



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 01:58 pm BST

PDB ID : 9TH8 / pdb_00009th8
EMDB ID : EMD-55918
Title : Cryo-EM structure of MCM2-7 DH bound to Sld3-Sld7, Cdc45 and DNA
Authors : Saleh, A.; Noguchi, Y.; Schneider, S.; Aramayo, R.; Speck, C.
Deposited on : 2025-12-03
Resolution : 2.90 Å(reported)
Based on initial models : 7PT6, 3WI3, 5BK4, 6U0M, 7P30, 3X38

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

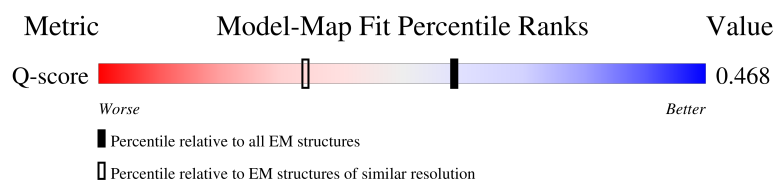
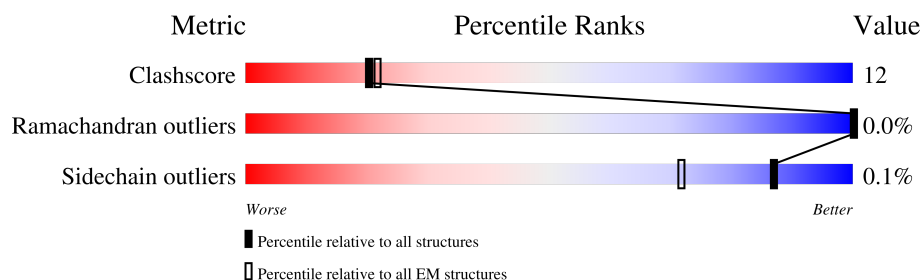
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



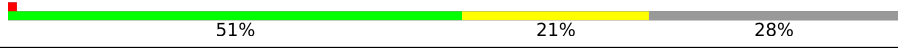
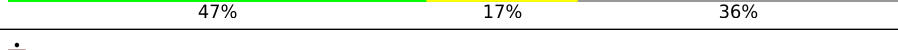
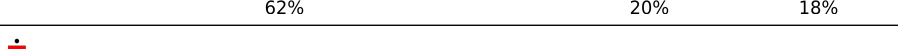
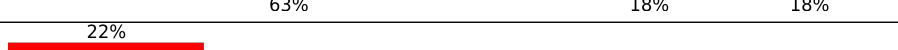
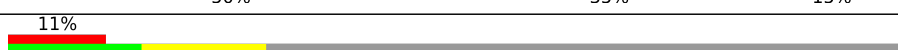
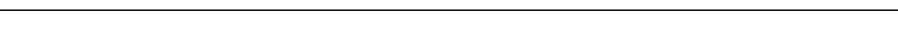
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	O	60	
2	S	60	
3	2	868	
3	B	868	

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Mol	Chain	Length	Quality of chain
4	3	971	
4	C	971	
5	4	933	
5	D	933	
6	5	775	
6	E	775	
7	6	1017	
7	F	1017	
8	7	845	
8	G	845	
9	X	668	
10	Z	650	
11	Y	257	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 72267 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 DNA chain called dsDNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	60	Total	C	N	O	P	0	0
			1230	585	225	360	60		

- Molecule 2 is a DNA chain called dsDNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	60	Total	C	N	O	P	0	0
			1230	585	225	360	60		

- Molecule 3 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	630	Total	C	N	O	S	0	0
			4989	3141	885	944	19		
3	2	630	Total	C	N	O	S	0	0
			4989	3141	885	944	19		

- Molecule 4 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	639	Total	C	N	O	S	0	0
			5009	3164	891	941	13		
4	3	639	Total	C	N	O	S	0	0
			5009	3164	891	941	13		

- Molecule 5 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	673	Total	C	N	O	S	0	0
			5358	3356	925	1047	30		
5	4	673	Total	C	N	O	S	0	0
			5358	3356	925	1047	30		

- Molecule 6 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	665	Total	C	N	O	S	0	0
			5197	3255	890	1027	25		
6	5	665	Total	C	N	O	S	0	0
			5197	3255	890	1027	25		

- Molecule 7 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	652	Total	C	N	O	S	0	0
			5160	3246	898	990	26		
7	6	652	Total	C	N	O	S	0	0
			5160	3246	898	990	26		

- Molecule 8 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	693	Total	C	N	O	S	0	0
			5457	3435	945	1047	30		
8	7	693	Total	C	N	O	S	0	0
			5457	3435	945	1047	30		

- Molecule 9 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	260	Total	C	N	O	S	0	0
			2148	1389	357	395	7		

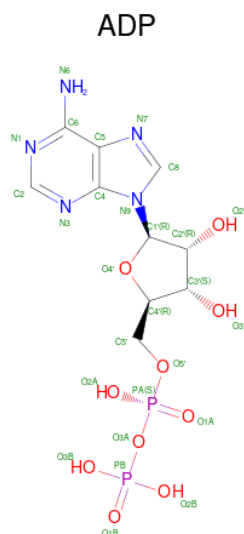
- Molecule 10 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	555	Total	C	N	O	S	0	0
			4493	2876	754	849	14		

- Molecule 11 is a protein called Mitochondrial morphogenesis protein SLD7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	74	Total	C	N	O	S	0	0
			600	370	108	121	1		

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 27	C 10	N 5	O 10	P 2	0
12	C	1	Total 27	C 10	N 5	O 10	P 2	0
12	E	1	Total 27	C 10	N 5	O 10	P 2	0
12	G	1	Total 27	C 10	N 5	O 10	P 2	0
12	2	1	Total 27	C 10	N 5	O 10	P 2	0
12	3	1	Total 27	C 10	N 5	O 10	P 2	0
12	5	1	Total 27	C 10	N 5	O 10	P 2	0
12	7	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total Zn 1 1	0
13	D	1	Total Zn 1 1	0
13	E	1	Total Zn 1 1	0

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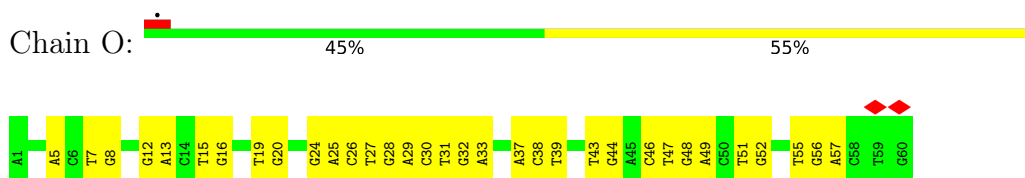
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Mol	Chain	Residues	Atoms		AltConf
13	F	1	Total 1	Zn 1	0
13	G	1	Total 1	Zn 1	0
13	2	1	Total 1	Zn 1	0
13	4	1	Total 1	Zn 1	0
13	5	1	Total 1	Zn 1	0
13	6	1	Total 1	Zn 1	0
13	7	1	Total 1	Zn 1	0

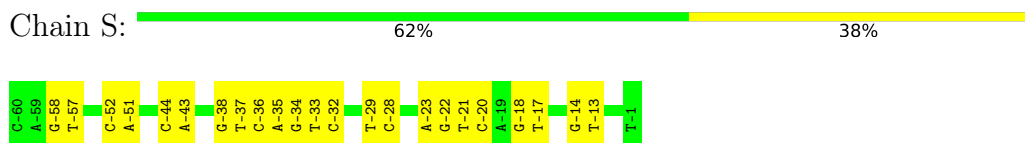
3 Residue-property plots

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

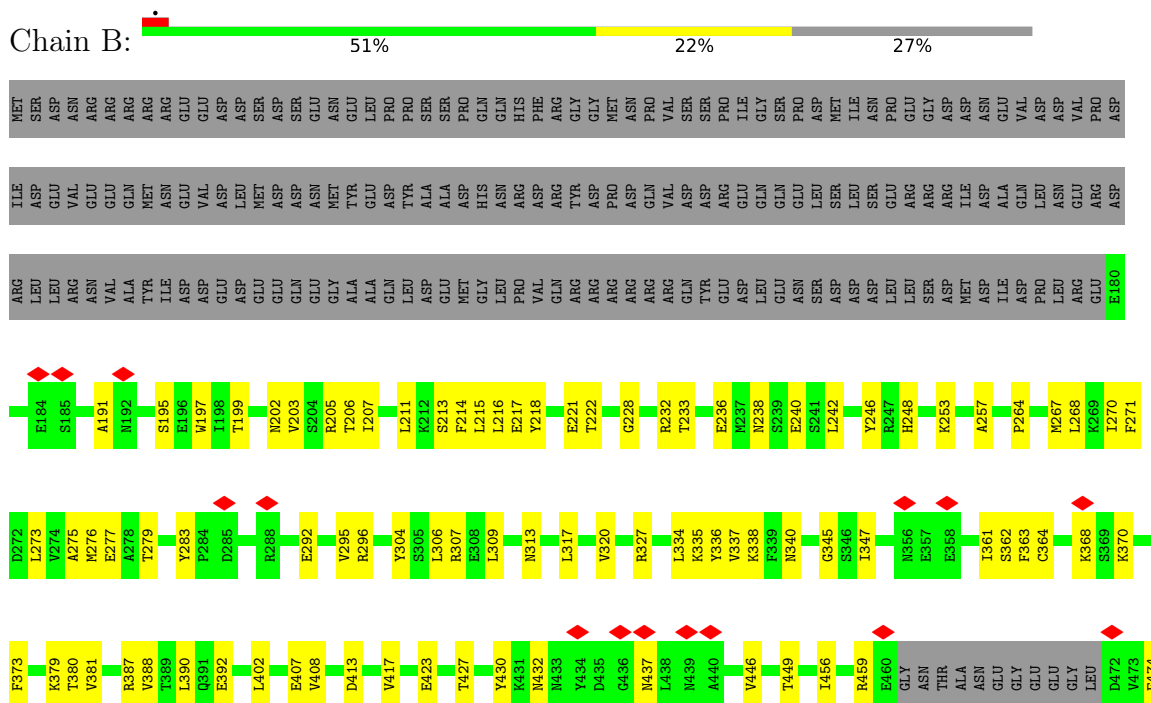
- Molecule 1: dsDNA (60-MER)



