100
64	T5	103/944 (11%)	99 (96%)	4 (4%)	28	64
64	t5	103/944 (11%)	99 (96%)	4 (4%)	28	64
All	All	35424/61136 (58%)	35351 (100%)	73 (0%)	85	96

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A2	464	THR
3	A2	490	LYS
4	A3	49	LEU

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Mol	Chain	Res	Type
4	A3	64	ARG
10	A9	199	GLN
11	AA	676	MET
11	AA	688	LYS
11	AA	692	ASP
12	AB	662	MET
18	AH	109	LYS
18	AH	130	ARG
19	AI	60	GLN
19	AI	61	ASP
19	AI	62	ILE
19	AI	77	LYS
19	AI	82	GLU
19	AI	84	VAL
19	AI	86	PHE
19	AI	102	VAL
19	AI	111	THR
28	AS	182	MET
28	AS	206	VAL
28	AS	236	LEU
50	SA	269	GLN
50	SA	270	TYR
9	SF	379	HIS
9	SF	401	LYS
3	B2	464	THR
3	B2	490	LYS
4	B3	49	LEU
4	B3	64	ARG
11	BA	676	MET
11	BA	688	LYS
11	BA	692	ASP
12	BB	662	MET
18	BH	109	LYS
18	BH	130	ARG
19	BI	60	GLN
19	BI	61	ASP
19	BI	62	ILE
19	BI	77	LYS
19	BI	82	GLU
19	BI	84	VAL
19	BI	86	PHE
19	BI	102	VAL

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Mol	Chain	Res	Type
19	BI	111	THR
28	BS	182	MET
28	BS	206	VAL
28	BS	236	LEU
50	sA	270	TYR
9	sF	379	HIS
9	sF	401	LYS
60	E3	409	LYS
60	E3	413	ILE
60	E3	939	THR
60	T3	833	ASN
60	T3	836	ILE
60	T3	837	TYR
60	T3	838	SER
64	T5	877	LYS
64	T5	919	ARG
64	T5	920	LYS
64	T5	931	GLN
61	T6	505	PRO
60	t3	833	ASN
60	t3	836	ILE
60	t3	837	TYR
60	t3	838	SER
64	t5	877	LYS
64	t5	919	ARG
64	t5	920	LYS
64	t5	931	GLN
61	t6	505	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (646) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	280	GLN
1	A0	283	GLN
1	A0	350	HIS
1	A0	577	GLN
1	A0	699	GLN
2	A1	258	ASN
2	A1	273	ASN
2	A1	277	ASN
2	A1	417	ASN
2	A1	425	ASN

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Mol	Chain	Res	Type
2	A1	500	ASN
2	A1	513	GLN
2	A1	567	HIS
2	A1	621	ASN
2	A1	638	ASN
3	A2	8	HIS
3	A2	22	GLN
3	A2	69	ASN
3	A2	251	GLN
3	A2	261	GLN
3	A2	356	GLN
3	A2	500	GLN
4	A3	9	ASN
4	A3	100	ASN
4	A3	107	ASN
5	A4	62	ASN
5	A4	145	GLN
6	A5	22	GLN
6	A5	43	ASN
7	A6	146	HIS
7	A6	339	HIS
8	A7	116	HIS
8	A7	229	HIS
8	A7	243	GLN
8	A7	247	ASN
8	A7	347	HIS
8	A7	349	ASN
8	A7	434	ASN
8	A7	539	ASN
8	A7	598	HIS
8	A7	633	GLN
8	A7	641	GLN
8	A7	644	GLN
10	A9	213	ASN
11	AA	68	GLN
11	AA	71	GLN
11	AA	109	HIS
11	AA	209	ASN
11	AA	213	HIS
11	AA	287	HIS
11	AA	299	HIS
11	AA	306	ASN

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Mol	Chain	Res	Type
11	AA	311	GLN
11	AA	339	ASN
11	AA	445	ASN
11	AA	451	HIS
11	AA	490	HIS
11	AA	510	GLN
11	AA	517	ASN
11	AA	525	GLN
11	AA	587	HIS
11	AA	650	GLN
11	AA	660	ASN
11	AA	736	ASN
11	AA	741	ASN
11	AA	742	ASN
11	AA	757	ASN
11	AA	802	ASN
11	AA	854	ASN
11	AA	935	GLN
11	AA	975	HIS
11	AA	1008	GLN
11	AA	1048	ASN
11	AA	1312	ASN
11	AA	1378	GLN
12	AB	73	GLN
12	AB	350	GLN
12	AB	357	GLN
12	AB	395	GLN
12	AB	465	ASN
12	AB	499	ASN
12	AB	572	HIS
12	AB	583	ASN
12	AB	770	GLN
12	AB	958	GLN
12	AB	984	HIS
12	AB	1015	HIS
12	AB	1025	HIS
12	AB	1065	GLN
12	AB	1161	HIS
12	AB	1177	HIS
13	AC	7	GLN
13	AC	73	GLN
15	AE	101	GLN

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Mol	Chain	Res	Type
15	AE	113	GLN
17	AG	10	ASN
17	AG	97	HIS
17	AG	102	GLN
17	AG	122	ASN
18	AH	134	ASN
19	AI	23	ASN
19	AI	79	HIS
19	AI	83	ASN
19	AI	108	HIS
20	AJ	53	HIS
21	AK	76	GLN
21	AK	89	ASN
22	AL	53	HIS
25	AO	91	ASN
25	AO	179	HIS
26	AQ	122	GLN
26	AQ	140	HIS
26	AQ	331	GLN
26	AQ	369	ASN
26	AQ	399	ASN
27	AR	88	HIS
27	AR	265	HIS
28	AS	220	ASN
28	AS	252	ASN
28	AS	255	ASN
28	AS	304	ASN
30	AU	272	ASN
30	AU	277	GLN
30	AU	280	GLN
31	AV	17	ASN
32	AW	72	GLN
32	AW	116	ASN
33	AX	123	HIS
33	AX	145	ASN
34	Ma	10	GLN
34	Ma	56	ASN
34	Ma	159	ASN
34	Ma	201	HIS
35	Mb	42	GLN
35	Mb	45	HIS
35	Mb	157	ASN

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Mol	Chain	Res	Type
36	Mc	51	HIS
36	Mc	54	GLN
36	Mc	76	ASN
36	Mc	93	GLN
36	Mc	101	GLN
37	Md	120	ASN
37	Md	296	ASN
37	Md	310	ASN
38	Me	3	GLN
38	Me	4	GLN
38	Me	51	ASN
38	Me	176	ASN
38	Me	258	ASN
38	Me	294	GLN
39	Mf	75	ASN
39	Mf	94	ASN
39	Mf	141	ASN
40	Mg	61	GLN
40	Mg	68	ASN
40	Mg	103	GLN
41	Mh	119	ASN
42	Mi	160	HIS
42	Mi	181	GLN
43	Mj	13	GLN
43	Mj	68	HIS
43	Mj	81	ASN
43	Mj	123	GLN
44	Mk	68	ASN
44	Mk	109	GLN
45	Ml	89	GLN
45	Ml	160	HIS
45	Ml	178	ASN
45	Ml	188	ASN
45	Ml	192	ASN
45	Ml	402	HIS
45	Ml	502	GLN
45	Ml	523	GLN
45	Ml	631	HIS
45	Ml	787	ASN
45	Ml	831	GLN
46	Mm	27	GLN
47	Mn	7	GLN

