



Full wwPDB EM Validation Report ⓘ

Oct 8, 2026 – 04:41 PM EDT

PDB ID : 9PDK / pdb_00009pdk
EMDB ID : EMD-71536
Title : Composite map of closed 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:

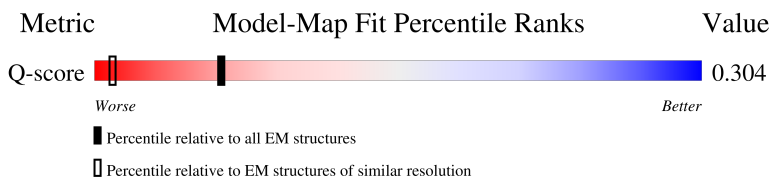
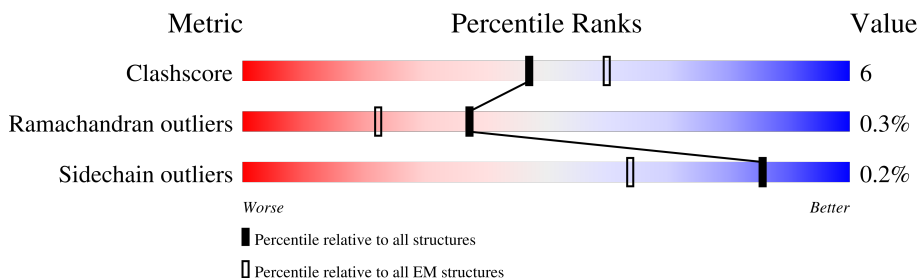
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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.



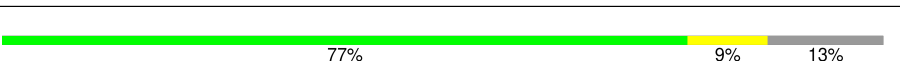
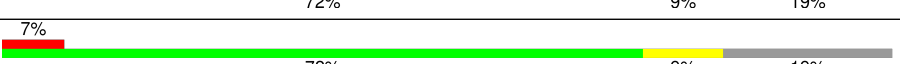
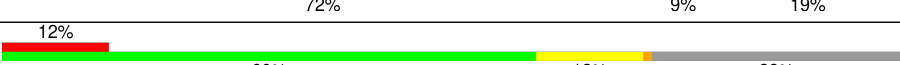
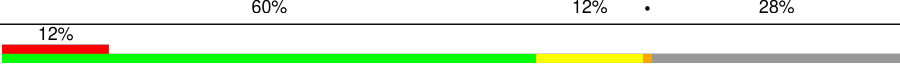
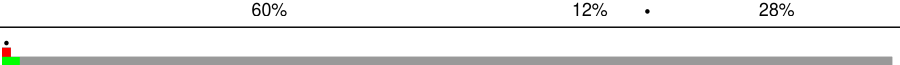
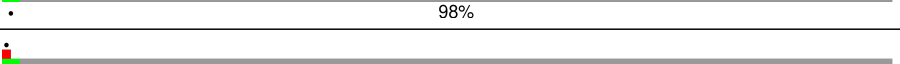
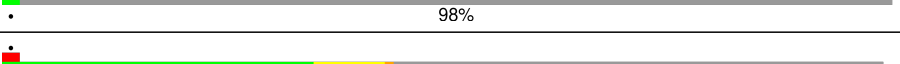
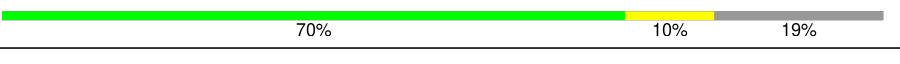
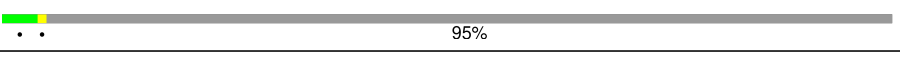
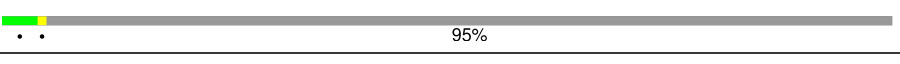
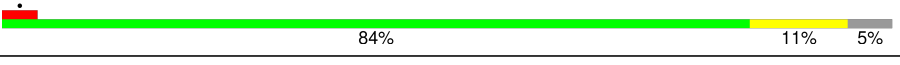
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	

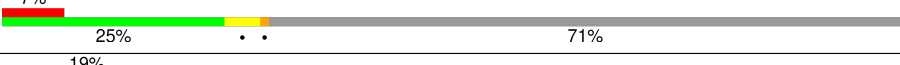
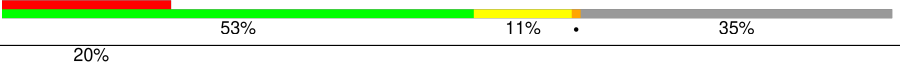
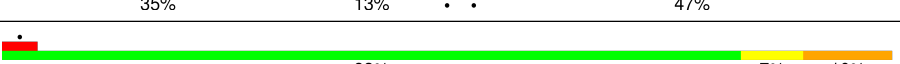
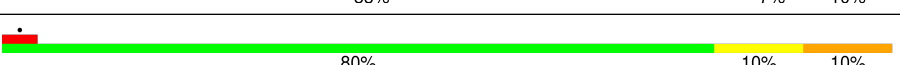
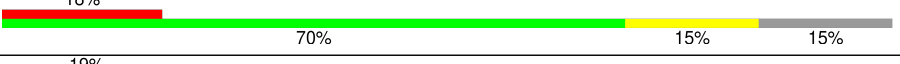
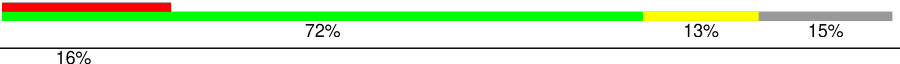
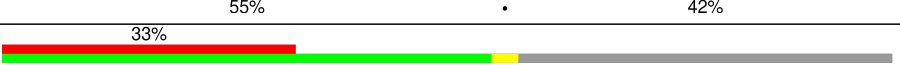
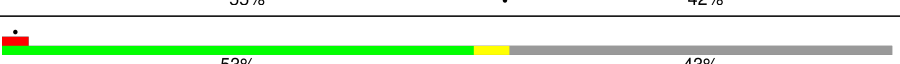
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Mol	Chain	Length	Quality of chain
13	BC	318	
14	AD	221	
14	BD	221	
15	AE	215	
15	BE	215	
16	AF	155	
16	BF	155	
17	AG	171	
17	BG	171	
18	AH	146	
18	BH	146	
19	AI	122	
19	BI	122	
20	AJ	70	
20	BJ	70	
21	AK	120	
21	BK	120	
22	AL	70	
22	BL	70	
23	AM	345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

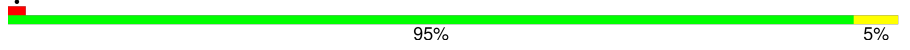
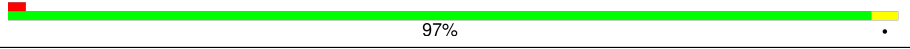
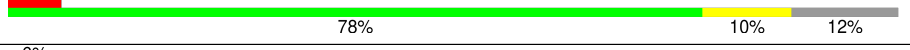
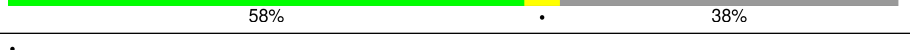
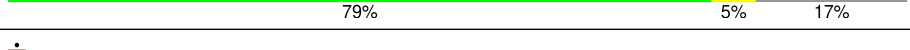
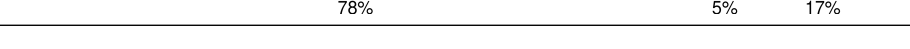
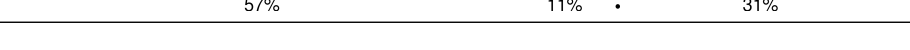
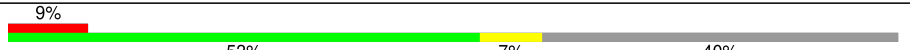
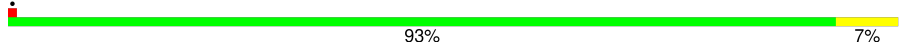
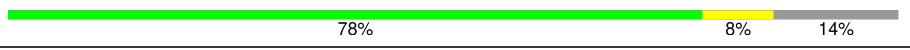
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Mol	Chain	Length	Quality of chain
26	AQ	735	
26	BQ	735	
27	AR	400	
27	BR	400	
28	AS	309	
28	BS	309	
29	AT	69	
29	BT	69	
30	AU	286	
30	BU	286	
31	AV	122	
31	BV	122	
32	AW	482	
32	BW	482	
33	AX	328	
33	BX	328	
34	Ma	295	
34	ma	295	
35	Mb	223	
35	mb	223	
36	Mc	115	
36	mc	115	
37	Md	687	
37	md	687	
38	Me	307	

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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	T1	431	
60	t1	431	
61	T2	397	

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Mol	Chain	Length	Quality of chain
61	t2	397	5%22%5%72%
62	T3	1132	6%57%9%33%
62	t3	1132	6%57%9%33%
63	T5	1081	7%90%
63	t5	1081	7%90%
64	T6	974	82%13%
64	t6	974	82%12%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 305572 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	B0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		
1	A0	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	B1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		
2	A1	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	B2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		
3	A2	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	B3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		
4	A3	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	B4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		
5	A4	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	B5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		
6	A5	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	B6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		
7	A6	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	B7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		
8	A7	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	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		
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		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		
12	AB	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	BC	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		
13	AC	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	BD	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		
14	AD	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	BE	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		
15	AE	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	BF	83	Total	C	N	O	S	0	0
			670	428	114	125	3		
16	AF	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	BG	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		
17	AG	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	BH	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		
18	AH	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	BI	116	Total	C	N	O	S	0	0
			944	581	172	181	10		
19	AI	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	BJ	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	AJ	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	BK	115	Total	C	N	O	S	0	0
			924	593	157	172	2		
21	AK	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	BL	45	Total	C	N	O	S	0	0
			359	221	71	63	4		
22	AL	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	BM	276	Total	C	N	O	S	0	0
			2097	1328	359	393	17		
23	AM	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	BN	69	Total	C	N	O	P	0	0
			1413	679	248	417	69		
24	AN	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	BO	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		
25	AO	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	BQ	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		
26	AQ	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	BR	261	Total	C	N	O	S	0	0
			2173	1369	383	411	10		
27	AR	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	BS	164	Total	C	N	O	S	0	0
			1301	812	230	251	8		
28	AS	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	BT	69	Total	C	N	O	P	0	0
			1416	679	257	411	69		
29	AT	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	BU	102	Total	C	N	O	S	0	0
			843	531	142	167	3		
30	AU	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	BV	104	Total	C	N	O	S	0	0
			815	511	136	164	4		
31	AV	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	BW	226	Total	C	N	O	S	0	0
			1836	1168	317	344	7		
32	AW	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	BX	191	Total	C	N	O	S	0	0
			1530	980	256	289	5		
33	AX	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	ml	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		
45	MI	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 2.

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

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 3.

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

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	T3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	t3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

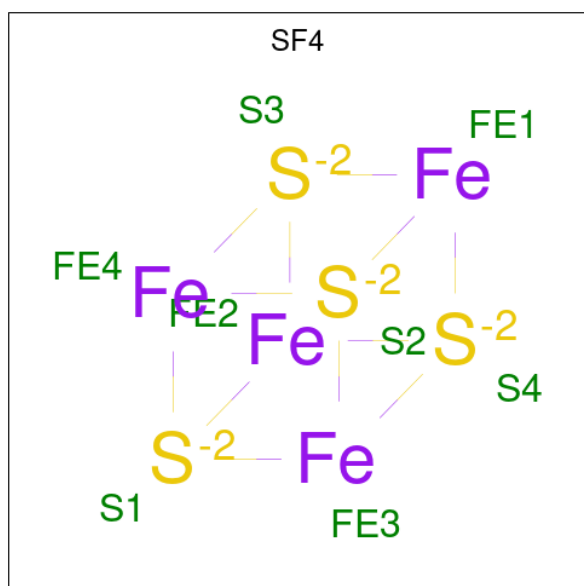
- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 16.

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

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



Mol	Chain	Residues	Atoms			AltConf
65	B0	1	Total	Fe	S	0
			8	4	4	
65	A0	1	Total	Fe	S	0
			8	4	4	

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

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

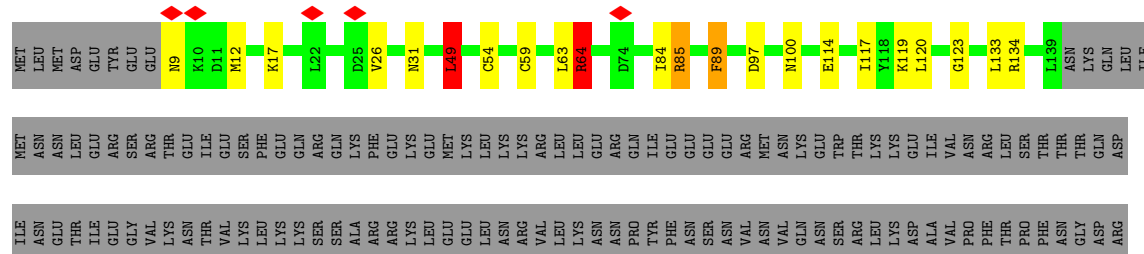
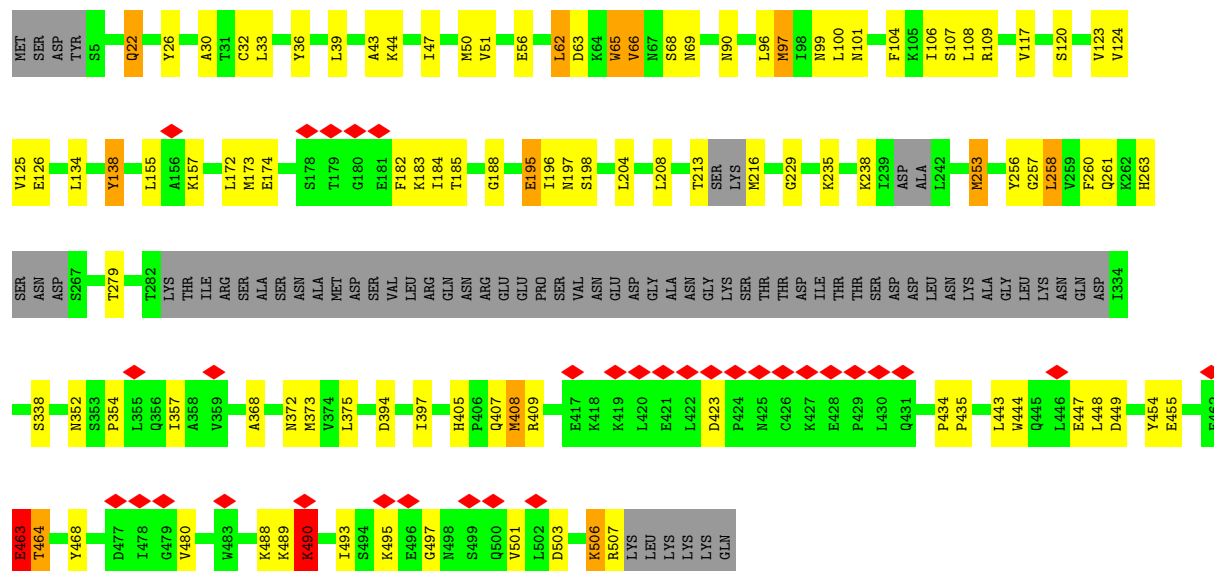
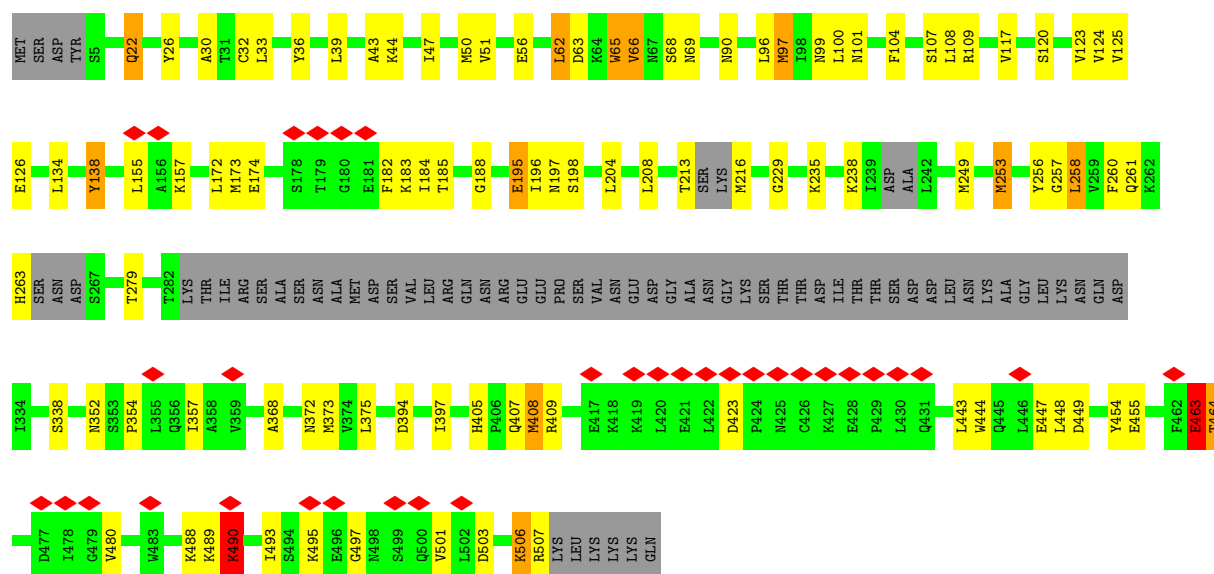
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Mol	Chain	Residues	Atoms		AltConf
66	AM	1	Total 1	Zn 1	0
66	AS	1	Total 1	Zn 1	0
66	AW	1	Total 1	Zn 1	0

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

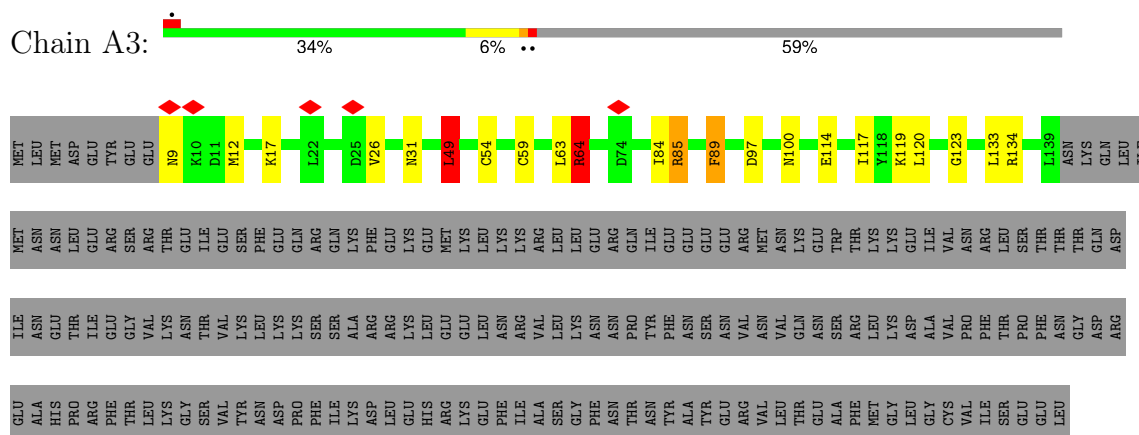
Mol	Chain	Residues	Atoms		AltConf
67	BA	1	Total 1	Mg 1	0
67	AA	1	Total 1	Mg 1	0



GLU
ALA
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GLU
PRO
ASP
ARG
PHE
THR
LEU
LYS
SER
GLY
VAL
TVR
ASN
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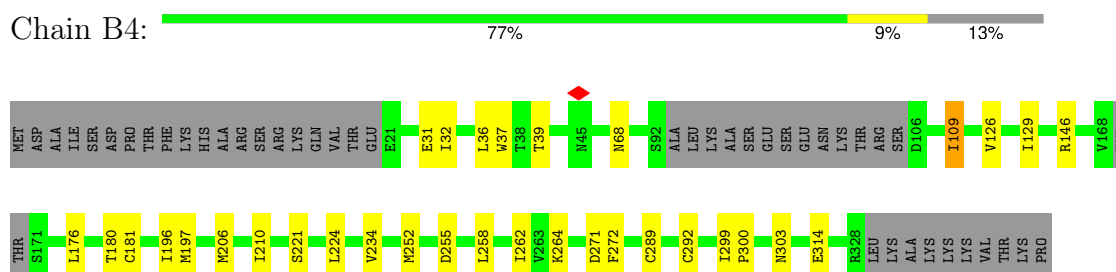
- Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain A3:



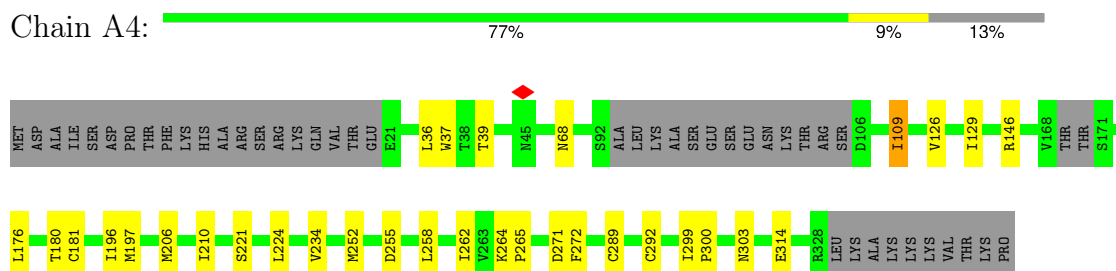
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain B4:



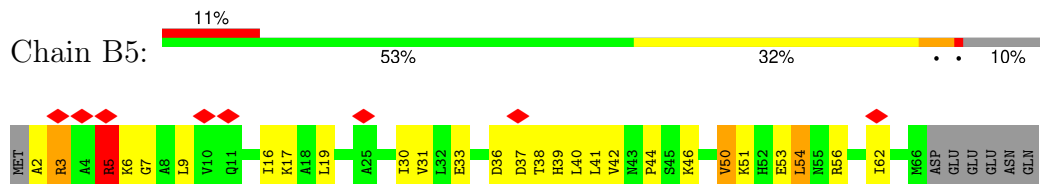
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain A4:



- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

Chain B5:



- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

Chain A5:





GLN	ASN	THR	ILE	ALA	HIS	THR	VAL	THR	ASN	SER	PRO	ASN	PRO	GLN	VAL	ILE	PRO	GLY	GLY	ALA	ALA	SER	LYS	SER	VAL	PRO	THR	PRO	SER	LEU	PRO	ILE	ALA	PRO	PRO	VAL	ALA	ALA	PRO	HIS	ASP	SER	GLU	ALA	THR	LEU	LEU	THR	ASN	SER	ASN	GLY	SER	ASN	ASN	THR
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- Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5

Chain sF:

[illegible]

GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR	SER	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	ILE	ALA	ASN	GLN	SER	SER	GLN	PRO	ILE	ALA	ALA	ALA	THR	SER	THR	PRO	PRO	PRO	PRO	PRO	ALA	ALA	HIS	HIS	LEU	HIS	PRO	GLN	GLN	ILE	GLE	GLN	VAL	PRO	PRO	LEU	ALA	LEU	PRO
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PRO	ILE	ASN	PRO	PRO	GLN	ILE	ALA	GLN	LEU	PRO	LEU	LEU	ASN	LYS	LEU	ARG	GLN	GLN	ALA	ALA	ILE	ALA	LYS	ASN	ASN	PRO	PRO	GLN	GLN	VAL	VAL	ASN	ASN	ALA	ALA	ILE	THR	THR	VAL	VAL	ALA	GLN	GLN	ARG	GLN	ILE	GLU	GLU	GLN	GLN	LYS	GLY	GLY	THR	ALA	ALA
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[illegible]

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VAL
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GLN
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F299

L301	P302	L303	L304	N305	L306	P307	K308	Y309	T310	T311	T312	T313	Y314	D315	P316	P317	E318	T319	K320	K321	P322		D333	T334	D335	T336		Q341	T342	T343			T357		Y360	D361		H379	T380	L381	K382	Y383		N389	T390	R391	M392	K393		T398	S399	Q400	K401	L402	P403	S404			N410			P435
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S666			E599	Q600	A601	H602	M603	A609	G617	D624	S627	R628	M629	I633	L653	A657	P662	K665	D666	LYS	ASP	ARG	ASP	THR	THR	ARG	ARG	LYS	ARG	ARG	ARG	GLN	GLY	GLY	SER	ASW	ARG	ARG	ARG	GLY	MET	LEU	ALA	LEU	SER	SER	ASN	THR	SER	SER	MET
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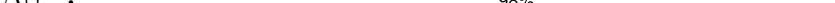
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GLY	HIS	SER	LEU	LEU	LEU	ILE	LYS	LEU	PRO	GLY	LYS	VAL	ASN	THR	LYS	GLU	GLU	PHE	ALA	ALA	ALA	PRO	ASN	ASP	THR	SER	SER	GLY	THR	ASN	LYS	LEU	LEU	ASN	SER	ASN	ILE	ARG	ALA	GLY	VAL	THR	ILE	PRO	SER	ILE	PRO	ASN
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[illegible]

THR
GLN
ASN
THR

- Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5

Chain A8:  98%

[illegible]

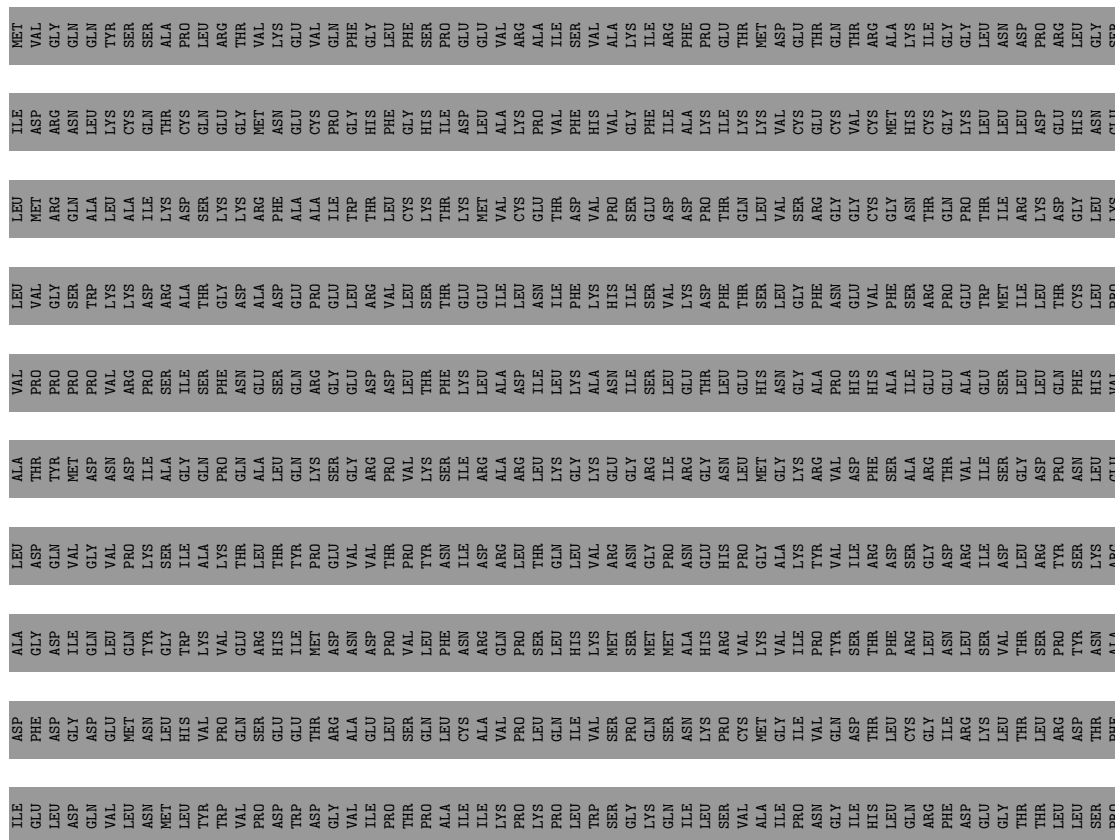
- Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5

[illegible]

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

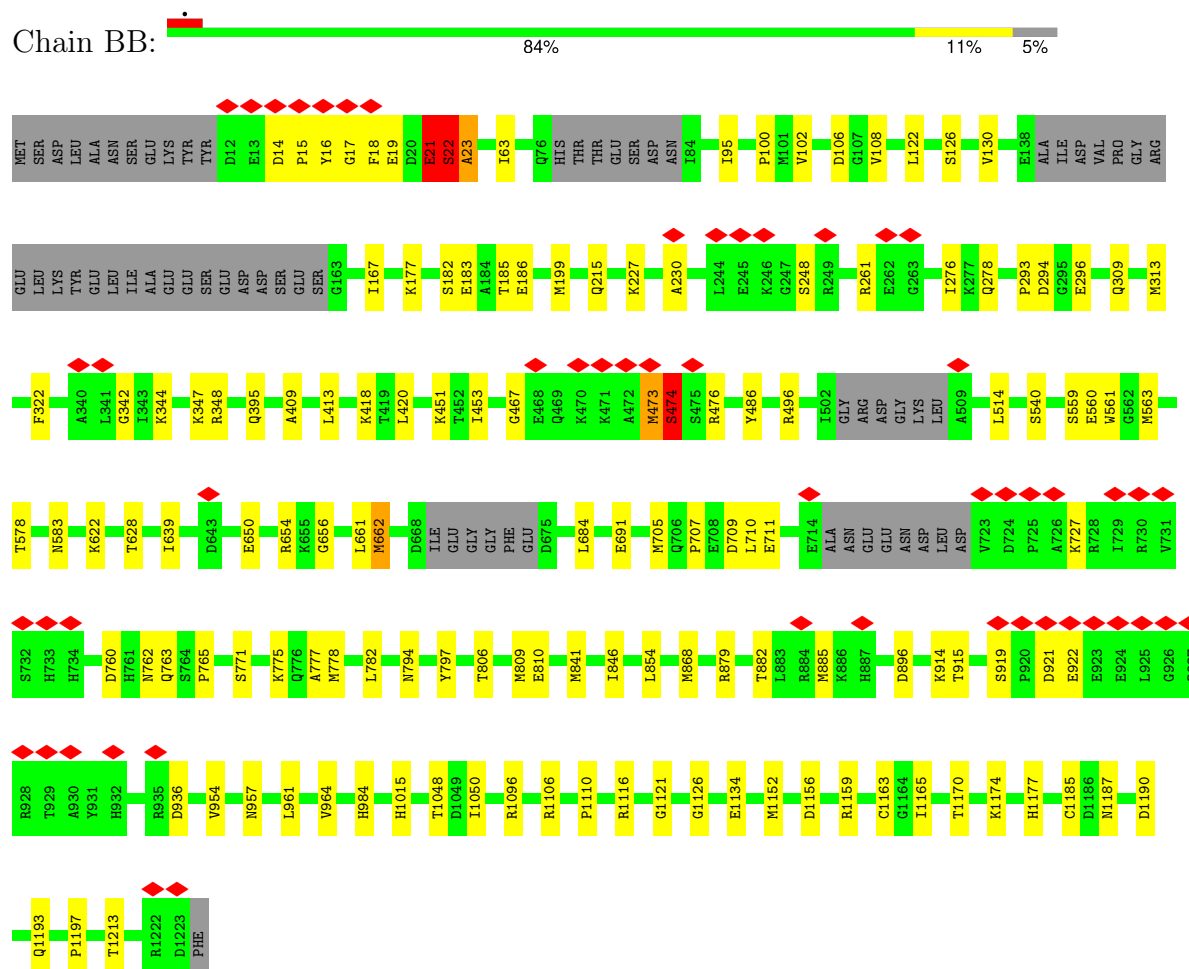
Chain mA: 95%

[illegible]



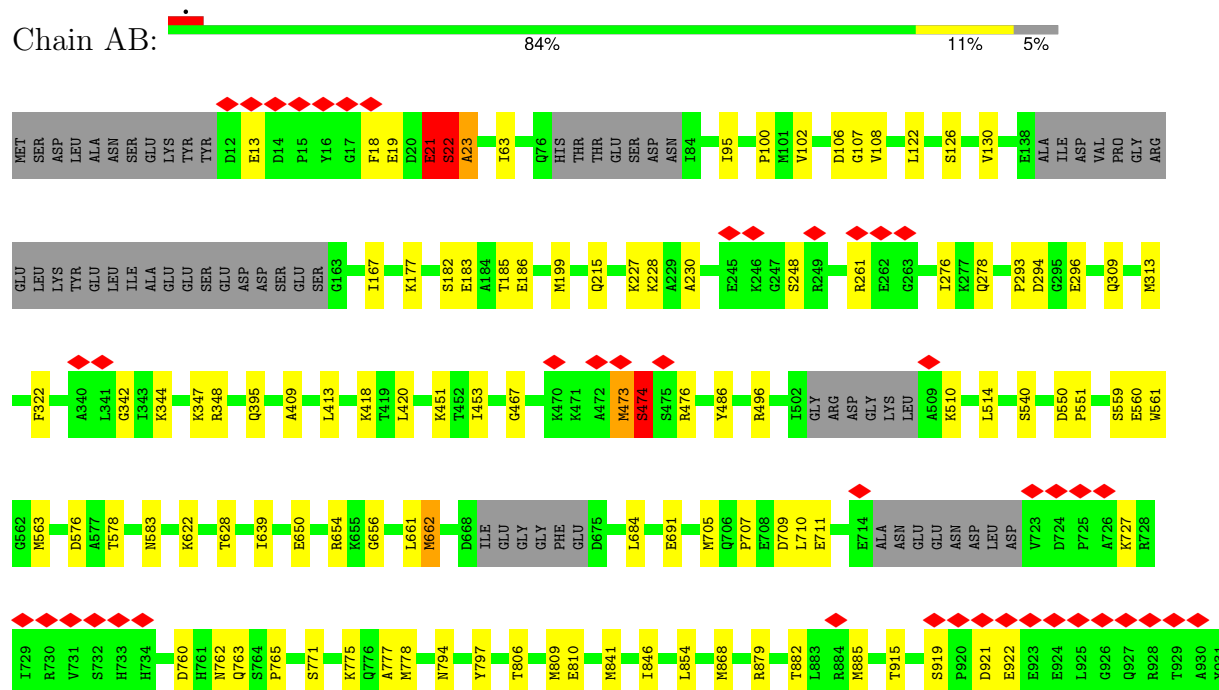
- Molecule 12: DNA-directed RNA polymerase II subunit RPB2

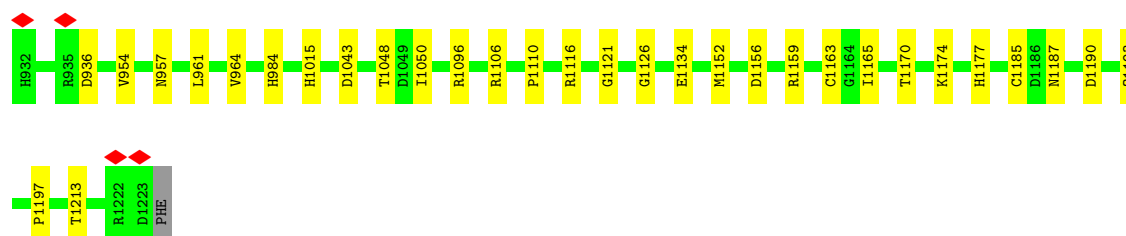
Chain BB:



- Molecule 12: DNA-directed RNA polymerase II subunit RPB2

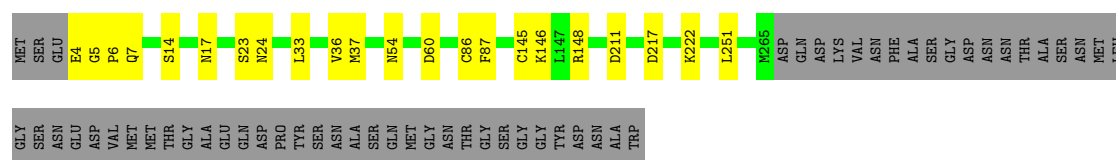
Chain AB:





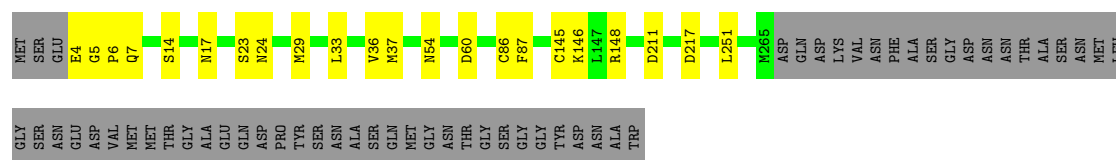
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain BC: 75% 7% 18%



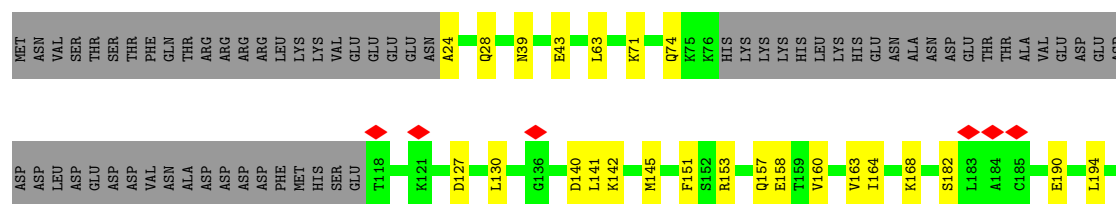
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain AC: 75% 7% 18%



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

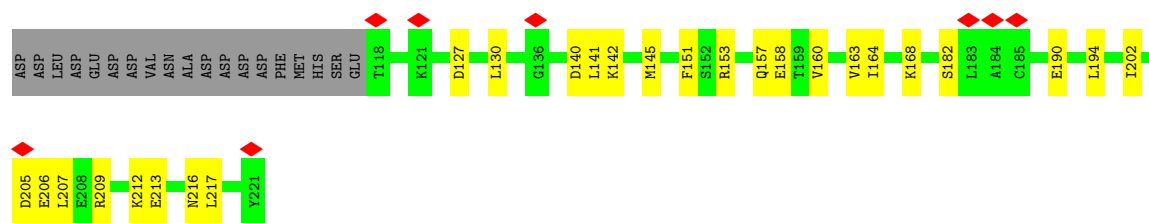
Chain BD: 56% 15% 29%



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

Chain AD: 56% 15% 29%





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

Chain BE: 90% 8% ..