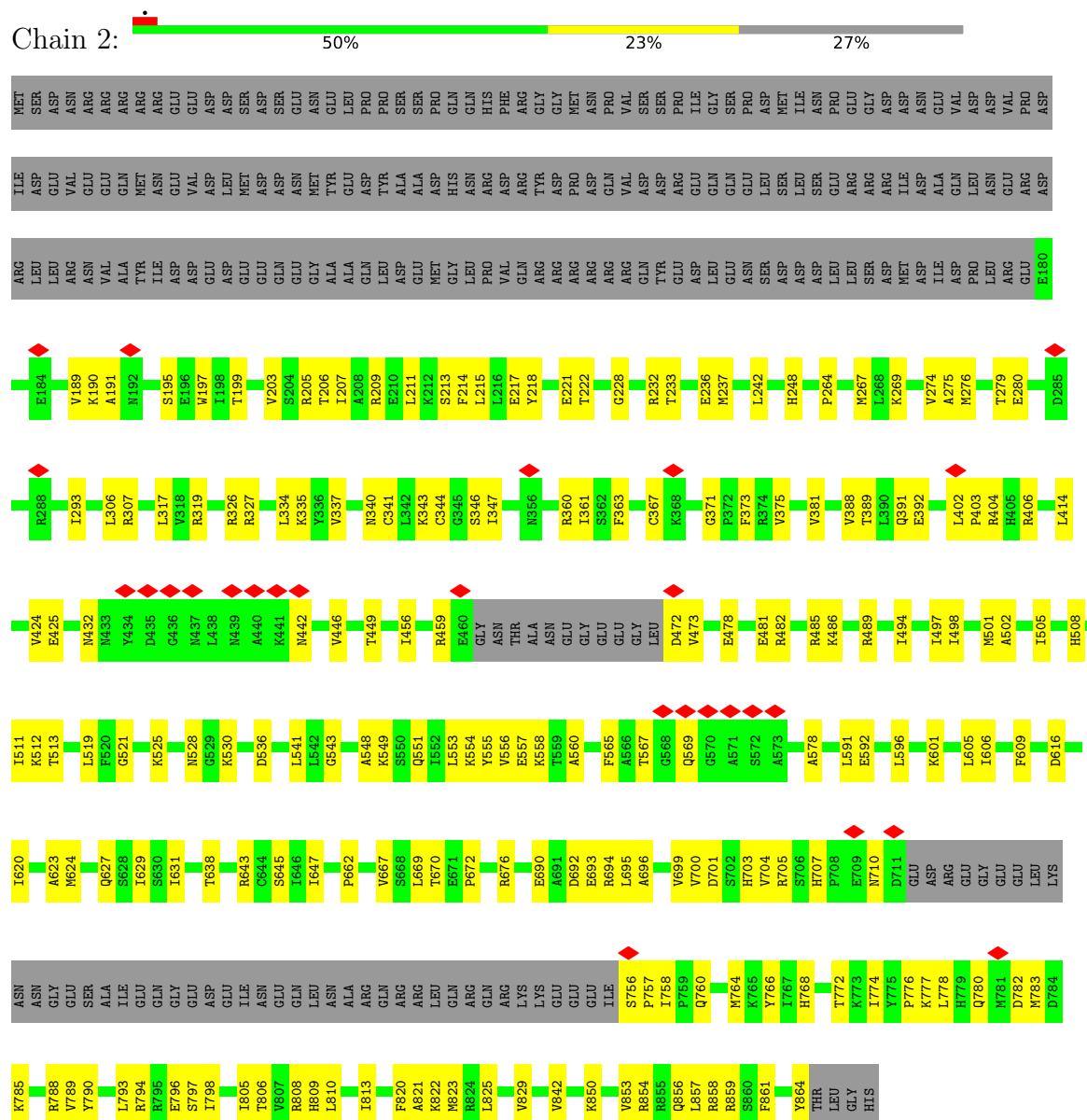
- Molecule 2: dsDNA (60-MER)



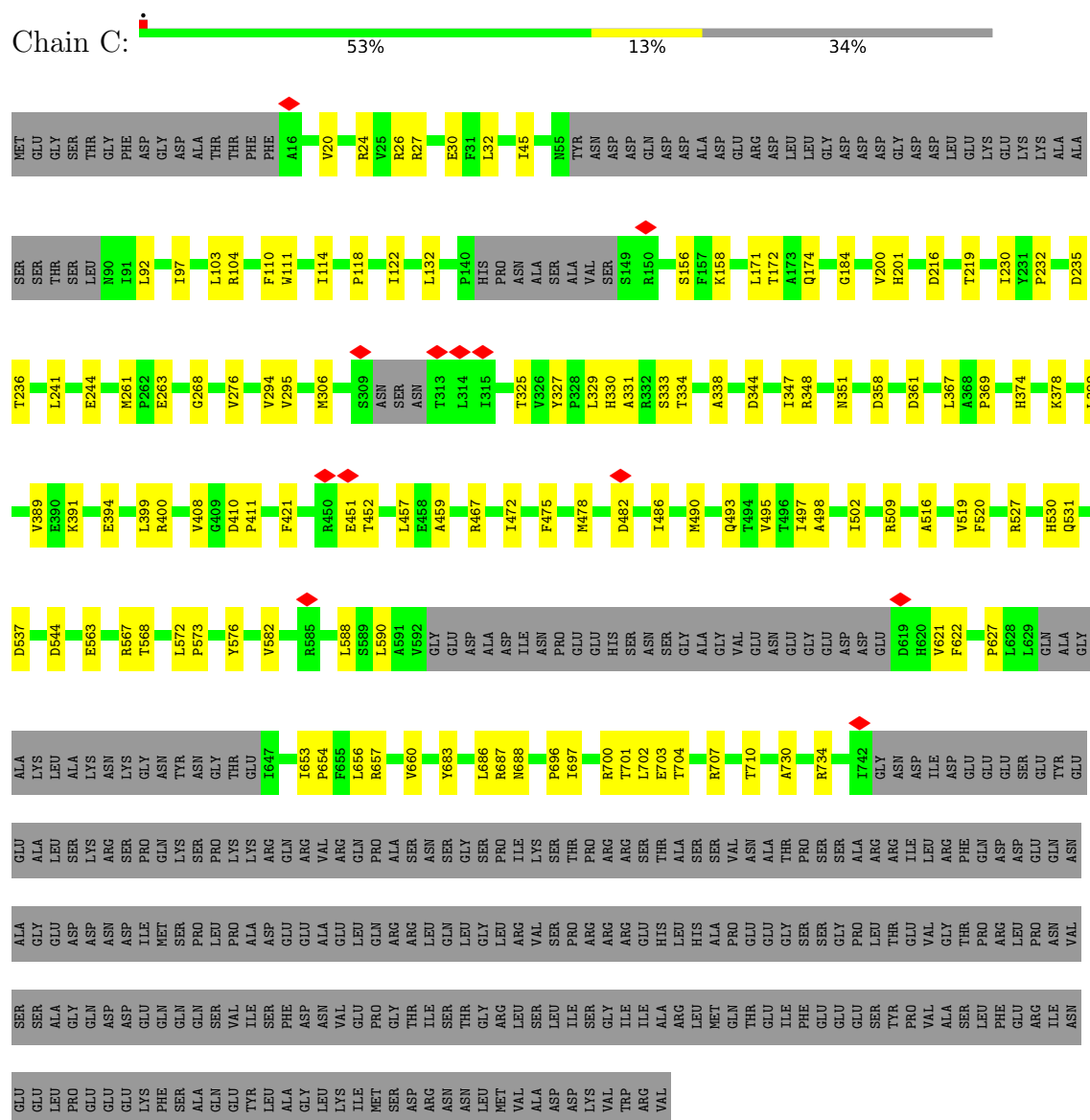
- Molecule 3: DNA replication licensing factor MCM2