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Mol	Chain	Res	Type
47	Mn	29	ASN
49	Mp	106	ASN
49	Mp	118	HIS
49	Mp	157	ASN
49	Mp	247	ASN
49	Mp	332	ASN
49	Mp	536	HIS
50	SA	169	GLN
50	SA	384	GLN
50	SA	549	ASN
51	SB	370	ASN
51	SB	522	GLN
51	SB	605	ASN
51	SB	619	ASN
51	SB	624	GLN
51	SB	680	ASN
51	SB	718	GLN
51	SB	732	ASN
51	SB	766	GLN
52	SC	78	GLN
52	SC	92	ASN
52	SC	110	ASN
51	SD	320	HIS
51	SD	359	ASN
51	SD	445	ASN
51	SD	552	ASN
51	SD	587	ASN
51	SD	605	ASN
51	SD	669	HIS
51	SD	678	GLN
51	SD	690	GLN
51	SD	699	ASN
51	SD	730	ASN
51	SD	769	HIS
53	SE	280	GLN
53	SE	452	ASN
53	SE	471	HIS
53	SE	498	GLN
53	SE	532	ASN
53	SE	538	ASN
9	SF	341	GLN
9	SF	349	ASN

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Mol	Chain	Res	Type
9	SF	389	ASN
9	SF	410	ASN
9	SF	482	ASN
9	SF	525	GLN
9	SF	534	GLN
9	SF	556	GLN
9	SF	560	GLN
9	SF	600	GLN
9	SF	651	ASN
9	SF	756	ASN
55	SH	466	GLN
55	SH	491	HIS
55	SH	584	GLN
56	SI	675	ASN
56	SI	805	ASN
56	SI	915	ASN
56	SI	917	GLN
56	SI	970	ASN
56	SI	981	ASN
56	SI	1095	ASN
56	SI	1100	ASN
56	SI	1213	ASN
56	SI	1216	ASN
56	SI	1288	ASN
56	SI	1294	GLN
56	SI	1297	ASN
56	SI	1300	GLN
58	SK	209	ASN
58	SK	261	GLN
58	SK	266	GLN
58	SK	445	ASN
59	SL	167	HIS
59	SL	179	GLN
59	SL	433	GLN
1	B0	280	GLN
1	B0	283	GLN
1	B0	350	HIS
1	B0	577	GLN
2	B1	258	ASN
2	B1	417	ASN
2	B1	425	ASN
2	B1	500	ASN

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Mol	Chain	Res	Type
2	B1	513	GLN
2	B1	567	HIS
2	B1	621	ASN
2	B1	638	ASN
3	B2	8	HIS
3	B2	69	ASN
3	B2	251	GLN
3	B2	261	GLN
3	B2	356	GLN
3	B2	500	GLN
4	B3	9	ASN
4	B3	100	ASN
4	B3	107	ASN
5	B4	62	ASN
6	B5	22	GLN
6	B5	43	ASN
7	B6	114	ASN
7	B6	146	HIS
7	B6	339	HIS
8	B7	116	HIS
8	B7	229	HIS
8	B7	243	GLN
8	B7	247	ASN
8	B7	331	GLN
8	B7	347	HIS
8	B7	349	ASN
8	B7	434	ASN
8	B7	539	ASN
8	B7	598	HIS
8	B7	633	GLN
8	B7	641	GLN
8	B7	644	GLN
10	B9	213	ASN
11	BA	68	GLN
11	BA	71	GLN
11	BA	109	HIS
11	BA	209	ASN
11	BA	213	HIS
11	BA	287	HIS
11	BA	299	HIS
11	BA	306	ASN
11	BA	311	GLN

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Mol	Chain	Res	Type
11	BA	445	ASN
11	BA	451	HIS
11	BA	490	HIS
11	BA	510	GLN
11	BA	517	ASN
11	BA	525	GLN
11	BA	587	HIS
11	BA	650	GLN
11	BA	660	ASN
11	BA	736	ASN
11	BA	741	ASN
11	BA	757	ASN
11	BA	802	ASN
11	BA	854	ASN
11	BA	935	GLN
11	BA	975	HIS
11	BA	1008	GLN
11	BA	1048	ASN
11	BA	1312	ASN
11	BA	1378	GLN
12	BB	73	GLN
12	BB	300	HIS
12	BB	350	GLN
12	BB	357	GLN
12	BB	395	GLN
12	BB	465	ASN
12	BB	572	HIS
12	BB	583	ASN
12	BB	770	GLN
12	BB	958	GLN
12	BB	984	HIS
12	BB	1015	HIS
12	BB	1025	HIS
12	BB	1065	GLN
12	BB	1161	HIS
12	BB	1177	HIS
13	BC	7	GLN
13	BC	73	GLN
13	BC	135	GLN
15	BE	101	GLN
15	BE	113	GLN
17	BG	10	ASN

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Mol	Chain	Res	Type
17	BG	97	HIS
17	BG	102	GLN
17	BG	122	ASN
18	BH	134	ASN
19	BI	23	ASN
19	BI	79	HIS
19	BI	83	ASN
19	BI	108	HIS
20	BJ	53	HIS
21	BK	76	GLN
21	BK	89	ASN
22	BL	53	HIS
25	BO	91	ASN
25	BO	179	HIS
26	BQ	122	GLN
26	BQ	140	HIS
26	BQ	160	GLN
26	BQ	369	ASN
26	BQ	399	ASN
27	BR	88	HIS
27	BR	265	HIS
28	BS	220	ASN
28	BS	252	ASN
28	BS	255	ASN
28	BS	283	GLN
28	BS	304	ASN
30	BU	272	ASN
30	BU	277	GLN
30	BU	280	GLN
32	BW	72	GLN
32	BW	116	ASN
33	BX	123	HIS
33	BX	145	ASN
34	ma	10	GLN
34	ma	56	ASN
34	ma	159	ASN
34	ma	180	HIS
34	ma	201	HIS
35	mb	42	GLN
35	mb	45	HIS
35	mb	85	HIS
35	mb	106	HIS

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Mol	Chain	Res	Type
35	mb	157	ASN
36	mc	19	GLN
36	mc	51	HIS
36	mc	54	GLN
36	mc	76	ASN
36	mc	93	GLN
36	mc	101	GLN
37	md	120	ASN
37	md	296	ASN
37	md	310	ASN
38	me	3	GLN
38	me	4	GLN
38	me	51	ASN
38	me	176	ASN
38	me	258	ASN
39	mf	75	ASN
39	mf	94	ASN
39	mf	141	ASN
40	mg	61	GLN
40	mg	68	ASN
40	mg	103	GLN
41	mh	119	ASN
42	mi	160	HIS
42	mi	181	GLN
43	mj	13	GLN
43	mj	68	HIS
43	mj	81	ASN
43	mj	123	GLN
44	mk	68	ASN
44	mk	109	GLN
45	ml	89	GLN
45	ml	160	HIS
45	ml	178	ASN
45	ml	188	ASN
45	ml	192	ASN
45	ml	402	HIS
45	ml	502	GLN
45	ml	523	GLN
45	ml	631	HIS
45	ml	741	ASN
45	ml	787	ASN
45	ml	801	HIS