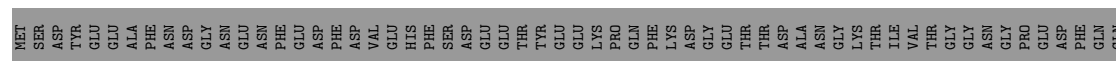
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain AE: 90% 8% ..



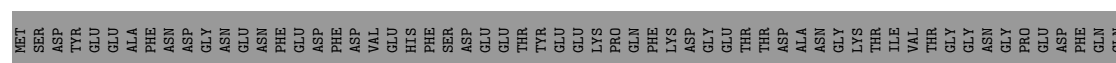
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain BF: 50% 46%



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

Chain AF: 49% 5% 46%

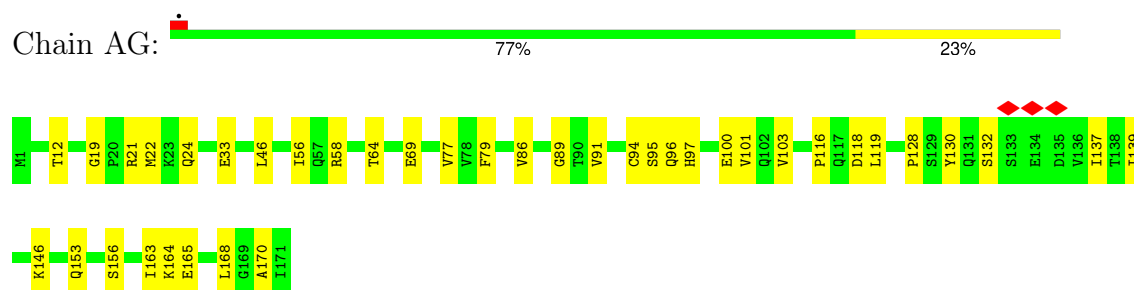


- Molecule 17: DNA-directed RNA polymerase II subunit RPB7

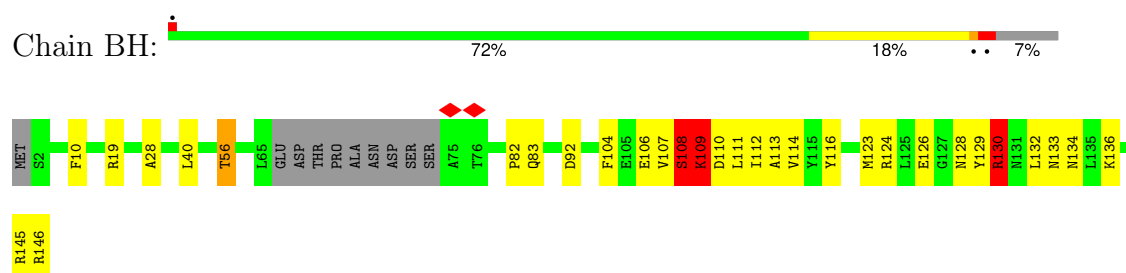
Chain BG: 75% 25%



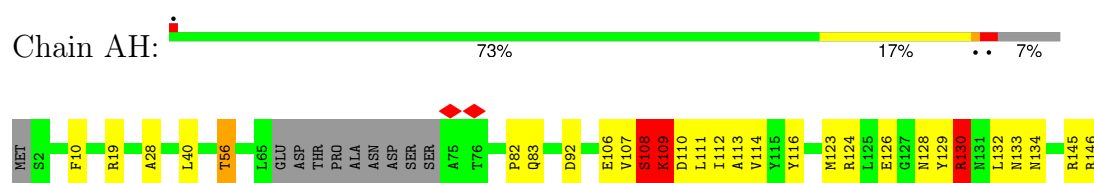
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



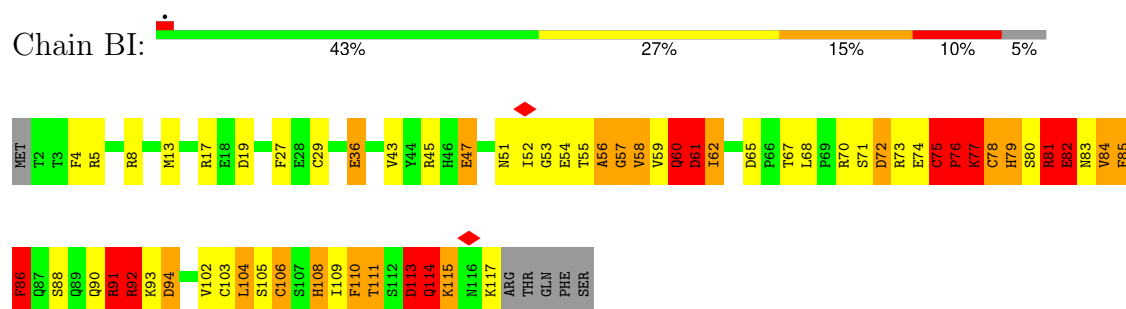
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



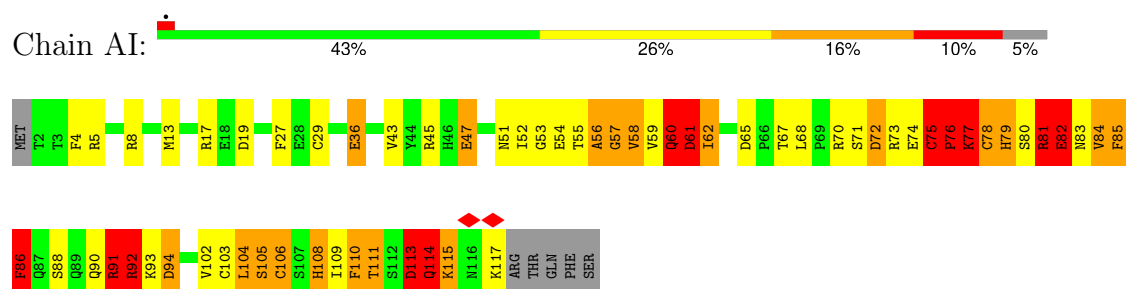
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- 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

Chain BJ:  79% 19% ..



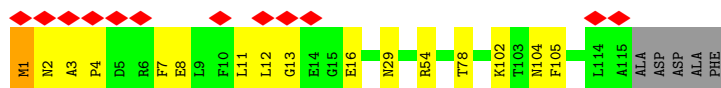
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain AJ:  79% 19% ..



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

Chain BK:  10% 82% 12% ..



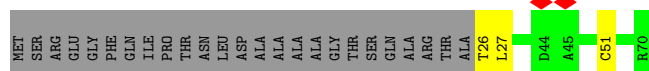
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11

Chain AK:  7% 82% 13% ..



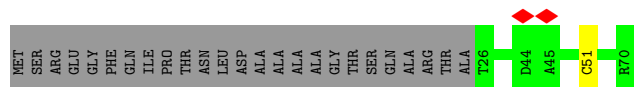
- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain BL:  60% 36%



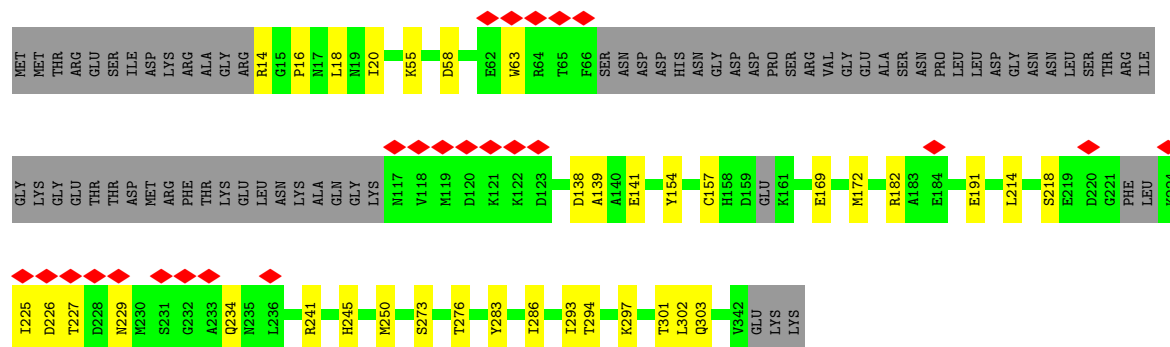
- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain AL:  63% 36%

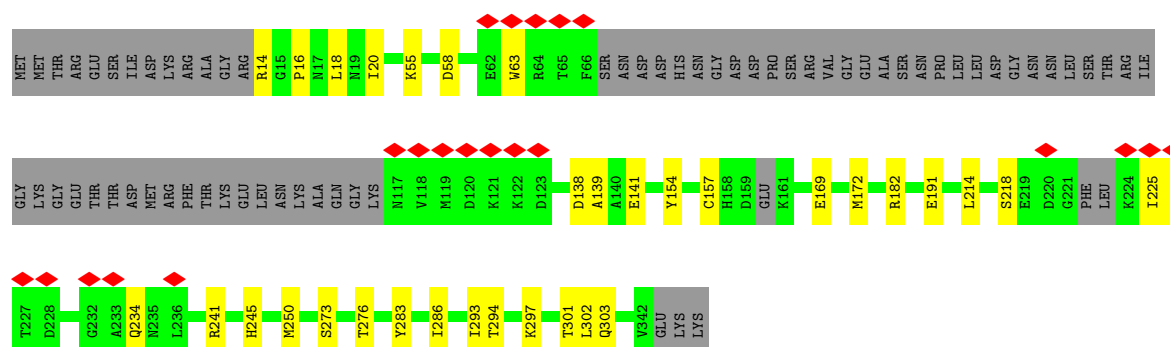


- Molecule 23: Transcription initiation factor IIB

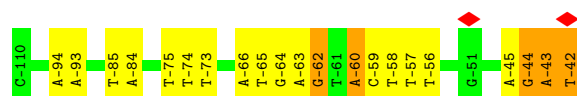
Chain BM:  7% 70% 10% 20%



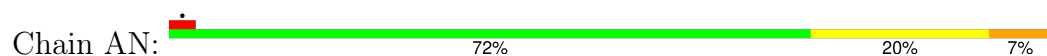
• Molecule 23: Transcription initiation factor IIB



• Molecule 24: promoter DNA

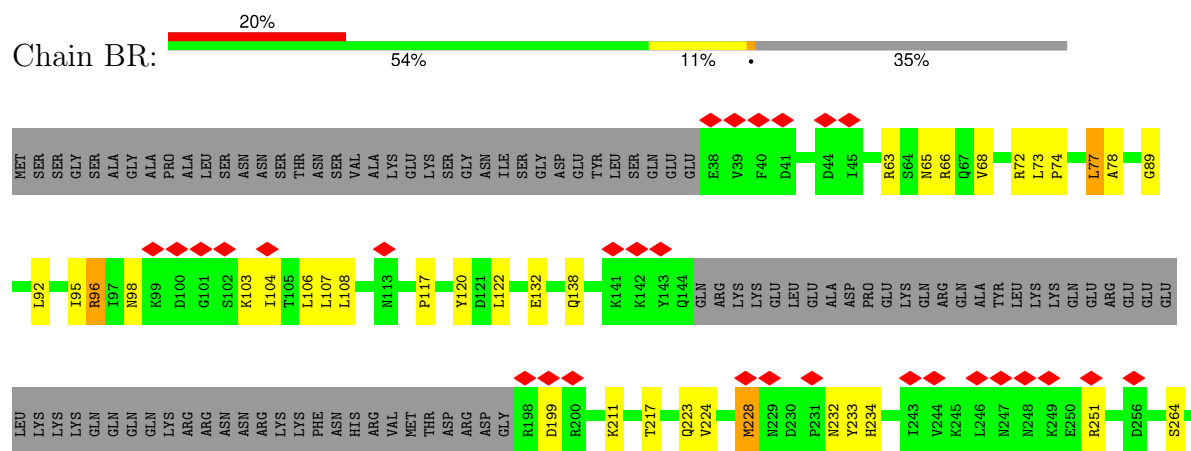
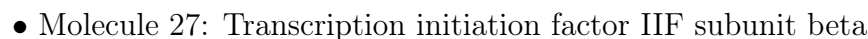


• Molecule 24: promoter DNA

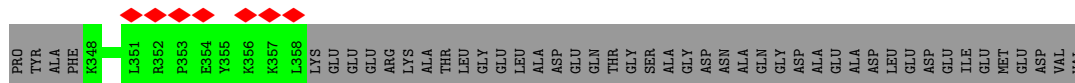
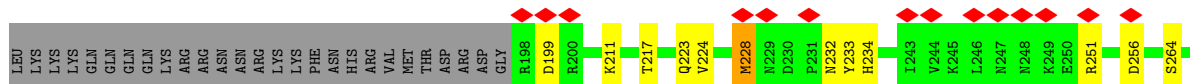
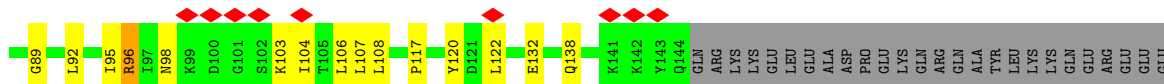
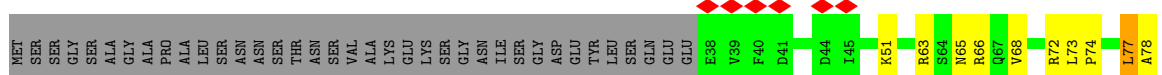


• Molecule 25: TATA-box-binding protein

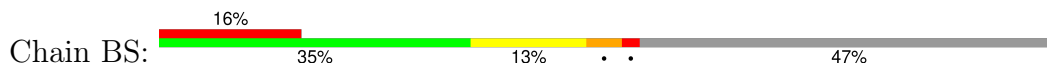




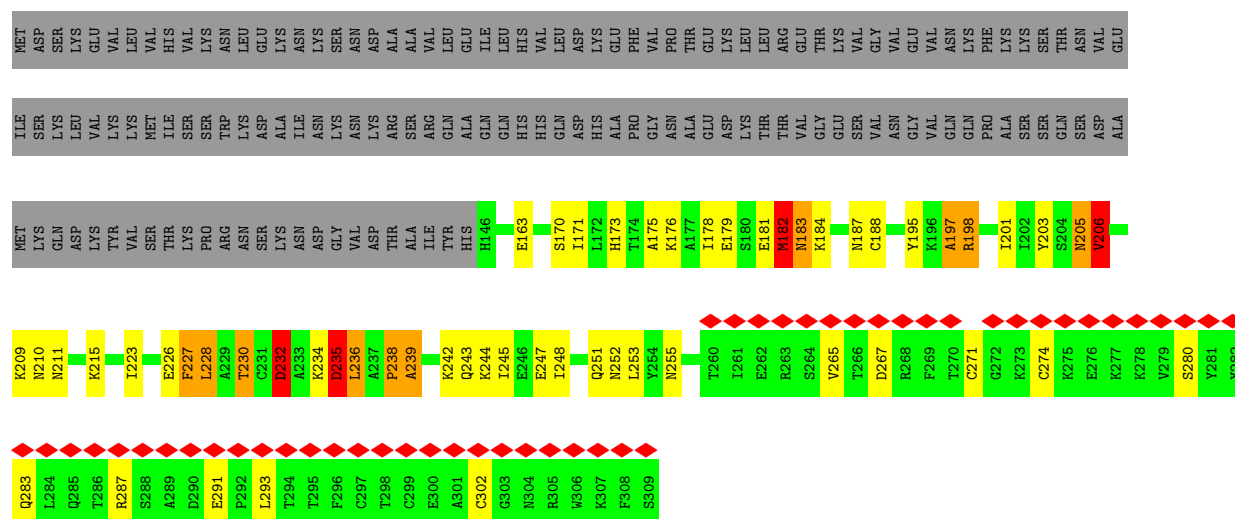
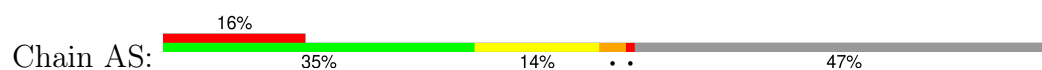
- Molecule 27: Transcription initiation factor IIF subunit beta



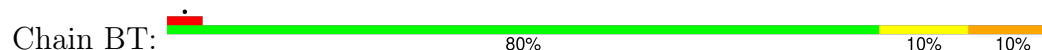
- Molecule 28: Transcription elongation factor S-II



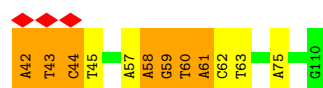
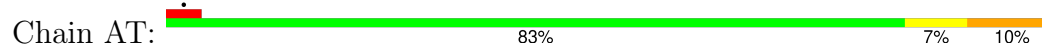
- Molecule 28: Transcription elongation factor S-II



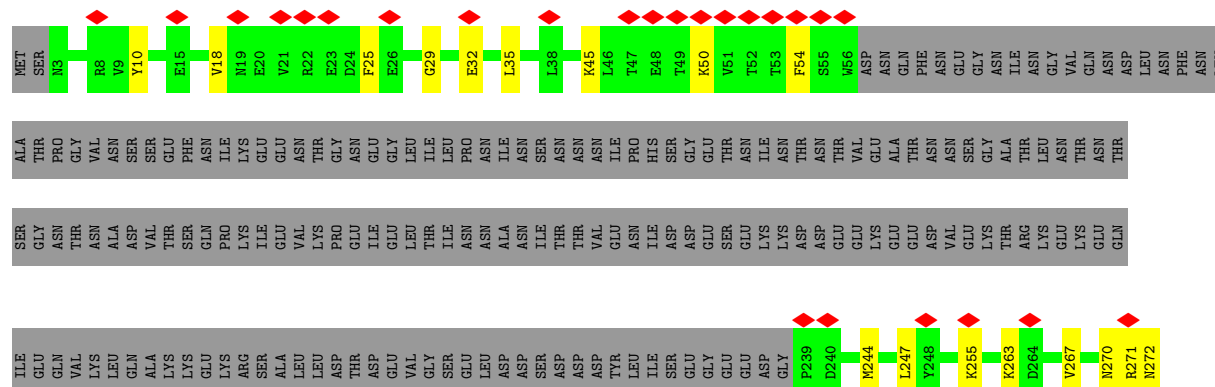
• Molecule 29: promoter DNA

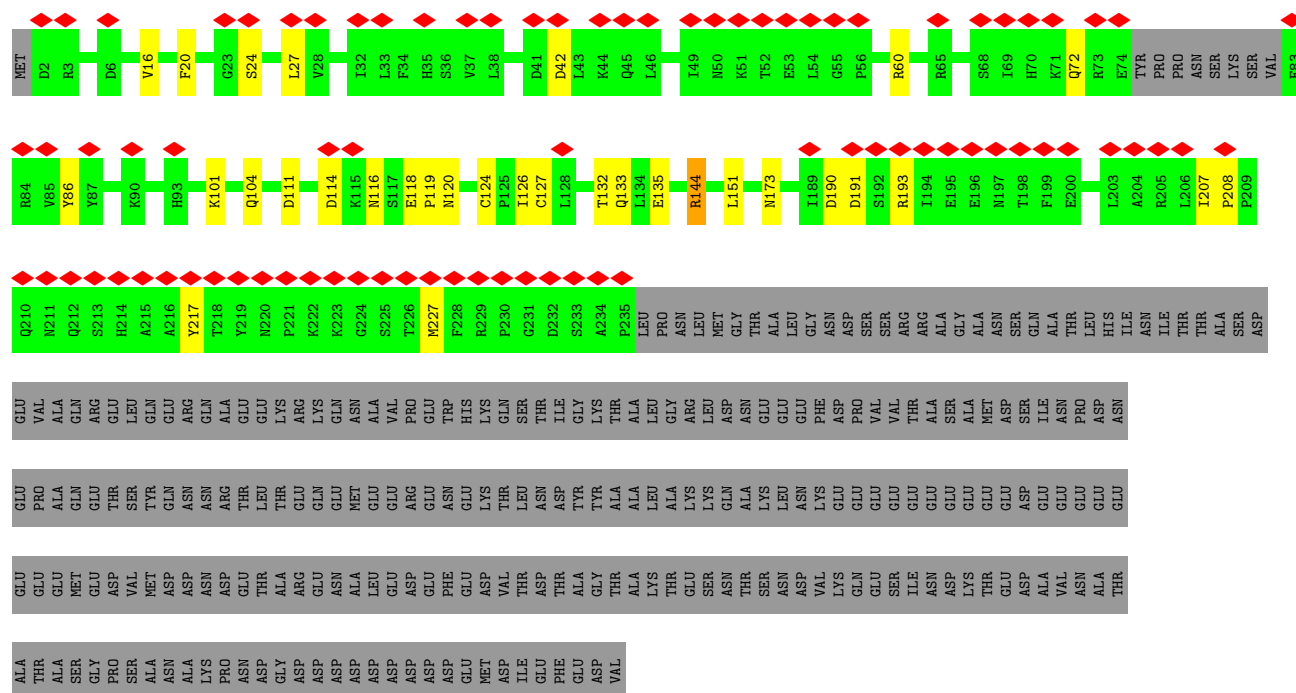


• Molecule 29: promoter DNA

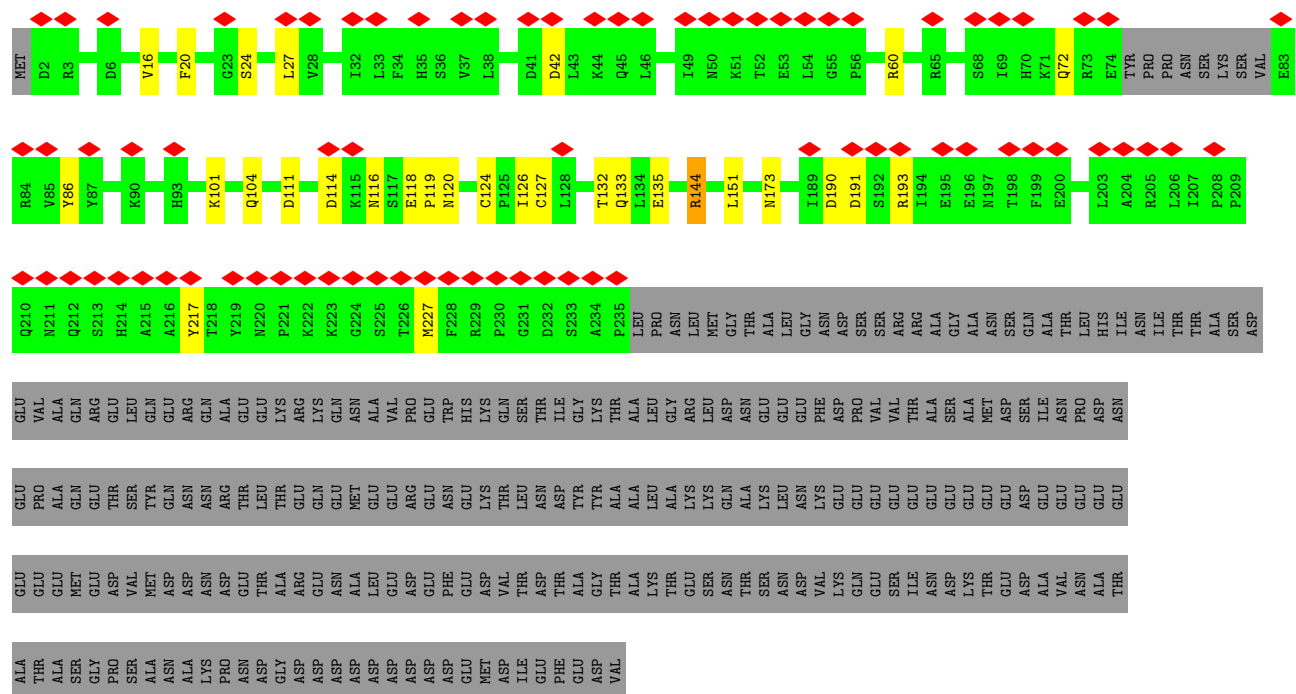
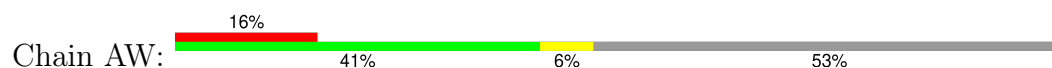


• Molecule 30: Transcription initiation factor IIA large subunit





• Molecule 32: Transcription initiation factor IIE subunit alpha



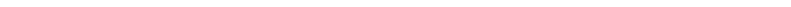
• Molecule 33: Transcription initiation factor IIE subunit beta



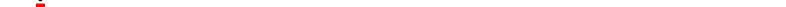


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-

- Chain mb:
- 61% 9% 30%
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 THR
 ALA
 SER
 LEU
 VAL
 PRO
 GLY
 GLY
 ASN
 GLN
 SER
 LEU
 GLN
 GLU
 ASP
 VAL
 SER
 PHE
 ASP
 PHE
 ASP
 ASN
 GLY
 VAL
 PRO
 G30
 L33
 D34
 V34
 A35
 M38
 R39
 Q42
 H45
 R49
 K56
 L59
 P60
 T80
 P97
 L98
 R115
 V122
 M126
- G134
 VAL
 THR
 THR
 ALA
 LEU
 LEU
 LYS
 E143
 E144
 I145
 R153
 T156
 N157
 K173
 ASN
 GLU
 GLU
 SER
 SER
 LEU
 SER
 GLU
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 SER
 SER
 LEU
 LEU
 VAL
 PRO
 S193
 I213
 THR
 GLY
 SER
 SER
 THR
 SER
 THR
 SER
 SER
 SER
 SER
 ASN

- Chain Mb: 
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|
| MET | SER | GLN | SER | THR | ALA | SER | LEU | VAL | PRO | GLY | GLY | ASN | GLN | SER | LEU | GLN | GLU | ASP | VAL | ASN | SER | PHE | ASP | PHE | ASN | GLY | VAL | PRO | G30 | L33 | D34 | A35 | M38 | R39 | Q42 | H45 | R49 | K56 | L59 | P60 | T80 | P97 | L98 | P99 | K100 | R115 | V122 |
| M126 | G134 | VAL | THR | THR | ALA | LEU | LEU | LYS | ASP | E143 | E144 | I145 | R153 | T156 | N157 | K173 | GLU | GLU | SER | LEU | SER | GLU | HIS | ALA | SER | LEU | LEU | VAL | ARG | ASP | SER | LYS | PRO | S193 | T213 | THR | GLY | SER | THR | THR | SER | SER | ASN | | | | |

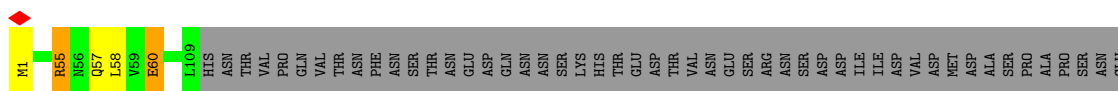
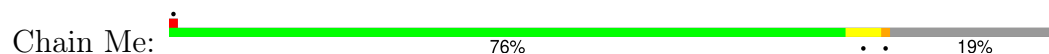
- Chain mc: 
- 

- Chain Mc:  83% 10% 6%
- 

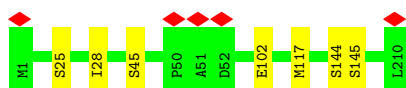
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



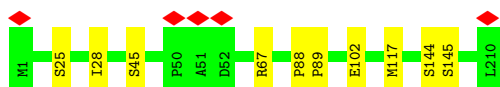
- Molecule 38: Mediator of RNA polymerase II transcription subunit 18



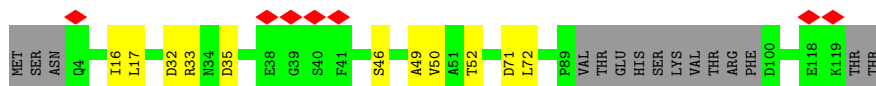
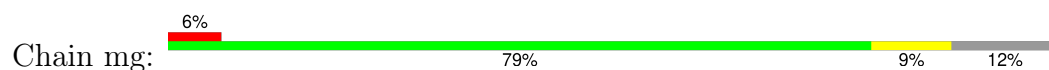
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



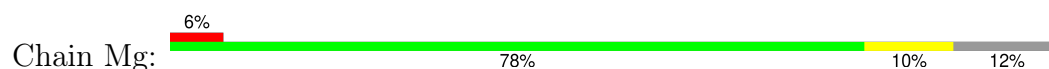
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



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

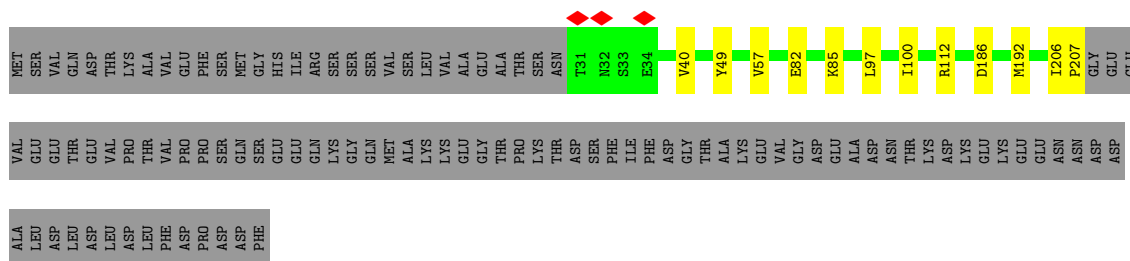


- Molecule 40: Mediator of RNA polymerase II transcription subunit 22

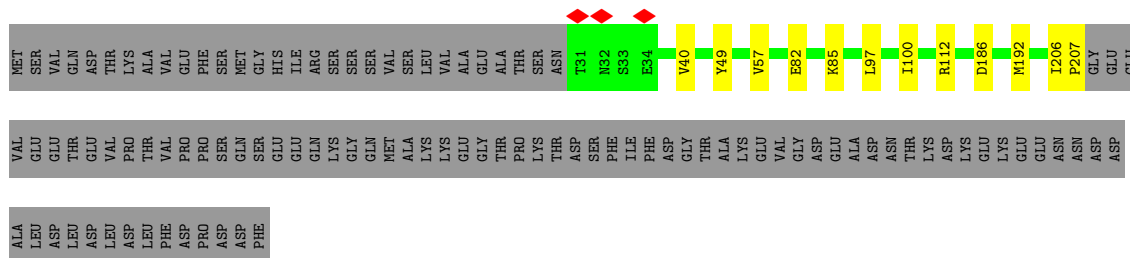


- Molecule 41: Mediator of RNA polymerase II transcription subunit 4

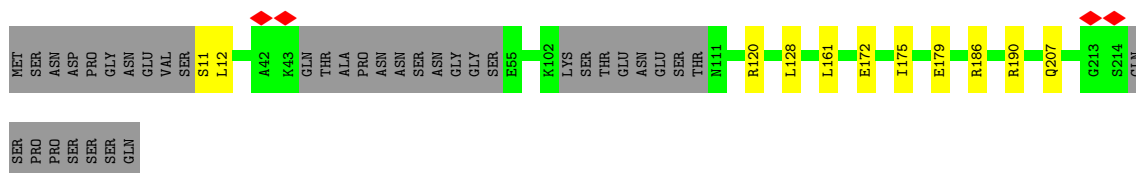
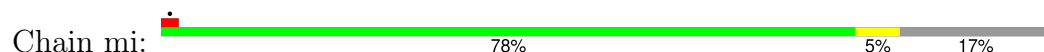