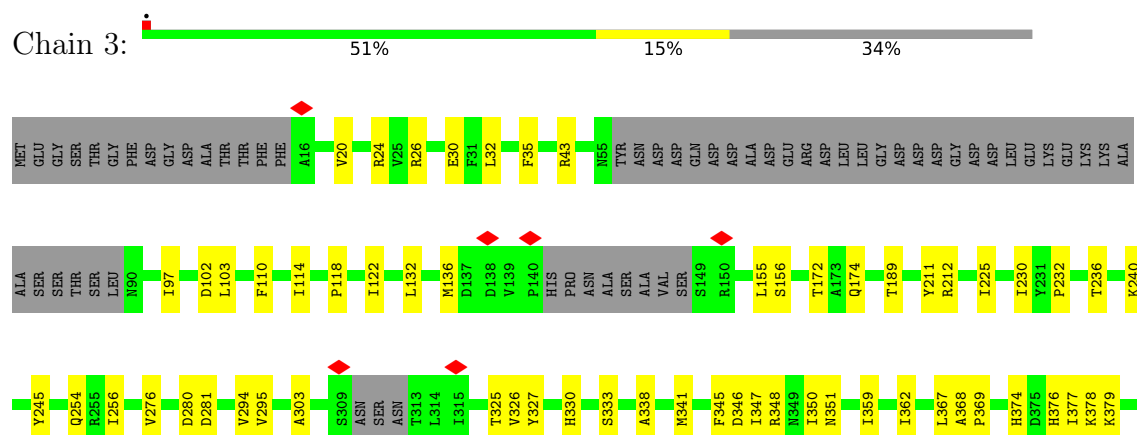
- Molecule 3: DNA replication licensing factor MCM2

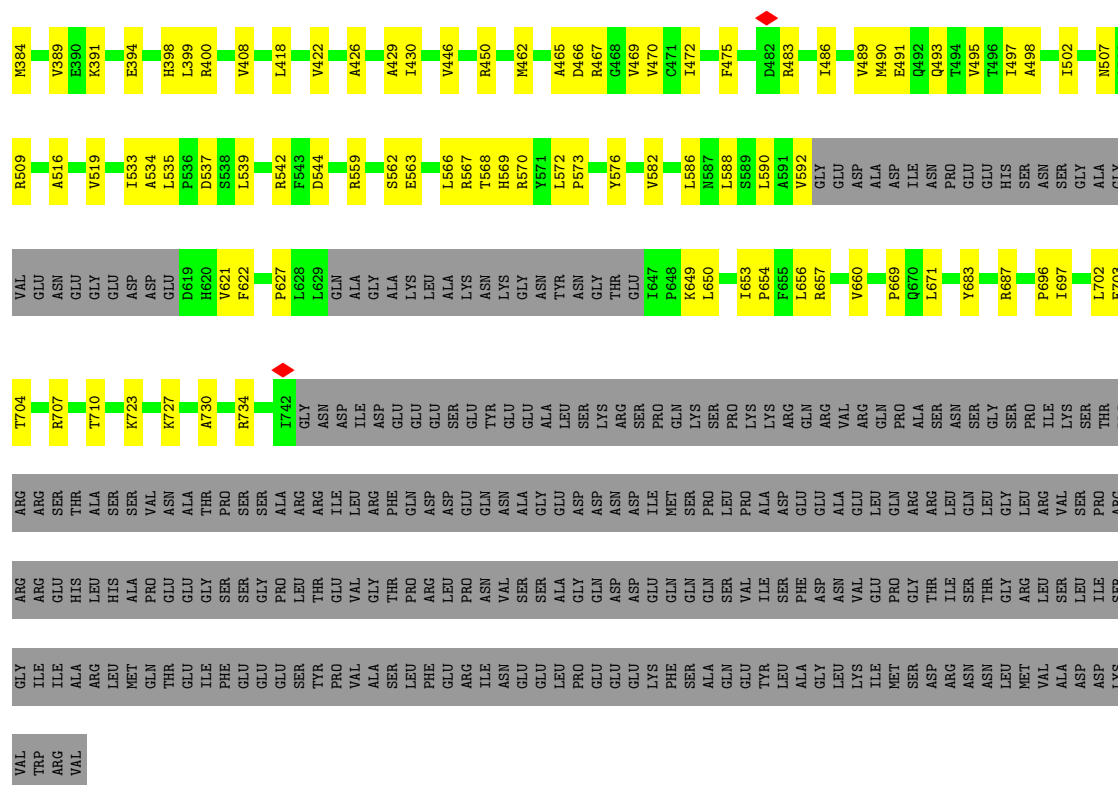


• Molecule 4: DNA replication licensing factor MCM3

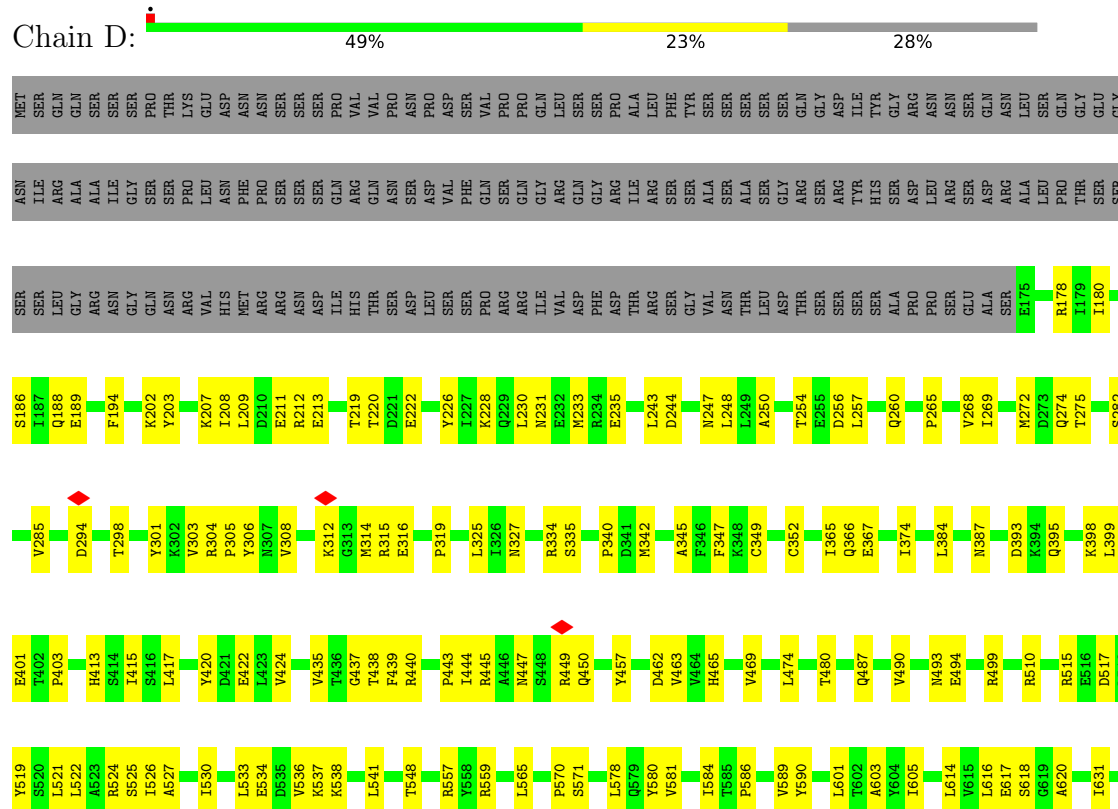


• Molecule 4: DNA replication licensing factor MCM3





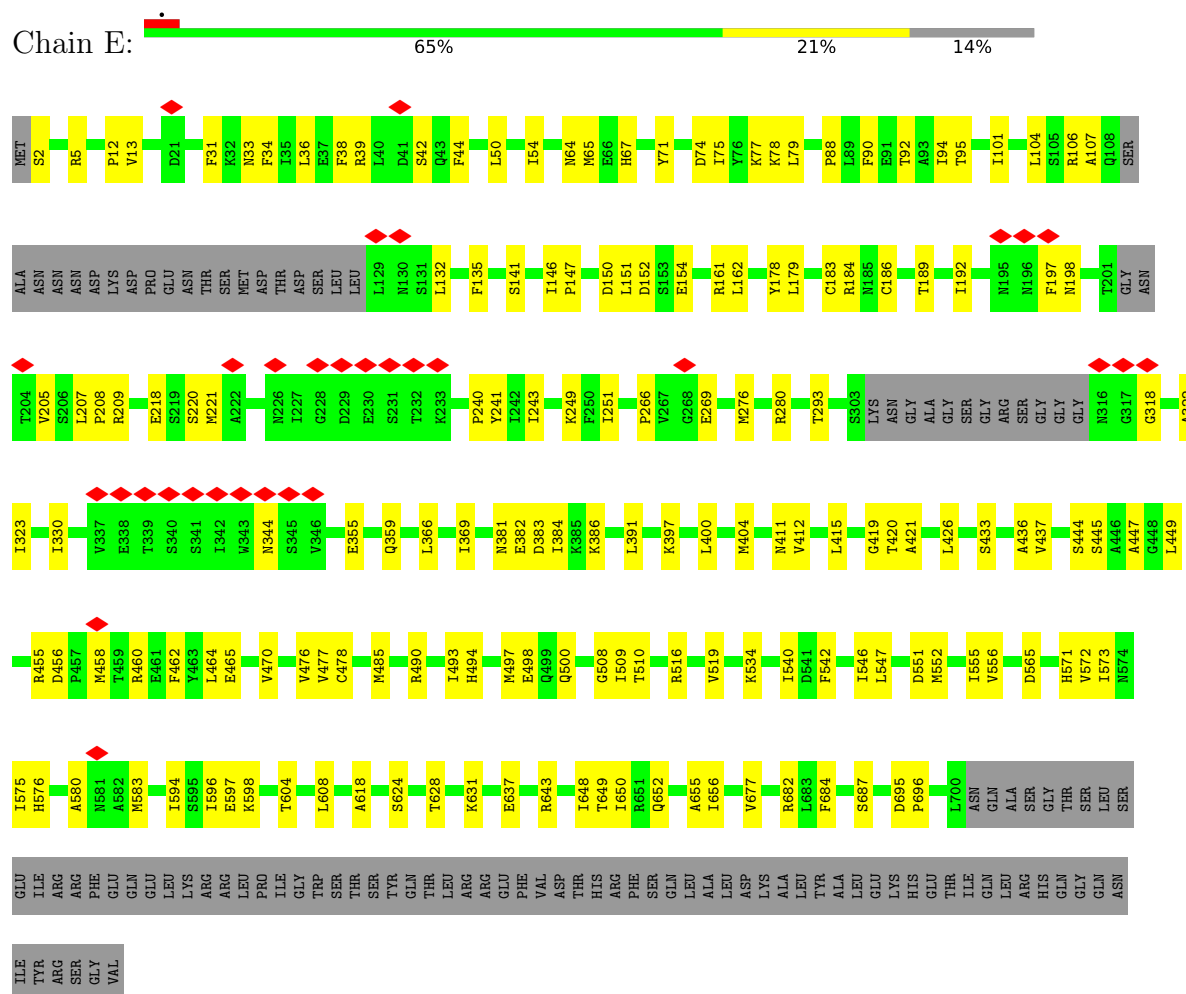
• Molecule 5: DNA replication licensing factor MCM4