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Mol	Chain	Res	Type
47	mn	7	GLN
49	mp	106	ASN
49	mp	118	HIS
49	mp	157	ASN
49	mp	247	ASN
49	mp	332	ASN
49	mp	536	HIS
50	sA	169	GLN
50	sA	384	GLN
50	sA	549	ASN
51	sB	370	ASN
51	sB	522	GLN
51	sB	605	ASN
51	sB	619	ASN
51	sB	624	GLN
51	sB	680	ASN
51	sB	718	GLN
51	sB	732	ASN
51	sB	766	GLN
52	sC	78	GLN
52	sC	92	ASN
52	sC	110	ASN
51	sD	320	HIS
51	sD	359	ASN
51	sD	445	ASN
51	sD	552	ASN
51	sD	587	ASN
51	sD	605	ASN
51	sD	647	GLN
51	sD	669	HIS
51	sD	678	GLN
51	sD	690	GLN
51	sD	699	ASN
51	sD	730	ASN
51	sD	769	HIS
53	sE	452	ASN
53	sE	471	HIS
53	sE	498	GLN
53	sE	532	ASN
9	sF	341	GLN
9	sF	349	ASN
9	sF	389	ASN

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Mol	Chain	Res	Type
9	sF	410	ASN
9	sF	482	ASN
9	sF	525	GLN
9	sF	534	GLN
9	sF	556	GLN
9	sF	560	GLN
9	sF	651	ASN
9	sF	756	ASN
55	sH	466	GLN
55	sH	491	HIS
56	sI	675	ASN
56	sI	805	ASN
56	sI	915	ASN
56	sI	917	GLN
56	sI	941	ASN
56	sI	970	ASN
56	sI	981	ASN
56	sI	1093	ASN
56	sI	1095	ASN
56	sI	1100	ASN
56	sI	1213	ASN
56	sI	1216	ASN
56	sI	1260	ASN
56	sI	1284	GLN
56	sI	1288	ASN
56	sI	1294	GLN
56	sI	1297	ASN
56	sI	1300	GLN
58	sK	209	ASN
58	sK	261	GLN
58	sK	266	GLN
58	sK	445	ASN
59	sL	167	HIS
59	sL	179	GLN
59	sL	433	GLN
60	E3	356	ASN
60	E3	516	HIS
60	E3	556	ASN
60	E3	708	GLN
60	E3	720	ASN
60	E3	831	GLN
60	E3	872	ASN

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Mol	Chain	Res	Type
60	E3	901	ASN
60	E3	1093	HIS
60	E3	1099	ASN
60	E3	1113	ASN
61	E6	155	ASN
61	E6	223	GLN
61	E6	418	GLN
61	E6	480	GLN
61	E6	523	GLN
61	E6	654	ASN
61	E6	676	ASN
61	E6	679	GLN
61	E6	693	GLN
61	E6	715	GLN
61	E6	800	ASN
61	E6	808	GLN
63	T2	46	GLN
63	T2	52	GLN
63	T2	82	ASN
63	T2	96	GLN
60	T3	333	GLN
60	T3	352	GLN
60	T3	356	ASN
60	T3	363	ASN
60	T3	421	ASN
60	T3	485	GLN
60	T3	528	ASN
60	T3	537	GLN
60	T3	608	ASN
60	T3	632	ASN
60	T3	690	ASN
60	T3	702	ASN
60	T3	728	GLN
60	T3	769	GLN
60	T3	901	ASN
60	T3	1099	ASN
60	T3	1105	ASN
60	T3	1113	ASN
45	T4	893	ASN
45	T4	913	ASN
45	T4	919	HIS
45	T4	1002	HIS

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Mol	Chain	Res	Type
45	T4	1021	GLN
45	T4	1025	GLN
45	T4	1070	HIS
64	T5	871	HIS
64	T5	931	GLN
61	T6	6	HIS
61	T6	25	ASN
61	T6	40	ASN
61	T6	44	HIS
61	T6	47	GLN
61	T6	100	GLN
61	T6	109	HIS
61	T6	129	ASN
61	T6	137	GLN
61	T6	162	HIS
61	T6	187	ASN
61	T6	266	GLN
61	T6	293	GLN
61	T6	317	ASN
61	T6	327	ASN
61	T6	530	GLN
61	T6	548	ASN
61	T6	675	ASN
61	T6	687	GLN
61	T6	693	GLN
61	T6	697	HIS
61	T6	726	ASN
61	T6	757	GLN
61	T6	771	ASN
61	T6	800	ASN
61	T6	864	ASN
61	T6	894	ASN
63	t2	46	GLN
63	t2	52	GLN
63	t2	82	ASN
63	t2	96	GLN
60	t3	333	GLN
60	t3	352	GLN
60	t3	356	ASN
60	t3	363	ASN
60	t3	421	ASN
60	t3	485	GLN

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Mol	Chain	Res	Type
60	t3	537	GLN
60	t3	608	ASN
60	t3	632	ASN
60	t3	690	ASN
60	t3	702	ASN
60	t3	769	GLN
60	t3	901	ASN
60	t3	1099	ASN
60	t3	1105	ASN
60	t3	1113	ASN
45	t4	893	ASN
45	t4	913	ASN
45	t4	919	HIS
45	t4	1002	HIS
45	t4	1021	GLN
45	t4	1025	GLN
45	t4	1070	HIS
64	t5	871	HIS
64	t5	931	GLN
61	t6	6	HIS
61	t6	25	ASN
61	t6	40	ASN
61	t6	44	HIS
61	t6	47	GLN
61	t6	100	GLN
61	t6	109	HIS
61	t6	129	ASN
61	t6	137	GLN
61	t6	162	HIS
61	t6	187	ASN
61	t6	222	GLN
61	t6	266	GLN
61	t6	273	GLN
61	t6	293	GLN
61	t6	327	ASN
61	t6	530	GLN
61	t6	548	ASN
61	t6	675	ASN
61	t6	687	GLN
61	t6	693	GLN
61	t6	697	HIS
61	t6	726	ASN