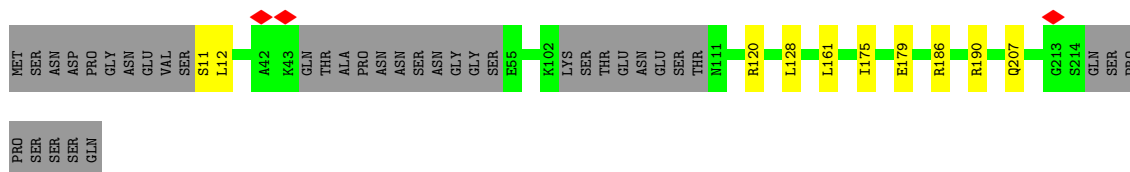
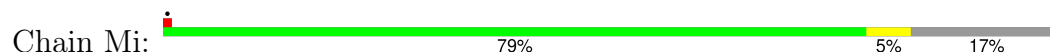
- Molecule 41: Mediator of RNA polymerase II transcription subunit 4



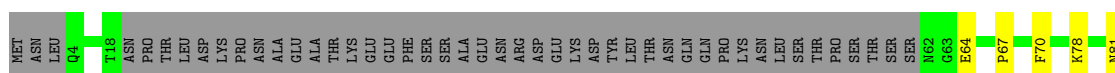
- Molecule 42: Mediator of RNA polymerase II transcription subunit 7



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

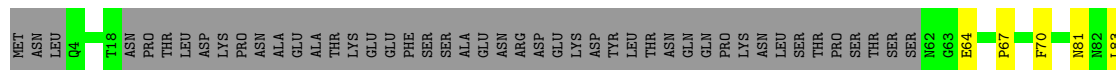


- Molecule 43: Mediator of RNA polymerase II transcription subunit 9

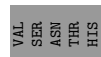
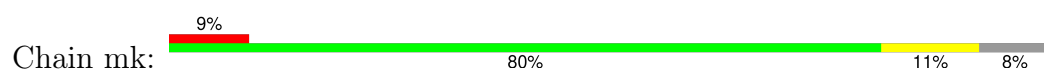




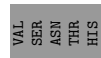
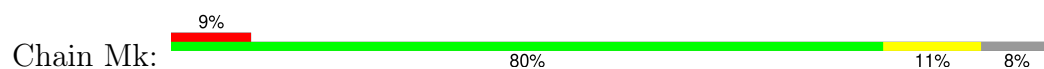
- Molecule 43: Mediator of RNA polymerase II transcription subunit 9



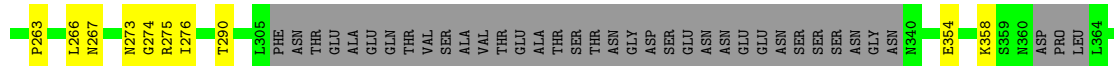
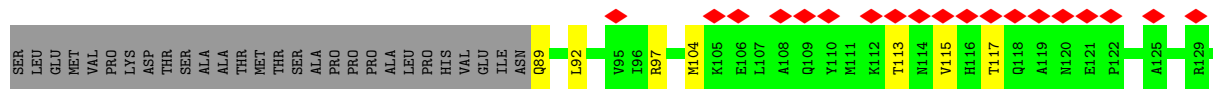
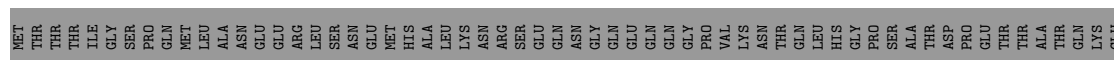
- Molecule 44: Mediator of RNA polymerase II transcription subunit 10



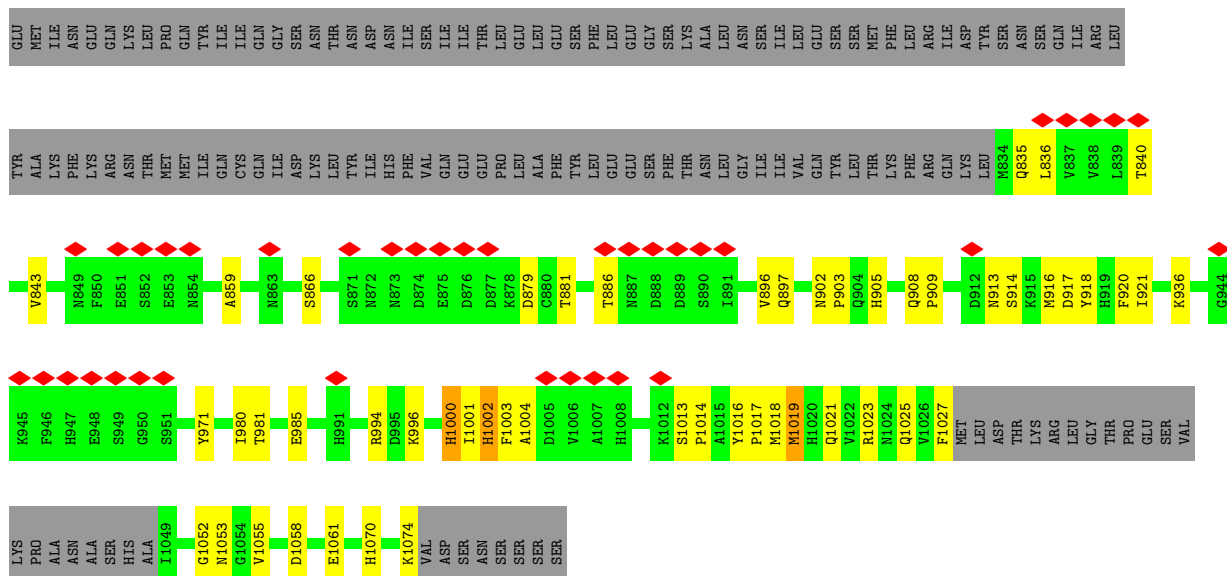
- Molecule 44: Mediator of RNA polymerase II transcription subunit 10



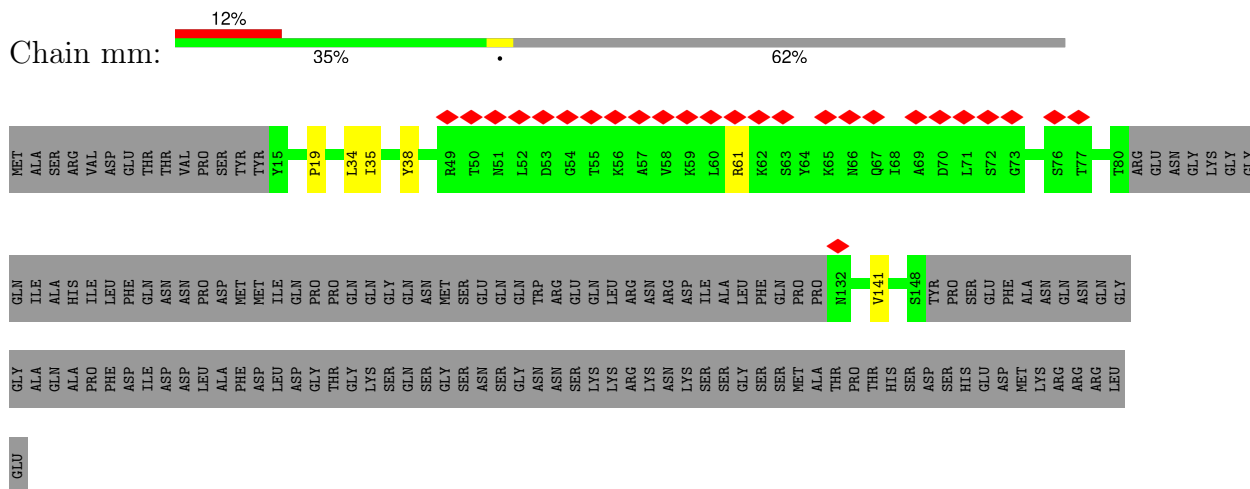
- Molecule 45: Mediator of RNA polymerase II transcription subunit 14



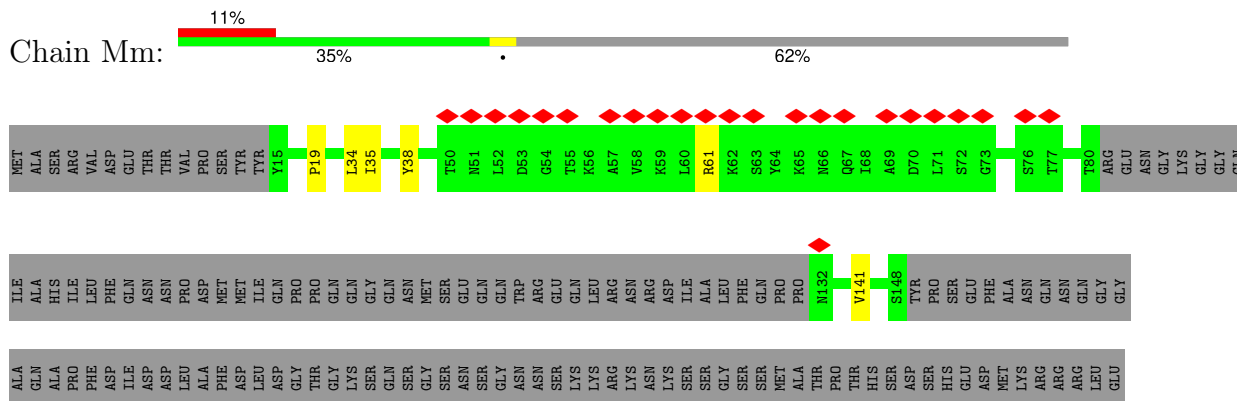




- Molecule 46: Mediator of RNA polymerase II transcription subunit 19



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

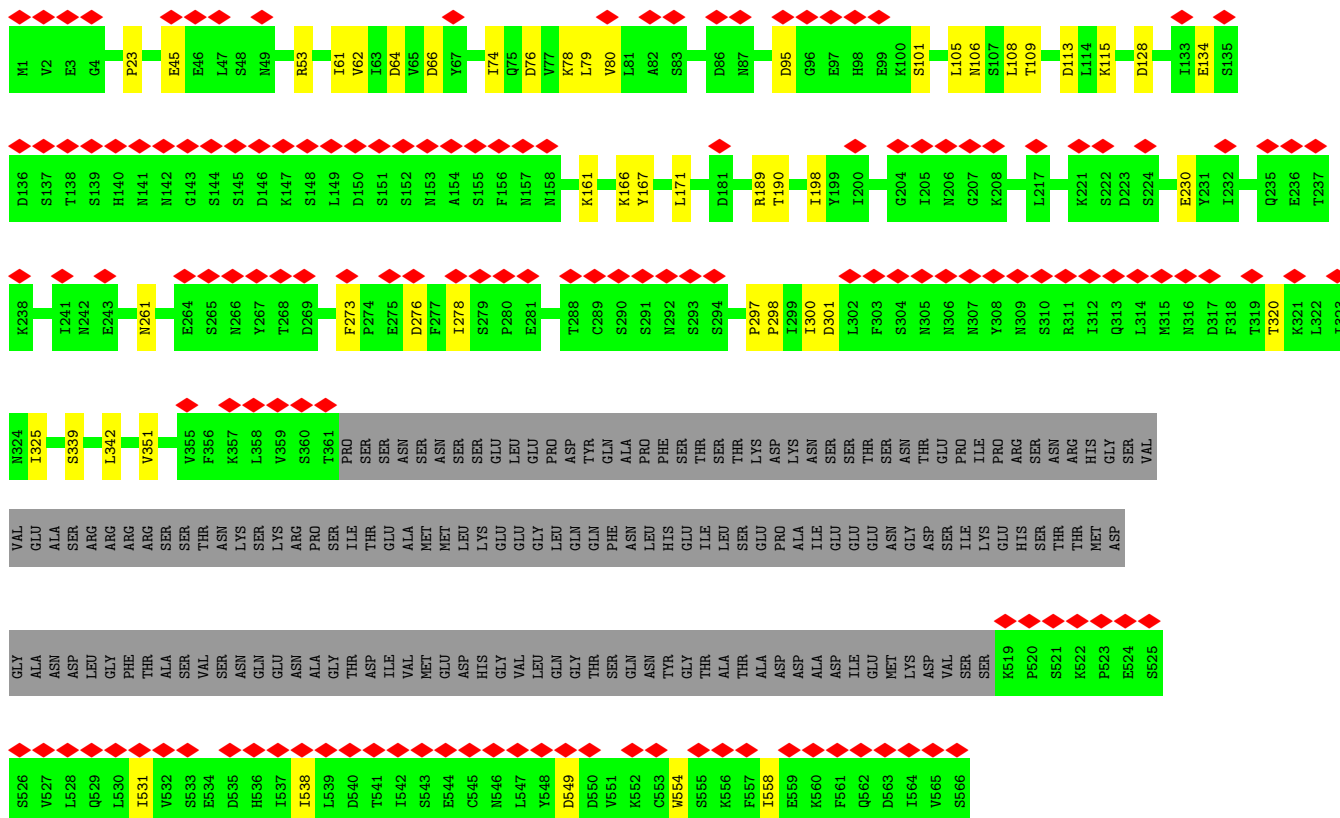


- Molecule 47: Mediator of RNA polymerase II transcription subunit 21

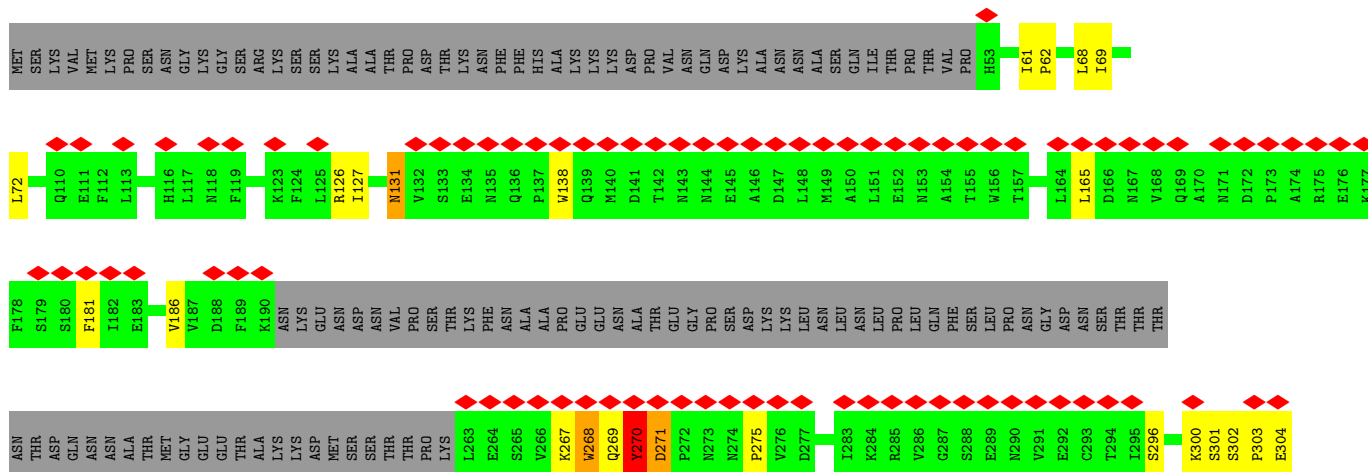


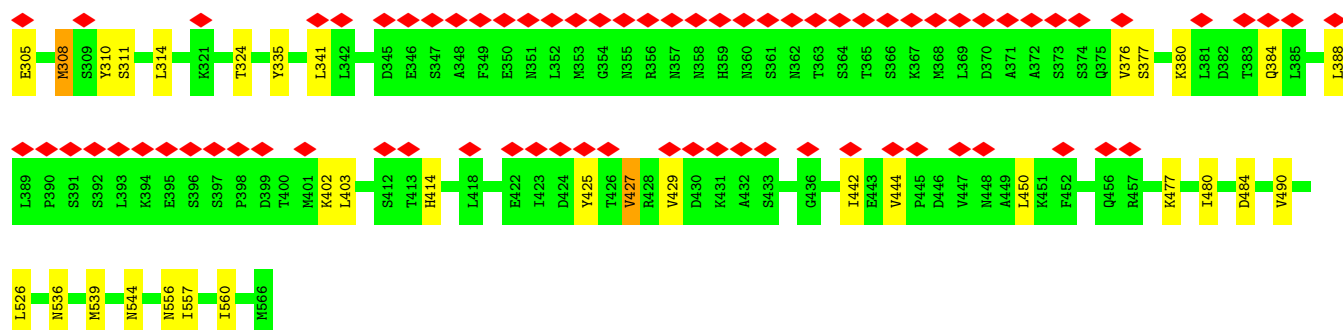


• Molecule 49: Mediator of RNA polymerase II transcription subunit 1

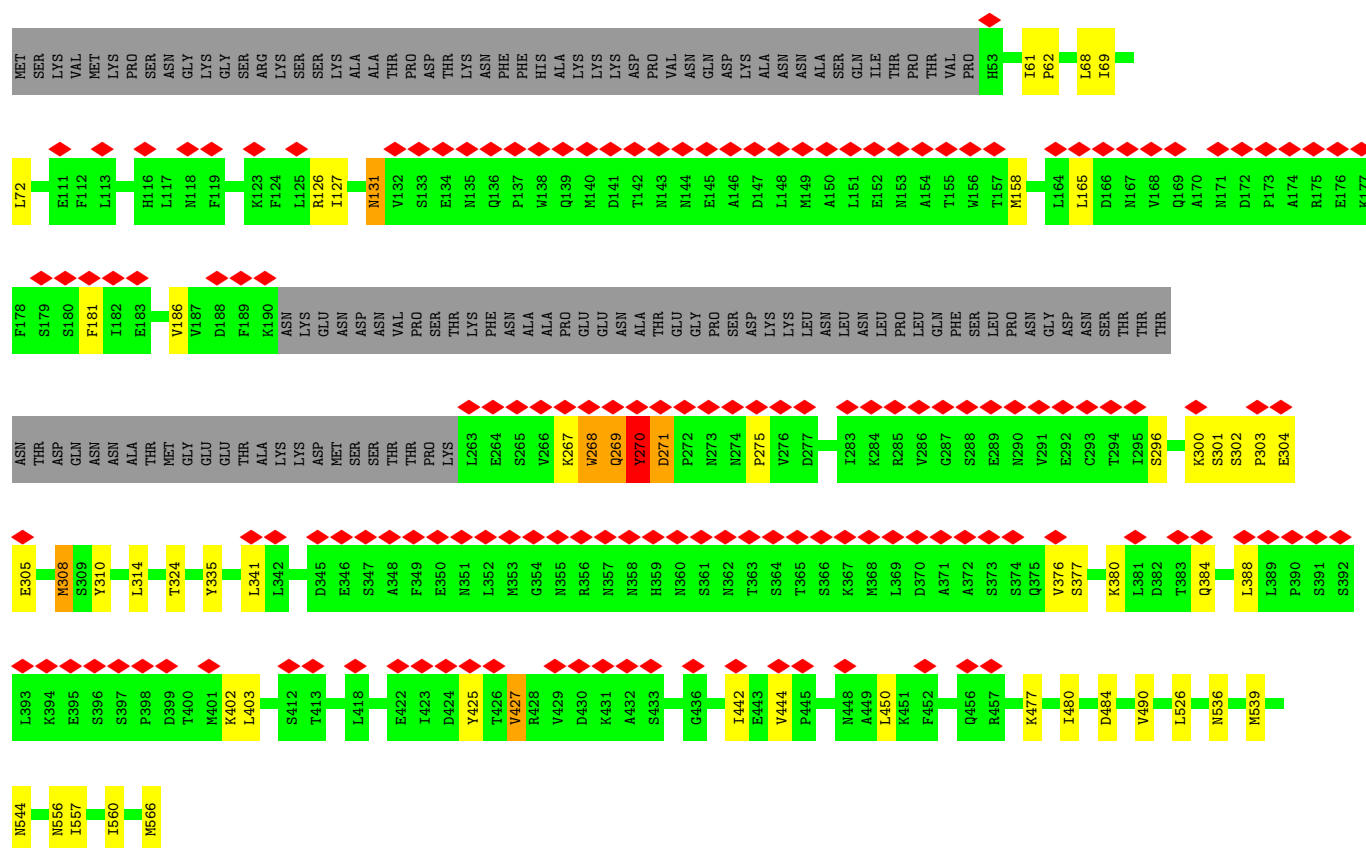


• Molecule 50: Transcription regulatory protein SNF12

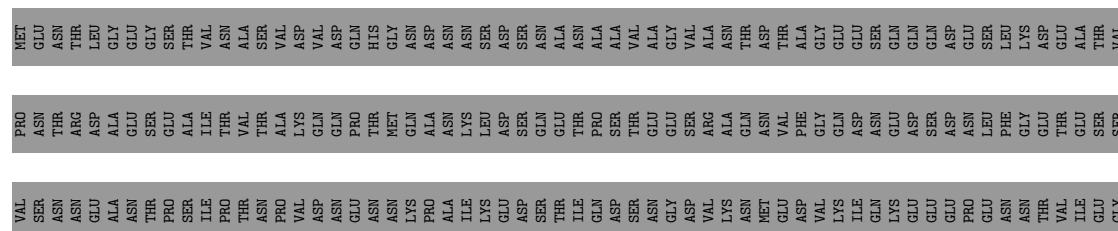


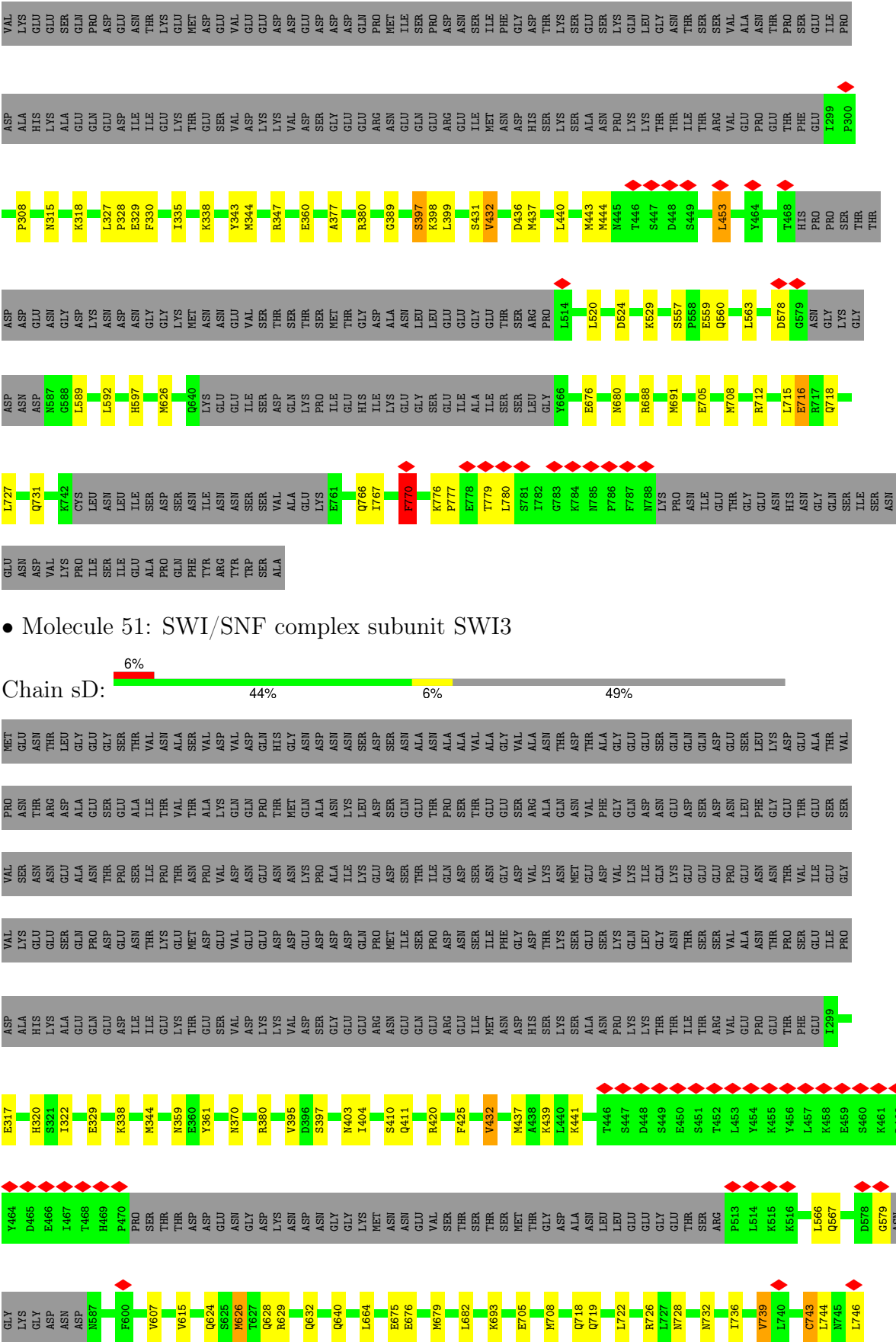


• Molecule 50: Transcription regulatory protein SNF12



• Molecule 51: SWI/SNF complex subunit SWI3

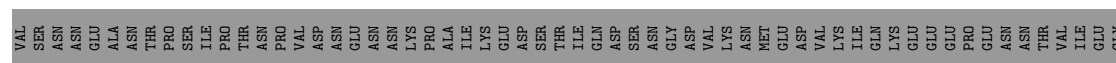
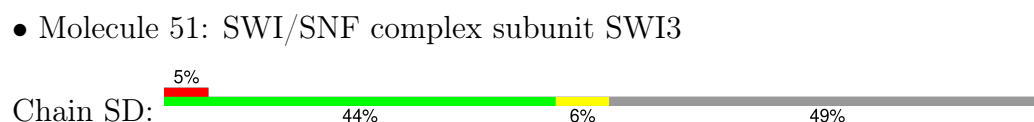




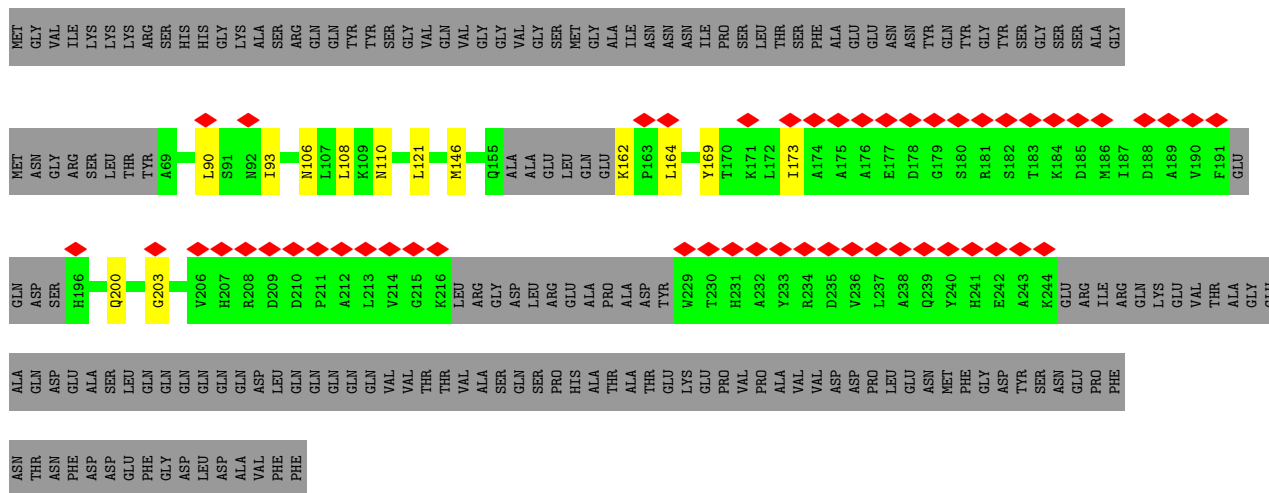
- Molecule 51: SWI/SNF complex subunit SWI3



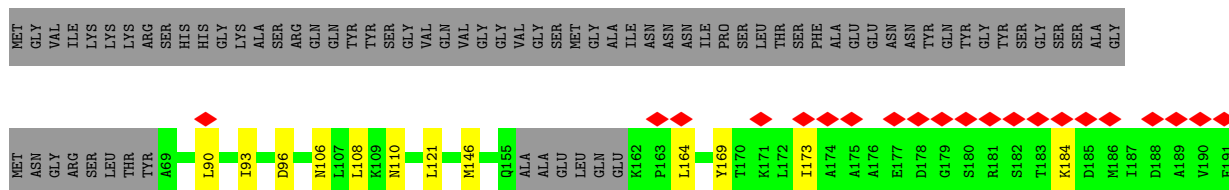
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TYR
TRP
SER
ALA



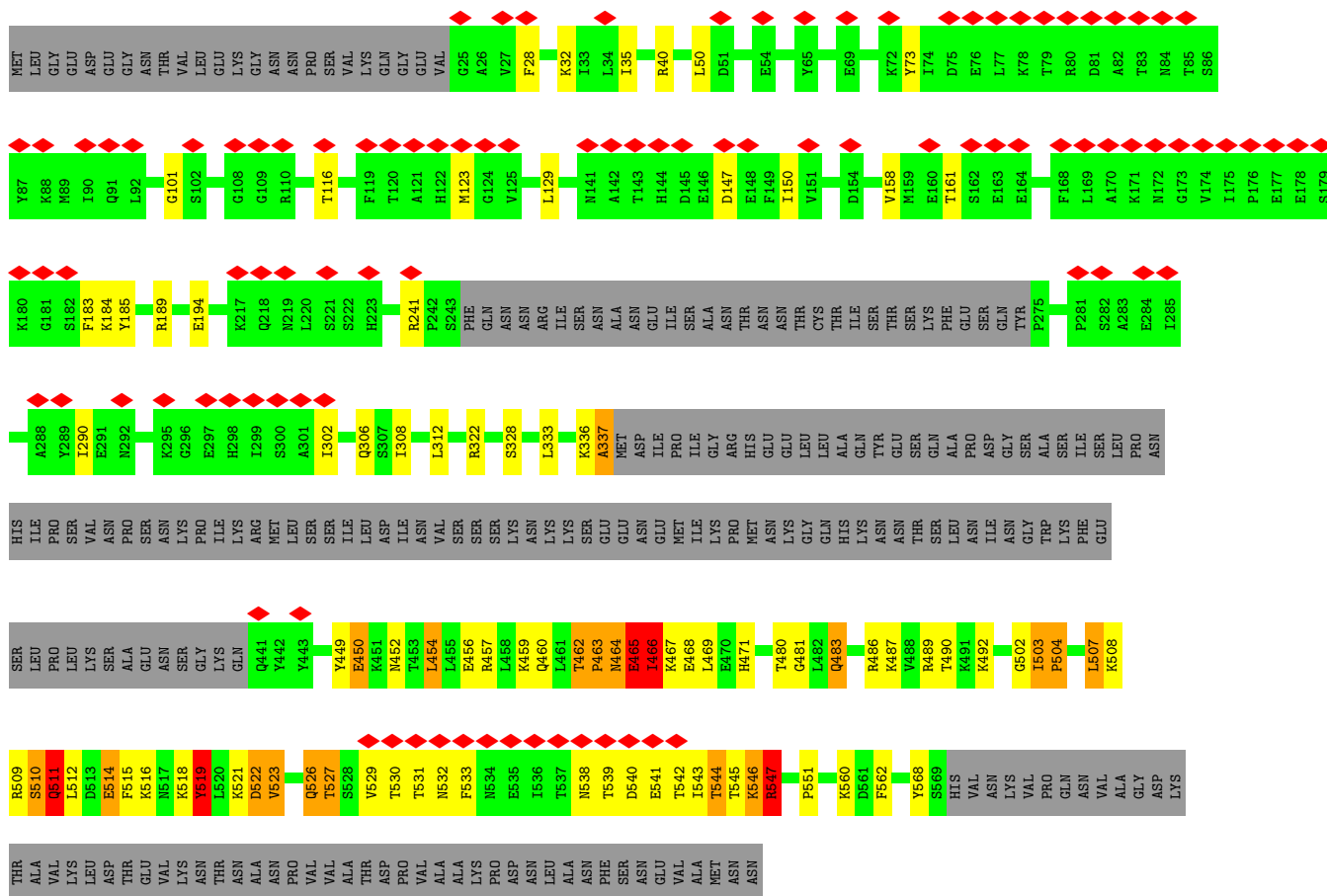
- Molecule 52: Transcription regulatory protein SNF6