GLY
VAL
ARG
ARG
SER
VAL
ARG
LEU
ASN
ARG
VAL

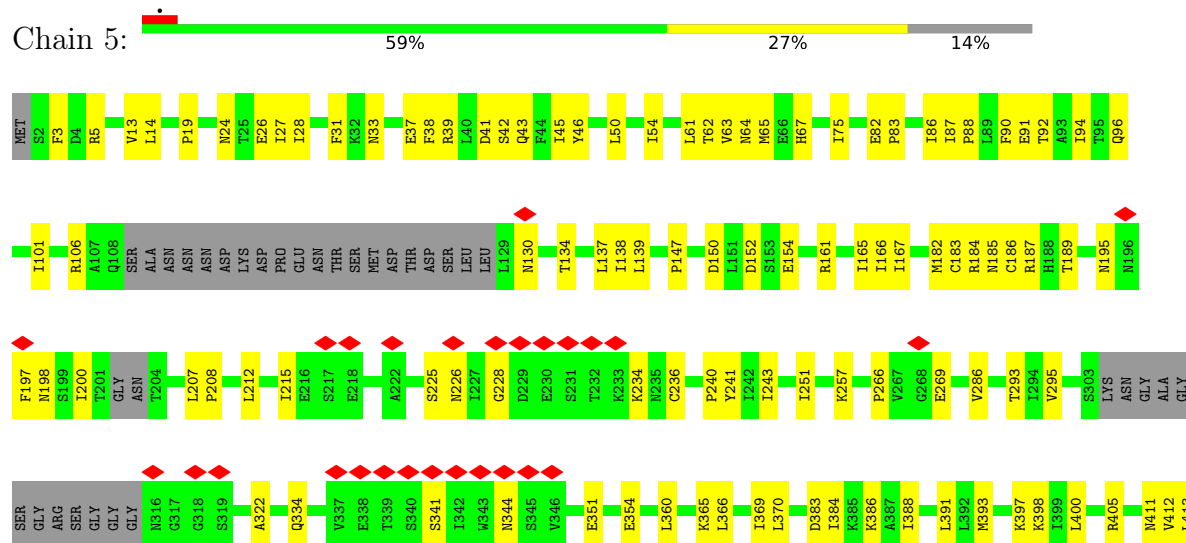
• Molecule 6: Minichromosome maintenance protein 5

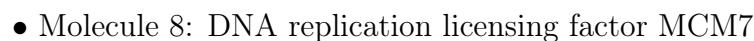
Chain E:

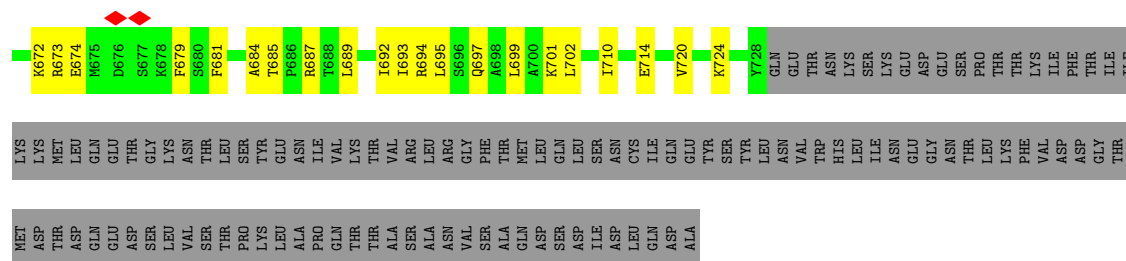


• Molecule 6: Minichromosome maintenance protein 5

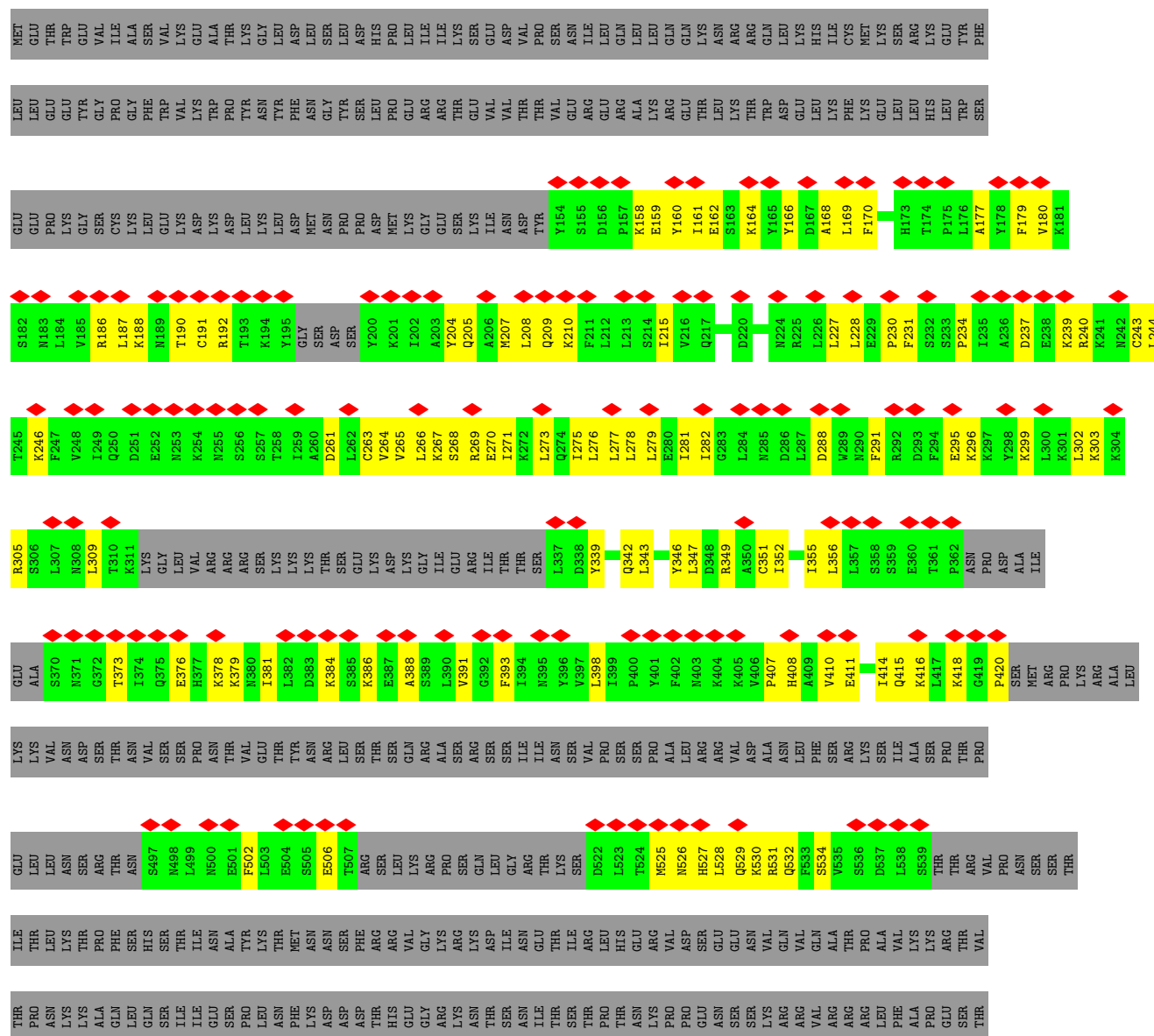
Chain 5:





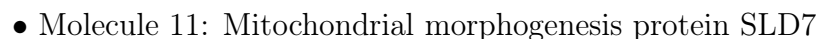


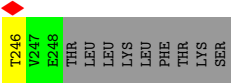
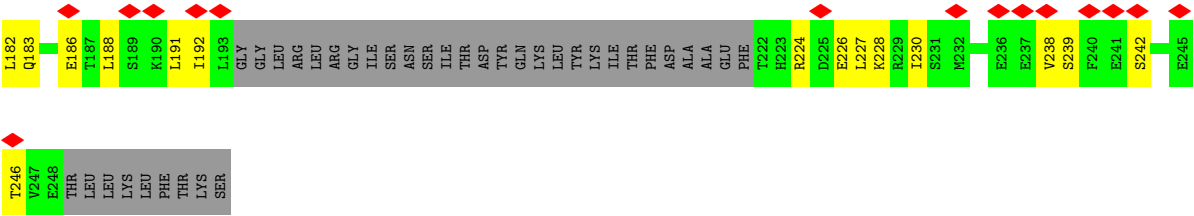
• Molecule 9: DNA replication regulator SLD3