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Mol	Chain	Res	Type
61	t6	733	HIS
61	t6	771	ASN
61	t6	800	ASN
61	t6	808	GLN
61	t6	864	ASN
61	t6	894	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 38 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
65	SF4	B0	801	1	0,12,12	-	-	-		
65	SF4	A0	801	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	SF4	B0	801	1	-	-	0/6/5/5
65	SF4	A0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	T3	4
60	t3	4
53	SE	3
53	sE	3
54	SG	2
54	sG	2
11	MA	2
11	mA	2
27	AR	2
27	BR	2
56	SI	1
56	sI	1
45	T4	1
45	t4	1
23	AM	1
23	BM	1
12	AB	1
12	BB	1
55	SH	1
55	sH	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SG	95:UNK	C	118:ARG	N	72.09
1	sG	95:UNK	C	118:ARG	N	72.09
1	SG	66:UNK	C	82:UNK	N	34.38
1	sG	66:UNK	C	82:UNK	N	34.38
1	MA	1652:PRO	C	1667:SER	N	32.61
1	mA	1652:PRO	C	1667:SER	N	32.61
1	MA	1614:PRO	C	1629:THR	N	25.71
1	mA	1614:PRO	C	1629:THR	N	25.71
1	SI	1099:ASN	C	1100:ASN	N	6.53
1	sI	1099:ASN	C	1100:ASN	N	6.53
1	T4	1003:PHE	C	1004:ALA	N	4.95
1	t4	1003:PHE	C	1004:ALA	N	4.95
1	AM	65:THR	C	66:PHE	N	4.70
1	BM	65:THR	C	66:PHE	N	4.70
1	SE	441:GLN	C	442:TYR	N	4.11
1	sE	441:GLN	C	442:TYR	N	4.11
1	T3	333:GLN	C	334:ASN	N	3.85
1	t3	333:GLN	C	334:ASN	N	3.85
1	AR	56:SER	C	57:LEU	N	3.73
1	BR	56:SER	C	57:LEU	N	3.73
1	T3	676:GLU	C	677:SER	N	3.42
1	t3	676:GLU	C	677:SER	N	3.42
1	SE	568:TYR	C	569:SER	N	3.35
1	sE	568:TYR	C	569:SER	N	3.35
1	SE	449:TYR	C	450:GLU	N	3.27
1	sE	449:TYR	C	450:GLU	N	3.27
1	T3	580:SER	C	581:PHE	N	3.27
1	t3	580:SER	C	581:PHE	N	3.27
1	AB	1155:SER	C	1156:ASP	N	3.25
1	BB	1155:SER	C	1156:ASP	N	3.25
1	T3	667:ASN	C	668:VAL	N	3.25
1	t3	667:ASN	C	668:VAL	N	3.25
1	AR	227:SER	C	228:MET	N	3.03
1	BR	227:SER	C	228:MET	N	3.03
1	SH	587:LYS	C	588:ASN	N	2.81
1	sH	587:LYS	C	588:ASN	N	2.81

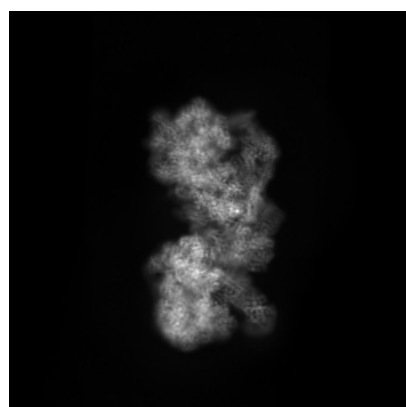
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71535. These allow visual inspection of the internal detail of the map and identification of artifacts.

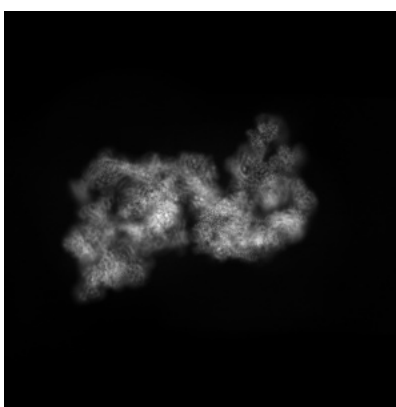
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

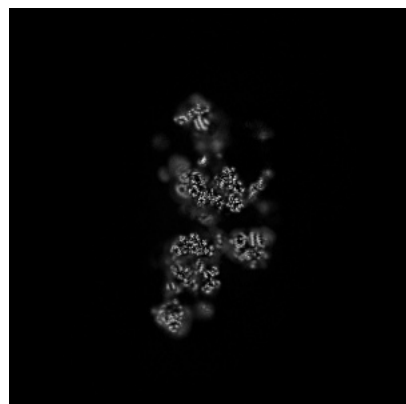


Z

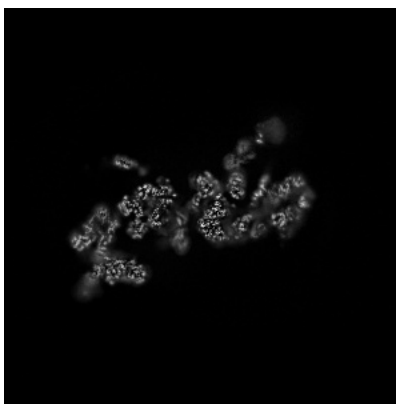
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

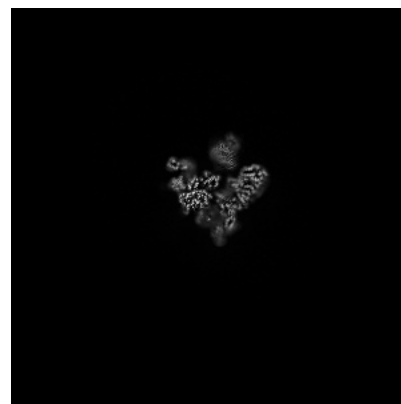
6.2.1 Primary map



X Index: 320



Y Index: 320

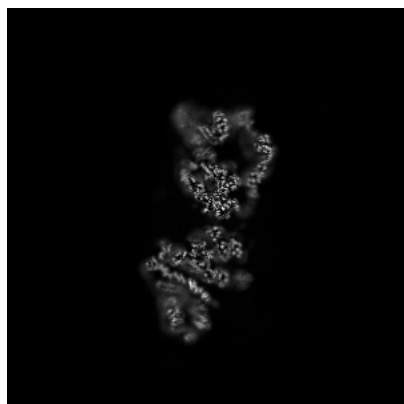


Z Index: 320

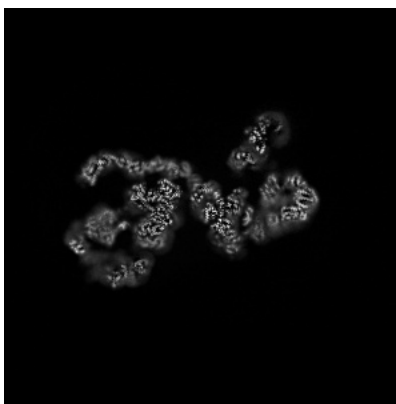
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