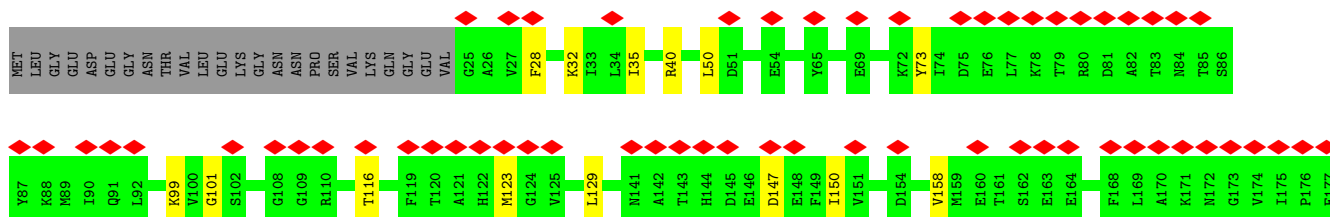
- Molecule 52: Transcription regulatory protein SNF6



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



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





TTR	PRO	VAL	PHE	ASP	ASN	ILE	ASN	THR	HIS	ILE	GLU	LEU	ALA	TYR	ASN	SER	LEU	LYS	THR	THR	LEU	GLN	ASP	PHE	ASP	HIS	ILE	PHE	SER	ASN	ARG	ILE	TTR	TTR	ASN	THR	GLY	ASP	SER	LEU	GLU	GLY	LYS	VAL	VAL	THR	THR	LYS	LYS	TTR	CYS
GLU	ILE	MET	GLY	ASP	ASN	SER	GLN	LEU	ASP	PHE	THR	GLY	GLU	GLN	TYR	THR	GLY	ARG	PRO	PRO	VAL	VAL	VAL	THR	THR	SER	SER	VAL	ALA	ALA	GLU	SER	PHE	THR	THR	ASP	GLU	ALA	ASP	SER	SER	SER	MET	THR	THR	GLY	ALA	GLA	SER	VAL	

- Molecule 55: Transcription regulatory protein SNF2



MET	ASN	ILE	PRO	GLN	ARG	GLN	PHE	SER	ASN	GLU	VAL	ASN	ARG	CYS	TYR	LEU	ARG	TRP	GLN	HIS	GLY	MET	ASN	ALA	PRO	SER	VAL	PRO	GLU	PHE	ILE	TYR	LEU	THR	LYS	VAL	LEU	GLN	PHE	ALA	LYS	ARG	GLN	GLU	GLN	LEU	GLN	MET	GLN	ARG	GLN	GLN
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GLN	GLY	ILE	GLY	GLY	SER	GLN	GLN	ASN	ASN	VAL	PRO	ASN	SER	SER	ASP	GLN	ALA	ALA	GLU	LEU	PRO	ASN	ASN	ASN	ALA	SER	SER	HIS	ILE	SER	SER	ALA	ALA	SER	ALA	ALA	SER	SER	PRO	PRO	GLY	ASN	ASN	GLU	THR	PHE	SER	SER	ALA	ALA	HIS	GLN	SER	PRO	ILE	MET	GLN	THR
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GLN	NET	PRO	PRO	LEU	ASN	SER	ASN	GLY	ASN	ASN	MET	LEU	PRO	GLN	GLN	SER	SER	VAL	GLY	SER	LEU	ASN	ALA	ALA	THR	ASN	ASN	PHE	SER	SER	PRO	PRO	THR	PRO	ALA	ALA	ASN	ASN	GLY	GLY	GLY	GLU	GLU	ASN	ASN	GLU	GLY	LYS	PRO	PRO	ASP	ASN	ASN	SER	SER	ASN	HIS	ASN	ASN	ASN	LEU	LEU	ASN	ASN	LEU	LEU	LEU	GLU	SER	SER	GLN	GLN	PRO
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[illegible]

ARG ARG LEU LEU PRO MET THR MET PHE LEU LEU GLN ALA ALA SER LEU LEU LEU LYS CYS LEU LEU VAL VAL ASN ARG LYS LYS PRO PRO PRO PHE PHE PHE GLN ALA VAL VAL ILE ILE LYS SER ASP ASP PHE HIS PRO PRO ASP PHE ARG MET LEU LEU SER SER LEU LEU GLN

ALA ARG ARG ARG GLN PRO THR ASP GLN ASN ASN GLN SER GLN LEU LEU GLY GLY ASN ASN THR THR GLN GLN PRO GLY THR ASN ASN HIS HIS TYR ASN ASN VAL VAL SER SER GLY GLY LEU LEU THR THR ARG ARG ASN ASN ALA ALA PRO PRO ASP ASP SER SER LYS LYS ASP ASP GLU GLU PHE PHE ALA ALA SER SER VAL VAL SER SER PRO PRO

GLY	PRO	SER	SER	VAL	HIS	ASN	ALA	LYS	ASN	GLY	THR	LEU	ASP	LYS	ASN	SER	SER	GLN	THR	VAL	SER	GLY	THR	PRO	ILE	THR	GLN	THR	GLU	SER	LYS	LYS	GLU	GLU	ASN	GLU	THR	ILE	SER	SER	ASN	VAL	ALA	LYS	THR	ALA	PRO	PRO	ASN	SER	ASN	LYS	THR	THR	HIS	THR	GLU	GLN	ASN	ASN	P418	P402
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Year	Score	Category
2013	432	Below Average
2014	435	Below Average
2015	439	Below Average
2016	443	Below Average
2017	447	Below Average
2018	448	Below Average
2019	449	Below Average
2020	453	Below Average
2021	454	Below Average
2022	455	Below Average
2023	468	Below Average
2024	472	Below Average
2025	475	Below Average
2026	482	Below Average
2027	505	Average
2028	517	Average
2029	518	Average
2030	526	Average
2031	534	Average
2032	535	Average
2033	536	Average
2034	537	Average
2035	538	Average
2036	539	Average
2037	553	Average
2038	562	Average
2039	584	Above Average
2040	585	Above Average
2041	586	Above Average
2042	587	Above Average
2043	588	Above Average
2044	590	Above Average
2045	591	Above Average
2046	592	Above Average
2047	593	Above Average
2048	594	Above Average
2049	595	Above Average
2050	596	Above Average
2051	597	Above Average
2052	598	Above Average
2053	599	Above Average

Amino Acid	Count	Type
A601	1	Standard
L605	1	Standard
M608	1	Standard
K609	1	Standard
K610	1	Standard
I613	1	Standard
K623	1	Standard
L627	1	Standard
K628	1	Standard
F629	1	Standard
L633	1	Standard
L634	1	Standard
K646	1	Modified
K653	1	Modified
E654	1	Modified
E655	1	Modified
L656	1	Modified
Q657	1	Modified
A658	1	Modified
LEU	1	Standard
LYS	1	Standard
ALA	1	Standard
ASN	1	Standard
ASP	1	Standard
GLU	1	Standard
GLY	1	Standard
ALA	1	Standard
TYR	1	Standard
ILE	1	Standard
LYS	1	Standard
LEU	1	Standard
LEU	1	Standard
ASP	1	Standard
GLN	1	Standard
THR	1	Standard
LYS	1	Standard
ASP	1	Standard
THR	1	Standard
ARG	1	Standard
ILE	1	Standard
THR	1	Standard
HIS	1	Standard
LEU	1	Standard
LEU	1	Standard
ARG	1	Standard
GLN	1	Standard
THR	1	Standard
ASN	1	Standard
ALA	1	Standard
ALA	1	Standard
PHE	1	Standard
LEU	1	Standard

LEU THR ARG ALA VAL LYS ASP GLN GLN LYS TYR THR TYR LYS GLU MET MET ILE ASP SER HIS ILE LYS GLU GLU ALA SER LEU LEU SER MET MET VAL PRO LYS LYS MET LYS ASP ASP ASP ASP ASN ASN ASN VAL VAL TYR TYR TYR TYR TYR TYR TYR TYR TYR

GLU ASP ILE LYS LYS GLN PRO SER ILE VAL GLY GLY THR LEU LYS ASP TYR GLN ILE LYS GLY LEU LEU ASN PHE ASN ASN HIS LEU ASN GLY ILE LEU LEU ALA ASP ASP MET GLY LEU LYS GLY THR ILE GLN THR ILE SER SER LEU LEU THR TYR TYR MET

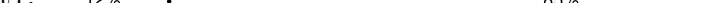
LYS ASN
ILE LEU
ARG ARG
GLY GLY
PRO PRO
TYR TYR
LEU LEU
VAL VAL
ILE ILE
VAL VAL
PRO PRO
LEU LEU
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THR THR
LEU LEU
SER SER
ASN ASN
TRP TRP
SER SER
SER SER
GLU GLU
PHE PHE
ALA ALA
LYS LYS
TRP TRP
ALA ALA
PRO PRO
PRO PRO
THR THR
LEU LEU
ARG ARG
THR THR
ILE ILE
SER SER
PHE PHE
LYS LYS
GLY GLY
SER SER
PRO PRO
ASN ASN
GLU GLU
ARG ARG
LYS LYS
ALA ALA
LYN LYN
GLN GLN
ALA ALA
LYS LYS
ILE ILE
ARG ARG
ALA ALA
GLY GLY
PHE PHE
ASP ASP
VAL VAL
LEU LEU
LEU LEU
THR THR

PHE GLU TYR ILE ILE LYS GLU ARG ALA LEU LEU SER LYS VAL VAL LYS HIS MET ILE ILE ASP GLU GLY HIS ARG MET LYS ASN ALA ALA GLN SER LYS LEU LEU SER THR THR TYR HIS ALA ASP TYR ARG ARG LEU LEU ILE LEU THR GLY PRO LEU GLN ASN ASN LEU LEU PRO

GLU	TRP	ALA	LEU	ASN	PHE	VAL	LEU	PRO	LYS	ILE	PHE	ASN	SER	VAL	LYS	SER	PHE	ASP	GLU	TRP	PHE	ASN	THR	PRO	PHE	ALA	ASN	GLY	GLN	ASP	LYS	ILE	LEU	LEU	SER	GLU	GLU	GLU	THR	LEU	LEU	VAL	ILE	ARG	ARG	LEU	HIS	LYS	VAL	LEU	ARG	PRO	PHE	PHE	LEU
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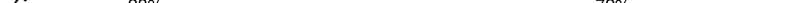
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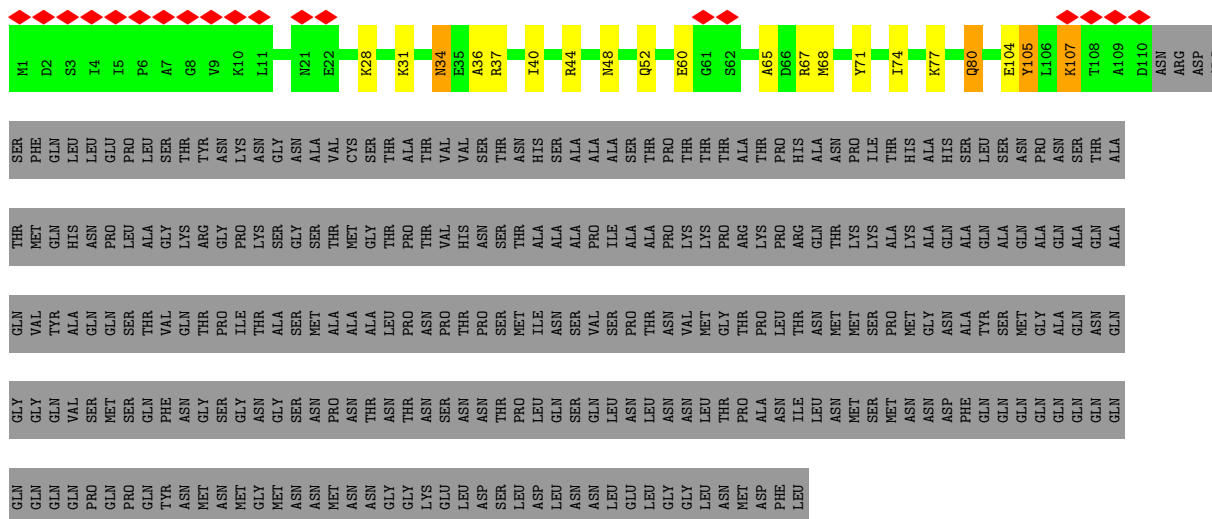
MET	GLN	LEU	LYS	LYS	ILE	CYS	ASN	HIS	PRO	PHE	VAL	PHE	GLU	GLU	VAL	GLU	ASP	GLN	ILE	ASN	PRO	THR	ARG	GLU	THR	ASN	ASP	ASP	ILE	TRP	TRP	VAL	ALA	ALA	LYS	LYS	ALA	THR	GLY	HIS	ARG	VAL	LEU	ILE	PHE	PHE	GLN	MET
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Chain t1:  12% . 85%

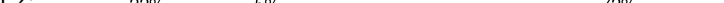


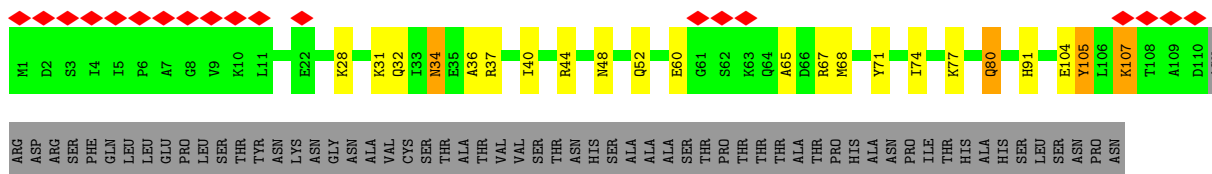
- Molecule 61: Mediator of RNA polymerase II transcription subunit 3

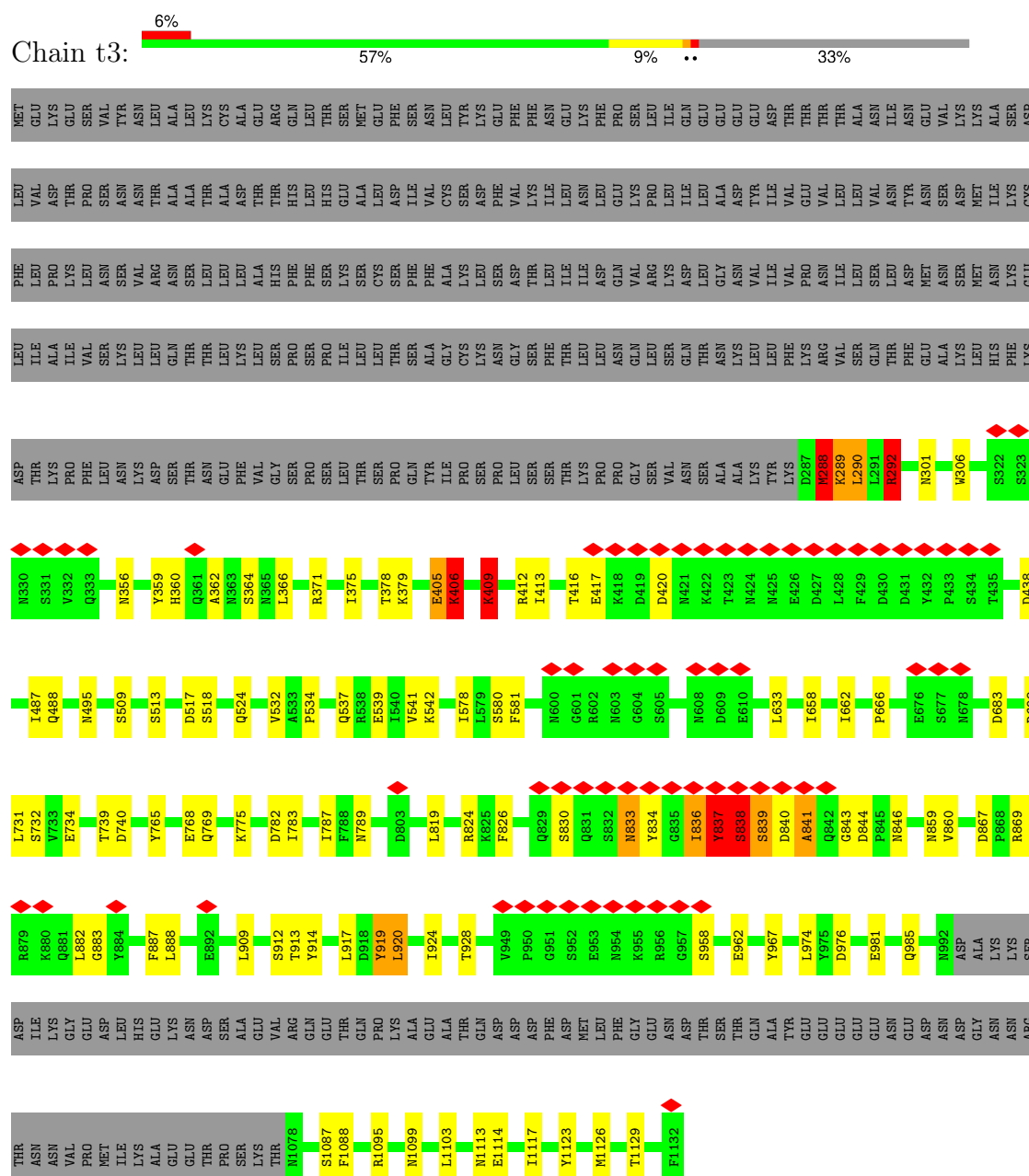
Chain T2:  5% 23% 72%



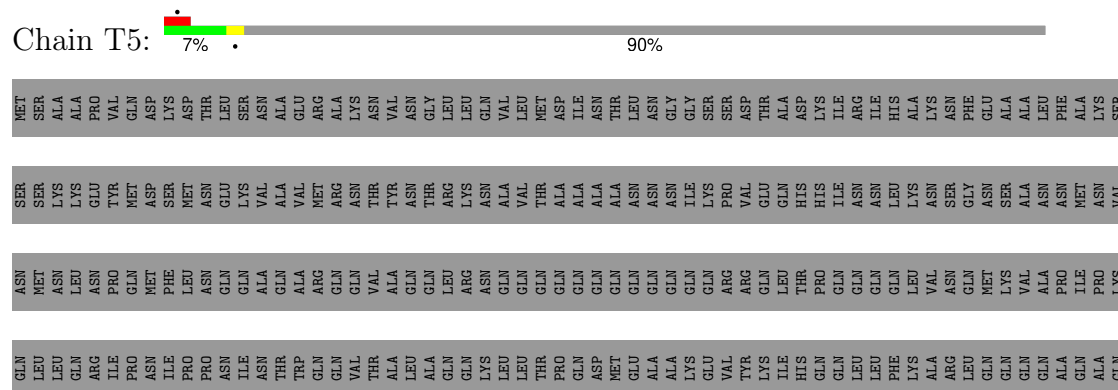
- Molecule 61: Mediator of RNA polymerase II transcription subunit 3

Chain t2: 

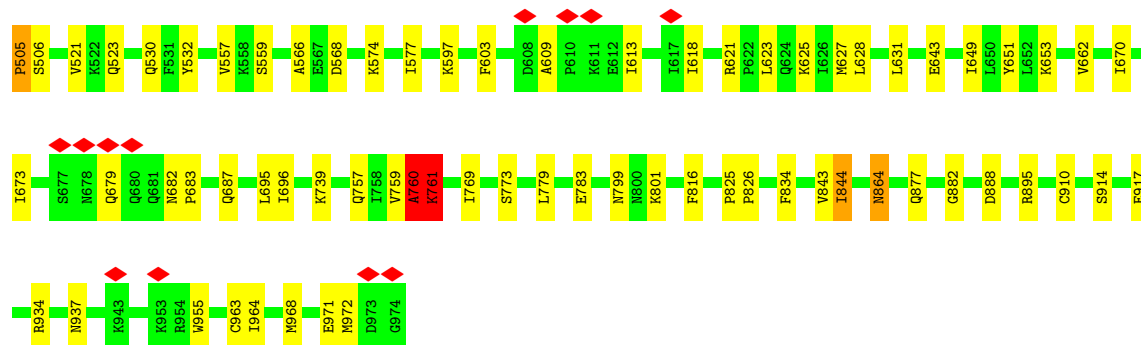




● Molecule 63: Mediator of RNA polymerase II transcription subunit 15

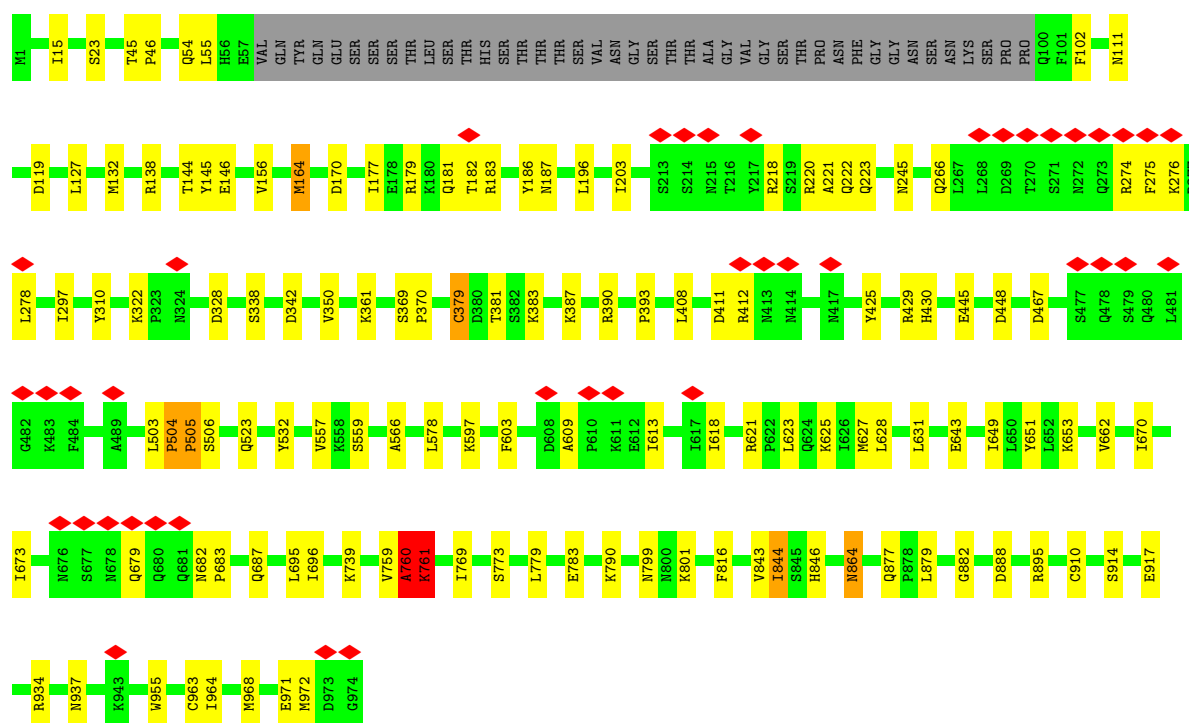






- Molecule 64: Mediator of RNA polymerase II transcription subunit 16

Chain t6: 82% 12%



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)	2700	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	0.054	Depositor
Recommended contour level	0.407	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	0.56	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	T1	0.68	2/520 (0.4%)	0.79	0/693
60	t1	0.68	2/520 (0.4%)	0.79	0/693
61	T2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
61	t2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
62	T3	0.64	17/6293 (0.3%)	0.97	36/8534 (0.4%)
62	t3	0.64	17/6293 (0.3%)	0.97	38/8534 (0.4%)
63	T5	1.28	16/904 (1.8%)	2.16	31/1202 (2.6%)
63	t5	1.29	16/904 (1.8%)	2.16	31/1202 (2.6%)
64	T6	0.46	9/7725 (0.1%)	0.71	10/10461 (0.1%)
64	t6	0.46	9/7725 (0.1%)	0.71	10/10461 (0.1%)
All	All	0.56	604/311402 (0.2%)	0.87	1277/421672 (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
9	A8	0	1
9	B8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
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
58	SK	0	3
58	sK	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
61	T2	0	1
61	t2	0	1
62	T3	1	6
62	t3	1	6
63	T5	1	2
63	t5	1	2
64	T6	0	1
64	t6	0	1
All	All	12	192