• Molecule 10: Cell division control protein 45



[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	292336	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 ($e^-/\text{\AA}^2$)	58.4, 62.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	32.615	Depositor
Minimum map value	-16.285	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.984	Depositor
Recommended contour level	4.61	Depositor
Map size ($\text{\AA}$)	407.96002, 407.96002, 407.96002	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality

5.1 Standard geometry

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

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	O	0.16	0/1379	0.36	0/2126
2	S	0.18	0/1379	0.37	0/2126
3	2	0.15	0/5076	0.40	0/6859
3	B	0.15	0/5076	0.40	0/6859
4	3	0.14	0/5096	0.34	0/6910
4	C	0.13	0/5096	0.32	0/6910
5	4	0.15	0/5435	0.38	0/7347
5	D	0.15	0/5435	0.39	0/7347
6	5	0.15	0/5271	0.41	2/7129 (0.0%)
6	E	0.16	0/5271	0.40	0/7129
7	6	0.15	0/5240	0.39	0/7072
7	F	0.15	0/5240	0.40	0/7072
8	7	0.14	0/5541	0.36	0/7487
8	G	0.14	0/5541	0.35	0/7487
9	X	0.20	0/2183	0.51	0/2932
10	Z	0.17	0/4578	0.50	0/6199
11	Y	0.19	0/603	0.59	0/804
All	All	0.15	0/73440	0.39	2/99795 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	228	GLY	CA-C-N	5.41	131.86	121.54
6	5	228	GLY	C-N-CA	5.41	131.86	121.54

There are no chirality outliers.

There are no planarity outliers.

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	O	1230	0	676	26	0
2	S	1230	0	676	21	0
3	2	4989	0	5029	157	0
3	B	4989	0	5029	145	0
4	3	5009	0	5086	105	0
4	C	5009	0	5086	91	0
5	4	5358	0	5405	138	0
5	D	5358	0	5405	165	0
6	5	5197	0	5237	147	0
6	E	5197	0	5237	127	0
7	6	5160	0	5180	128	0
7	F	5160	0	5180	138	0
8	7	5457	0	5525	121	0
8	G	5457	0	5525	121	0
9	X	2148	0	2209	84	0
10	Z	4493	0	4489	181	0
11	Y	600	0	609	34	0
12	2	27	0	12	4	0
12	3	27	0	12	0	0
12	5	27	0	12	0	0
12	7	27	0	12	0	0
12	B	27	0	12	2	0
12	C	27	0	12	0	0
12	E	27	0	12	1	0
12	G	27	0	12	1	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	G	1	0	0	0	0
All	All	72267	0	71679	1749	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 12.