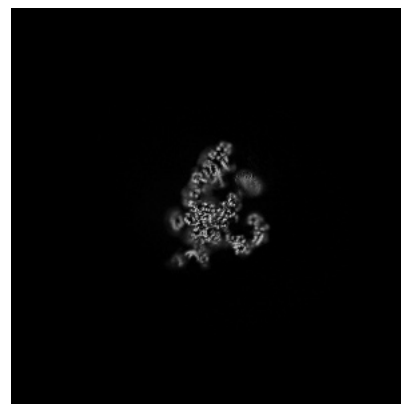
6.3.1 Primary map



X Index: 293



Y Index: 303

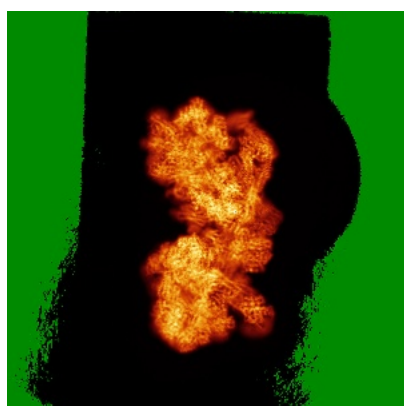


Z Index: 247

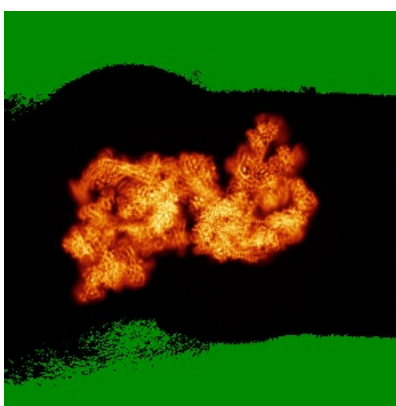
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

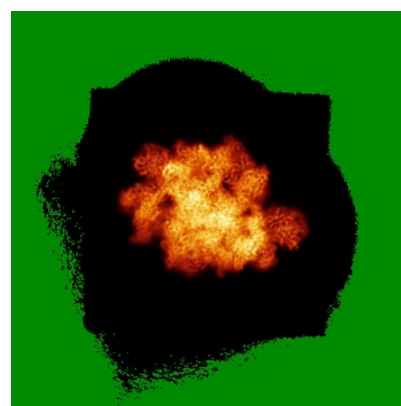
6.4.1 Primary map



X



Y



Z

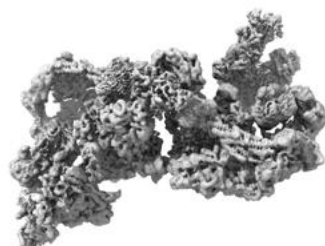
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

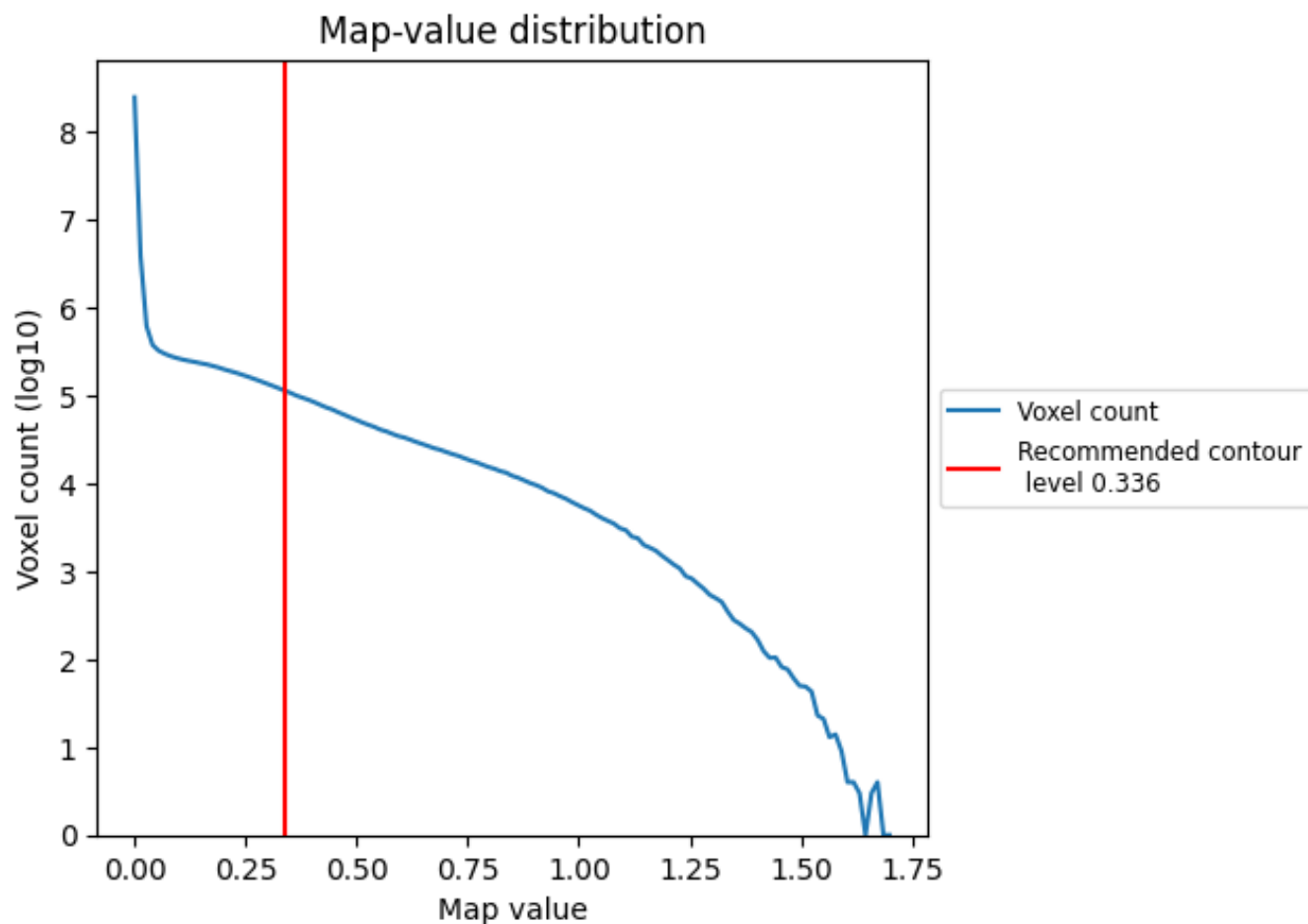
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