All (604) 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
62	t3	837	TYR	CG-CD2	19.70	1.80	1.39
62	T3	837	TYR	CG-CD2	19.69	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
9	sF	485	LEU	CG-CD1	-17.27	0.95	1.52
9	SF	485	LEU	CG-CD1	-17.27	0.95	1.52
63	t5	920	LYS	CB-CG	-16.19	1.03	1.52
63	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B3	49	LEU	CB-CG	-13.98	1.25	1.53
4	A3	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
62	T3	289	LYS	CG-CD	-12.17	1.16	1.52
62	t3	289	LYS	CG-CD	-12.15	1.16	1.52
20	BJ	58	GLU	CB-CG	-12.15	1.16	1.52
10	A9	209	MET	CB-CG	-12.12	1.16	1.52
10	B9	209	MET	CB-CG	-12.09	1.16	1.52
62	T3	289	LYS	CB-CG	11.99	1.88	1.52
62	t3	289	LYS	CB-CG	11.97	1.88	1.52
19	AI	86	PHE	CG-CD1	-11.66	1.14	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	t2	34	ASN	CG-OD1	-11.64	1.01	1.23
19	BI	86	PHE	CG-CD1	-11.62	1.14	1.38
12	AB	22	SER	C-N	11.60	1.50	1.33
61	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	B5	50	VAL	CB-CG1	-10.74	1.17	1.52
6	A5	50	VAL	CB-CG1	-10.74	1.17	1.52
10	B9	199	GLN	CD-NE2	10.71	1.55	1.33
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
53	SE	523	VAL	CB-CG2	-10.55	1.17	1.52
55	SH	455	MET	SD-CE	-10.52	1.53	1.79
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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	-9.04	1.25	1.52
45	t4	1018	MET	CB-CG	-9.03	1.25	1.52
58	SK	303	LEU	CG-CD1	-9.02	1.22	1.52
62	t3	836	ILE	C-N	9.02	1.46	1.33
62	T3	836	ILE	C-N	9.01	1.46	1.33
58	sK	303	LEU	CG-CD1	-9.01	1.22	1.52
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
50	sA	269	GLN	CB-CG	-8.96	1.25	1.52
7	A6	384	MET	SD-CE	-8.96	1.57	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
28	BS	198	ARG	CB-CG	-8.83	1.25	1.52
53	SE	483	GLN	CD-OE1	-8.83	1.06	1.23
53	sE	483	GLN	CD-OE1	-8.82	1.06	1.23
62	T3	289	LYS	CA-CB	8.81	1.67	1.53
62	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
64	T6	864	ASN	CG-ND2	-8.67	1.15	1.33
64	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
62	T3	288	MET	C-N	8.59	1.45	1.33
29	BT	45	DT	P-O5'	8.59	1.68	1.59
62	t3	288	MET	C-N	8.59	1.45	1.33
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	BI	84	VAL	CA-CB	-8.49	1.44	1.54
19	AI	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
3	A2	408	MET	SD-CE	-8.45	1.58	1.79
11	BA	455	MET	SD-CE	-8.44	1.58	1.79
53	SE	507	LEU	CG-CD2	-8.44	1.24	1.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
63	T5	919	ARG	NE-CZ	-8.28	1.24	1.33
63	t5	919	ARG	NE-CZ	-8.26	1.24	1.33
63	T5	943	LEU	CG-CD1	-8.23	1.25	1.52
64	t6	132	MET	SD-CE	-8.23	1.58	1.79
63	t5	943	LEU	CG-CD1	-8.23	1.25	1.52
64	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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
6	B5	3	ARG	CD-NE	-7.63	1.35	1.46
57	SJ	1	MET	SD-CE	-7.63	1.60	1.79
57	sJ	1	MET	SD-CE	-7.62	1.60	1.79
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
62	T3	289	LYS	CA-C	-7.59	1.43	1.52
63	T5	920	LYS	CA-C	-7.59	1.42	1.52
62	t3	289	LYS	CA-C	-7.59	1.43	1.52
63	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
62	t3	290	LEU	N-CA	-7.44	1.37	1.46
5	B4	109	ILE	CB-CG2	-7.43	1.28	1.52
62	T3	290	LEU	N-CA	-7.41	1.37	1.46
1	B0	537	MET	SD-CE	-7.37	1.61	1.79
10	B9	217	GLU	CD-OE1	-7.37	1.11	1.25
1	A0	537	MET	SD-CE	-7.37	1.61	1.79
63	t5	923	LYS	CE-NZ	-7.35	1.27	1.49
10	A9	217	GLU	CD-OE1	-7.35	1.11	1.25
63	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
3	B2	69	ASN	N-CA	-7.31	1.37	1.46
28	BS	205	ASN	C-N	-7.31	1.23	1.33
28	AS	205	ASN	C-N	-7.31	1.23	1.33
2	B1	197	GLU	CD-OE1	-7.31	1.11	1.25
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
3	B2	69	ASN	CB-CG	-7.12	1.34	1.52
3	A2	69	ASN	CB-CG	-7.10	1.34	1.52
63	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
63	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
64	t6	972	MET	SD-CE	-6.97	1.62	1.79
64	T6	972	MET	SD-CE	-6.96	1.62	1.79
8	A7	338	LEU	C-O	-6.96	1.15	1.24
50	SA	269	GLN	C-O	6.96	1.29	1.23
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
61	t2	80	GLN	CD-OE1	-6.91	1.10	1.23
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	T2	80	GLN	CD-OE1	-6.86	1.10	1.23
53	SE	527	THR	CB-OG1	-6.86	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	t1	40	LEU	CG-CD1	-6.84	1.29	1.52
53	sE	527	THR	CB-OG1	-6.83	1.32	1.43
60	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	BE	121	MET	SD-CE	-6.80	1.62	1.79
15	AE	121	MET	SD-CE	-6.80	1.62	1.79
62	T3	919	TYR	CD2-CE2	-6.80	1.18	1.38
62	t3	919	TYR	CD2-CE2	-6.80	1.18	1.38
62	t3	838	SER	CA-C	6.79	1.61	1.52
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
62	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
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
53	SE	519	TYR	CD2-CE2	-6.64	1.18	1.38
64	T6	971	GLU	CD-OE1	-6.62	1.12	1.25
64	t6	971	GLU	CD-OE1	-6.60	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
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
55	sH	453	PHE	CE2-CZ	-6.45	1.19	1.38
55	SH	453	PHE	CE2-CZ	-6.45	1.19	1.38
4	B3	64	ARG	CA-C	-6.44	1.44	1.52
50	SA	269	GLN	CD-OE1	-6.44	1.11	1.23
4	A3	64	ARG	CA-C	-6.43	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
26	BQ	147	LEU	CG-CD2	-6.27	1.31	1.52
28	BS	206	VAL	N-CA	-6.26	1.38	1.46
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
62	t3	837	TYR	CB-CG	-6.15	1.38	1.51
51	sD	626	MET	SD-CE	-6.15	1.64	1.79
62	T3	837	TYR	CB-CG	-6.14	1.38	1.51
19	AI	84	VAL	CB-CG2	-6.14	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
62	T3	837	TYR	N-CA	6.09	1.54	1.46
53	sE	511	GLN	CD-OE1	-6.07	1.12	1.23
62	t3	837	TYR	N-CA	6.05	1.54	1.46
53	SE	511	GLN	CD-OE1	-6.05	1.12	1.23
63	T5	923	LYS	CG-CD	-6.04	1.34	1.52
63	t5	923	LYS	CG-CD	-6.04	1.34	1.52
20	AJ	58	GLU	CD-OE1	-6.03	1.13	1.25
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
62	t3	920	LEU	CG-CD1	-6.01	1.32	1.52
62	T3	920	LEU	CG-CD1	-6.00	1.32	1.52
62	T3	406	LYS	CA-C	5.98	1.60	1.52
62	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
58	SK	237	GLN	CG-CD	-5.95	1.37	1.52
28	BS	182	MET	N-CA	5.95	1.53	1.46
63	T5	877	LYS	CD-CE	-5.94	1.34	1.52
63	t5	877	LYS	CD-CE	-5.93	1.34	1.52
12	BB	22	SER	CA-C	5.92	1.60	1.52
11	BA	542	GLU	CD-OE1	-5.92	1.14	1.25
8	A7	723	GLN	CD-OE1	-5.92	1.12	1.23
45	t4	1016	TYR	C-N	5.92	1.41	1.33
8	B7	723	GLN	CD-OE1	-5.90	1.12	1.23
45	T4	1016	TYR	C-N	5.89	1.41	1.33
53	sE	503	ILE	CB-CG2	-5.89	1.33	1.52
12	AB	22	SER	CA-C	5.88	1.60	1.52
58	sK	228	ILE	CG1-CD1	-5.87	1.28	1.51
53	SE	503	ILE	CB-CG2	-5.87	1.33	1.52
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
63	t5	872	ARG	CZ-NH2	-5.84	1.25	1.33
11	BA	688	LYS	N-CA	-5.83	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A0	167	VAL	CB-CG2	-5.83	1.33	1.52
3	B2	464	THR	CB-CG2	5.83	1.71	1.52
53	SE	519	TYR	CE2-CZ	-5.82	1.24	1.38
1	B0	167	VAL	CB-CG2	-5.81	1.33	1.52
3	A2	464	THR	CB-CG2	5.81	1.71	1.52
11	AA	688	LYS	N-CA	-5.81	1.38	1.46
60	T1	70	GLN	CD-OE1	-5.80	1.12	1.23
24	BN	-62	DG	O3'-P	5.80	1.68	1.61
60	t1	70	GLN	CD-OE1	-5.80	1.12	1.23
53	sE	522	ASP	C-N	5.79	1.40	1.33
63	T5	872	ARG	CZ-NH2	-5.79	1.25	1.33
24	AN	-62	DG	O3'-P	5.78	1.68	1.61
53	SE	522	ASP	C-N	5.78	1.40	1.33
55	sH	482	GLY	C-O	-5.77	1.17	1.23
63	t5	877	LYS	CA-C	-5.77	1.45	1.52
19	AI	60	GLN	CD-OE1	-5.75	1.12	1.23
63	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
64	t6	955	TRP	C-N	5.73	1.40	1.34
64	T6	955	TRP	C-N	5.73	1.40	1.34
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
63	T5	931	GLN	CB-CG	-5.70	1.35	1.52
63	t5	931	GLN	CB-CG	-5.69	1.35	1.52
3	B2	490	LYS	CD-CE	-5.68	1.35	1.52
6	A5	62	ILE	CG1-CD1	-5.68	1.29	1.51
45	t4	1000	HIS	C-O	-5.68	1.15	1.23
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
62	t3	289	LYS	C-N	-5.67	1.26	1.33
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
62	T3	289	LYS	C-N	-5.65	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	T4	1000	HIS	C-O	-5.64	1.15	1.23
56	sI	1306	LYS	CD-CE	-5.64	1.35	1.52
19	AI	111	THR	CB-CG2	5.64	1.71	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
64	T6	532	TYR	CD1-CE1	-5.62	1.21	1.38
3	B2	490	LYS	CG-CD	-5.62	1.35	1.52
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	A2	253	MET	SD-CE	-5.62	1.65	1.79
63	T5	877	LYS	CE-NZ	-5.62	1.32	1.49
63	t5	877	LYS	CE-NZ	-5.61	1.32	1.49
64	t6	532	TYR	CD1-CE1	-5.61	1.21	1.38
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
19	AI	60	GLN	CD-NE2	5.58	1.45	1.33
28	AS	228	LEU	CG-CD2	-5.58	1.34	1.52
62	T3	633	LEU	CG-CD1	-5.57	1.34	1.52
28	BS	228	LEU	CG-CD2	-5.57	1.34	1.52
62	t3	633	LEU	CG-CD1	-5.57	1.34	1.52
19	BI	60	GLN	CD-NE2	5.56	1.45	1.33
24	AN	-59	DC	C1'-N1	5.55	1.55	1.47
53	SE	510	SER	C-N	5.53	1.41	1.33
64	T6	761	LYS	CD-CE	-5.53	1.35	1.52
64	t6	761	LYS	CD-CE	-5.53	1.35	1.52
63	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
63	t5	923	LYS	CB-CG	-5.50	1.35	1.52
63	t5	931	GLN	CG-CD	-5.50	1.38	1.52
63	T5	931	GLN	CG-CD	-5.49	1.38	1.52
9	sF	400	GLN	C-O	-5.48	1.17	1.24
19	AI	115	LYS	CG-CD	-5.47	1.36	1.52
6	B5	3	ARG	CZ-NH1	5.47	1.40	1.32
28	AS	182	MET	CA-C	-5.47	1.45	1.52
9	SF	400	GLN	C-O	-5.46	1.17	1.24
64	T6	164	MET	SD-CE	-5.46	1.65	1.79
28	BS	182	MET	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BI	115	LYS	CG-CD	-5.46	1.36	1.52
55	sH	449	MET	CG-SD	-5.46	1.67	1.80
64	t6	164	MET	SD-CE	-5.46	1.66	1.79
55	SH	449	MET	CG-SD	-5.45	1.67	1.80
64	t6	54	GLN	CD-NE2	-5.43	1.21	1.33
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
64	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
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
6	B5	54	LEU	CG-CD1	-5.33	1.34	1.52
63	t5	931	GLN	CD-NE2	5.33	1.44	1.33
63	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
62	T3	917	LEU	CG-CD2	-5.28	1.35	1.52
58	SK	147	LEU	CB-CG	-5.27	1.43	1.53
62	t3	917	LEU	CG-CD2	-5.26	1.35	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
11	BA	692	ASP	CA-C	5.07	1.59	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
53	sE	519	TYR	CB-CG	-5.05	1.40	1.51
19	BI	85	PHE	N-CA	5.05	1.51	1.45
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
63	t5	877	LYS	CG-CD	-5.03	1.37	1.52
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
63	T5	877	LYS	CG-CD	-5.01	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 (1277) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A2	69	ASN	CB-CG-ND2	-32.11	68.24	116.40
63	T5	920	LYS	CB-CG-CD	29.86	179.98	111.30
63	t5	920	LYS	CB-CG-CD	29.85	179.95	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
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
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	B9	200	MET	CA-CB-CG	24.83	163.75	114.10
10	A9	200	MET	CA-CB-CG	24.83	163.76	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
62	T3	837	TYR	CB-CG-CD2	-22.98	86.33	120.80
62	t3	837	TYR	CB-CG-CD2	-22.98	86.34	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
63	T5	919	ARG	CD-NE-CZ	21.03	153.84	124.40
63	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
63	t5	923	LYS	CB-CG-CD	20.44	158.30	111.30
63	T5	923	LYS	CB-CG-CD	20.43	158.29	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
19	BI	92	ARG	CG-CD-NE	20.29	156.65	112.00
19	AI	92	ARG	CG-CD-NE	20.29	156.64	112.00
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
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
63	t5	923	LYS	CG-CD-CE	-18.79	68.08	111.30
63	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	BI	78	CYS	CB-CA-C	-18.20	73.24	110.38
19	AI	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	688	LYS	N-CA-C	-17.32	92.15	113.28
45	T4	1018	MET	N-CA-CB	17.16	134.96	109.91
45	t4	1018	MET	N-CA-CB	17.15	134.95	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
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
63	t5	920	LYS	CA-CB-CG	16.42	146.94	114.10
63	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	BI	86	PHE	CB-CG-CD2	-15.78	93.88	120.70
19	AI	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
62	T3	837	TYR	CD1-CG-CD2	-15.03	95.55	118.10
62	t3	837	TYR	CD1-CG-CD2	-15.01	95.58	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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SF	401	LYS	N-CA-CB	-14.23	86.44	110.49
63	t5	877	LYS	CG-CD-CE	14.18	143.92	111.30
63	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	BA	692	ASP	OD1-CG-OD2	-13.90	89.53	122.90
11	AA	692	ASP	OD1-CG-OD2	-13.90	89.54	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
63	t5	919	ARG	CA-CB-CG	13.26	140.62	114.10
63	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
62	T3	837	TYR	CG-CD1-CE1	12.80	140.40	121.20
62	t3	837	TYR	CG-CD1-CE1	12.80	140.40	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
63	T5	931	GLN	CB-CG-CD	12.73	134.24	112.60
19	AI	113	ASP	CA-CB-CG	12.71	125.31	112.60
63	t5	931	GLN	CB-CG-CD	12.70	134.18	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	SE	547	ARG	NE-CZ-NH2	12.54	130.49	119.20
63	t5	931	GLN	CG-CD-NE2	-12.52	97.62	116.40
63	T5	920	LYS	CG-CD-CE	-12.51	82.52	111.30
9	sF	401	LYS	CG-CD-CE	-12.51	82.54	111.30
63	t5	920	LYS	CG-CD-CE	-12.51	82.53	111.30
63	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	B9	217	GLU	CA-CB-CG	12.50	139.10	114.10
10	A9	217	GLU	OE1-CD-OE2	-12.50	92.91	122.90
10	A9	217	GLU	CA-CB-CG	12.48	139.07	114.10
10	B9	209	MET	CB-CA-C	12.45	131.00	110.22
10	A9	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
62	t3	837	TYR	N-CA-CB	-12.25	91.86	111.22
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
62	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
62	t3	837	TYR	CB-CG-CD1	12.10	138.95	120.80
62	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	60	GLN	C-N-CA	-11.86	103.82	122.67
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
63	t5	920	LYS	CB-CA-C	11.56	125.64	109.92
63	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
62	T3	406	LYS	CA-C-N	11.18	138.96	120.62
62	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
62	t3	406	LYS	CA-C-N	11.16	138.92	120.62
62	t3	406	LYS	C-N-CA	11.16	138.92	120.62
55	sH	594	LEU	CD1-CG-CD2	-11.15	86.26	110.80
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
45	t4	1018	MET	CB-CA-C	-10.94	94.11	110.96
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
12	AB	22	SER	CA-C-O	-10.91	104.91	120.51
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
63	t5	919	ARG	CG-CD-NE	-10.80	88.23	112.00
63	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
45	t4	1018	MET	CB-CG-SD	10.76	144.99	112.70
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
19	AI	104	LEU	CD1-CG-CD2	-10.75	87.15	110.80
19	BI	104	LEU	CD1-CG-CD2	-10.75	87.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	93	LYS	CA-CB-CG	-10.73	92.65	114.10
53	SE	463	PRO	CA-N-CD	-10.71	97.01	112.00
55	sH	594	LEU	CA-CB-CG	10.70	153.76	116.30
55	SH	594	LEU	CA-CB-CG	10.70	153.75	116.30
64	T6	760	ALA	CA-C-N	10.70	141.98	121.54
64	T6	760	ALA	C-N-CA	10.70	141.98	121.54
64	t6	760	ALA	CA-C-N	10.70	141.97	121.54
64	t6	760	ALA	C-N-CA	10.70	141.97	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
12	BB	662	MET	CB-CG-SD	10.24	143.43	112.70
12	AB	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
29	BT	60	DT	O4'-C1'-N1	10.22	115.16	108.00
9	SF	389	ASN	N-CA-C	-10.22	99.08	112.68
9	sF	389	ASN	N-CA-C	-10.21	99.10	112.68
29	AT	60	DT	O4'-C1'-N1	10.21	115.14	108.00
24	AN	-43	DA	O4'-C1'-C2'	-10.14	97.78	105.90
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
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
62	T3	836	ILE	N-CA-CB	9.66	131.01	110.64
62	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
62	T3	837	TYR	CA-CB-CG	9.59	131.16	113.90
62	t3	837	TYR	CA-CB-CG	9.59	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	BI	62	ILE	CB-CA-C	-9.42	93.79	111.79
19	AI	62	ILE	CB-CA-C	-9.42	93.79	111.79
3	B2	490	LYS	N-CA-CB	-9.42	94.22	111.37
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
62	t3	409	LYS	N-CA-CB	9.34	126.27	110.49
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
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
55	SH	592	LEU	CD1-CG-CD2	-9.32	90.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	T3	409	LYS	N-CA-CB	9.32	126.25	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
63	t5	920	LYS	CD-CE-NZ	9.03	140.80	111.90
53	SE	510	SER	CA-C-O	-9.02	110.81	120.92
63	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
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
3	B2	490	LYS	CA-CB-CG	8.80	131.70	114.10
28	AS	232	ASP	OD1-CG-OD2	-8.80	101.78	122.90
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
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
62	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
62	t3	292	ARG	CD-NE-CZ	8.74	136.64	124.40
62	t3	289	LYS	N-CA-CB	8.73	122.90	110.07
62	T3	289	LYS	N-CA-CB	8.72	122.89	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
64	t6	761	LYS	CB-CG-CD	8.58	131.02	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
64	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
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
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
9	sF	485	LEU	CD1-CG-CD2	-8.42	92.27	110.80
19	AI	114	GLN	CG-CD-NE2	-8.42	103.77	116.40
63	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
63	t5	931	GLN	OE1-CD-NE2	-8.39	114.20	122.60
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
61	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
53	sE	454	LEU	CD1-CG-CD2	-8.37	92.38	110.80
61	T2	107	LYS	O-C-N	-8.37	110.91	122.46
63	t5	931	GLN	CG-CD-OE1	8.34	137.47	120.80
9	SF	389	ASN	N-CA-CB	-8.33	96.34	110.33
9	sF	389	ASN	N-CA-CB	-8.32	96.35	110.33
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
63	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-8.15	82.96	100.90
45	t4	1018	MET	CG-SD-CE	-8.15	82.97	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
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
63	t5	919	ARG	CB-CG-CD	7.80	129.24	111.30
28	AS	230	THR	OG1-CB-CG2	7.80	124.89	109.30
63	T5	919	ARG	CB-CG-CD	7.79	129.22	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
19	BI	115	LYS	CD-CE-NZ	-7.74	87.13	111.90
53	SE	527	THR	CA-CB-OG1	-7.74	97.99	109.60
19	AI	115	LYS	CD-CE-NZ	-7.73	87.16	111.90
63	T5	919	ARG	CA-C-N	7.71	136.18	122.08
63	T5	919	ARG	C-N-CA	7.71	136.18	122.08
6	B5	3	ARG	CB-CA-C	-7.70	94.10	109.35
6	A5	3	ARG	CB-CA-C	-7.70	94.11	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
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
62	T3	836	ILE	CB-CG1-CD1	-7.67	97.69	113.80
63	t5	919	ARG	CA-C-N	7.67	136.12	122.08
63	t5	919	ARG	C-N-CA	7.67	136.12	122.08
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
63	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
62	t3	836	ILE	CB-CG1-CD1	-7.65	97.73	113.80
19	AI	60	GLN	CG-CD-OE1	7.64	136.09	120.80
62	t3	919	TYR	CZ-CE2-CD2	7.64	133.35	119.60
62	T3	919	TYR	CZ-CE2-CD2	7.64	133.35	119.60
63	t5	919	ARG	N-CA-C	7.64	120.95	109.95
10	A9	199	GLN	CG-CD-NE2	-7.63	104.95	116.40
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	BI	104	LEU	CB-CG-CD1	7.61	133.52	110.70
19	AI	104	LEU	CB-CG-CD1	7.61	133.51	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
9	sF	448	GLN	CG-CD-NE2	7.43	127.54	116.40
62	T3	838	SER	CB-CA-C	-7.42	98.37	110.77
63	T5	877	LYS	CD-CE-NZ	7.42	135.65	111.90
62	t3	838	SER	CB-CA-C	-7.42	98.38	110.77
63	t5	877	LYS	CD-CE-NZ	7.42	135.64	111.90
19	BI	86	PHE	CD1-CE1-CZ	-7.41	106.66	120.00
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
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
61	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
61	t2	34	ASN	CB-CG-ND2	7.24	127.26	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BI	68	LEU	CB-CG-CD1	7.23	132.38	110.70
4	A3	64	ARG	N-CA-CB	7.23	120.68	109.48
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
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
62	T3	836	ILE	CB-CA-C	-7.04	100.73	111.08
62	t3	836	ILE	CB-CA-C	-7.04	100.73	111.08
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
62	T3	289	LYS	N-CA-C	-7.02	102.19	111.24
28	BS	198	ARG	N-CA-CB	6.98	121.10	110.28
62	t3	289	LYS	N-CA-C	-6.98	102.23	111.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
63	t5	920	LYS	N-CA-CB	6.88	120.34	110.77
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	6.87	118.46	110.97
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
50	SA	427	VAL	CG1-CB-CG2	-6.86	95.71	110.80
63	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
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
28	AS	223	ILE	CA-CB-CG1	6.81	121.97	110.40
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
61	t2	105	TYR	CB-CG-CD2	-6.78	110.63	120.80
19	AI	94	ASP	CB-CA-C	6.77	121.98	111.02
61	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	sH	590	GLU	CG-CD-OE2	-6.73	102.93	118.40
19	BI	78	CYS	N-CA-C	6.72	120.70	112.23
19	AI	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
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
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
62	t3	837	TYR	CB-CA-C	6.53	124.82	111.11
62	T3	837	TYR	CB-CA-C	6.53	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AH	108	SER	C-N-CA	-6.52	111.14	122.36
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
64	T6	379	CYS	CA-C-N	6.51	133.97	121.54
64	T6	379	CYS	C-N-CA	6.51	133.97	121.54
64	t6	379	CYS	CA-C-N	6.50	133.96	121.54
64	t6	379	CYS	C-N-CA	6.50	133.96	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
63	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
63	t5	919	ARG	CB-CA-C	6.48	123.86	111.48
28	AS	209	LYS	CB-CG-CD	-6.48	96.40	111.30
62	t3	838	SER	N-CA-C	-6.47	98.64	108.67
62	T3	838	SER	N-CA-C	-6.46	98.66	108.67
38	me	60	GLU	CA-CB-CG	6.44	126.98	114.10
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
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
19	BI	108	HIS	CB-CG-CD2	6.42	139.54	131.20
38	Me	60	GLU	CA-CB-CG	6.42	126.93	114.10
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
28	BS	243	GLN	N-CA-C	-6.40	104.92	114.64
51	SD	607	VAL	CG1-CB-CG2	-6.40	96.73	110.80
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
19	AI	114	GLN	CG-CD-OE1	6.35	133.50	120.80
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
62	t3	840	ASP	CA-CB-CG	6.31	118.91	112.60
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
62	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
51	sD	739	VAL	CB-CA-C	6.27	120.23	112.02
9	SF	310	GLN	CA-CB-CG	6.27	126.64	114.10
58	sK	91	TYR	OH-CZ-CE2	6.27	138.70	119.90
1	A0	557	MET	CB-CG-SD	6.27	131.50	112.70
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	t5	923	LYS	CA-CB-CG	-6.17	101.77	114.10
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
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
12	AB	19	GLU	N-CA-CB	-6.15	100.75	110.22
63	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
63	t5	922	THR	CA-C-N	6.14	133.26	121.54
63	t5	922	THR	C-N-CA	6.14	133.26	121.54
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
63	T5	922	THR	CA-C-N	6.13	133.25	121.54
63	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
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
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
63	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
63	t5	877	LYS	N-CA-C	6.09	118.70	111.33
19	BI	67	THR	N-CA-CB	-6.08	101.21	110.33
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
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
3	B2	97	MET	N-CA-CB	-6.05	101.12	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
62	t3	405	GLU	CA-C-N	-6.01	112.22	120.28
62	t3	405	GLU	C-N-CA	-6.01	112.22	120.28
62	T3	405	GLU	CA-C-N	-6.01	112.22	120.28
62	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
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
64	t6	971	GLU	CG-CD-OE2	5.97	132.14	118.40
64	T6	971	GLU	CG-CD-OE2	5.97	132.12	118.40
61	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
61	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
62	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
62	t3	836	ILE	CG1-CB-CG2	5.93	128.49	110.70
29	AT	61	DA	C3'-C2'-C1'	-5.93	95.39	102.50
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
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
63	T5	927	ARG	N-CA-CB	5.91	119.77	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
63	t5	931	GLN	N-CA-CB	-5.91	101.42	110.16
24	BN	-45	DA	OP1-P-O3'	-5.90	90.29	108.00
19	AI	91	ARG	CB-CG-CD	5.90	124.87	111.30
19	BI	91	ARG	CB-CG-CD	5.89	124.86	111.30
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
63	t5	927	ARG	N-CA-CB	5.89	119.73	109.72
4	B3	64	ARG	CA-CB-CG	5.89	125.88	114.10
63	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
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
62	t3	409	LYS	CB-CA-C	-5.84	98.79	110.42
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
62	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	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
3	A2	66	VAL	N-CA-C	5.82	117.09	108.65
15	AE	116	ILE	CG1-CB-CG2	-5.82	93.25	110.70
1	B0	451	GLU	CG-CD-OE1	-5.80	105.06	118.40
1	A0	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
29	BT	59	DG	O4'-C1'-N9	5.78	112.05	108.00
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
64	t6	504	PRO	N-CA-C	5.76	117.73	110.70
19	BI	67	THR	OG1-CB-CG2	5.76	120.82	109.30
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
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
64	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	BT	44	DC	O3'-P-O5'	5.73	114.89	104.00
29	AT	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
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
62	t3	288	MET	CA-C-N	5.69	130.10	120.88
62	t3	288	MET	C-N-CA	5.69	130.10	120.88
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
62	T3	288	MET	CA-C-N	5.68	130.08	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	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
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
24	BN	-43	DA	P-O3'-C3'	-5.64	112.93	119.70
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
35	Mb	49	ARG	N-CA-C	5.64	118.15	111.33
31	BV	12	ARG	CA-C-N	5.64	132.31	121.54
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
23	BM	234	GLN	CA-CB-CG	5.63	125.36	114.10
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BR	77	LEU	CA-CB-CG	5.55	135.73	116.30
29	BT	58	DA	O4'-C1'-N9	5.55	111.89	108.00
27	AR	77	LEU	CA-CB-CG	5.55	135.73	116.30
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
19	BI	72	ASP	CB-CA-C	-5.54	100.07	109.38
56	SI	1251	LYS	CG-CD-CE	5.54	124.05	111.30
27	BR	96	ARG	CG-CD-NE	5.54	124.18	112.00
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
55	SH	590	GLU	CB-CG-CD	5.54	122.01	112.60
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
51	sB	432	VAL	CA-CB-CG2	5.53	119.80	110.40
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
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
23	BM	141	GLU	CA-CB-CG	5.52	125.14	114.10
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
61	t2	105	TYR	CB-CA-C	-5.51	101.64	110.79
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
61	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BA	1221	LYS	CA-CB-CG	5.46	125.02	114.10
63	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
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
63	t5	920	LYS	CA-C-O	-5.43	114.49	119.76
43	mj	87	LEU	CA-C-N	5.43	127.87	120.54
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
45	t4	1052	GLY	CA-C-N	5.42	131.89	121.54
45	t4	1052	GLY	C-N-CA	5.42	131.89	121.54
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
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
63	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
63	t5	927	ARG	CB-CG-CD	5.39	123.71	111.30
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
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
62	T3	412	ARG	CA-C-N	5.36	127.31	120.56
62	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
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
62	t3	412	ARG	CA-C-N	5.35	127.30	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	t3	412	ARG	C-N-CA	5.35	127.30	120.56
62	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
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
62	t3	292	ARG	CA-CB-CG	5.33	124.76	114.10
62	t3	860	VAL	N-CA-C	5.33	115.96	110.36
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
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
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
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
62	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
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
29	BT	42	DA	P-O3'-C3'	-5.30	113.34	119.70
55	SH	594	LEU	N-CA-CB	-5.30	102.31	110.20
50	SA	269	GLN	OE1-CD-NE2	-5.30	117.30	122.60
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	t4	1017	PRO	CA-C-N	-5.27	113.69	120.65
45	t4	1017	PRO	C-N-CA	-5.27	113.69	120.65
11	AA	204	THR	OG1-CB-CG2	-5.27	98.77	109.30
55	sH	595	GLU	OE1-CD-OE2	-5.26	110.27	122.90
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	110.28	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
11	BA	204	THR	OG1-CB-CG2	-5.25	98.81	109.30
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
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
62	t3	843	GLY	CA-C-N	5.24	134.58	121.80
62	t3	843	GLY	C-N-CA	5.24	134.58	121.80
62	T3	843	GLY	CA-C-N	5.24	134.58	121.80
62	T3	843	GLY	C-N-CA	5.24	134.58	121.80
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
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
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	BS	232	ASP	CB-CG-OD2	-5.21	106.42	118.40
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SF	756	ASN	C-N-CA	-5.20	115.50	122.42
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
19	AI	77	LYS	N-CA-C	-5.20	107.11	113.50
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
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
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
12	AB	21	GLU	O-C-N	-5.18	115.70	122.59
56	SI	1248	LEU	CB-CG-CD1	5.17	126.22	110.70
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
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
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
62	t3	859	ASN	CA-C-N	5.16	127.25	120.60
62	t3	859	ASN	C-N-CA	5.16	127.25	120.60
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	sB	453	LEU	CB-CG-CD1	-5.14	95.28	110.70
51	SB	453	LEU	CB-CG-CD1	-5.14	95.28	110.70
62	T3	859	ASN	CA-C-N	5.14	127.23	120.60
62	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
9	sF	315	ASP	CB-CG-OD1	5.13	130.19	118.40
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
9	SF	392	MET	CA-CB-CG	5.13	124.36	114.10
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
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
28	BS	205	ASN	O-C-N	-5.09	116.34	122.15
20	AJ	58	GLU	OE1-CD-OE2	-5.09	110.67	122.90
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
61	t2	105	TYR	CB-CG-CD1	5.08	128.42	120.80
3	A2	66	VAL	CA-CB-CG2	5.08	119.03	110.40
43	mj	88	GLU	CA-CB-CG	5.07	124.25	114.10
61	T2	105	TYR	CB-CG-CD1	5.07	128.41	120.80
9	SF	380	THR	N-CA-C	-5.07	106.93	113.01
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
11	AA	1160	SER	N-CA-C	5.07	117.82	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	SI	1194	LEU	CB-CG-CD2	-5.07	95.50	110.70
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
19	AI	86	PHE	CA-C-O	-5.07	116.03	121.45
53	sE	511	GLN	CB-CA-C	5.06	120.50	110.42
3	B2	66	VAL	CA-CB-CG2	5.06	119.00	110.40
53	SE	523	VAL	N-CA-CB	5.06	119.93	110.77
53	sE	463	PRO	CA-C-O	-5.06	111.40	120.60
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
53	sE	523	VAL	N-CA-CB	5.05	119.91	110.77
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
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
24	BN	-42	DT	C4-C5-C7	-5.04	114.83	122.40
55	SH	592	LEU	CB-CG-CD1	-5.04	95.57	110.70
64	T6	759	VAL	CA-C-N	-5.04	115.99	123.05
64	T6	759	VAL	C-N-CA	-5.04	115.99	123.05
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
28	BS	198	ARG	CB-CG-CD	-5.04	99.72	111.30
28	AS	198	ARG	CB-CG-CD	-5.04	99.71	111.30
3	B2	253	MET	CB-CG-SD	-5.04	97.59	112.70
63	t5	919	ARG	NE-CZ-NH2	-5.04	114.67	119.20
24	AN	-42	DT	C4-C5-C7	-5.03	114.85	122.40
62	T3	289	LYS	CA-C-O	5.03	126.08	120.80
62	T3	859	ASN	N-CA-C	5.03	117.50	111.71
19	AI	53	GLY	N-CA-C	5.03	125.10	113.18
63	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
62	t3	859	ASN	N-CA-C	5.03	117.49	111.71
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
64	t6	759	VAL	CA-C-N	-5.02	116.02	123.05
64	t6	759	VAL	C-N-CA	-5.02	116.02	123.05
19	BI	65	ASP	CB-CA-C	5.02	115.74	110.17
62	t3	289	LYS	CA-C-O	5.02	126.07	120.80
53	sE	123	MET	CA-CB-CG	5.02	124.14	114.10
37	Md	255	ASN	N-CA-C	5.02	119.65	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
62	t3	841	ALA	CA-C-N	5.01	131.11	121.54
62	t3	841	ALA	C-N-CA	5.01	131.11	121.54
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
64	T6	971	GLU	CG-CD-OE1	-5.00	106.90	118.40
64	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	B9	199	GLN	CA
28	BS	206	VAL	CA
50	sA	269	GLN	CA
9	sF	398	THR	CB
10	A9	199	GLN	CA
28	AS	206	VAL	CA
50	SA	269	GLN	CA
9	SF	398	THR	CB
62	T3	836	ILE	CB
63	T5	920	LYS	CA
62	t3	836	ILE	CB
63	t5	920	LYS	CA

All (192) 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

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide
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
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	Peptide,Sidechain
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

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Mol	Chain	Res	Type	Group
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
10	B9	217	GLU	Sidechain
11	BA	1277	GLU	Mainchain,Peptide
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	Peptide,Sidechain
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

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Mol	Chain	Res	Type	Group
28	BS	232	ASP	Sidechain
28	BS	236	LEU	Mainchain
31	BV	33	GLU	Peptide
32	BW	144	ARG	Sidechain
37	Md	206	ASP	Peptide
38	Me	55	ARG	Peptide,Sidechain
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
61	T2	105	TYR	Sidechain
62	T3	288	MET	Mainchain
62	T3	292	ARG	Sidechain
62	T3	406	LYS	Mainchain
62	T3	409	LYS	Mainchain
62	T3	837	TYR	Sidechain
62	T3	912	SER	Peptide

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Mol	Chain	Res	Type	Group
45	T4	1002	HIS	Sidechain
63	T5	923	LYS	Mainchain
63	T5	931	GLN	Sidechain
64	T6	760	ALA	Peptide
37	md	206	ASP	Peptide
38	me	55	ARG	Peptide,Sidechain
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
61	t2	105	TYR	Sidechain
62	t3	288	MET	Mainchain
62	t3	292	ARG	Sidechain
62	t3	406	LYS	Mainchain
62	t3	409	LYS	Mainchain
62	t3	837	TYR	Sidechain
62	t3	912	SER	Peptide