All (1749) 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)
5:D:781:GLY:HA2	5:D:790:ARG:HH22	1.32	0.94
5:D:571:SER:H	8:G:687:ARG:HH12	1.16	0.90
7:F:517:LYS:HE2	11:Y:153:ILE:HD13	1.56	0.87
4:C:156:SER:HB2	4:C:325:THR:HB	1.58	0.85
4:C:527:ARG:HD3	4:C:531:GLN:HE21	1.41	0.85
3:2:306:LEU:HB2	3:2:392:GLU:HG3	1.58	0.83
5:D:180:ILE:HD13	9:X:528:LEU:HD22	1.60	0.83
4:C:306:MET:HE1	6:E:179:LEU:HD11	1.59	0.83
2:S:-29:DT:H5"	6:E:209:ARG:HH22	1.46	0.81
6:E:161:ARG:HH21	6:E:293:THR:HG21	1.45	0.81
8:G:132:ILE:HG13	8:G:144:ASN:HD22	1.47	0.80
10:Z:78:ILE:HG13	10:Z:118:ARG:HH12	1.46	0.80
5:D:474:LEU:HD23	5:D:748:THR:HG23	1.64	0.79
6:5:161:ARG:HG2	6:5:295:VAL:HG22	1.63	0.79
10:Z:633:ARG:HE	10:Z:634:ARG:H	1.30	0.79
10:Z:328:LEU:HD21	10:Z:331:HIS:HB2	1.63	0.79
3:B:806:THR:HG22	3:B:808:ARG:H	1.47	0.78
10:Z:383:SER:HA	10:Z:386:ARG:HG2	1.64	0.78
10:Z:500:GLN:HB3	10:Z:504:ARG:NH1	1.99	0.77
5:D:718:ARG:HD3	8:G:665:ILE:HD11	1.66	0.77
5:4:349:CYS:HB3	5:4:352:CYS:HB2	1.68	0.76
10:Z:301:ARG:HG2	10:Z:302:LEU:HD12	1.68	0.76
5:4:522:LEU:HB3	5:4:541:LEU:HD11	1.68	0.75
7:F:519:MET:HE1	7:F:750:GLN:HB2	1.69	0.75
8:G:586:LEU:HB3	8:G:590:LEU:HD21	1.69	0.74
9:X:264:VAL:HA	9:X:267:LYS:HG2	1.69	0.74
4:3:156:SER:HB2	4:3:325:THR:HB	1.67	0.74
3:B:283:TYR:HE1	10:Z:364:ALA:HB1	1.52	0.74
6:5:185:ASN:HD22	6:5:236:CYS:HA	1.52	0.74
10:Z:546:LEU:HB2	10:Z:584:LEU:HD21	1.69	0.74
3:B:327:ARG:HG2	3:B:388:VAL:HG12	1.69	0.74
10:Z:74:LEU:HD13	10:Z:78:ILE:HD11	1.70	0.74
3:2:233:THR:HA	3:2:236:GLU:HG2	1.68	0.73
6:5:27:ILE:HG23	6:5:75:ILE:HD11	1.70	0.73
8:G:685:THR:HG22	8:G:687:ARG:H	1.53	0.73
10:Z:235:GLY:HA2	10:Z:238:GLU:HG2	1.70	0.73
8:7:61:PRO:HG2	8:7:64:MET:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:803:PHE:H	3:B:849:GLN:HE21	1.37	0.72
3:2:264:PRO:HG3	3:2:317:LEU:HB2	1.70	0.72
10:Z:250:SER:HB3	10:Z:280:LEU:HD11	1.71	0.72
5:D:474:LEU:HB2	5:D:586:PRO:HD3	1.72	0.72
6:E:383:ASP:HA	6:E:386:LYS:HD3	1.72	0.72
5:D:366:GLN:HE22	8:G:297:GLN:HG3	1.54	0.72
10:Z:100:PRO:HA	10:Z:103:TYR:HD1	1.55	0.72
8:G:581:LEU:HD21	8:G:591:LEU:HD13	1.71	0.71
7:6:497:ASN:HB3	7:6:503:VAL:HG11	1.72	0.71
4:3:491:GLU:HG3	4:3:542:ARG:HH11	1.55	0.71
7:F:348:VAL:HG13	7:F:349:THR:HG23	1.70	0.71
6:E:77:LYS:HZ1	10:Z:382:HIS:H	1.39	0.71
5:4:618:SER:HA	7:6:373:MET:HE3	1.70	0.71
7:6:340:ASN:HD21	7:6:343:PHE:HB2	1.55	0.71
10:Z:153:GLY:HA2	10:Z:156:LYS:HE2	1.71	0.71
10:Z:538:LEU:HD21	10:Z:574:GLU:H	1.56	0.71
10:Z:92:LEU:HD23	10:Z:140:ILE:HG21	1.73	0.70
5:D:571:SER:N	8:G:687:ARG:HH12	1.88	0.70
4:3:367:LEU:HD23	4:3:656:LEU:HD11	1.73	0.70
10:Z:3:TYR:HD1	10:Z:7:GLN:HB3	1.56	0.70
6:5:50:LEU:HD22	6:5:101:ILE:HD12	1.74	0.70
6:5:13:VAL:HG23	6:5:14:LEU:HG	1.73	0.70
7:6:304:LEU:HG	7:6:323:GLN:HG2	1.73	0.70
8:7:206:PRO:HD3	8:7:352:THR:HG21	1.73	0.70
9:X:264:VAL:HG13	9:X:378:LYS:NZ	2.07	0.70
4:3:723:LYS:HE3	4:3:727:LYS:HE3	1.73	0.70
6:5:405:ARG:HH12	6:5:500:GLN:HB2	1.56	0.70
11:Y:162:GLN:HA	11:Y:165:ILE:HG12	1.74	0.69
10:Z:26:GLN:HA	10:Z:78:ILE:HG22	1.74	0.69
7:F:517:LYS:HA	7:F:520:VAL:HG22	1.72	0.69
10:Z:521:HIS:HB3	10:Z:562:LYS:HE3	1.75	0.69
5:D:219:THR:HG23	5:D:220:THR:HG23	1.74	0.69
7:6:737:LYS:HD3	7:6:740:GLU:HB3	1.75	0.69
6:E:266:PRO:HG2	6:E:269:GLU:HB3	1.75	0.69
8:G:590:LEU:HB2	8:G:594:PHE:CE2	2.27	0.69
5:D:589:VAL:HG21	5:D:620:ALA:HB1	1.75	0.68
5:4:330:GLY:HA3	5:4:399:LEU:HD21	1.74	0.68
5:4:515:ARG:HG2	5:4:517:ASP:H	1.58	0.68
8:7:589:ALA:HB1	8:7:593:ARG:HH21	1.58	0.68
10:Z:621:ARG:HH22	10:Z:630:ILE:HD12	1.58	0.68
5:4:234:ARG:HD3	5:4:284:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:806:THR:HG21	3:B:808:ARG:HE	1.59	0.68
5:D:178:ARG:HB2	5:D:188:GLN:HE22	1.58	0.68
3:2:690:GLU:HA	3:2:693:GLU:HG2	1.76	0.68
10:Z:331:HIS:HE1	10:Z:419:ILE:HD13	1.59	0.68
7:F:508:LEU:HD23	7:F:512:GLU:HG3	1.76	0.68
5:D:515:ARG:HG2	5:D:517:ASP:H	1.59	0.67
6:5:266:PRO:HG2	6:5:269:GLU:HB3	1.75	0.67
10:Z:388:LEU:HA	10:Z:391:ILE:HG12	1.74	0.67
5:D:480:THR:HG22	7:F:370:THR:HG21	1.76	0.67
8:7:396:ASP:HB2	8:7:400:ARG:HH12	1.59	0.67
8:G:578:LEU:HD22	8:G:583:ASN:HB3	1.76	0.67
6:E:411:ASN:HD22	6:E:519:VAL:H	1.42	0.67
5:D:304:ARG:HB3	5:D:465:HIS:HB2	1.77	0.67
5:4:219:THR:HG23	5:4:220:THR:HG23	1.76	0.67
9:X:378:LYS:HA	9:X:381:ILE:HG22	1.76	0.67
3:2:809:HIS:O	3:2:813:ILE:HG13	1.94	0.67
7:6:773:LEU:HD21	7:6:804:ILE:HG12	1.76	0.66
3:B:667:VAL:HG12	3:B:669:LEU:H	1.59	0.66
3:2:789:VAL:HG13	3:2:864:TYR:HE2	1.61	0.66
5:4:251:TYR:HB3	5:4:254:THR:HG22	1.76	0.66
2:S:-18:DG:H2"	2:S:-17:DT:H5"	1.78	0.66
3:B:334:LEU:HG	6:E:322:ALA:HB1	1.78	0.66
3:B:854:ARG:HG3	3:B:858:ARG:HH12	1.59	0.66
4:C:367:LEU:HD23	4:C:656:LEU:HD11	1.78	0.66
7:F:591:PHE:HZ	7:F:751:LEU:HD22	1.61	0.66
8:G:444:VAL:HG12	8:G:446:ASP:H	1.60	0.66
7:6:800:LEU:O	7:6:804:ILE:HG13	1.95	0.66
3:B:211:LEU:HD13	3:B:271:PHE:HD1	1.61	0.66
6:E:542:PHE:HB2	6:E:546:ILE:HD12	1.78	0.66
7:6:773:LEU:HD12	7:6:803:MET:HE2	1.77	0.66
9:X:240:ARG:HH21	9:X:244:LEU:HB3	1.60	0.66
5:4:769:GLU:HG3	5:4:819:LEU:HD13	1.77	0.65
3:B:605:LEU:HD23	3:B:647:ILE:HB	1.78	0.65
8:G:230:ILE:HD12	8:G:239:ILE:HD12	1.79	0.65
4:3:391:LYS:HB2	4:3:399:LEU:HB2	1.79	0.65
8:G:432:LEU:HD23	8:G:473:ILE:HG13	1.78	0.65
5:4:589:VAL:HG21	5:4:620:ALA:HB1	1.77	0.65
5:4:712:VAL:HG22	8:7:672:LYS:HZ2	1.60	0.65
10:Z:513:ILE:HG23	10:Z:518:LEU:HB2	1.77	0.65
4:3:669:PRO:HG2	4:3:710:THR:HG23	1.77	0.65
4:3:462:MET:HG2	4:3:470:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:487:ASN:C	7:F:487:ASN:HD22	2.03	0.65
11:Y:226:GLU:HG2	11:Y:238:VAL:HG22	1.79	0.65
3:2:233:THR:HB	3:2:237:MET:HE1	1.79	0.65
5:4:841:LYS:HG3	5:4:842:THR:HG23	1.79	0.65
6:E:147:PRO:HG2	6:E:150:ASP:HB2	1.78	0.65
5:4:373:ARG:HD3	5:4:375:ASP:HB2	1.79	0.65
10:Z:354:ASN:HA	10:Z:357:LYS:HG2	1.79	0.65
3:B:486:LYS:HA	3:B:489:ARG:HD2	1.79	0.64
6:E:2:SER:HA	6:E:221:MET:HG2	1.79	0.64
7:F:518:GLU:HA	7:F:521:LYS:HE3	1.79	0.64
4:3:486:ILE:O	4:3:490:MET:HG2	1.97	0.64
3:B:488:SER:HB2	3:B:825:LEU:HD12	1.78	0.64
8:7:230:ILE:HD12	8:7:239:ILE:HD12	1.80	0.64
8:7:652:MET:HE2	8:7:657:ASN:HB3	1.79	0.64
5:D:701:ARG:HH21	5:D:796:ARG:HD3	1.63	0.64