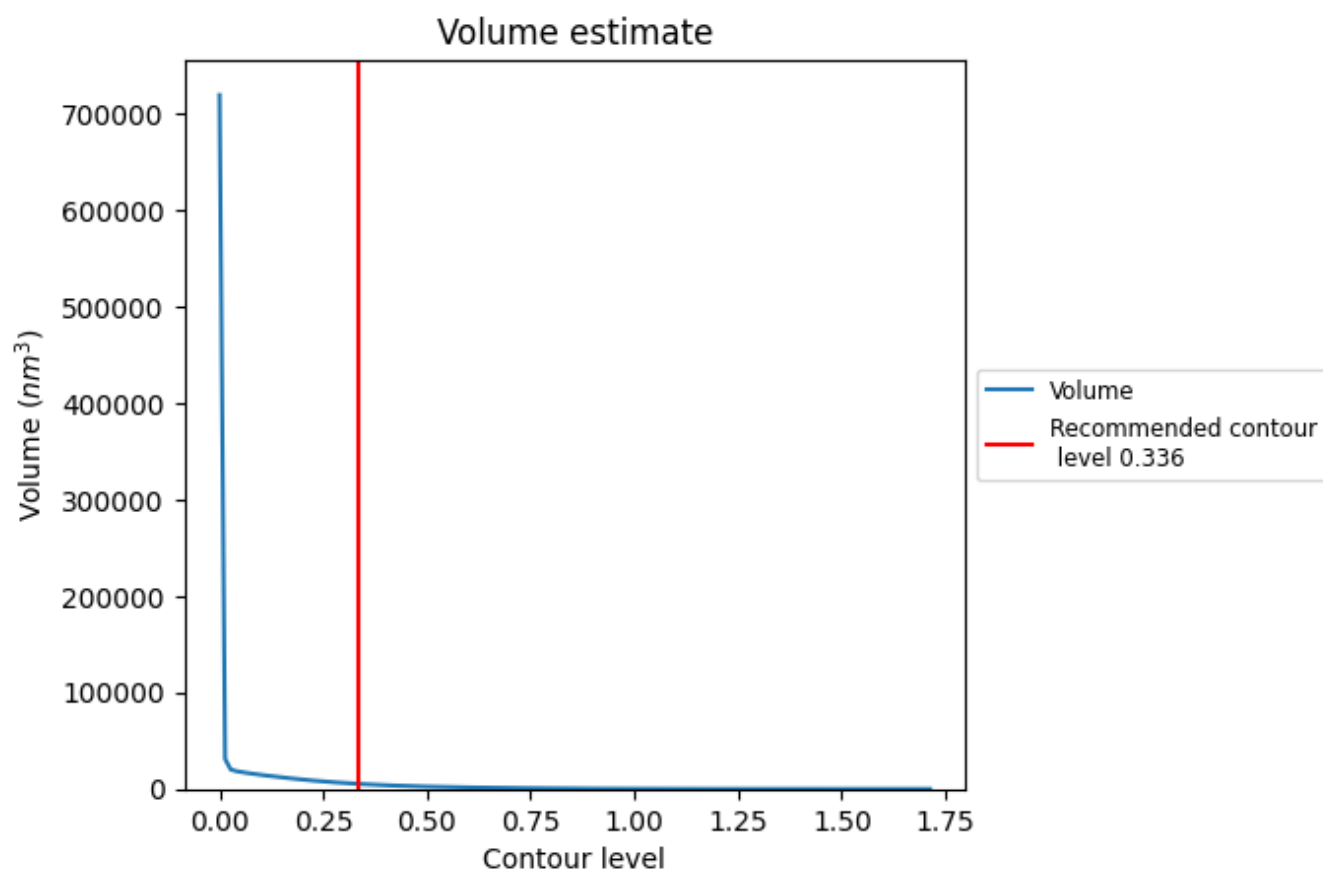
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

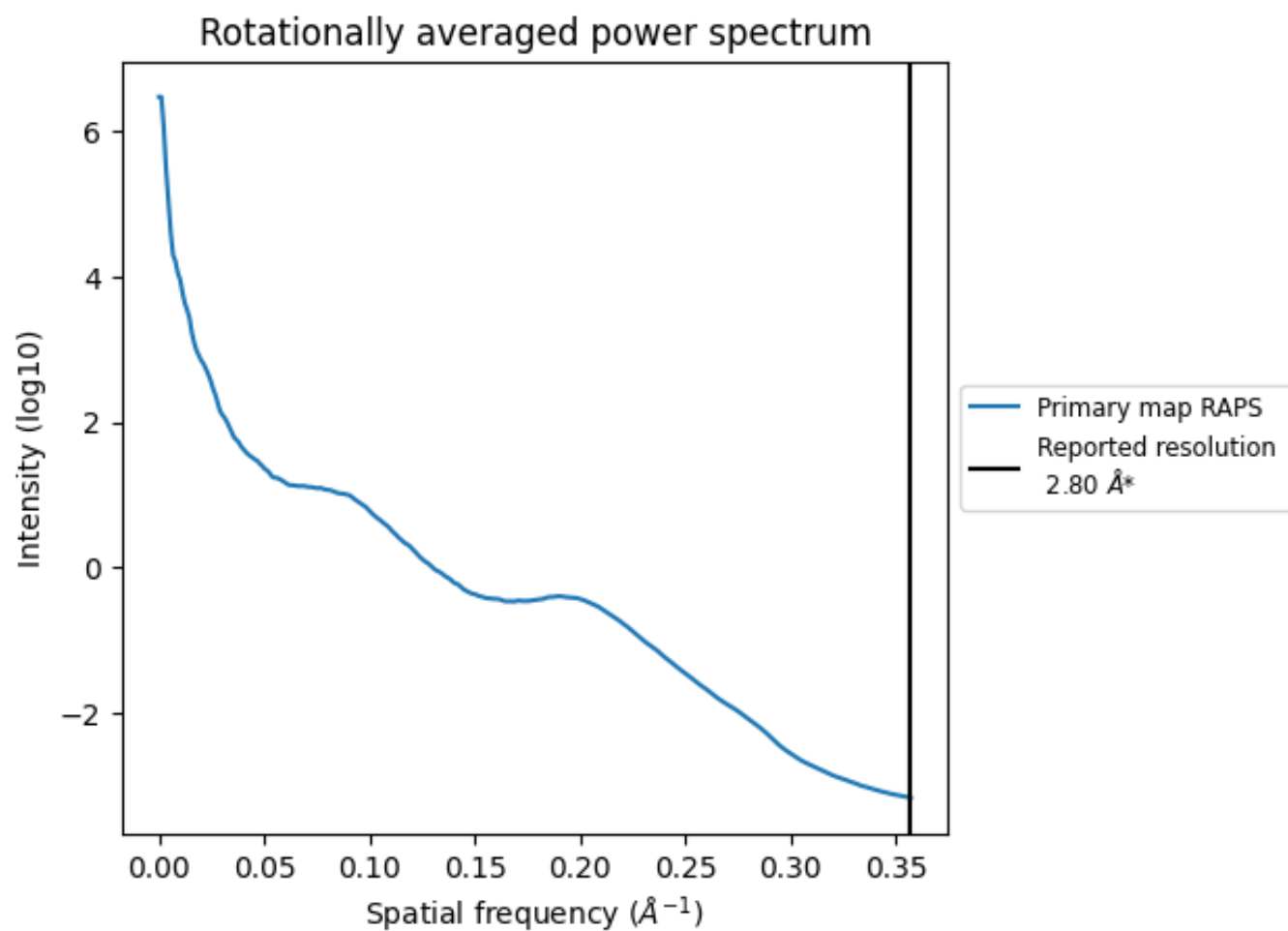
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5251 nm^3 ; this corresponds to an approximate mass of 4744 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