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Mol	Chain	Res	Type	Group
45	t4	1002	HIS	Sidechain
63	t5	923	LYS	Mainchain
63	t5	931	GLN	Sidechain
64	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	143	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	108	0
13	AC	2061	0	2029	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	69	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	55	0
45	T4	1780	0	1765	31	0
45	ml	5367	0	5607	47	0
45	t4	1780	0	1765	37	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	3243	27	0
49	mp	3330	0	3243	46	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	T1	516	0	527	9	0
60	t1	516	0	527	10	0
61	T2	891	0	907	14	0
61	t2	891	0	907	15	0
62	T3	6173	0	6169	73	0
62	t3	6173	0	6169	90	0
63	T5	894	0	930	23	0
63	t5	894	0	928	36	0
64	T6	7551	0	7605	86	0
64	t6	7551	0	7605	101	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
66	BW	1	0	0	0	0
67	AA	1	0	0	0	0
67	BA	1	0	0	0	0
All	All	305572	0	305164	3655	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 (3655) 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)
62:T3:837:TYR:CD2	62:T3:837:TYR:CG	1.80	1.68
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
62:t3:837:TYR:CD2	62:t3:837:TYR:CG	1.80	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
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
3:A2:506:LYS:NZ	3:A2:506:LYS:CE	1.68	1.55
19:BI:117:LYS:CD	64:t6:801:LYS:HZ3	0.94	1.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:t3:289:LYS:CB	62:t3:289:LYS:CG	1.88	1.50
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:AM:302:LEU:C	27:AR:270:MET:CE	1.86	1.49
23:BM:16:PRO:HG3	32:BW:151:LEU:CD2	1.43	1.48
49:mp:153:ASN:HB3	62:t3:739:THR:CG2	1.37	1.48
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
62:T3:289:LYS:CG	62: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:BI:75:CYS:CB	19:BI:75:CYS:SG	2.07	1.43
19:AI:75:CYS:SG	19:AI:75:CYS:CB	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
19:BI:117:LYS:CD	64:t6:801:LYS:NZ	1.82	1.39
4:A3:100:ASN:ND2	34:Ma:140:GLY:HA3	1.40	1.35
49:mp:153:ASN:CB	62:t3:739:THR:CG2	2.03	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
4:B3:100:ASN:ND2	34:ma:140:GLY:HA3	1.40	1.34
55:SH:594:LEU:CD2	55:SH:594:LEU:CB	2.04	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
19:BI:117:LYS:HD2	64:t6:801:LYS:NZ	1.40	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:BM:303:GLN:HG3	27:BR:270:MET:SD	1.70	1.29
23:AM:301:THR:HG23	27:AR:271:ARG:NH2	1.42	1.29
49:mp:153:ASN:CA	62:t3:739:THR:HG21	1.38	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:BA:420:ARG:CD	38:me:60:GLU:OE1	1.81	1.27
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
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
23:BM:303:GLN:CG	27:BR:270:MET:SD	2.24	1.25
19:AI:86:PHE:CD2	19:AI:86:PHE:CD1	1.98	1.25
62:t3:837:TYR:CD2	62:t3:837:TYR:CB	2.20	1.25
62:T3:837:TYR:CD2	62: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:B3:100:ASN:CB	34:ma:140:GLY:HA2	1.54	1.22
4:A3:100: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
4:A3:49:LEU:HD23	17:AG:164:LYS:CE	1.70	1.20
62:t3:837:TYR:CD2	62:t3:837:TYR:HB3	1.73	1.20
18:AH:128:ASN:HD21	43:Mj:81:ASN:ND2	1.41	1.19
62:T3:837:TYR:CD2	62: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:B3:100:ASN:CA	34:ma:140:GLY:HA2	1.72	1.18
4:A3:100:ASN:CA	34:Ma:140:GLY:HA2	1.72	1.18
55:SH:585:LEU:O	55:SH:589:HIS:N	1.76	1.17
49:mp:153:ASN:HB3	62:t3:739:THR:HG22	1.26	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
23:BM:16:PRO:CG	32:BW:151:LEU:CD2	2.07	1.15
11:AA:678:GLU:OE2	64:T6:761:LYS:NZ	1.76	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:BM:302:LEU:HA	27:BR:270:MET:HE3	1.22	1.13
23:AM:302:LEU:C	27:AR:270:MET:HE2	1.71	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B8:790:LYS:HB3	9:sF:763:ARG:HH21	1.09	1.13
9:A8:790:LYS:HB3	9:SF:763:ARG:HH21	1.09	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
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
45:MI:797:LYS:HB3	45:t4:836:LEU:CD2	1.80	1.10
19:BI:81:ARG:HH22	64:t6:790:LYS:HE3	1.16	1.10
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
11:AA:68:GLN:CG	32:AW:151:LEU:CD1	2.30	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
49:mp:153:ASN:CB	62:t3:739:THR:HG21	1.69	1.08
23:AM:302:LEU:HA	27:AR:270:MET:HE3	1.22	1.08
62:t3:837:TYR:CD2	62:t3:837:TYR:CD1	2.33	1.08
23:BM:245:HIS:HD2	27:BR:264:SER:HB2	1.13	1.07
11:AA:68:GLN:HG3	32:AW:151:LEU:HD11	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
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
19:BI:117:LYS:CG	64:t6:801:LYS:NZ	2.20	1.04
4:A3:64:ARG:NH2	17:AG:165:GLU:OE1	1.89	1.04
4:B3:100:ASN:HB3	34:ma:140:GLY:HA2	1.09	1.04
19:BI:117:LYS:CE	64:t6:801:LYS:HZ3	1.71	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:HB3	34:Ma:140:GLY:N	1.71	1.04
12:AB:868:MET:HE1	23:AM:182:ARG:O	1.57	1.04
19:BI:74:GLU:HG3	64:t6:846:HIS:NE2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:mp:156:PHE:HD2	62:t3:740:ASP:HB2	1.14	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
19:BI:74:GLU:HG3	64:t6:846:HIS:CD2	1.93	1.03
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
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
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
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
19:BI:104:LEU:CD2	19:BI:104:LEU:HD13	1.88	1.03
23:AM:16:PRO:HG2	32:AW:151:LEU:HD21	1.36	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
19:BI:117:LYS:CE	64:t6:801:LYS:NZ	2.20	1.02
23:BM:303:GLN:CD	27:BR:270:MET:SD	2.42	1.02
55:sH:592:LEU:CD1	55:sH:592:LEU:CB	2.36	1.02
6:A5:7:GLY:HA3	6:A5:41:LEU:HD11	1.42	1.02
19:BI:104:LEU:CD2	19:BI:104:LEU:CB	2.37	1.02
4:A3:100:ASN:ND2	34:Ma:140:GLY:CA	2.23	1.02
23:BM:301:THR:HG23	27:BR:271:ARG:HH22	0.91	1.01
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
4:B3:100:ASN:ND2	34:ma:140:GLY:CA	2.23	1.01
4:B3:49:LEU:HG	17:BG:164:LYS:CB	1.90	1.01
49:mp:153:ASN:CA	62:t3:739:THR:CG2	2.28	1.01
62:T3:837:TYR:CD2	62: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
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
49:mp:157:ASN:OD1	62:t3:740:ASP:OD1	1.79	1.00
55:SH:594:LEU:CD2	55:SH:594:LEU:CD1	2.38	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: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
11:AA:420:ARG:CG	38:Me:60:GLU:OE1	2.09	1.00
17:AG:100:GLU:HG3	32:AW:144:ARG:NH2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:BI:117:LYS:CG	64:t6:801:LYS:HZ3	1.75	0.99
28:BS:274:CYS:HB3	28:BS:302:CYS:SG	2.02	0.99
28:AS:274:CYS:HB3	28:AS:302:CYS:SG	2.03	0.98
19:BI:117:LYS:HG2	64:t6:801:LYS:HZ1	1.29	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
59:SL:430:LEU:HA	59:SL:433:GLN:HE21	1.25	0.98
23:BM:245:HIS:CD2	27:BR:264:SER:HB2	1.97	0.98
49:mp:156:PHE:CD2	62:t3:740:ASP:HB2	1.98	0.97
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
49:mp:153:ASN:HB3	62:t3:739:THR:HG23	1.44	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
9:sF:400:GLN:O	9:sF:402:ILE:HG13	1.66	0.96
4:B3:100:ASN:HD22	34:ma:140:GLY:HA3	1.19	0.96
4:A3:100:ASN:HA	34:Ma:140:GLY:HA2	1.46	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
55:sH:586:TYR:O	55:sH:590:GLU:CA	2.15	0.94
9:B8:790:LYS:HB3	9:sF:763:ARG:NH2	1.82	0.94
12:BB:16:TYR:O	63:t5:927:ARG:CZ	2.14	0.94
4:A3:49:LEU:HD23	17:AG:164:LYS:HD2	1.01	0.94
11:BA:420:ARG:HG3	38:me:60:GLU:OE1	1.68	0.94
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
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
11:BA:420:ARG:HD3	38:me:60:GLU:OE2	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:463:GLU:O	9:SF:402:ILE:CG1	2.16	0.93
49:mp:153:ASN:CB	62:t3:739:THR:HG22	1.81	0.93
53:sE:523:VAL:CA	53:sE:547:ARG:NH1	2.31	0.93
19:BI:74:GLU:CG	64:t6:846:HIS:NE2	2.32	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:B3:49:LEU:CD2	17:BG:164:LYS:CD	2.20	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
11:BA:420:ARG:CD	38:me:60:GLU:CD	2.38	0.93
12:BB:15:PRO:C	63:t5:931:GLN:HG2	1.94	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:B3:49:LEU:CG	17:BG:164:LYS:HD2	2.00	0.92
4:A3:49:LEU:HD23	17:AG:164:LYS:HE2	1.50	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
18:AH:128:ASN:HD21	43:Mj:81:ASN:HD21	0.97	0.92
55:sH:584:GLN:O	55:sH:588:ASN:HB3	1.70	0.92
23:AM:301:THR:CG2	27:AR:271:ARG:HH22	1.80	0.92
4:A3:100:ASN:HB3	34:Ma:140:GLY:HA2	1.10	0.92
19:BI:117:LYS:HE3	64:t6:801:LYS:NZ	1.85	0.92
45:MI:797:LYS:CB	45:t4:836:LEU:HD21	1.99	0.92
4:B3:100:ASN:HD22	34:ma:140:GLY:C	1.76	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
1:B0:544:TYR:H	2:B1:358:MET:HE1	1.32	0.91
19:BI:117:LYS:HD2	64:t6:801:LYS:CE	1.99	0.90
19:BI:74:GLU:CD	64:t6:846:HIS:NE2	2.29	0.90
11:BA:110:CYS:HB3	11:BA:167:CYS:SG	2.11	0.90
4:A3:49:LEU:CG	17:AG:164:LYS:HD2	1.99	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
53:sE:523:VAL:HA	53:sE:547:ARG:HH11	1.36	0.89
11:AA:110:CYS:HB3	11:AA:167:CYS:SG	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AM:14:ARG:HH22	32:AW:126:ILE:HD13	1.14	0.89
12:BB:15:PRO:O	63:t5:927:ARG:HG3	1.71	0.89
49:mp:156:PHE:HD2	62:t3:740:ASP:CB	1.85	0.89
24:AN:-62:DG:N2	29:AT:62:DC:O2	2.06	0.89
45:MI:797:LYS:CB	45:t4:836:LEU:CD2	2.50	0.88
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
11:BA:420:ARG:HH21	38:me:58:LEU:HD23	1.38	0.88
4:A3:100:ASN:HD22	34:Ma:140:GLY:HA3	1.19	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:16:TYR:O	63:t5:927:ARG:NE	2.06	0.87
19:BI:117:LYS:HD2	64:t6:801:LYS:HZ3	0.70	0.87
23:BM:302:LEU:N	27:BR:270:MET:HE1	1.90	0.87
11:AA:420:ARG:HH21	38:Me:58:LEU:HD23	1.38	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
19:BI:117:LYS:HG2	64:t6:801:LYS:NZ	1.84	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
23:BM:16:PRO:HG3	32:BW:151:LEU:HD21	0.93	0.86
19:AI:78:CYS:SG	19:AI:106:CYS:HB3	2.16	0.86
28:AS:187:ASN:HB2	28:AS:228:LEU:HD21	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
3:B2:261:GLN:HG2	3:B2:263:HIS:H	1.41	0.85
3:A2:253:MET:HE2	3:A2:258:LEU:HD23	1.58	0.85
9:SF:321:LEU:HD23	55:SH:449:MET:SD	2.16	0.85
3:B2:253:MET:HE2	3:B2:258:LEU:HD23	1.58	0.85
12:BB:14:ASP:HB3	63:t5:927:ARG:HH22	1.42	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
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
28:AS:271:CYS:HB3	28:AS:274:CYS:SG	2.17	0.85
12:BB:14:ASP:HB3	63:t5:927:ARG:NH2	1.91	0.84
12:BB:15:PRO:O	63:t5:931:GLN:HG2	1.77	0.84
53:sE:533:PHE:HA	53:sE:540:ASP:HA	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BI:78:CYS:SG	19:BI:106:CYS:HB3	2.16	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
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
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
18:BH:128:ASN:ND2	43:mj:81:ASN:ND2	2.26	0.82
3:A2:463:GLU:O	9:sF:402:ILE:HG13	1.78	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
64:t6:503:LEU:HG	64:t6:505:PRO:HD2	1.63	0.81
3:B2:463:GLU:O	9:sF:402:ILE:HG13	1.78	0.81
64:T6:503:LEU:HG	64: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
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
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
1:B0:104:ARG:NH2	1:B0:202:LEU:O	2.14	0.80
58:SK:237:GLN:HG2	58:SK:307:TYR:HE1	1.45	0.80
53:SE:468:GLU:HA	53:SE:471:HIS:HD2	1.45	0.80
11:BA:68:GLN:CG	32:BW:151:LEU:HD13	2.07	0.79
17:AG:100:GLU:HG3	32:AW:144:ARG:HH21	1.42	0.79
12:BB:16:TYR:O	63:t5:927:ARG:CD	2.31	0.79
12:AB:13:GLU:HB2	63:T5:919:ARG:NH2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:BH:109:LYS:O	43:mj:83:LEU:CB	2.30	0.78
24:AN:-75:DT:H3	29:AT:75:DA:H61	1.28	0.78
24:BN:-75:DT:H3	29:BT:75:DA:H61	1.28	0.78
3:A2:454:TYR:HB2	6:A5:9:LEU:HB3	1.64	0.78
12:AB:13:GLU:HB2	63: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
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
14:BD:151:PHE:O	14:BD:153:ARG:NH1	2.17	0.77
28:BS:184:LYS:HD2	28:BS:228:LEU:HD13	1.64	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
53:sE:523:VAL:CA	53:sE:547:ARG:HH12	1.94	0.77
14:AD:151:PHE:O	14:AD:153:ARG:NH1	2.17	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
4:B3:49:LEU:HB3	17:BG:164:LYS:CD	2.15	0.77
18:AH:128:ASN:ND2	43:Mj:81:ASN:ND2	2.26	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
49:mp:153:ASN:HA	62:t3:739:THR:HG21	1.59	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
45:MI:797:LYS:HB3	45:t4:836:LEU:HD22	1.64	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
63:T5:855:LEU:HD22	64:T6:769:ILE:HD11	1.68	0.76
1:B0:536:GLY:O	1:B0:537:MET:HE2	1.86	0.75
63:t5:855:LEU:HD22	64:t6:769:ILE:HD11	1.68	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
12:BB:16:TYR:O	63:t5:927:ARG:HD3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
55:sH:585:LEU:CD2	55:sH:589:HIS:CD2	2.70	0.73
19:AI:5:ARG:NH2	19:AI:36:GLU:OE1	2.21	0.73
11:AA:73:GLY:HA3	11:AA:76:GLU:HG2	1.71	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
19:BI:74:GLU:CG	64:t6:846:HIS:CD2	2.71	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
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
4:B3:49:LEU:HB3	17:BG:164:LYS:HD2	1.71	0.72
14:AD:209:ARG:NH2	35:Mb:34:ASP:OD2	2.22	0.72
8:B7:224:LYS:HD3	8:B7:338:LEU:O	1.90	0.72
23:AM:14:ARG:NH2	32:AW:126:ILE:HA	2.03	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
63:T5:868:ARG:HG2	63:T5:872:ARG:HD2	1.72	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
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
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
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
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
63:t5:868:ARG:HG2	63:t5:872:ARG:HD2	1.72	0.71
4:B3:49:LEU:CD2	17:BG:164:LYS:CB	2.68	0.71
14:AD:158:GLU:OE1	35:Mb:45:HIS:CE1	2.43	0.71
4:B3:49:LEU:HD23	17:BG:164:LYS:CG	2.19	0.71
12:BB:15:PRO:O	63:t5:927:ARG:CG	2.39	0.71
23:BM:157:CYS:SG	23:BM:214:LEU:HD21	2.30	0.71
4:A3:100:ASN:HB3	34:Ma:140:GLY:HA3	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:BA:465:TYR:HE1	21:BK:3:ALA:HA	1.55	0.70
23:AM:303:GLN:CB	27:AR:270:MET:SD	2.79	0.70
17:BG:100:GLU:CD	32:BW:144:ARG:NE	2.49	0.70
19:AI:59:VAL:HG13	19:AI:61:ASP:H	1.55	0.70
18:BH:106:GLU:OE2	43:mj:83:LEU:HD13	1.91	0.70
27:AR:73:LEU:HD12	27:AR:74:PRO:HD2	1.72	0.70
45:ml:89:GLN:HE21	45:ml:159:PHE:H	1.39	0.70
23:AM:245:HIS:CD2	27:AR:264:SER:CB	2.72	0.70
1:A0:125:LYS:NZ	1:A0:127:THR:OG1	2.21	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
63:T5:936:ILE:HG23	63:T5:943:LEU:HD11	1.74	0.70
62:t3:360:HIS:CD2	62:t3:919:TYR:HE2	2.10	0.70
19:BI:74:GLU:OE2	64:t6:846:HIS:CD2	2.44	0.70
18:AH:106:GLU:OE2	43:Mj:83:LEU:HD13	1.91	0.69
64:t6:218:ARG:HH22	64:t6:220:ARG:HB2	1.57	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
49:mp:154:ALA:HA	62:t3:739:THR:HB	1.75	0.69
50:sA:335:TYR:HD1	51:sB:727:LEU:HD11	1.58	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
45:t4:981:THR:HG1	45:t4:1004:ALA:N	1.90	0.69
62:T3:360:HIS:CD2	62:T3:919:TYR:HE2	2.10	0.69
4:B3:49:LEU:CD2	17:BG:164:LYS:HE2	2.21	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
62:T3:360:HIS:HD2	62:T3:919:TYR:HE2	1.41	0.69
64:T6:218:ARG:HH22	64:T6:220:ARG:HB2	1.57	0.69
19:BI:117:LYS:HE3	64:t6:801:LYS:HZ2	1.55	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
45:T4:981:THR:HG1	45:T4:1004:ALA:N	1.90	0.69
62:t3:360:HIS:HD2	62:t3:919:TYR:HE2	1.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:sE:530:THR:HG22	53:sE:532:ASN:HD21	1.59	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
14:AD:213:GLU:CG	35:Mb:38:MET:HE1	2.23	0.68
1:B0:125:LYS:NZ	1:B0:127:THR:OG1	2.21	0.68
1:A0:554:TRP:HA	1:A0:557:MET:SD	2.34	0.68
63:t5:936:ILE:HG23	63:t5:943:LEU:HD11	1.74	0.68
63:t5:913:ILE:HD11	63:t5:943:LEU:HD13	1.74	0.68
23:BM:16:PRO:HB3	32:BW:151:LEU:CD2	2.23	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
6:B5:5:ARG:NH2	6:B5:33:GLU:OE2	2.26	0.68
53:SE:530:THR:HG22	53:SE:532:ASN:HD21	1.59	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:AA:107:CYS:HB3	11:AA:110:CYS:SG	2.34	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	64:T6:757:GLN:NE2	2.27	0.67
23:AM:16:PRO:HB3	32:AW:151:LEU:CD2	2.23	0.67
60:t1:46:MET:HE1	60:t1:66:SER:H	1.60	0.67
62:t3:837:TYR:HB3	62:t3:837:TYR:HD2	1.50	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
60:T1:46:MET:HE1	60:T1:66:SER:H	1.59	0.67
61:T2:65:ALA:HA	61:T2:68:MET:HE2	1.76	0.67
63:T5:913:ILE:HD11	63:T5:943:LEU:HD13	1.74	0.67
1:B0:554:TRP:HA	1:B0:557:MET:SD	2.34	0.67
62:T3:837:TYR:HB3	62:T3:837:TYR:HD2	1.50	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:810:GLU:OE1	26:AQ:24:ARG:NH1	2.27	0.67
7:B6:399:ARG:NH2	7:B6:434:GLN:HA	2.10	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
8:B7:711:LYS:HA	8:B7:716:MET:HE3	1.76	0.67
4:A3:31:ASN:HD22	4:A3:63:LEU:HD12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A7:711:LYS:HA	8:A7:716:MET:HE3	1.76	0.67
3:B2:155:LEU:HD12	3:B2:157:LYS:H	1.60	0.67
51:SD:675:GLU:O	51:SD:679:MET:HE3	1.95	0.67
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
1:A0:537:MET:HE1	1:A0:619:THR:N	2.10	0.66
61:t2:65:ALA:HA	61:t2:68:MET:HE2	1.76	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
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
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
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
1:B0:533:THR:HG21	1:B0:537:MET:HE3	1.76	0.66
20:AJ:7:CYS:HA	20:AJ:49:MET:HE2	1.76	0.66
63:T5:874:GLU:OE1	63:T5:874:GLU:N	2.28	0.66
4:B3:54:CYS:HB3	4:B3:59:CYS:SG	2.34	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
3:B2:480:VAL:HG11	3:B2:497:GLY:HA3	1.78	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
1:A0:418:LEU:HD13	1:A0:435:MET:HE1	1.78	0.66
19:BI:104:LEU:CD2	19:BI:104:LEU:HB2	2.25	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
9:sF:391:ARG:NH2	56:sI:701:GLU:OE1	2.29	0.66
1:B0:537:MET:HE1	1:B0:619:THR:N	2.11	0.65
11:BA:150:THR:HA	11:BA:166:GLY:HA2	1.78	0.65
53:sE:450:GLU:HB2	53:sE:454:LEU:HD23	1.78	0.65
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
4:B3:49:LEU:HD22	17:BG:164:LYS:HD2	1.70	0.65
8:B7:719:SER:O	8:B7:722:ARG:N	2.29	0.65
51:SB:688:ARG:HA	51:SB:691:MET:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
31:BV:35:SER:HB2	31:BV:39:ARG:HH21	1.62	0.65
18:AH:114:VAL:HG13	18:AH:132:LEU:HD12	1.79	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
64:T6:643:GLU:OE1	64:T6:864:ASN:ND2	2.30	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
45:Ml:797:LYS:HB2	45:t4:836:LEU:HD21	1.77	0.65
3:A2:463:GLU:HB2	9:SF:401:LYS:C	2.23	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
1:A0:494:PRO:O	1:A0:495:MET:HE2	1.97	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
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
8:B7:181:TYR:CZ	8:B7:336:PRO:HB2	2.33	0.64
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
14:AD:158:GLU:OE1	35:Mb:45:HIS:HE1	1.80	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
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
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
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
64:T6:651:TYR:HH	64:T6:910:CYS:HG	1.46	0.64
23:BM:301:THR:HG23	27:BR:271:ARG:CZ	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:t6:643:GLU:OE1	64:t6:864:ASN:ND2	2.30	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
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
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
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
11:AA:150:THR:HA	11:AA:166:GLY:HA2	1.78	0.63
19:AI:17:ARG:HH21	19:AI:19:ASP:HB2	1.62	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
58:sK:262:GLU:O	58:sK:266:GLN:NE2	2.30	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
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
55:sH:592:LEU:HA	55:sH:595:GLU:HG3	1.80	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
3:B2:463:GLU:HB2	9:sF:401:LYS:C	2.23	0.63
12:BB:14:ASP:CB	63:t5:927:ARG:NH2	2.62	0.63
53:sE:531:THR:HA	53:sE:542:THR:HA	1.80	0.63
6:B5:36:ASP:HB2	6:B5:39:HIS:HB2	1.81	0.63
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
60:t1:85:ASP:OD1	61:t2:44:ARG:NH2	2.32	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
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
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
31:BV:36:LEU:HA	31:BV:39:ARG:HG2	1.81	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
63:t5:874:GLU:OE1	63:t5:874:GLU:N	2.28	0.62
12:BB:1106:ARG:NH2	12:BB:1110:PRO:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
26:AQ:352:MET:HB3	26:AQ:361:TRP:HB2	1.80	0.62
64:T6:963:CYS:SG	64:T6:964:ILE:N	2.72	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
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
64:t6:963:CYS:SG	64:t6:964:ILE:N	2.72	0.62
23:BM:14:ARG:O	32:BW:126:ILE:HG23	2.00	0.62
3:A2:66:VAL:HG12	5:A4:262:ILE:HA	1.81	0.62
9:SF:389:ASN:O	9:SF:392:MET:N	2.33	0.62
60:T1:85:ASP:OD1	61:T2:44:ARG:NH2	2.32	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
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
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
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
12:BB:15:PRO:O	63:t5:931:GLN:CG	2.48	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
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
5:B4:255:ASP:HB3	5:B4:258:LEU:HB2	1.82	0.61
58:SK:36:ILE:HG23	58:SK:54:MET:HE3	1.82	0.61
26:BQ:144:THR:HA	26:BQ:147:LEU:HD21	1.81	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
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
1:A0:539:VAL:HG12	1:A0:621:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A7:242:LEU:HB2	8:A7:313:VAL:HB	1.82	0.61
56:sI:1251:LYS:HD2	56:sI:1255:PHE:CZ	2.35	0.61
12:AB:13:GLU:CB	63:T5:919:ARG:NH2	2.62	0.61
51:SB:436:ASP:C	51:SB:437:MET:HE2	2.24	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
3:A2:443:LEU:O	3:A2:447:GLU:HG2	2.00	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
5:A4:271:ASP:OD1	5:A4:272:PHE:N	2.34	0.61
11:BA:91:PHE:CE1	11:BA:204:THR:HG22	2.35	0.61
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
49:mp:156:PHE:CD2	62:t3:740:ASP:CB	2.73	0.60
55:sH:585:LEU:CD2	55:sH:589:HIS:HD2	2.10	0.60
14:AD:206:GLU:HA	14:AD:209:ARG:HG2	1.82	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
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
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
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
4:B3:100:ASN:HA	34:ma:140:GLY:CA	2.25	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
45:Ml:797:LYS:CD	45:t4:836:LEU:HD21	2.32	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
11:BA:465:TYR:CE1	21:BK:4:PRO:HD2	2.37	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
11:AA:465:TYR:CE1	21:AK:4:PRO:HD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
64:T6:145:TYR:HB2	64:T6:968:MET:HE3	1.83	0.60
63:t5:909:VAL:HA	63:t5:912:HIS:HB2	1.84	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
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
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
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
63:t5:923:LYS:O	63:t5:926:GLN:N	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
63:T5:909:VAL:HA	63:T5:912:HIS:HB2	1.84	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
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
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
64:t6:503:LEU:HD12	64:t6:504:PRO:HD2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
64:T6:127:LEU:HD21	64:T6:182:THR:HG21	1.85	0.59
64:t6:145:TYR:HB2	64:t6:968:MET:HE3	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
43:mj:145:ARG:O	43:mj:149:ARG:NH1	2.36	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:B0:464: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
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
11:BA:1278:ASN:N	11:BA:1279:ILE:HD12	2.15	0.59
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
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
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
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
45:ml:184:LYS:O	45:ml:188:ASN:ND2	2.36	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
64:T6:503:LEU:HD12	64:T6:504:PRO:HD2	1.84	0.58
13:BC:148:ARG:HD3	20:BJ:65:PRO:HG3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
63:T5:923:LYS:O	63:T5:926:GLN:N	2.34	0.58
11:BA:68:GLN:CG	32:BW:151:LEU:HD11	2.09	0.58
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
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
64:t6:127:LEU:HD21	64:t6:182:THR:HG21	1.85	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:678:GLU:CD	64:T6:761:LYS:NZ	2.58	0.58
18:AH:106:GLU:OE2	43:Mj:83:LEU:HD11	2.03	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
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
62:t3:406:LYS:O	62:t3:409:LYS:N	2.29	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
60:T1:67:GLN:HA	60:T1:70:GLN:OE1	2.04	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
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:B0:541: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
9:SF:551:VAL:HG22	9:SF:556:GLN:HG3	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
11:AA:1158:PRO:HB3	11:AA:1188:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:337:ALA:HB1	53:SE:462:THR:HB	1.86	0.57
18:BH:109:LYS:O	43:mj:83:LEU:HD12	2.05	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
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
12:BB:15:PRO:O	63:t5:931:GLN:CD	2.41	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
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
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
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
9:sF:551:VAL:HG22	9:sF:556:GLN:HG3	1.85	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
53:sE:503:ILE:HD12	53:sE:503:ILE:H	1.70	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
62:T3:406:LYS:O	62:T3:409:LYS:N	2.29	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
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
63:t5:934:ILE:HG23	63:t5:945:MET:HE1	1.86	0.57
1:B0:252:LEU:HB2	1:B0:435:MET:HB3	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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	63: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
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
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
61:t2:36:ALA:O	61:t2:40:ILE:HG12	2.05	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
19:BI:74:GLU:CD	64:t6:846:HIS:CD2	2.83	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
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
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
58:sK:202:LYS:HB3	58:sK:207:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:t1:67:GLN:HA	60:t1:70:GLN:OE1	2.04	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
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
45:T4:903:PRO:HG3	45:T4:936:LYS:HB2	1.87	0.56
63:T5:934:ILE:HG23	63:T5:945:MET:HE1	1.86	0.56
9:sF:662:ARG:HA	9:sF:665:LYS:HE2	1.88	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:Ml:490:GLN:HG2	45:Ml:502:GLN:HE21	1.70	0.56
51:SB:329:GLU:HB3	9:SF:537:LEU:HD23	1.88	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
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
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
11:AA:465:TYR:CE1	21:AK:3:ALA:HA	2.38	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
44:Mk:12:GLN:OE1	45:Ml:152:ARG:NH2	2.39	0.56
62:t3:289:LYS:CB	62:t3:289:LYS:CD	2.67	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
28:BS:227:PHE:HA	28:BS:230:THR:HG23	1.88	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
53:SE:468:GLU:HA	53:SE:471:HIS:CD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
62:T3:301:ASN:ND2	62: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
61:t2:71:TYR:HA	61:t2:74:ILE:HG12	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
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
62:T3:289:LYS:CB	62:T3:289:LYS:CD	2.67	0.55
62:t3:541:VAL:HG11	62:t3:581:PHE:HB2	1.87	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
12:BB:16:TYR:C	63:t5:927:ARG:HD3	2.31	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
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
61:T2:36:ALA:O	61:T2:40:ILE:HG12	2.05	0.55
62:T3:769:GLN:NE2	64:T6:338:SER:O	2.39	0.55
45:t4:903:PRO:HG3	45:t4:936:LYS:HB2	1.87	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:237:GLN:CD	58:SK:303:LEU:HD11	2.31	0.55
61:T2:71:TYR:HA	61:T2:74:ILE:HG12	1.88	0.55
62:t3:888:LEU:HD21	64:t6:274:ARG:HD3	1.88	0.55
12:BB:496:ARG:NH2	12:BB:540:SER:O	2.39	0.55
49:mp:153:ASN:HB2	62:t3:739:THR:HG22	1.80	0.55
51:sB:705:GLU:HA	51:sB:708:MET:HG2	1.89	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
62:T3:541:VAL:HG11	62:T3:581:PHE:HB2	1.87	0.55
62:T3:888:LEU:HD21	64:T6:274:ARG:HD3	1.88	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
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
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
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
62:t3:416:THR:O	62:t3:420:ASP:HB2	2.06	0.55
64:t6:651:TYR:OH	64:t6:910:CYS:SG	2.61	0.55
5:B4:221:SER:OG	5:B4:224:LEU:HD23	2.07	0.55
19:BI:81:ARG:NH2	64:t6:790:LYS:HE3	2.02	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
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
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
45:T4:835:GLN:HG2	45:T4:886:THR:HG21	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
64:T6:618:ILE:O	64:T6:653:LYS:NZ	2.39	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
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
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
62:t3:301:ASN:ND2	62:t3:974:LEU:O	2.38	0.55
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
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
62:T3:416:THR:O	62:T3:420:ASP:HB2	2.06	0.54
64:T6:429:ARG:NH1	64:T6:430:HIS:O	2.40	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
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
45:t4:971:TYR:HB2	45:t4:980:ILE:HB	1.89	0.54
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
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
64:t6:381:THR:HG22	64:t6:383:LYS:H	1.72	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
28:AS:248:ILE:HG13	28:AS:252:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:t4:835:GLN:HG2	45:t4:886:THR:HG21	1.89	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:A2:372: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
63:t5:922:THR:OG1	63:t5:923:LYS:N	2.41	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
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
62:T3:1126:MET:HA	62:T3:1129:THR:HG22	1.90	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:523:VAL:CG1	53:SE:523:VAL:HG21	2.35	0.54
62:t3:769:GLN:NE2	64:t6:338:SER:O	2.39	0.54
45:t4:1000:HIS:O	45:t4:1002:HIS:HD2	1.90	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
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
64:t6:429:ARG:NH1	64:t6:430:HIS:O	2.40	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
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
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
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
64:T6:381:THR:HG22	64:T6:383:LYS:H	1.72	0.53
62:t3:360:HIS:CD2	62:t3:919:TYR:CE2	2.95	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
12:AB:248:SER:H	12:AB:418:LYS:HE3	1.73	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:sH:443:ILE:HD11	56:sI:662:ARG:HD2	1.91	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:Ml:438:LEU:HG	45:Ml:460:ILE:HG13	1.91	0.53
45:Ml:461:VAL:HG13	45:Ml:463:ASN:H	1.73	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
11:AA:68:GLN:HE21	32:AW:151:LEU:HD13	1.74	0.53
19:AI:117:LYS:HG2	64: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
62:t3:1126:MET:HA	62:t3:1129:THR:HG22	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
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
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:B0:577:GLN:NE2	2:B1:330:LEU:HD11	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
19:AI:117:LYS:HG2	64: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
64:T6:679:GLN:O	64:T6:682:ASN:ND2	2.42	0.53
14:BD:63:LEU:HB3	14:BD:130:LEU:HD22	1.91	0.53
9:sF:544:ILE:HG22	9:sF:629:MET:HE1	1.91	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
64:T6:23:SER:O	64:T6:179:ARG:NH2	2.41	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
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
64:T6:361:LYS:HB3	64:T6:370:PRO:HA	1.91	0.53
64:t6:23:SER:O	64:t6:179:ARG:NH2	2.41	0.53
3:B2:22:GLN:HG3	3:B2:26:TYR:CZ	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
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
64:t6:679:GLN:O	64:t6:682:ASN:ND2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:sL:98:ASN:HB3	59:sL:101:ALA:HB2	1.90	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
63:T5:922:THR:OG1	63:T5:923:LYS:N	2.41	0.52
45:t4:881:THR:HB	45:t4:897:GLN:HB2	1.92	0.52
64:t6:618:ILE:O	64:t6:653:LYS:NZ	2.39	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
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
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
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
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
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
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
45:t4:879:ASP:O	45:t4:902:ASN:ND2	2.39	0.52
64:t6:683:PRO:O	64:t6:687:GLN:NE2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
64:T6:445:GLU:OE1	64:T6:448:ASP:HB2	2.10	0.52
45:t4:896:VAL:O	45:t4:908:GLN:NE2	2.38	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
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
62:T3:360:HIS:CD2	62:T3:919:TYR:CE2	2.95	0.52
64:T6:696:ILE:HG13	64:T6:773:SER:HB3	1.92	0.52
64:t6:445:GLU:OE1	64:t6:448:ASP:HB2	2.10	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
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
45:T4:1021:GLN:OE1	45:T4:1025:GLN:NE2	2.43	0.52
62:t3:981:GLU:OE1	62:t3:985:GLN:NE2	2.43	0.52
64:t6:361:LYS:HB3	64:t6:370:PRO:HA	1.90	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
45:T4:881:THR:HB	45:T4:897:GLN:HB2	1.92	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
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
64:T6:220:ARG:NH1	64:T6:221:ALA:O	2.43	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
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
64:T6:557:VAL:HG22	64:T6:603:PHE:CE1	2.46	0.51
45:t4:1021:GLN:OE1	45:t4:1025:GLN:NE2	2.43	0.51
64:t6:369:SER:O	64:t6:390:ARG:NH1	2.43	0.51
1:B0:210:TYR:OH	1:B0:235:ASP:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:BI:74:GLU:OE2	64:t6:846:HIS:NE2	2.41	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
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
51:SB:770:PHE:CZ	51:SD:743:CYS:HB2	2.45	0.51
64:T6:369:SER:O	64:T6:390:ARG:NH1	2.44	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
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
50:SA:384:GLN:HE22	51:SB:731:GLN:HA	1.75	0.51
64:T6:683:PRO:O	64:T6:687:GLN:NE2	2.43	0.51
64:t6:218:ARG:HH12	64:t6:220:ARG:HB2	1.76	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
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
63:t5:871:HIS:HA	63:t5:874:GLU:OE2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:sL:189:MET:HE3	59:sL:305:LEU:HD12	1.93	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:MI:505:THR:HA	45:MI: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
64:T6:218:ARG:HH12	64:T6:220:ARG:HB2	1.76	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
2:A1:336:ILE:HG23	2:A1:337:ILE:HG23	1.93	0.51
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
45:T4:879:ASP:O	45:T4:902:ASN:ND2	2.39	0.51
62:t3:782:ASP:OD1	62:t3:783:ILE:N	2.44	0.51
64:t6:218:ARG:NH2	64:t6:220:ARG:HB2	2.26	0.51
64:t6:557:VAL:HG22	64:t6:603:PHE:CE1	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Ml: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
63:T5:857:ASP:OD2	63:T5:954:ARG:NH2	2.43	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
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
3:B2:124:VAL:HG22	3:B2:126:GLU:H	1.77	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
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	64:T6:834:PHE:CE1	2.46	0.50
21:AK:7:PHE:HB2	21:AK:11:LEU:HD12	1.93	0.50
45:Ml:252:THR:HG21	45:Ml:290:THR:HG21	1.93	0.50
50:SA:556:ASN:ND2	55:SH:553:GLU:OE1	2.41	0.50
63:T5:871:HIS:HA	63:T5:874:GLU:OE2	2.11	0.50
64:T6:914:SER:OG	64:T6:917:GLU:OE1	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
64:t6:220:ARG:NH1	64:t6:221:ALA:O	2.43	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
3:A2:138:TYR:CE2	3:A2:260:PHE:CD1	2.99	0.50
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
62:T3:405:GLU:O	62:T3:406:LYS:C	2.53	0.50
62:T3:981:GLU:OE1	62:T3:985:GLN:NE2	2.43	0.50
64:t6:696:ILE:HG13	64:t6:773:SER:HB3	1.92	0.50
64:t6:888:ASP:O	64:t6:895:ARG:NH2	2.45	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
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
62:T3:782:ASP:OD1	62:T3:783:ILE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:AB:763:GLN:HG2	12:AB:765:PRO:HD2	1.93	0.50
63:t5:857:ASP:OD2	63:t5:954:ARG:NH2	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
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
45:T4:918:TYR:HA	45:T4:921:ILE:HD12	1.93	0.50
64:T6:888:ASP:O	64:T6:895:ARG:NH2	2.45	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
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
64:t6:877:GLN:NE2	64:t6:882:GLY:O	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:T4:994:ARG:HH12	45:T4:996:LYS:HG2	1.77	0.50
64:T6:328:ASP:N	64:T6:328:ASP:OD1	2.44	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
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
64:T6:218:ARG:NH2	64:T6:220:ARG:HB2	2.26	0.50
64:T6:877:GLN:NE2	64:T6:882:GLY:O	2.44	0.50
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:A2:204: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
62:t3:913:THR:OG1	62:t3:914:TYR:N	2.44	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
56:sI:1099:ASN:HB3	56:sI:1100:ASN:HD21	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:MI:158:ASN:ND2	46:Mm:38:TYR:O	2.45	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
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
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
61:T2:28:LYS:HA	61:T2:31:LYS:HE2	1.94	0.49
62:T3:289:LYS:CG	62:T3:289:LYS:CA	2.88	0.49
64:t6:914:SER:OG	64:t6:917:GLU:OE1	2.29	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
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
62:t3:289:LYS:CG	62:t3:289:LYS:CA	2.88	0.49
4:B3:85:ARG:HE	4:B3:117:ILE:HD13	1.77	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:t4:994:ARG:HH12	45:t4:996:LYS:HG2	1.77	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
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:MI:263:PRO:HD2	45:MI:266:LEU:HD12	1.93	0.49
45:MI:480:ARG:NH1	45:MI:496:SER:O	2.45	0.49
45:MI:508:VAL:HG22	45:MI: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
61:T2:60:GLU:O	61:T2:67:ARG:NH2	2.46	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
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
62:t3:869:ARG:HH21	62:t3:882:LEU:HD23	1.76	0.49
45:t4:909:PRO:O	45:t4:913:ASN:ND2	2.46	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
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
60:t1:92:SER:HA	61:t2:37:ARG:HH22	1.78	0.49
61:t2:28:LYS:HA	61:t2:31:LYS:HE2	1.93	0.49
62:t3:301:ASN:HD22	62:t3:974:LEU:HB3	1.78	0.49
64:t6:467:ASP:OD1	64:t6:467:ASP:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
35:Mb:97:PRO:HA	37:Md:254:LEU:HD23	1.95	0.49
45:MI:797:LYS:HB3	45:t4:836:LEU:HD21	1.62	0.49
50:SA:68:LEU:HD23	50:SA:69:ILE:HG13	1.94	0.49
45:t4:1070:HIS:O	45:t4:1074:LYS:N	2.46	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
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
61:t2:60:GLU:O	61:t2:67:ARG:NH2	2.46	0.49
45:t4:918:TYR:HA	45:t4:921:ILE:HD12	1.93	0.49
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
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
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
64:t6:328:ASP:N	64:t6:328:ASP:OD1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:MI:641:SER:HB2	45:MI:652:GLU:HB2	1.95	0.48
9:SF:473:LEU:HD21	9:SF:499:TYR:CE2	2.49	0.48
45:T4:1070:HIS:O	45:T4:1074:LYS:N	2.46	0.48
62:t3:438:ASP:OD1	62:t3:441:HIS:ND1	2.44	0.48
64:t6:266:GLN:NE2	64:t6:276:LYS:O	2.46	0.48
64:t6:342:ASP:OD2	64:t6:387:LYS:NZ	2.46	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
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
64:T6:934:ARG:HG2	64:T6:937:ASN:HD21	1.78	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
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
62:T3:1095:ARG:O	62:T3:1099:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:T6:266:GLN:NE2	64:T6:276:LYS:O	2.46	0.48
64:T6:342:ASP:OD2	64:T6:387:LYS:NZ	2.46	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
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
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
62:T3:869:ARG:HH21	62:T3:882:LEU:HD23	1.76	0.48
62:t3:405:GLU:O	62:t3:406:LYS:C	2.53	0.48
62:t3:1095:ARG:O	62:t3:1099:ASN:ND2	2.46	0.48
64:t6:55:LEU:O	64:t6:164:MET:HE1	2.14	0.48
64:t6:779:LEU:O	64:t6:783:GLU:HB2	2.14	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
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
60:T1:92:SER:HA	61:T2:37:ARG:HH22	1.78	0.48
64:T6:55:LEU:O	64:T6:164:MET:HE1	2.14	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
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:B0:108: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
62:T3:698:ASP:HA	62:T3:702:ASN:HD22	1.79	0.48
45:T4:981:THR:OG1	45:T4:1004:ALA:N	2.46	0.48
62:t3:698:ASP:HA	62:t3:702:ASN:HD22	1.79	0.48
62:t3:1087:SER:OG	62:t3:1088:PHE:N	2.47	0.48
64:t6:559:SER:OG	64:t6:566:ALA:HB2	2.14	0.48
64:t6:609:ALA:HB1	64:t6:613:ILE:HD12	1.96	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
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
62:T3:1087:SER:OG	62:T3:1088:PHE:N	2.47	0.48
62:t3:539:GLU:OE1	62:t3:542:LYS:NZ	2.47	0.48
64:t6:627:MET:SD	64:t6:649:ILE:HD11	2.54	0.48
64:t6:934:ARG:HG2	64:t6:937:ASN:HD21	1.78	0.48
2:B1:472:GLN:HE22	5:B4:37:TRP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:ML:734:GLN:O	45:ML:770:ARG:NH1	2.44	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
45:T4:909:PRO:O	45:T4:913:ASN:ND2	2.46	0.48
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
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
62:T3:438:ASP:OD1	62:T3:441:HIS:ND1	2.44	0.47
62:T3:1114:GLU:HA	62:T3:1117:ILE:HG22	1.95	0.47
11:BA:1148:ILE:HD12	11:BA:1196:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
62:T3:539:GLU:OE1	62:T3:542:LYS:NZ	2.47	0.47
62:t3:1103:LEU:HD22	62:t3:1113:ASN:HD22	1.80	0.47
62:t3:1114:GLU:HA	62:t3:1117:ILE:HG22	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:A0:550: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
62:t3:371:ARG:O	62:t3:375:ILE:HG12	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
57:SJ:27:TYR:CE2	57:SJ:61:LYS:HD2	2.49	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
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:MI:722:MET:HE2	45:MI:727:LYS:HB3	1.96	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
62:T3:371:ARG:O	62:T3:375:ILE:HG12	2.14	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
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
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:MI:246:LEU:HD21	45:MI: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
62:T3:360:HIS:HD2	62:T3:919:TYR:CE2	2.26	0.47
45:T4:896:VAL:O	45:T4:908:GLN:NE2	2.38	0.47
64:T6:297:ILE:HB	64:T6:310:TYR:HB2	1.96	0.47
64:t6:506:SER:OG	64:t6:523:GLN:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
63:T5:849:ARG:O	63:T5:853:LEU:HD23	2.15	0.47
64:T6:467:ASP:N	64:T6:467:ASP:OD1	2.46	0.47
64:T6:609:ALA:HB1	64:T6:613:ILE:HD12	1.96	0.47
62:t3:518:SER:O	62:t3:524:GLN:NE2	2.47	0.47
45:t4:902:ASN:O	45:t4:905:HIS:ND1	2.44	0.47
45:t4:1001:ILE:HG23	45:t4:1055:VAL:HB	1.97	0.47
64:t6:297:ILE:HB	64:t6:310:TYR:HB2	1.96	0.47
1:B0:68:LYS:HD2	1:B0:204:ASN:HA	1.97	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:951:LEU:HD23	56:SI:975:LEU:HD11	1.97	0.47
64:T6:559:SER:OG	64:T6:566:ALA:HB2	2.14	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
19:BI:117:LYS:CE	64:t6:801:LYS:HZ2	2.13	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
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
62:T3:301:ASN:HD22	62:T3:974:LEU:HB3	1.78	0.47
45:T4:1001:ILE:HG23	45:T4:1055:VAL:HB	1.97	0.47
64:T6:393:PRO:HA	64:T6:425:TYR:HA	1.97	0.47
62:t3:783:ILE:O	62:t3:787:ILE:HG12	2.15	0.47
63:t5:896:ASP:OD1	63:t5:896:ASP: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
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
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
64:T6:203:ILE:HA	64:T6:223:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:T6:627:MET:SD	64:T6:649:ILE:HD11	2.54	0.47
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
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
62:T3:783:ILE:O	62:T3:787:ILE:HG12	2.15	0.46
45:T4:917:ASP:HB3	45:T4:920:PHE:HD2	1.81	0.46
64:T6:411:ASP:OD1	64:T6:411:ASP:N	2.48	0.46
64:T6:779:LEU:O	64:T6:783:GLU:HB2	2.14	0.46
62:t3:920:LEU:O	62:t3:924:ILE:HG12	2.14	0.46
64:t6:670:ILE:HA	64:t6:673:ILE:HD12	1.97	0.46
6:B5:6:LYS:HB3	6:B5:44:PRO:HG2	1.97	0.46
19:BI:117:LYS:HD2	64:t6:801:LYS:CD	2.44	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:T5:896:ASP:N	63:T5:896:ASP:OD1	2.48	0.46
62:t3:483:ASN:OD1	62:t3:487:ILE:N	2.47	0.46
45:t4:917:ASP:HB3	45:t4:920:PHE:HD2	1.81	0.46
64:t6:662:VAL:HB	64:t6:695:LEU:HD21	1.98	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
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
62:T3:920:LEU:O	62:T3:924:ILE:HG12	2.14	0.46
64:T6:651:TYR:OH	64:T6:910:CYS:SG	2.61	0.46
62:t3:830:SER:HB2	62:t3:841:ALA:HB1	1.96	0.46
62:t3:869:ARG:NH2	62:t3:882:LEU:HD23	2.31	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
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
56:SI:1020:SER:OG	56:SI:1021:GLU:N	2.48	0.46
62:T3:306:TRP:HD1	62:T3:580:SER:HA	1.80	0.46
62:T3:541:VAL:HG22	62:T3:578:ILE:HD13	1.98	0.46
45:t4:1023:ARG:NH1	45:t4:1027:PHE:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
61:T2:77:LYS:HA	61:T2:80:GLN:NE2	2.30	0.46
62:T3:483:ASN:OD1	62:T3:487:ILE:N	2.47	0.46
64:T6:670:ILE:HA	64:T6:673:ILE:HD12	1.97	0.46
61:t2:77:LYS:HA	61:t2:80:GLN:NE2	2.30	0.46
64:t6:203:ILE:HA	64:t6:223:GLN:HA	1.96	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
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
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:ML:92:LEU:HD21	45:ML: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
62:T3:830:SER:HB2	62:T3:841:ALA:HB1	1.96	0.46
62:t3:306:TRP:HD1	62:t3:580:SER:HA	1.80	0.46
45:t4:981:THR:OG1	45:t4:1004:ALA:N	2.46	0.46
63:t5:950:ASN:HB3	63:t5:954:ARG:HD2	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
64:T6:408:LEU:O	64:T6:412:ARG:NH2	2.48	0.46
64:t6:138:ARG:HD3	64:t6:138:ARG:HA	1.79	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
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:B2:455: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
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
62:T3:518:SER:O	62:T3:524:GLN:NE2	2.47	0.46
62:t3:775:LYS:HB2	62:t3:826:PHE:HE1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
62:T3:1103:LEU:HD22	62:T3:1113:ASN:HD22	1.80	0.46
45:T4:1023:ARG:NH1	45:T4:1027:PHE:O	2.48	0.46
62:t3:289:LYS:HB3	62:t3:290:LEU:HD22	1.98	0.46
64:t6:393:PRO:HA	64:t6:425:TYR:HA	1.97	0.46
64:t6:408:LEU:O	64:t6:412:ARG:NH2	2.48	0.46
64:t6:411:ASP:OD1	64:t6:411:ASP:N	2.48	0.46
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
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
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:MI: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:239:SER:HB3	58:SK:307:TYR:CZ	2.51	0.45
45:T4:1058:ASP:OD1	45:T4:1061:GLU:HG2	2.17	0.45
64:T6:506:SER:OG	64:T6:523:GLN:OE1	2.31	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
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
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
63:T5:937:SER:O	63:T5:943:LEU:HD12	2.17	0.45
63:T5:950:ASN:HB3	63:T5:954:ARG:HD2	1.98	0.45
62:t3:364:SER:HB2	62:t3:366:LEU:HD13	1.98	0.45
63:t5:849:ARG:O	63:t5:853:LEU:HD23	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
62:T3:869:ARG:NH2	62:T3:882:LEU:HD23	2.31	0.45
1:B0:523:GLY:O	1:B0:527:VAL:HG23	2.16	0.45
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
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
62:T3:364:SER:HB2	62:T3:366:LEU:HD13	1.98	0.45
64:T6:322:LYS:HD3	64:T6:322:LYS:HA	1.74	0.45
62:t3:288:MET:HG2	62:t3:292:ARG:NH1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:934:ASN:HB3	56:SI:938:MET:HE2	1.97	0.45
62:T3:289:LYS:HB3	62:T3:290:LEU:HD22	1.97	0.45
62:t3:360:HIS:HD2	62:t3:919:TYR:CE2	2.26	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
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
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
62:t3:833:ASN:HB2	62:t3:834:TYR:H	1.70	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
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
61:T2:48:ASN:O	61:T2:52:GLN:NE2	2.50	0.45
64:t6:187:ASN:HB3	64:t6:245:ASN:HB3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B6:246:ASP:N	7:B6:246:ASP:OD1	2.49	0.45
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
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:ML:354:GLU:OE1	45:ML: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
63:T5:922:THR:HG23	63:T5:925:ALA:H	1.82	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
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
64:T6:176:ASN:OD1	64:T6:176:ASN:N	2.49	0.45
64:T6:825:PRO:HA	64:T6:826:PRO:HD3	1.85	0.45
61:t2:48:ASN:O	61:t2:52:GLN:NE2	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
64:T6:181:GLN:HB2	64:T6:183:ARG:HH11	1.82	0.45
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
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
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
62:T3:288:MET:HG2	62:T3:292:ARG:NH1	2.32	0.44
62:T3:775:LYS:HB2	62:T3:826:PHE:HE1	1.81	0.44
64:T6:187:ASN:HB3	64:T6:245:ASN:HB3	1.99	0.44
62:t3:578:ILE:O	62:t3:581:PHE:N	2.50	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:T4:1003:PHE:CZ	45:T4:1019:MET:HG3	2.52	0.44
60:t1:40:LEU:HA	60:t1:40:LEU:HD13	1.69	0.44
62:t3:532:VAL:HB	62:t3:537:GLN:HE21	1.82	0.44
62:t3:541:VAL:HG22	62:t3:578:ILE:HD13	1.98	0.44
64:t6:739:LYS:HZ3	64:t6:799:ASN:CG	2.26	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:T4:985:GLU:OE1	45:T4:1002:HIS:NE2	2.50	0.44
45:t4:1003:PHE:CZ	45:t4:1019:MET:HG3	2.52	0.44
64:t6:181:GLN:HB2	64:t6:183:ARG:HH11	1.82	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: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
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
45:t4:985:GLU:OE1	45:t4:1002:HIS:NE2	2.50	0.44
45:t4:1058:ASP:OD1	45:t4:1061:GLU:HG2	2.17	0.44
64:t6:170:ASP:OD1	64:t6:170:ASP:N	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:sI:1207:LEU:HA	56:sI:1210:ILE:HG12	2.00	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
62:T3:532:VAL:HB	62:T3:537:GLN:HE21	1.82	0.44
64:t6:222:GLN:NE2	64:t6:223:GLN:O	2.51	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
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
61:T2:34:ASN:N	61:T2:34:ASN:OD1	2.46	0.44
61:T2:77:LYS:HA	61:T2:80:GLN:CD	2.42	0.44
64:T6:662:VAL:HB	64:T6:695:LEU:HD21	1.98	0.44
64:T6:739:LYS:HZ3	64:T6:799:ASN:CG	2.26	0.44
63:t5:937:SER:O	63:t5:943:LEU:HD12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
62:T3:731:LEU:HD23	62:T3:731:LEU:HA	1.86	0.44
45:T4:902:ASN:O	45:T4:905:HIS:ND1	2.44	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
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
64:T6:222:GLN:NE2	64:T6:223:GLN:O	2.51	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
62:T3:578:ILE:O	62:T3:581:PHE:N	2.50	0.43
62:t3:789:ASN:OD1	62:t3:846:ASN:ND2	2.47	0.43
45:t4:840:THR:HA	45:t4:843:VAL:HG12	2.00	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
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
64:t6:350:VAL:HG23	64:t6:379:CYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
60:T1:40:LEU:HA	60:T1:40:LEU:HD13	1.69	0.43
64:T6:350:VAL:HG23	64:T6:379:CYS:HB3	1.99	0.43
61:t2:77:LYS:HA	61:t2:80:GLN:CD	2.42	0.43
62:t3:658:ILE:O	62:t3:662:ILE:HG12	2.18	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
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
61:T2:104:GLU:HA	61:T2:107:LYS:HG2	2.00	0.43
62:T3:789:ASN:OD1	62:T3:846:ASN:ND2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
62:T3:658:ILE:O	62:T3:662:ILE:HG12	2.18	0.43
62:T3:732:SER:O	62:T3:734:GLU:N	2.51	0.43
62:T3:833:ASN:HB2	62:T3:834:TYR:H	1.70	0.43
61:t2:34:ASN:N	61:t2:34:ASN:OD1	2.46	0.43
62:t3:359:TYR:HE2	62:t3:913:THR:HB	1.83	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
62:T3:869:ARG:HG2	62:T3:876:ASP:OD2	2.19	0.43
45:T4:1003:PHE:CE1	45:T4:1019:MET:HE2	2.54	0.43
64:T6:138:ARG:HD3	64:T6:138:ARG:HA	1.79	0.43
64:t6:127:LEU:HD13	64:t6:186:TYR:CE2	2.54	0.43
64:t6:739:LYS:HZ3	64:t6:799:ASN:HD21	1.66	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
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
62:T3:378:THR:HG22	62:T3:379:LYS:HD3	2.01	0.43
63:t5:922:THR:HG23	63:t5:925:ALA:H	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
45:t4:1003:PHE:CE2	45:t4:1019:MET:HG3	2.54	0.43
64:t6:119:ASP:OD1	64:t6:119:ASP:N	2.52	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:15:PRO:C	63:t5:931:GLN:CG	2.56	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
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
62:T3:888:LEU:HA	64:T6:278:LEU:HD21	2.00	0.43
45:T4:1000:HIS:ND1	45:T4:1002:HIS:CD2	2.87	0.43
64:T6:119:ASP:OD1	64:T6:119:ASP:N	2.52	0.43
61:t2:104:GLU:HA	61:t2:107:LYS:HG2	2.00	0.43
64:t6:739:LYS:HZ3	64:t6:799:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
64:T6:111:ASN:HD21	64:T6:119:ASP:H	1.67	0.43
62:t3:480:PHE:HB3	62:t3:488:GLN:HB3	2.01	0.43
62:t3:883:GLY:HA2	64:t6:275:PHE:HE1	1.84	0.43
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
62:T3:480:PHE:HB3	62:T3:488:GLN:HB3	2.01	0.42
45:T4:1003:PHE:CE2	45:T4:1019:MET:HG3	2.54	0.42
64:T6:102:PHE:HD1	64:T6:177:ILE:HG22	1.84	0.42
64:T6:739:LYS:HZ3	64:T6:799:ASN:ND2	2.17	0.42
62:t3:378:THR:HG22	62:t3:379:LYS:HD3	2.01	0.42
62:t3:909:LEU:HG	62:t3:967:TYR:HE2	1.84	0.42
45:t4:1000:HIS:ND1	45:t4:1002:HIS:CD2	2.87	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
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
62:T3:359:TYR:HE2	62:T3:913:THR:HB	1.83	0.42
64:T6:597:LYS:HG3	64:T6:816:PHE:HE2	1.84	0.42
60:t1:31:LYS:HA	60:t1:34:VAL:HG12	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:A7:457:TYR:OH	8:A7:488:ASP:O	2.32	0.42
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
62:T3:958:SER:O	62:T3:962:GLU:HB2	2.20	0.42
62:t3:869:ARG:HG2	62:t3:876:ASP:OD2	2.19	0.42
64:t6:144:THR:OG1	64:t6:146:GLU:OE2	2.19	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:16:TYR:O	63:t5:927:ARG:NH1	2.47	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
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
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
64:T6:621:ARG:O	64:T6:625:LYS:NZ	2.52	0.42
62:t3:824:ARG:NH1	62:t3:870:ILE:O	2.42	0.42
62:t3:958:SER:O	62:t3:962:GLU:HB2	2.20	0.42
64:t6:322:LYS:HD3	64:t6:322:LYS:HA	1.74	0.42
64:t6:621:ARG:O	64:t6:625:LYS:NZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
62:T3:482:ARG:HH22	62:T3:517:ASP:HA	1.85	0.42
62:T3:867:ASP:HB3	62:T3:870:ILE:HG12	2.00	0.42
62:T3:887:PHE:HE1	62:T3:919:TYR:HD1	1.67	0.42
60:t1:95:SER:OG	61:t2:37:ARG:NH2	2.53	0.42
62:t3:683:ASP:OD1	62:t3:683:ASP:N	2.53	0.42
62:t3:867:ASP:HB3	62:t3:870:ILE:HG12	2.00	0.42
62:t3:888:LEU:HA	64:t6:278:LEU:HD21	2.00	0.42
64:t6:843:VAL:HG22	64:t6:844:ILE:H	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
60:T1:31:LYS:HA	60:T1:34:VAL:HG12	2.00	0.42
62:t3:732:SER:O	62:t3:734:GLU:N	2.51	0.42
62:t3:838:SER:O	62:t3:839:SER:C	2.62	0.42
45:t4:1003:PHE:CE1	45:t4:1019:MET:HE2	2.54	0.42
63:t5:880:PRO:HA	63:t5:883:LEU:HG	2.01	0.42
64:t6:597:LYS:HG3	64:t6:816:PHE:HE2	1.84	0.42
64:t6:643:GLU:H	64:t6:643:GLU:HG2	1.52	0.42
1:B0:260:ALA:HB2	1:B0:398:ALA:HB3	2.00	0.42
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:226:THR:HG23	58:SK:227:TRP:HD1	1.83	0.42
62:T3:838:SER:O	62:T3:839:SER:C	2.62	0.42
62:T3:883:GLY:HA2	64:T6:275:PHE:HE1	1.84	0.42
45:T4:914:SER:HB2	45:T4:916:MET:HE2	2.01	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
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
45:MI:797:LYS:HD3	45:t4:836:LEU:HD21	2.01	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
45:T4:840:THR:HA	45:T4:843:VAL:HG12	2.00	0.42
64:T6:127:LEU:HD13	64:T6:186:TYR:CE2	2.54	0.42
64:T6:218:ARG:HH12	64:T6:220:ARG:CB	2.33	0.42
64:T6:628:LEU:HD23	64:T6:631:LEU:HD12	2.01	0.42
61:t2:31:LYS:HA	61:t2:34:ASN:HD21	1.85	0.42
62:t3:482:ARG:HH22	62:t3:517:ASP:HA	1.85	0.42
64:t6:218:ARG:HH12	64:t6:220:ARG:CB	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
64:T6:196:LEU:HD23	64:T6:196:LEU:HA	1.92	0.42
64:t6:102:PHE:HD1	64:t6:177:ILE:HG22	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
63:T5:880:PRO:HA	63:T5:883:LEU:HG	2.01	0.42
64:t6:45:THR:HA	64:t6:46:PRO:HD3	1.92	0.42
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
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
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:MI:769:LEU:HB3	45:MI:780:LEU:HD12	2.02	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
62:T3:909:LEU:HG	62:T3:967:TYR:HE2	1.84	0.41
64:T6:653:LYS:HE2	64:T6:653:LYS:HB2	1.81	0.41
45:t4:914:SER:HB2	45:t4:916:MET:HE2	2.01	0.41
64:t6:111:ASN:HD21	64:t6:119:ASP:H	1.67	0.41
64:t6:760:ALA:O	64:t6:761:LYS:HG3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
63:T5:869:PHE:O	63:T5:873:GLN:HG3	2.20	0.41
63:T5:913:ILE:HG21	63:T5:938:ILE:HB	2.02	0.41
64:T6:623:LEU:HD11	64:T6:653:LYS:HE3	2.02	0.41
64:T6:739:LYS:HZ3	64:T6:799:ASN:HD21	1.66	0.41
62:t3:731:LEU:HD23	62:t3:731:LEU:HA	1.86	0.41
63:t5:913:ILE:HG21	63:t5:938:ILE:HB	2.02	0.41
64:t6:628:LEU:HD23	64:t6:631:LEU:HD12	2.02	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
1:A0:549:SER:O	1:A0:553:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
61:T2:31:LYS:HA	61:T2:34:ASN:HD21	1.85	0.41
62:T3:534:PRO:HA	62:T3:537:GLN:HG3	2.02	0.41
45:T4:859:ALA:HB3	45:T4:866:SER:HB2	2.02	0.41
64:T6:625:LYS:H	64:T6:625:LYS:HG2	1.66	0.41
64:T6:843:VAL:HG22	64:T6:844:ILE:H	1.83	0.41
62:t3:509:SER:O	62:t3:513:SER:OG	2.38	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
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
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
62:t3:768:GLU:OE1	62:t3:819:LEU:HD23	2.20	0.41
62:t3:976:ASP:OD2	62:t3:1123:TYR:OH	2.38	0.41
64:t6:196:LEU:HD23	64:t6:196:LEU:HA	1.92	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
7:A6:227:HIS:CD2	7:A6:318:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
60:T1:95:SER:OG	61:T2:37:ARG:NH2	2.53	0.41
62:T3:683:ASP:OD1	62:T3:683:ASP:N	2.53	0.41
62:T3:768:GLU:OE1	62:T3:819:LEU:HD23	2.20	0.41
64:T6:170:ASP:OD1	64:T6:170:ASP:N	2.48	0.41
64:T6:480:GLN:NE2	64:T6:486:ASN:OD1	2.41	0.41
63:t5:869:PHE:O	63:t5:873:GLN:HG3	2.20	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:522:ASP:C	53:SE:547:ARG:NH1	2.79	0.41
45:T4:1023:ARG:HA	45:T4:1027:PHE:HB2	2.02	0.41
64:t6:623:LEU:HD11	64:t6:653:LYS:HE3	2.02	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
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
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
62:T3:666:PRO:HA	62:T3:765:TYR:HB3	2.02	0.41
60:t1:76:LYS:HA	60:t1:76:LYS:HD2	1.93	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
4:A3:97:ASP:N	4:A3:97:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
62:T3:509:SER:O	62:T3:513:SER:OG	2.38	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: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
59:sL:161:ILE:HG22	59:sL:334:ILE:HB	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
62:T3:1082:ILE:HD11	64:T6:380:ASP:HB3	2.03	0.41
45:T4:1010:THR:O	45:T4:1013:SER:OG	2.27	0.41
64:T6:760:ALA:O	64:T6:761:LYS:HG3	2.20	0.41
60:t1:31:LYS:HZ3	60:t1:83:ILE:HD12	1.86	0.41
62:t3:356:ASN:O	62:t3:360:HIS:ND1	2.52	0.41
62:t3:534:PRO:HA	62:t3:537:GLN:HG3	2.02	0.41
45:t4:859:ALA:HB3	45:t4:866:SER:HB2	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
60:t1:101:LEU:HD12	60:t1:102:THR:HG23	2.03	0.41
62:t3:887:PHE:HE1	62:t3:919:TYR:HD1	1.67	0.41
64:t6:15:ILE:HD11	64:t6:145:TYR:HB3	2.03	0.41
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
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
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
62:t3:495:ASN:OD1	62:t3:495:ASN:N	2.54	0.40
45:t4:1013:SER:HA	45:t4:1014:PRO:HD3	1.93	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)
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
64:T6:574:LYS:HA	64:T6:577:ILE:HG22	2.04	0.40
62:t3:413:ILE:O	62:t3:417:GLU:HG3	2.22	0.40
64:t6:653:LYS:HB2	64:t6:653:LYS:HE2	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
60:T1:47:MET:O	60:T1:51:GLN:N	2.55	0.40
62:T3:976:ASP:OD2	62:T3:1123:TYR:OH	2.38	0.40
62:T3:1126:MET:HE3	62:T3:1126:MET:HB2	1.95	0.40
62:t3:666:PRO:HA	62:t3:765:TYR:HB3	2.02	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
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
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
60:T1:31:LYS:HZ3	60:T1:83:ILE:HD12	1.86	0.40
62:T3:824:ARG:NH1	62:T3:870:ILE:O	2.42	0.40
64:T6:568:ASP:N	64:T6:568:ASP:OD1	2.54	0.40
61:t2:32:GLN:NE2	61:t2:91:HIS:O	2.55	0.40
45:t4:1023:ARG:HA	45:t4:1027:PHE:HB2	2.02	0.40
64:t6:578:LEU:HD22	64:t6:879:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
62:T3:413:ILE:O	62:T3:417:GLU:HG3	2.22	0.40
64:T6:521:VAL:HB	64:T6:530:GLN:HE21	1.87	0.40
63:t5:934:ILE:CG2	63:t5:945:MET:HE1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	T1	61/431 (14%)	61 (100%)	0	0	100	100
60	t1	61/431 (14%)	61 (100%)	0	0	100	100
61	T2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
61	t2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	T3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55
62	t3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55
63	T5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23
63	t5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23
64	T6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
64	t6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
All	All	36516/65810 (56%)	34690 (95%)	1700 (5%)	126 (0%)	37	66