6:E:411:ASN:ND2	6:E:519:VAL:HG12	2.12	0.64
10:Z:567:MET:HE1	10:Z:569:LEU:HB2	1.79	0.64
7:F:521:LYS:HB3	11:Y:149:LYS:HZ1	1.60	0.64
8:G:161:ILE:HD12	8:G:185:VAL:HG12	1.78	0.64
7:6:199:THR:HA	7:6:261:ARG:HE	1.62	0.64
6:E:624:SER:O	6:E:628:THR:HG23	1.98	0.64
6:5:152:ASP:HB3	6:5:154:GLU:HG2	1.80	0.64
10:Z:272:LEU:HD23	10:Z:275:LEU:HD12	1.80	0.64
10:Z:321:GLN:HE22	10:Z:323:ASP:HB3	1.63	0.64
5:4:471:ASP:HB2	5:4:745:GLU:HG2	1.80	0.64
5:4:602:THR:HG22	5:4:654:ILE:HD13	1.78	0.64
9:X:420:PRO:HA	10:Z:521:HIS:CE1	2.32	0.64
8:7:542:GLU:HG3	8:7:543:GLN:HG3	1.80	0.63
5:D:268:VAL:O	5:D:272:MET:HG3	1.97	0.63
5:D:794:THR:HG21	7:F:578:SER:HB3	1.79	0.63
9:X:349:ARG:HA	9:X:352:ILE:HG22	1.80	0.63
5:D:401:GLU:HG2	5:D:403:PRO:HD3	1.80	0.63
3:2:189:VAL:HG22	3:2:191:ALA:H	1.62	0.63
3:2:766:TYR:HE2	3:2:825:LEU:HD11	1.61	0.63
5:4:692:ILE:HG21	5:4:699:LEU:HD21	1.81	0.63
8:7:485:GLY:HA2	8:7:529:MET:HE3	1.80	0.63
8:G:581:LEU:HD12	8:G:678:LYS:HE3	1.81	0.63
5:D:422:GLU:HB2	5:D:493:ASN:HA	1.81	0.63
1:O:31:DT:H2"	1:O:32:DG:C8	2.33	0.63
7:F:800:LEU:O	7:F:804:ILE:HG13	1.98	0.63
3:B:402:LEU:HD23	7:F:391:PRO:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:590:LEU:HB2	8:G:594:PHE:HE2	1.63	0.63
3:2:850:LYS:O	3:2:854:ARG:HG2	1.99	0.63
9:X:420:PRO:HA	10:Z:521:HIS:HE1	1.63	0.63
5:4:348:LYS:HG2	5:4:385:ILE:HD11	1.80	0.62
8:7:452:GLY:H	8:7:694:ARG:NH1	1.97	0.62
5:D:601:LEU:HD23	5:D:620:ALA:HB3	1.81	0.62
8:G:396:ASP:HB2	8:G:400:ARG:HH12	1.64	0.62
3:2:424:VAL:HG22	3:2:425:GLU:H	1.64	0.62
5:4:794:THR:HG22	5:4:796:ARG:H	1.63	0.62
6:5:182:MET:HE2	6:5:187:ARG:HE	1.64	0.62
4:3:563:GLU:O	4:3:567:ARG:HG3	1.99	0.62
8:7:685:THR:HG22	8:7:687:ARG:H	1.65	0.62
6:E:50:LEU:HD22	6:E:101:ILE:HD12	1.80	0.62
7:F:596:VAL:HG12	7:F:631:ALA:HB2	1.81	0.62
8:G:359:PRO:HD3	6:5:3:PHE:HE2	1.63	0.62
9:X:205:GLN:O	9:X:209:GLN:HG2	1.99	0.62
3:B:271:PHE:HE2	3:B:295:VAL:HG11	1.64	0.62
6:E:650:ILE:H	6:E:650:ILE:HD12	1.64	0.62
8:G:452:GLY:H	8:G:694:ARG:HH12	1.45	0.62
9:X:386:LYS:HD3	9:X:388:ALA:H	1.65	0.62
5:D:571:SER:H	8:G:687:ARG:NH1	1.92	0.62
5:4:457:TYR:HB2	8:7:253:PRO:HG2	1.82	0.62
6:5:197:PHE:HD2	6:5:200:ILE:HD11	1.65	0.62
7:6:144:LYS:HA	7:6:196:LEU:HD13	1.80	0.62
5:D:457:TYR:HB2	8:G:253:PRO:HG2	1.80	0.62
6:5:420:THR:HG21	6:5:556:VAL:HG21	1.82	0.62
7:6:711:LEU:HD11	7:6:806:LEU:HD11	1.82	0.62
10:Z:434:VAL:HB	10:Z:498:LEU:HD21	1.82	0.62
4:C:486:ILE:O	4:C:490:MET:HG2	2.00	0.62
6:E:618:ALA:HB1	6:E:677:VAL:HG21	1.82	0.62
8:G:538:HIS:HD2	8:G:593:ARG:HD2	1.65	0.62
4:C:563:GLU:O	4:C:567:ARG:HG3	2.00	0.62
3:2:402:LEU:HD23	7:6:629:MET:HE1	1.80	0.62
10:Z:247:VAL:H	10:Z:284:TYR:HE2	1.47	0.62
6:E:5:ARG:HB3	4:3:240:LYS:HE2	1.82	0.61
3:2:662:PRO:HG3	3:2:850:LYS:HZ3	1.64	0.61
8:7:139:LEU:O	8:7:143:LEU:HG	2.00	0.61
8:7:443:ARG:HH12	8:7:447:GLY:HA2	1.65	0.61
9:X:351:CYS:O	9:X:355:ILE:HD12	2.00	0.61
3:B:337:VAL:HA	3:B:380:THR:HG23	1.82	0.61
8:7:668:ARG:HD2	8:7:684:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:621:VAL:HG23	4:3:622:PHE:HD1	1.64	0.61
6:5:50:LEU:O	6:5:54:ILE:HG12	2.01	0.61
6:5:161:ARG:HH21	6:5:293:THR:HG21	1.64	0.61
5:D:522:LEU:HB3	5:D:541:LEU:HD11	1.82	0.61
7:6:504:PHE:HD1	7:6:505:LEU:HD22	1.65	0.61
8:G:497:VAL:HG22	8:G:506:MET:HE3	1.81	0.61
3:2:854:ARG:HA	3:2:857:LEU:HB2	1.82	0.61
7:6:707:SER:HB2	7:6:798:ARG:NH1	2.15	0.61
8:7:452:GLY:H	8:7:694:ARG:HH12	1.48	0.61
7:F:312:ASP:HB2	7:F:343:PHE:HB3	1.82	0.61
11:Y:158:GLN:HA	11:Y:161:GLN:HG3	1.81	0.61
5:D:208:ILE:HA	5:D:213:GLU:HG3	1.83	0.61
5:4:666:ASN:O	5:4:666:ASN:ND2	2.33	0.61
8:7:495:ALA:HA	8:7:509:GLU:O	2.00	0.61
6:E:497:MET:HE2	6:E:519:VAL:HG11	1.83	0.61
5:4:198:LEU:HD11	5:4:276:ILE:HG12	1.81	0.61
7:F:275:ARG:HG2	7:F:278:ASP:OD2	2.00	0.60
3:2:343:LYS:NZ	3:2:371:GLY:HA3	2.16	0.60
4:3:400:ARG:HG3	4:3:493:GLN:NE2	2.15	0.60
6:5:370:LEU:HD12	6:5:666:LEU:HD11	1.82	0.60
6:E:186:CYS:HB2	4:3:230:ILE:HG23	1.82	0.60
8:G:206:PRO:HD3	8:G:352:THR:HG21	1.83	0.60
6:5:226:ASN:HA	6:5:234:LYS:HE3	1.83	0.60
1:O:38:DC:H1'	5:D:449:ARG:HH21	1.66	0.60
6:E:580:ALA:HA	6:E:583:MET:HE2	1.82	0.60
8:G:139:LEU:O	8:G:143:LEU:HG	2.01	0.60
3:2:191:ALA:HB3	3:2:197:TRP:HB2	1.84	0.60
6:E:104:LEU:HD12	8:7:166:LEU:HB2	1.84	0.60
5:D:306:TYR:HB3	5:D:465:HIS:ND1	2.16	0.60
8:G:363:PHE:HB2	8:G:366:LEU:HD12	1.84	0.60
8:G:621:MET:HE3	8:G:622:HIS:ND1	2.17	0.60
3:2:555:TYR:HD1	3:2:558:LYS:HE2	1.66	0.60
5:D:334:ARG:HG2	5:D:398:LYS:HB3	1.81	0.60
6:E:50:LEU:O	6:E:54:ILE:HG12	2.01	0.60
6:E:433:SER:HB3	6:E:436:ALA:HB2	1.83	0.60
8:G:537:ILE:HG22	8:G:541:MET:HE2	1.82	0.60
3:2:478:GLU:O	3:2:481:GLU:HG3	2.02	0.60
1:O:46:DC:H2'	1:O:47:DT:H71	1.84	0.60
4:C:276:VAL:HG11	4:C:294:VAL:HG11	1.84	0.60
6:5:618:ALA:HB1	6:5:677:VAL:HG21	1.82	0.60
10:Z:471:LYS:HA	10:Z:474:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:530:ILE:HD11	8:7:448:MET:HE2	1.83	0.59
8:G:575:ASN:HB3	8:G:583:ASN:HD22	1.67	0.59
3:2:557:GLU:OE2	3:2:565:PHE:HB2	2.02	0.59
4:3:327:TYR:HB3	4:3:590:LEU:HD11	1.84	0.59
6:5:571:HIS:O	6:5:575:ILE:HD12	2.02	0.59
5:D:186:SER:HB3	5:D:189:GLU:HB3	1.83	0.59
8:G:228:ARG:HG2	8:G:329:ARG:HD2	1.83	0.59
4:C:683:TYR:CZ	4:C:687:ARG:HD2	2.38	0.59
3:B:306:LEU:HD11	3:B:390:LEU:HD23	1.84	0.59
5:D:212:ARG:HG2	5:D:212:ARG:O	2.03	0.59
3:2:494:ILE:O	3:2:498:ILE:HG13	2.02	0.59
4:3:730:ALA:O	4:3:734:ARG:HG2	2.01	0.59
9:X:279:LEU:HD23	9:X:398:LEU:HD22	1.83	0.59
3:B:307:ARG:HD2	7:F:493:VAL:HG11	1.84	0.59
3:2:334:LEU:HD12	6:5:322:ALA:HB1	1.85	0.59
3:2:446:VAL:HG22	7:6:303:GLU:HB3	1.84	0.59
3:B:213:SER:O	3:B:217:GLU:HG3	2.03	0.59
8:G:567:ALA:HB3	8:G:586:LEU:HD11	1.85	0.59
6:5:542:PHE:HB2	6:5:546:ILE:HD12	1.85	0.59
8:7:162:ARG:HE	8:7:181:LEU:HD22	1.67	0.59
6:5:551:ASP:HB3	6:5:655:ALA:HB1	1.83	0.59
5:D:334:ARG:NE	5:D:398:LYS:HD2	2.17	0.59
7:F:156:GLN:O	7:F:160:MET:HG3	2.03	0.59
3:B:338:LYS:HD3	3:B:379:LYS:HB3	1.85	0.59
4:3:507:ASN:HD21	4:3:509:ARG:NH1	2.01	0.59
8:7:664:TYR:CD2	8:7:689:LEU:HB2	2.38	0.59
8:G:495:ALA:HB2	8:G:510:GLY:HA2	1.85	0.58
3:B:766:TYR:HE1	3:B:825:LEU:HD11	1.67	0.58
5:D:445:ARG:HB2	7:F:410:LEU:HD11	1.83	0.58