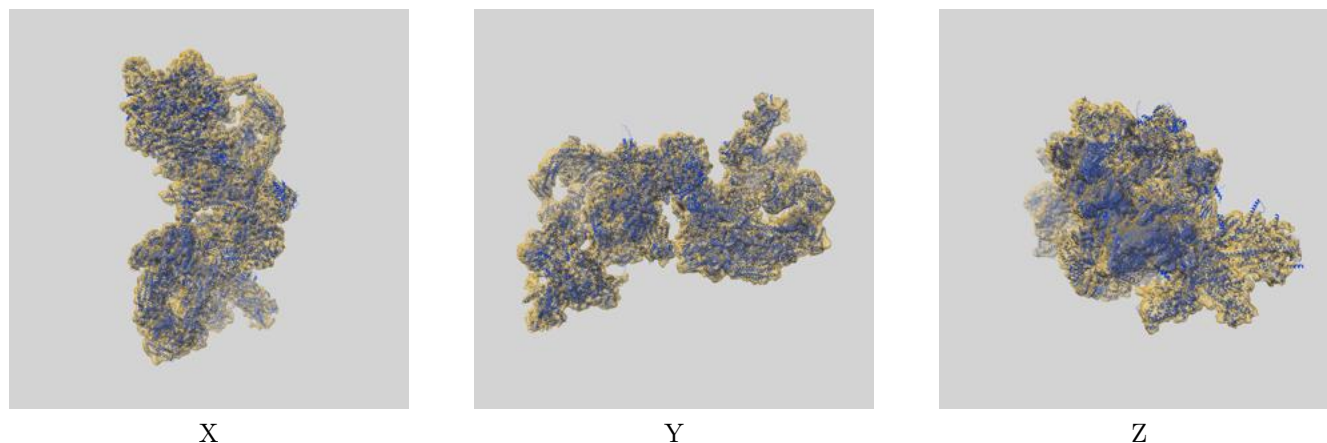
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

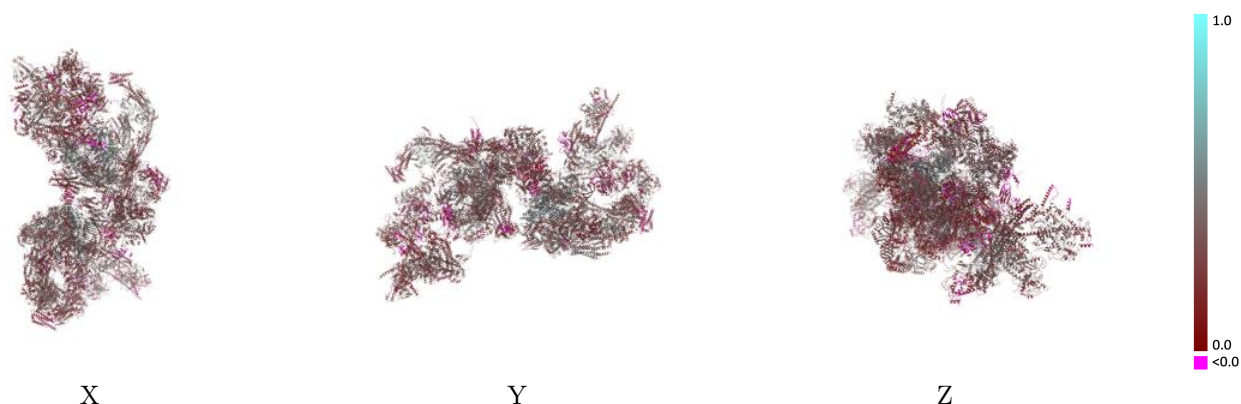
This section contains information regarding the fit between EMDB map EMD-71535 and PDB model 9PDJ. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



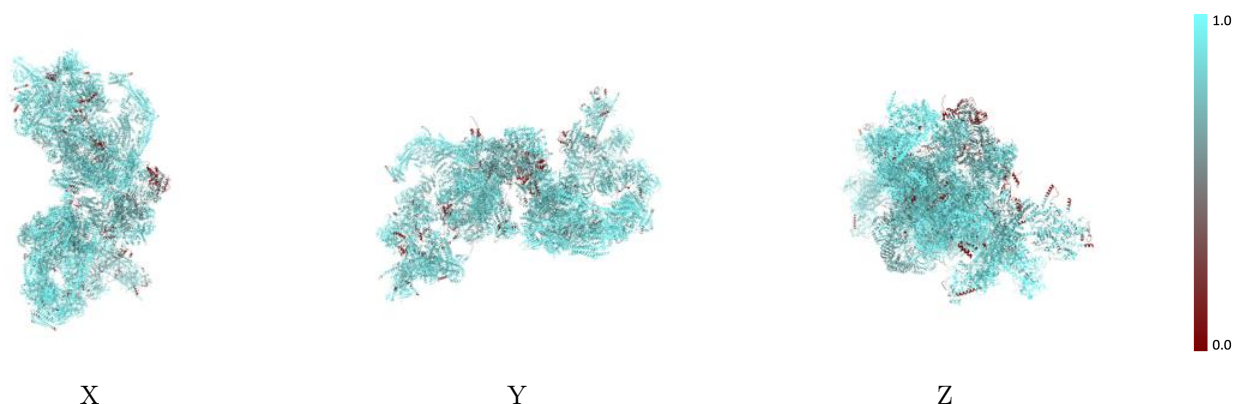
The images above show the 3D surface view of the map at the recommended contour level 0.336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