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
9	SF	361	ASP
62	T3	844	ASP
45	T4	1053	ASN
64	T6	761	LYS
62	t3	844	ASP
45	t4	1053	ASN
64	t6	761	LYS
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
3	A2	68	SER
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	Ml	646	LYS
50	SA	302	SER
59	SL	304	ASN
62	T3	839	SER
64	T6	156	VAL
62	t3	839	SER
64	t6	156	VAL
3	B2	235	LYS
28	BS	239	ALA
9	sF	357	THR
55	sH	592	LEU
56	sI	1051	LYS
3	A2	235	LYS
28	AS	239	ALA

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Mol	Chain	Res	Type
9	SF	357	THR
55	SH	592	LEU
56	SI	1051	LYS
63	T5	906	PRO
63	t5	906	PRO
11	BA	569	LYS
19	BI	47	GLU
19	BI	79	HIS
25	BO	128	SER
28	BS	235	ASP
11	mA	1574	SER
11	AA	569	LYS
19	AI	47	GLU
19	AI	79	HIS
25	AO	128	SER
28	AS	235	ASP
11	MA	1574	SER
62	T3	362	ALA
64	T6	844	ILE
62	t3	362	ALA
64	t6	844	ILE
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
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
63	T5	921	PRO
63	t5	921	PRO
11	mA	1584	TYR
46	mm	19	PRO
53	sE	504	PRO
19	AI	58	VAL
11	MA	1584	TYR

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Mol	Chain	Res	Type
46	Mm	19	PRO
53	SE	504	PRO
19	BI	58	VAL
46	mm	35	ILE
46	Mm	35	ILE
11	BA	464	PRO
11	AA	464	PRO
50	sA	62	PRO
56	sI	867	PRO
50	SA	62	PRO
56	SI	867	PRO
62	T3	928	THR
62	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A7	539/737 (73%)	539 (100%)	0	100	100
8	B7	539/737 (73%)	539 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	BK	99/102 (97%)	99 (100%)	0	100	100
22	AL	40/57 (70%)	40 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Mf	178/178 (100%)	178 (100%)	0	100	100
39	mf	178/178 (100%)	178 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	sC	141/288 (49%)	141 (100%)	0	100	100
53	SE	368/558 (66%)	368 (100%)	0	100	100
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	T1	60/389 (15%)	60 (100%)	0	100	100
60	t1	60/389 (15%)	60 (100%)	0	100	100
61	T2	100/339 (30%)	100 (100%)	0	100	100
61	t2	100/339 (30%)	100 (100%)	0	100	100
62	T3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
62	t3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
63	T5	103/944 (11%)	99 (96%)	4 (4%)	28	64
63	t5	103/944 (11%)	99 (96%)	4 (4%)	28	64
64	T6	861/897 (96%)	860 (100%)	1 (0%)	88	97
64	t6	861/897 (96%)	860 (100%)	1 (0%)	88	97
All	All	33862/59186 (57%)	33792 (100%)	70 (0%)	85	96

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B2	464	THR
3	B2	490	LYS
4	B3	49	LEU

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

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Mol	Chain	Res	Type
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
62	T3	833	ASN
62	T3	836	ILE
62	T3	837	TYR
62	T3	838	SER
63	T5	877	LYS
63	T5	919	ARG
63	T5	920	LYS
63	T5	931	GLN
64	T6	505	PRO
62	t3	833	ASN
62	t3	836	ILE
62	t3	837	TYR
62	t3	838	SER
63	t5	877	LYS
63	t5	919	ARG
63	t5	920	LYS
63	t5	931	GLN
64	t6	505	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (617) such sidechains are listed below:

Mol	Chain	Res	Type
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
2	B1	513	GLN
2	B1	567	HIS
2	B1	621	ASN
2	B1	638	ASN
3	B2	8	HIS

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Mol	Chain	Res	Type
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
11	BA	445	ASN
11	BA	451	HIS
11	BA	490	HIS
11	BA	510	GLN
11	BA	517	ASN

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Mol	Chain	Res	Type
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
17	BG	97	HIS
17	BG	102	GLN
17	BG	122	ASN
18	BH	134	ASN
19	BI	23	ASN

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Mol	Chain	Res	Type
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
35	mb	157	ASN
36	mc	19	GLN
36	mc	51	HIS
36	mc	54	GLN
36	mc	76	ASN

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Mol	Chain	Res	Type
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
47	mn	7	GLN
49	mp	106	ASN
49	mp	118	HIS
49	mp	153	ASN
49	mp	247	ASN

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Mol	Chain	Res	Type
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
9	sF	410	ASN
9	sF	482	ASN
9	sF	525	GLN
9	sF	534	GLN
9	sF	556	GLN

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Mol	Chain	Res	Type
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
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
2	A1	500	ASN
2	A1	513	GLN

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Mol	Chain	Res	Type
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
11	AA	311	GLN
11	AA	339	ASN

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Mol	Chain	Res	Type
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
15	AE	113	GLN
17	AG	10	ASN

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Mol	Chain	Res	Type
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
36	Mc	51	HIS
36	Mc	54	GLN

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Mol	Chain	Res	Type
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
46	Mm	27	GLN
47	Mn	7	GLN
47	Mn	29	ASN
49	Mp	106	ASN
49	Mp	118	HIS

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Mol	Chain	Res	Type
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
9	SF	389	ASN
9	SF	410	ASN
9	SF	482	ASN
9	SF	525	GLN

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Mol	Chain	Res	Type
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
61	T2	46	GLN
61	T2	52	GLN
61	T2	82	ASN
61	T2	96	GLN
62	T3	333	GLN
62	T3	352	GLN
62	T3	356	ASN
62	T3	363	ASN
62	T3	421	ASN
62	T3	485	GLN
62	T3	528	ASN
62	T3	537	GLN

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Mol	Chain	Res	Type
62	T3	608	ASN
62	T3	632	ASN
62	T3	690	ASN
62	T3	702	ASN
62	T3	728	GLN
62	T3	769	GLN
62	T3	901	ASN
62	T3	1099	ASN
62	T3	1105	ASN
62	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
63	T5	871	HIS
63	T5	931	GLN
64	T6	6	HIS
64	T6	25	ASN
64	T6	40	ASN
64	T6	44	HIS
64	T6	47	GLN
64	T6	100	GLN
64	T6	109	HIS
64	T6	129	ASN
64	T6	137	GLN
64	T6	162	HIS
64	T6	187	ASN
64	T6	266	GLN
64	T6	293	GLN
64	T6	317	ASN
64	T6	327	ASN
64	T6	530	GLN
64	T6	548	ASN
64	T6	675	ASN
64	T6	687	GLN
64	T6	693	GLN
64	T6	697	HIS
64	T6	726	ASN
64	T6	757	GLN

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Mol	Chain	Res	Type
64	T6	771	ASN
64	T6	800	ASN
64	T6	864	ASN
64	T6	894	ASN
61	t2	46	GLN
61	t2	52	GLN
61	t2	96	GLN
62	t3	333	GLN
62	t3	352	GLN
62	t3	356	ASN
62	t3	363	ASN
62	t3	421	ASN
62	t3	485	GLN
62	t3	528	ASN
62	t3	537	GLN
62	t3	608	ASN
62	t3	632	ASN
62	t3	635	GLN
62	t3	690	ASN
62	t3	702	ASN
62	t3	769	GLN
62	t3	901	ASN
62	t3	1099	ASN
62	t3	1105	ASN
62	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
63	t5	871	HIS
64	t6	6	HIS
64	t6	25	ASN
64	t6	40	ASN
64	t6	44	HIS
64	t6	47	GLN
64	t6	100	GLN
64	t6	109	HIS
64	t6	129	ASN
64	t6	137	GLN

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Mol	Chain	Res	Type
64	t6	162	HIS
64	t6	187	ASN
64	t6	266	GLN
64	t6	293	GLN
64	t6	327	ASN
64	t6	530	GLN
64	t6	548	ASN
64	t6	675	ASN
64	t6	687	GLN
64	t6	693	GLN
64	t6	697	HIS
64	t6	726	ASN
64	t6	771	ASN
64	t6	800	ASN
64	t6	864	ASN
64	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	A0	801	1	0,12,12	-	-	-		
65	SF4	B0	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	A0	801	1	-	-	0/6/5/5
65	SF4	B0	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
62	T3	4
62	t3	4
53	sE	3
53	SE	3
54	sG	2
54	SG	2
11	mA	2
11	MA	2
27	BR	2
27	AR	2

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Mol	Chain	Number of breaks
56	sI	1
56	SI	1
45	T4	1
45	t4	1
23	BM	1
23	AM	1
12	BB	1
12	AB	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	BM	65:THR	C	66:PHE	N	4.70
1	AM	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	BR	56:SER	C	57:LEU	N	3.73
1	AR	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	BB	1155:SER	C	1156:ASP	N	3.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	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	BR	227:SER	C	228:MET	N	3.03
1	AR	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

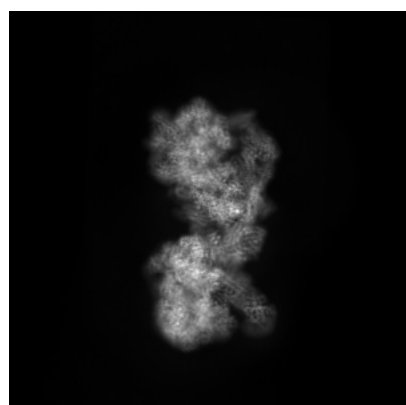
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71536. These allow visual inspection of the internal detail of the map and identification of artifacts.