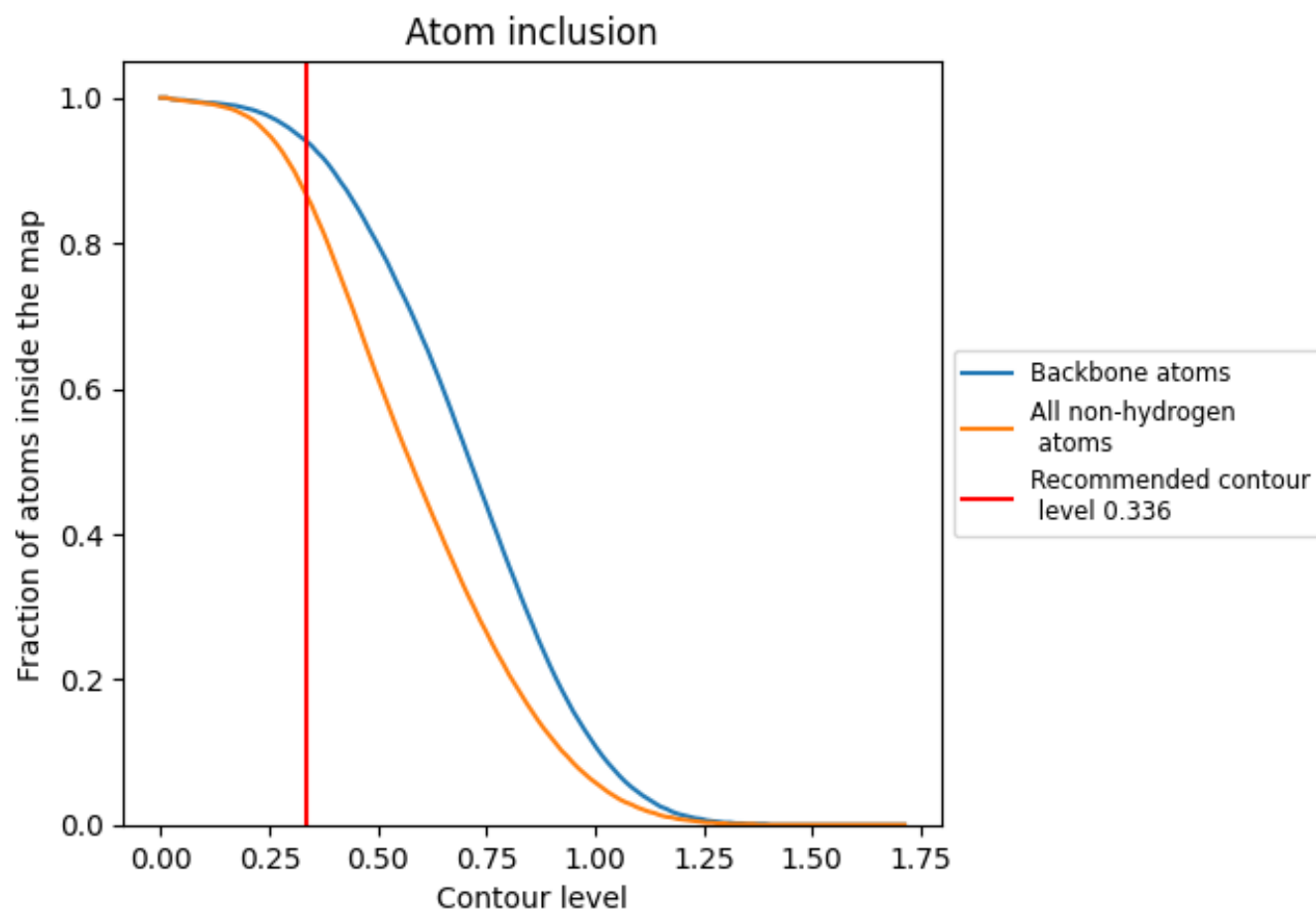
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.336).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.3020
A0	 0.9320	 0.2820
A1	 0.8710	 0.2400
A2	 0.9170	 0.2150
A3	 0.9170	 0.2280
A4	 0.9680	 0.3290
A5	 0.8720	 0.1310
A6	 0.8950	 0.3040
A7	 0.8760	 0.1860
A8	 0.6470	 -0.0200
A9	 0.1760	 0.0170
AA	 0.9450	 0.4490
AB	 0.9220	 0.4460
AC	 0.9690	 0.5110
AD	 0.9080	 0.2210
AE	 0.9610	 0.4330
AF	 0.9740	 0.4830
AG	 0.9610	 0.3400
AH	 0.9690	 0.4550
AI	 0.9470	 0.4080
AJ	 0.9510	 0.4740
AK	 0.9240	 0.4620
AL	 0.9600	 0.4220
AM	 0.8790	 0.3120
AN	 0.9210	 0.2410
AO	 0.8320	 0.3130
AQ	 0.7790	 0.2250
AR	 0.7990	 0.1870
AS	 0.7360	 0.2400
AT	 0.9150	 0.2440
AU	 0.6880	 0.2420
AV	 0.6840	 0.2430
AW	 0.7290	 0.1510
AX	 0.6150	 0.2020
B0	 0.9320	 0.2700



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Chain	Atom inclusion	Q-score
B1	 0.8700	 0.2280
B2	 0.9160	 0.2080
B3	 0.9180	 0.2190
B4	 0.9680	 0.3120
B5	 0.8800	 0.1310
B6	 0.8930	 0.2870
B7	 0.8780	 0.1780
B8	 0.6620	 -0.0210
B9	 0.1760	 0.0380
BA	 0.9380	 0.4200
BB	 0.9110	 0.4210
BC	 0.9660	 0.4830
BD	 0.9090	 0.2100
BE	 0.9600	 0.4070
BF	 0.9720	 0.4550
BG	 0.9580	 0.3220
BH	 0.9670	 0.4310
BI	 0.9430	 0.3900
BJ	 0.9490	 0.4460
BK	 0.9090	 0.4270
BL	 0.9630	 0.4070
BM	 0.8750	 0.2980
BN	 0.9250	 0.2400
BO	 0.8230	 0.2980
BQ	 0.7760	 0.2100
BR	 0.7960	 0.1830
BS	 0.7340	 0.2320
BT	 0.9160	 0.2430
BU	 0.6790	 0.2370
BV	 0.6820	 0.2370
BW	 0.7250	 0.1500
BX	 0.6080	 0.1950
E3	 0.6920	 0.2870
E6	 0.5600	 0.2520
MA	 0.9590	 0.4180
Ma	 0.9530	 0.3970
Mb	 0.9660	 0.3680
Mc	 0.9540	 0.3620
Md	 0.9350	 0.3330
Me	 0.9530	 0.4380
Mf	 0.9430	 0.4190
Mg	 0.9200	 0.3400

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Chain	Atom inclusion	Q-score
Mh	 0.9420	 0.3670
Mi	 0.9650	 0.3830
Mj	 0.9730	 0.3250
Mk	 0.9140	 0.1930
MI	 0.8790	 0.2320
Mm	 0.8310	 0.1900
Mn	 0.9610	 0.3180
Mo	 0.9540	 0.4110
Mp	 0.7120	 0.1990
SA	 0.6720	 0.1880
SB	 0.9170	 0.2980
SC	 0.7100	 0.2480
SD	 0.8620	 0.3050
SE	 0.8430	 0.1930
SF	 0.9010	 0.3390
SG	 0.9810	 0.3550
SH	 0.9010	 0.3230
SI	 0.8700	 0.3550
SJ	 0.7220	 0.2250
SK	 0.7970	 0.2880
SL	 0.7780	 0.3040
T1	 0.9070	 0.2340
T2	 0.8420	 0.2010
T3	 0.8770	 0.3060
T4	 0.8710	 0.2140
T5	 0.7480	 0.2210
T6	 0.9140	 0.3360
mA	 0.9560	 0.4040
ma	 0.9490	 0.3760
mb	 0.9650	 0.3450
mc	 0.9560	 0.3430
md	 0.9340	 0.3120
me	 0.9480	 0.4140
mf	 0.9420	 0.3990
mg	 0.9250	 0.3190
mh	 0.9410	 0.3470
mi	 0.9640	 0.3610
mj	 0.9740	 0.3100
mk	 0.9130	 0.1840
ml	 0.8770	 0.2240
mm	 0.8290	 0.1840
mn	 0.9590	 0.3010

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Chain	Atom inclusion	Q-score
mo	 0.9480	 0.3880
mp	 0.7150	 0.1920
sA	 0.6700	 0.1800
sB	 0.9140	 0.2850
sC	 0.6990	 0.2400
sD	 0.8540	 0.2920
sE	 0.8390	 0.1870
sF	 0.9010	 0.3210
sG	 0.9810	 0.3460
sH	 0.8950	 0.3070
sI	 0.8580	 0.3360
sJ	 0.7130	 0.2190
sK	 0.7940	 0.2740
sL	 0.7710	 0.2870
t1	 0.8990	 0.2300
t2	 0.8380	 0.1990
t3	 0.8690	 0.2990
t4	 0.8680	 0.2110
t5	 0.7370	 0.2130
t6	 0.9100	 0.3250