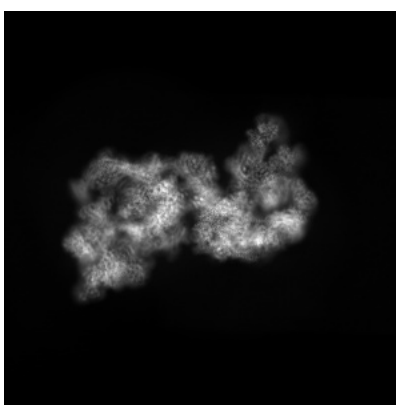
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

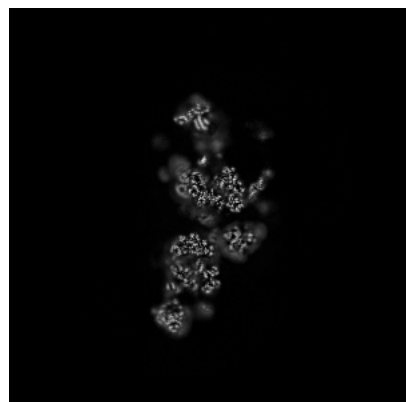


Z

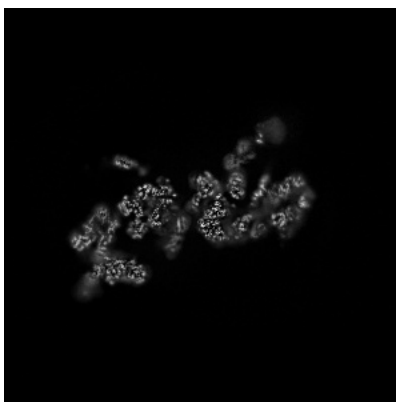
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

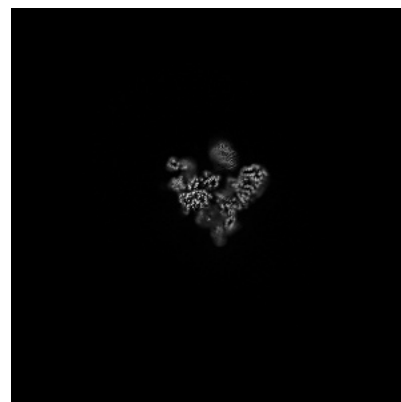
6.2.1 Primary map



X Index: 320



Y Index: 320

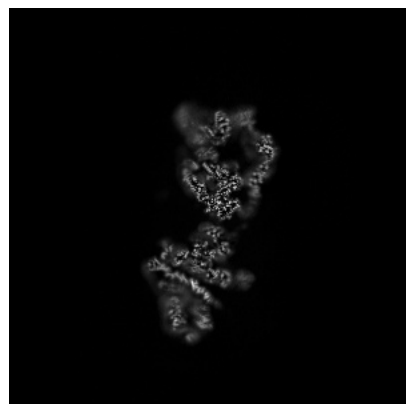


Z Index: 320

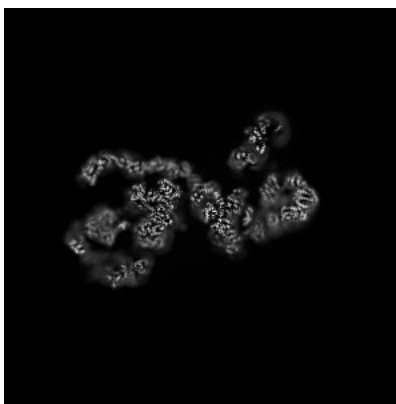
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

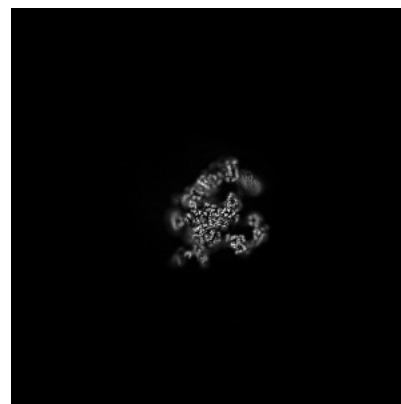
6.3.1 Primary map



X Index: 292



Y Index: 303

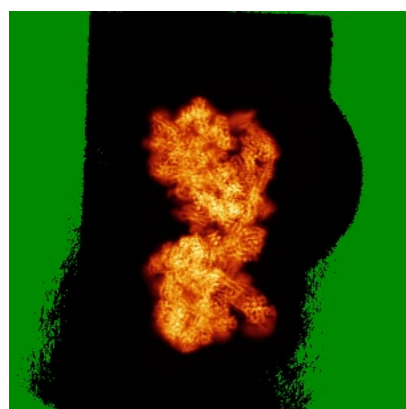


Z Index: 249

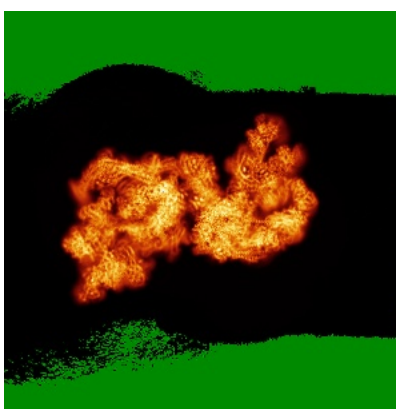
The images above show the largest variance slices of the map in three orthogonal directions.

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

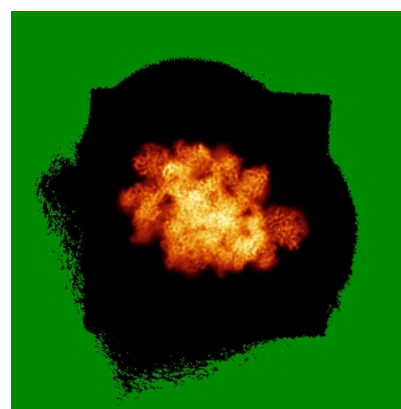
6.4.1 Primary map



X



Y



Z

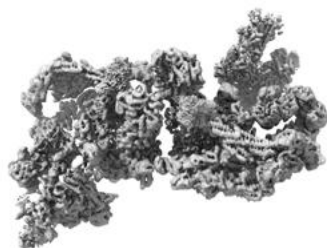
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

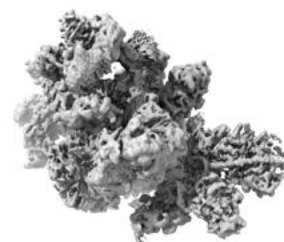
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.407. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

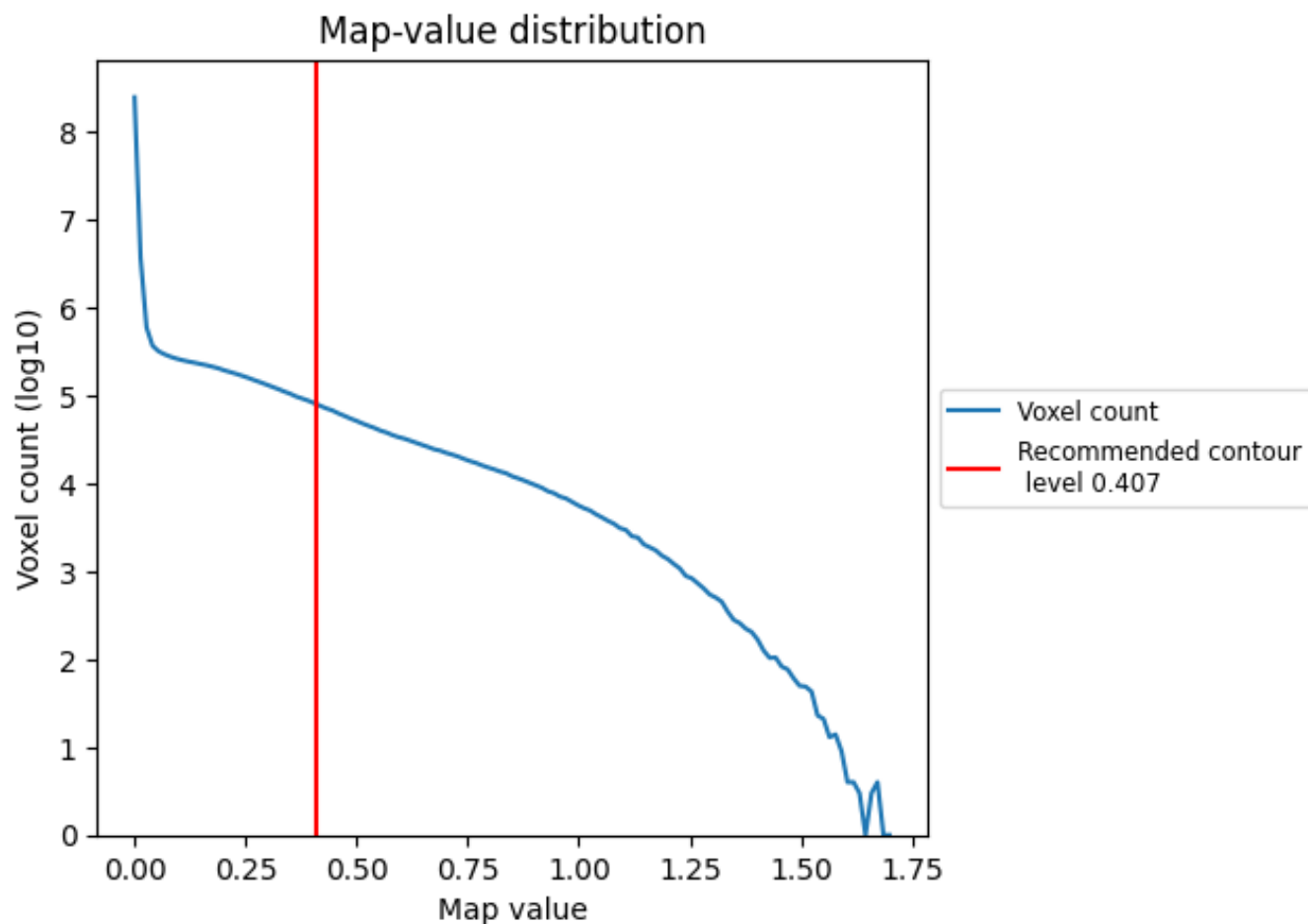
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

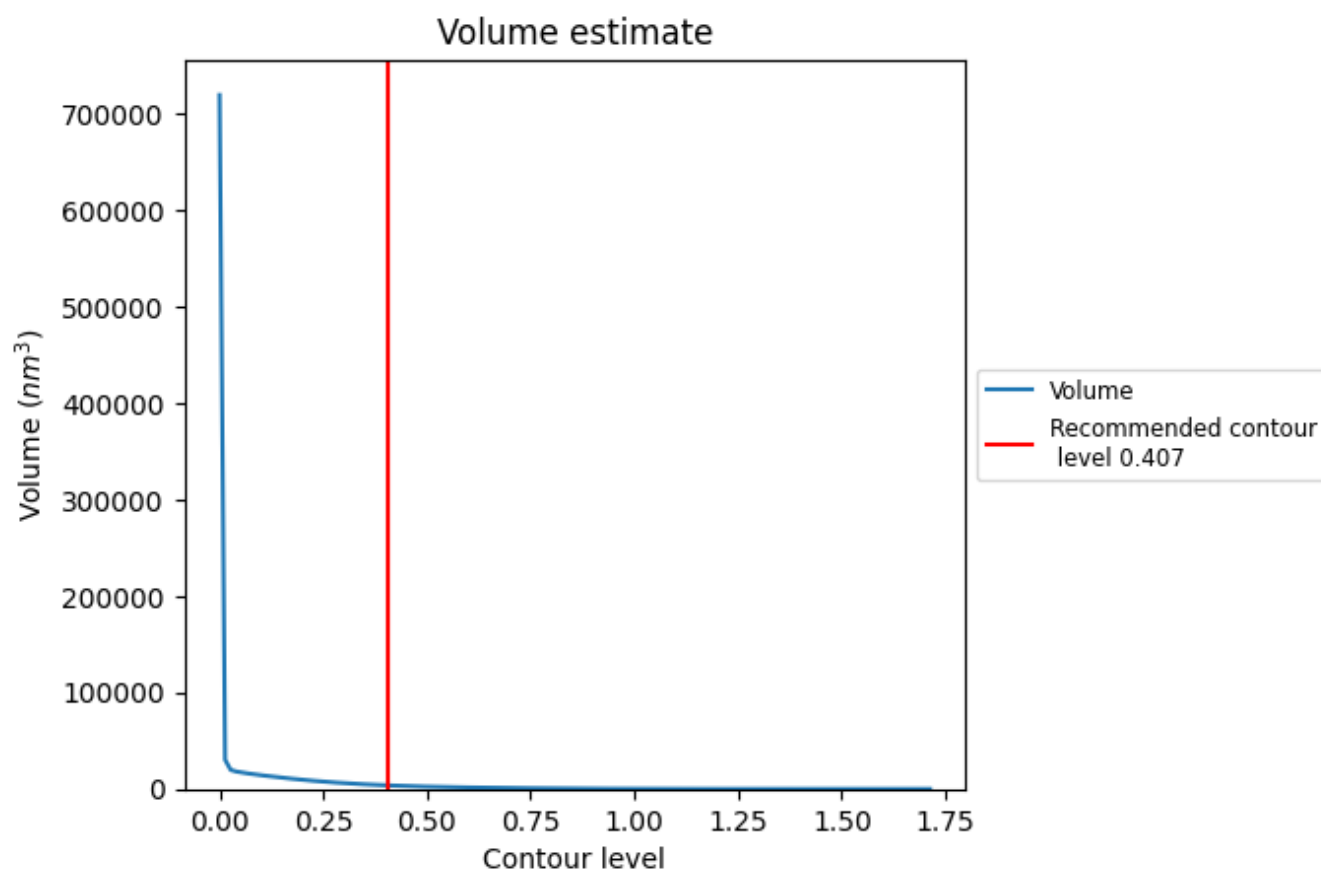
This section contains the results of statistical analysis of the map.

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.

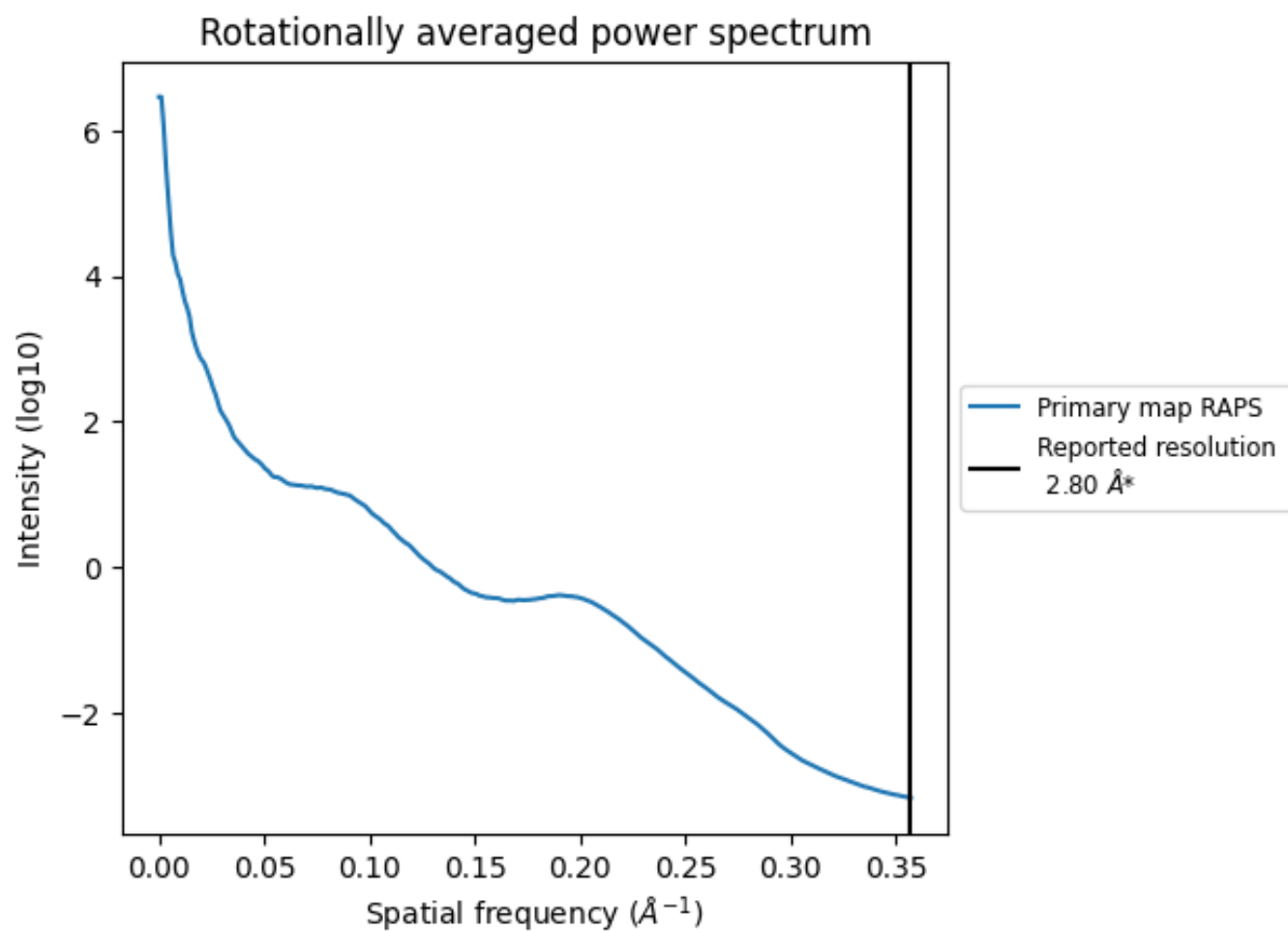
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3703 nm^3 ; this corresponds to an approximate mass of 3345 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

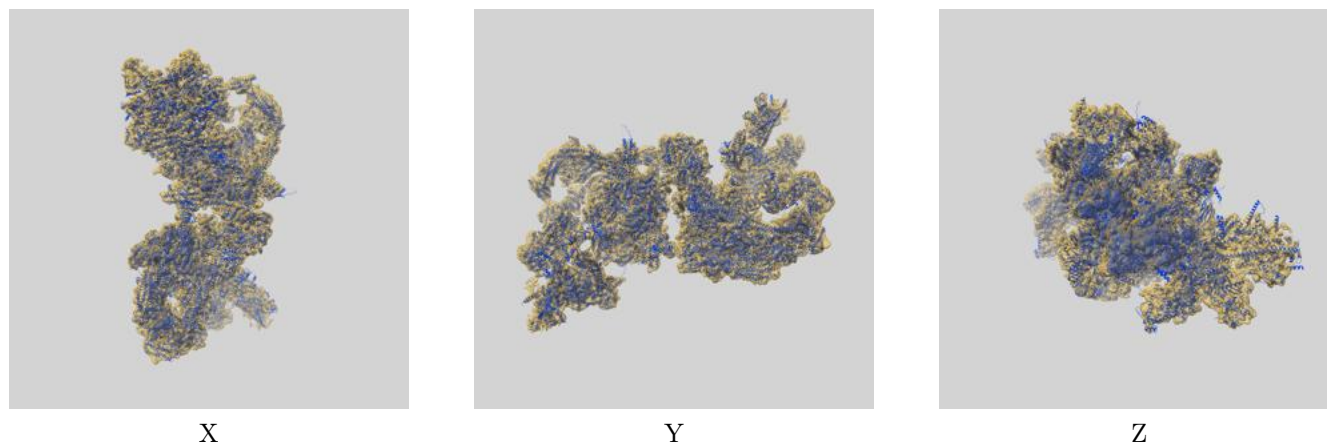
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

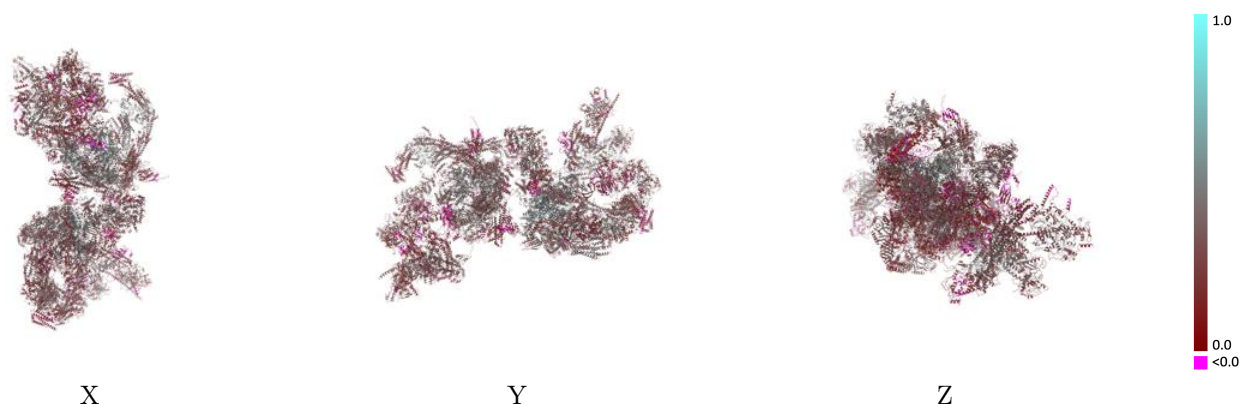
This section contains information regarding the fit between EMDB map EMD-71536 and PDB model 9PDK. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



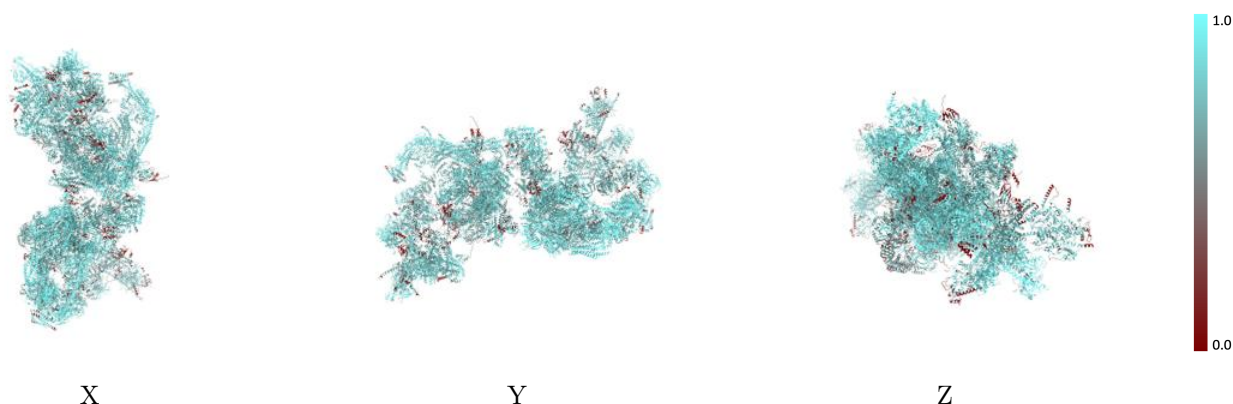
The images above show the 3D surface view of the map at the recommended contour level 0.407 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



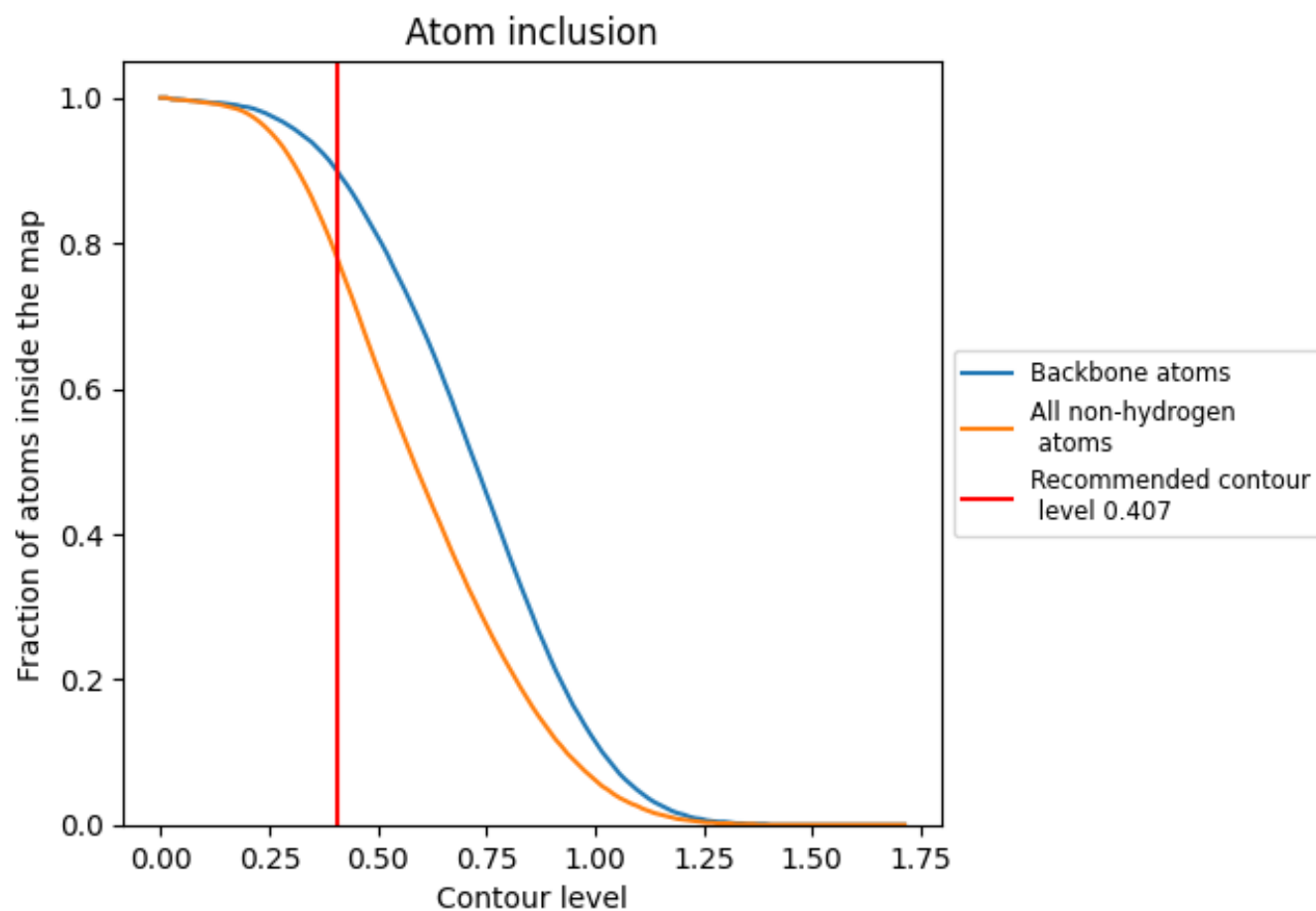
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.407).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.407) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.3040
A0	 0.8460	 0.2820
A1	 0.7670	 0.2400
A2	 0.8150	 0.2150
A3	 0.8120	 0.2280
A4	 0.9190	 0.3290
A5	 0.7260	 0.1310
A6	 0.8290	 0.3040
A7	 0.7210	 0.1860
A8	 0.2860	 -0.0200
A9	 0.0330	 0.0170
AA	 0.8970	 0.4490
AB	 0.8640	 0.4460
AC	 0.9440	 0.5110
AD	 0.7660	 0.2210
AE	 0.9230	 0.4330
AF	 0.9280	 0.4830
AG	 0.8860	 0.3400
AH	 0.9170	 0.4550
AI	 0.8820	 0.4080
AJ	 0.9040	 0.4740
AK	 0.8620	 0.4620
AL	 0.8990	 0.4220
AM	 0.7610	 0.3120
AN	 0.8520	 0.2410
AO	 0.7130	 0.3130
AQ	 0.6370	 0.2250
AR	 0.5880	 0.1870
AS	 0.6090	 0.2400
AT	 0.8510	 0.2440
AU	 0.5360	 0.2420
AV	 0.5710	 0.2430
AW	 0.5420	 0.1510
AX	 0.3750	 0.2020
B0	 0.8460	 0.2700



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Chain	Atom inclusion	Q-score
B1	 0.7610	 0.2280
B2	 0.8150	 0.2080
B3	 0.8150	 0.2190
B4	 0.9170	 0.3120
B5	 0.7300	 0.1310
B6	 0.8270	 0.2870
B7	 0.7190	 0.1780
B8	 0.2780	 -0.0210
B9	 0.0330	 0.0380
BA	 0.8800	 0.4200
BB	 0.8450	 0.4210
BC	 0.9280	 0.4830
BD	 0.7640	 0.2100
BE	 0.9120	 0.4070
BF	 0.9160	 0.4550
BG	 0.8800	 0.3220
BH	 0.8960	 0.4310
BI	 0.8630	 0.3900
BJ	 0.8970	 0.4460
BK	 0.8340	 0.4270
BL	 0.8900	 0.4070
BM	 0.7410	 0.2980
BN	 0.8480	 0.2400
BO	 0.6980	 0.2980
BQ	 0.6250	 0.2100
BR	 0.5770	 0.1830
BS	 0.6030	 0.2320
BT	 0.8450	 0.2430
BU	 0.5190	 0.2370
BV	 0.5500	 0.2370
BW	 0.5320	 0.1500
BX	 0.3470	 0.1950
MA	 0.8640	 0.4180
Ma	 0.8990	 0.3970
Mb	 0.9160	 0.3680
Mc	 0.8960	 0.3620
Md	 0.8550	 0.3330
Me	 0.9140	 0.4380
Mf	 0.9010	 0.4190
Mg	 0.8440	 0.3400
Mh	 0.8840	 0.3670
Mi	 0.9180	 0.3830

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Chain	Atom inclusion	Q-score
Mj	 0.9100	 0.3250
Mk	 0.8240	 0.1930
MI	 0.7650	 0.2320
Mm	 0.6940	 0.1900
Mn	 0.8810	 0.3180
Mo	 0.8990	 0.4110
Mp	 0.5570	 0.2010
SA	 0.5400	 0.1880
SB	 0.8160	 0.2980
SC	 0.5890	 0.2480
SD	 0.7650	 0.3050
SE	 0.6530	 0.1930
SF	 0.8290	 0.3390
SG	 0.9320	 0.3550
SH	 0.8070	 0.3230
SI	 0.7890	 0.3550
SJ	 0.6150	 0.2250
SK	 0.7180	 0.2880
SL	 0.6790	 0.3040
T1	 0.8050	 0.2380
T2	 0.7070	 0.2030
T3	 0.7820	 0.3130
T4	 0.7170	 0.2140
T5	 0.5920	 0.2240
T6	 0.8220	 0.3420
mA	 0.8580	 0.4040
ma	 0.8900	 0.3760
mb	 0.9120	 0.3450
mc	 0.8890	 0.3430
md	 0.8460	 0.3120
me	 0.9030	 0.4140
mf	 0.8900	 0.3990
mg	 0.8300	 0.3190
mh	 0.8740	 0.3470
mi	 0.9050	 0.3610
mj	 0.9070	 0.3100
mk	 0.8220	 0.1840
ml	 0.7600	 0.2240
mm	 0.6880	 0.1840
mn	 0.8720	 0.3010
mo	 0.8910	 0.3880
mp	 0.5480	 0.1910

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Chain	Atom inclusion	Q-score
sA	 0.5240	 0.1800
sB	 0.8070	 0.2850
sC	 0.5700	 0.2390
sD	 0.7540	 0.2920
sE	 0.6480	 0.1870
sF	 0.8160	 0.3210
sG	 0.9280	 0.3460
sH	 0.7950	 0.3070
sI	 0.7650	 0.3360
sJ	 0.6090	 0.2190
sK	 0.7080	 0.2740
sL	 0.6640	 0.2870
t1	 0.7980	 0.2280
t2	 0.7020	 0.1940
t3	 0.7700	 0.2990
t4	 0.7030	 0.2070
t5	 0.5670	 0.2070
t6	 0.8080	 0.3240