6:E:152:ASP:HB3	6:E:154:GLU:HG2	1.84	0.58
7:F:808:GLU:O	7:F:812:ARG:HG3	2.02	0.58
5:4:345:ALA:HB2	5:4:365:ILE:HD13	1.84	0.58
4:C:498:ALA:HB3	8:G:488:SER:HB2	1.84	0.58
5:D:618:SER:HA	7:F:373:MET:HE3	1.84	0.58
8:G:589:ALA:HB1	8:G:593:ARG:HH12	1.68	0.58
9:X:346:TYR:HA	9:X:349:ARG:HE	1.68	0.58
4:3:466:ASP:HB3	8:7:324:VAL:HG13	1.84	0.58
8:7:615:HIS:O	8:7:619:VAL:HG23	2.03	0.58
10:Z:469:LEU:HB3	10:Z:473:TRP:CZ3	2.38	0.58
10:Z:233:TYR:CE2	10:Z:237:LEU:HD21	2.38	0.58
1:O:56:DG:H2"	1:O:57:DA:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:327:TYR:HB3	4:C:590:LEU:HD11	1.85	0.58
6:E:39:ARG:HG2	10:Z:313:PRO:HG3	1.86	0.58
8:G:538:HIS:CD2	8:G:593:ARG:HD2	2.38	0.58
6:5:147:PRO:HG2	6:5:150:ASP:HB2	1.86	0.58
11:Y:227:LEU:HD13	11:Y:230:ILE:HD11	1.86	0.58
4:C:687:ARG:HH22	8:G:602:ASP:HB2	1.69	0.58
4:3:430:ILE:HD12	4:3:465:ALA:HB2	1.85	0.58
5:4:256:ASP:O	5:4:260:GLN:HG3	2.03	0.58
4:3:572:LEU:HD12	4:3:573:PRO:HD2	1.84	0.58
6:E:571:HIS:O	6:E:575:ILE:HD12	2.04	0.58
4:3:559:ARG:HH21	6:5:624:SER:HA	1.68	0.58
11:Y:159:GLN:O	11:Y:163:ARG:HG2	2.04	0.58
8:G:82:LEU:HD12	8:G:206:PRO:HA	1.85	0.58
4:3:703:GLU:O	4:3:707:ARG:HG3	2.04	0.58
5:4:465:HIS:HE1	5:4:467:LYS:HB2	1.69	0.58
5:4:688:VAL:O	5:4:692:ILE:HG12	2.04	0.58
10:Z:524:ILE:HG23	10:Z:525:TYR:CD1	2.39	0.58
10:Z:639:PRO:O	10:Z:643:LYS:HG2	2.04	0.58
3:2:707:HIS:HA	7:6:557:LYS:HG2	1.86	0.57
4:3:544:ASP:HB3	4:3:704:THR:HG23	1.85	0.57
5:4:527:ALA:HB1	5:4:530:ILE:HD12	1.84	0.57
2:S:-29:DT:H2"	2:S:-28:DC:C6	2.40	0.57
4:C:295:VAL:HB	4:C:325:THR:HG22	1.85	0.57
7:F:623:ILE:HD12	7:F:672:LEU:HD21	1.84	0.57
3:2:203:VAL:O	3:2:207:ILE:HG12	2.04	0.57
8:7:541:MET:HE1	8:7:594:PHE:CE2	2.39	0.57
10:Z:566:PRO:HA	10:Z:586:PRO:HD3	1.87	0.57
4:C:582:VAL:HG23	6:E:397:LYS:HZ2	1.68	0.57
6:E:444:SER:HB3	6:E:447:ALA:HB3	1.86	0.57
3:2:497:ILE:HG22	3:2:758:ILE:HD12	1.87	0.57
3:B:264:PRO:HG3	3:B:317:LEU:HB2	1.87	0.57
3:2:693:GLU:OE2	7:6:778:LYS:HE3	2.05	0.57
8:7:689:LEU:O	8:7:692:ILE:HG22	2.04	0.57
4:C:568:THR:HG23	6:E:400:LEU:HD21	1.87	0.57
4:C:730:ALA:O	4:C:734:ARG:HG2	2.04	0.57
5:D:721:ALA:HB1	8:G:661:VAL:HG22	1.85	0.57
6:E:411:ASN:HD22	6:E:519:VAL:HG12	1.70	0.57
9:X:527:HIS:O	9:X:531:ARG:HG3	2.05	0.57
4:3:225:ILE:HD11	6:5:184:ARG:HA	1.87	0.57
7:6:360:ARG:HE	7:6:376:THR:HG21	1.69	0.57
10:Z:598:LYS:NZ	10:Z:601:ILE:HG13	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:778:LEU:HA	3:B:829:VAL:HG22	1.87	0.57
5:D:758:ILE:HG22	5:D:760:PRO:HD3	1.86	0.57
3:2:567:THR:HG22	3:2:569:GLN:H	1.70	0.57
6:5:580:ALA:HA	6:5:583:MET:HE2	1.87	0.57
7:6:550:GLN:OE1	7:6:677:SER:HB3	2.05	0.57
6:5:38:PHE:CZ	6:5:67:HIS:HB3	2.40	0.57
3:B:525:LYS:HD2	6:E:576:HIS:ND1	2.20	0.57
6:E:88:PRO:O	6:E:92:THR:HG23	2.05	0.57
3:2:820:PHE:HA	3:2:823:MET:HG2	1.86	0.57
5:4:505:ASP:O	5:4:509:ILE:HG13	2.05	0.57
1:O:28:DG:H4'	3:2:360:ARG:HH22	1.70	0.56
3:B:211:LEU:HD22	3:B:271:PHE:CE1	2.39	0.56
5:D:282:SER:HA	5:D:285:VAL:HG22	1.87	0.56
5:D:557:ARG:HH12	5:D:652:GLN:HB2	1.69	0.56
4:3:446:VAL:HG13	4:3:502:ILE:HD12	1.86	0.56
6:5:690:ASP:O	6:5:694:GLN:HG2	2.05	0.56
10:Z:368:ILE:HD12	10:Z:369:PRO:HD2	1.87	0.56
11:Y:177:ILE:O	11:Y:181:ARG:HG2	2.05	0.56
8:G:158:THR:HG23	8:G:181:LEU:HD21	1.86	0.56
8:G:502:VAL:HG23	8:G:503:THR:HG23	1.86	0.56
3:2:760:GLN:O	3:2:764:MET:HG3	2.04	0.56
7:6:516:LEU:O	7:6:520:VAL:HG23	2.05	0.56
2:S:-29:DT:H5''	6:E:209:ARG:NH2	2.19	0.56
3:B:214:PHE:HD2	3:B:215:LEU:HD22	1.69	0.56
3:B:340:ASN:HD22	7:6:429:THR:HG21	1.70	0.56
3:B:707:HIS:CE1	7:F:762:LYS:HZ3	2.23	0.56
4:C:201:HIS:HB2	4:C:241:LEU:HD22	1.86	0.56
4:C:688:ASN:ND2	8:G:606:ARG:HD2	2.20	0.56
5:D:444:ILE:HD12	7:F:411:GLY:HA2	1.87	0.56
3:2:307:ARG:HD2	7:6:493:VAL:HG11	1.88	0.56
3:2:596:LEU:HD11	3:2:620:ILE:HD13	1.86	0.56
4:3:295:VAL:HB	4:3:325:THR:HG22	1.87	0.56
5:4:268:VAL:O	5:4:272:MET:HG3	2.06	0.56
7:6:306:LYS:HB3	7:6:320:ASN:HA	1.86	0.56
9:X:288:ASP:HA	9:X:291:PHE:HD1	1.70	0.56
9:X:526:ASN:O	9:X:530:LYS:HG2	2.05	0.56
11:Y:176:HIS:HB3	11:Y:180:LYS:NZ	2.20	0.56
3:B:347:ILE:HD11	7:6:429:THR:HB	1.87	0.56
3:2:242:LEU:HD21	3:2:275:ALA:HB1	1.87	0.56
3:2:511:ILE:HD12	3:2:541:LEU:HD22	1.88	0.56
4:3:498:ALA:HB3	8:7:488:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:649:THR:H	6:5:652:GLN:HG2	1.71	0.56
10:Z:125:ALA:HB1	10:Z:247:VAL:HG13	1.88	0.56
1:O:24:DG:H2"	1:O:25:DA:C8	2.41	0.56
6:E:38:PHE:CZ	6:E:67:HIS:HB3	2.40	0.56
8:G:87:GLN:O	8:G:91:GLU:HG3	2.06	0.56
5:4:204:LYS:O	5:4:208:ILE:HG13	2.05	0.56
8:7:596:ILE:HD12	8:7:598:PHE:HE2	1.69	0.56
8:7:697:GLN:O	8:7:701:LYS:HG3	2.04	0.56
5:D:447:ASN:HD22	5:D:450:GLN:HG3	1.71	0.56
7:F:144:LYS:HA	7:F:196:LEU:HD13	1.87	0.56
7:F:653:HIS:CE1	7:F:704:PRO:HB2	2.40	0.56
3:2:530:LYS:HZ2	6:5:596:ILE:HG12	1.71	0.56
10:Z:49:PHE:HD2	10:Z:56:SER:HB2	1.69	0.56
5:D:254:THR:HG23	5:D:257:LEU:HD23	1.87	0.56
3:2:391:GLN:HE21	3:2:403:PRO:HB2	1.71	0.56
9:X:379:LYS:HA	9:X:379:LYS:HE3	1.88	0.56
5:4:554:LYS:HE3	5:4:554:LYS:HA	1.86	0.56
8:7:411:TYR:CZ	8:7:430:LYS:HD3	2.41	0.56
10:Z:133:ASN:HB2	10:Z:140:ILE:HD11	1.86	0.56
10:Z:259:LEU:HD22	10:Z:269:ASN:ND2	2.21	0.56
11:Y:242:SER:O	11:Y:246:THR:HG23	2.06	0.56
3:B:335:LYS:HB3	3:B:381:VAL:HG13	1.88	0.56
4:3:426:ALA:HB3	4:3:429:ALA:HB2	1.88	0.56
5:4:202:LYS:HG3	5:4:204:LYS:HE2	1.87	0.56
7:6:157:HIS:HA	7:6:160:MET:HE2	1.88	0.56
9:X:347:LEU:HB3	9:X:416:LYS:HG3	1.88	0.56
5:4:443:PRO:HG3	5:4:457:TYR:CZ	2.41	0.56
7:6:612:VAL:HG11	7:6:668:ILE:HG13	1.88	0.56
7:F:340:ASN:HD21	7:F:343:PHE:HB2	1.71	0.55
3:2:478:GLU:O	3:2:482:ARG:HG2	2.06	0.55
8:7:544:GLN:HG2	8:7:560:ARG:HA	1.88	0.55
3:2:605:LEU:HD23	3:2:647:ILE:HB	1.88	0.55
5:4:315:ARG:HH21	5:4:413:HIS:HD2	1.54	0.55
6:E:494:HIS:NE2	6:E:546:ILE:HG12	2.21	0.55
7:F:429:THR:HB	3:2:347:ILE:HD11	1.87	0.55
4:C:230:ILE:HG23	6:5:186:CYS:HB2	1.88	0.55
4:3:189:THR:HB	4:3:254:GLN:HE21	1.71	0.55
7:6:591:PHE:HZ	7:6:751:LEU:HD22	1.71	0.55
10:Z:61:ILE:HD11	10:Z:86:PHE:CZ	2.42	0.55
8:7:537:ILE:HG23	8:7:563:ILE:HD13	1.89	0.55
9:X:170:PHE:HZ	9:X:231:PHE:HE1	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:299:VAL:HG11	10:Z:409:PHE:CE1	2.41	0.55
3:B:267:MET:O	3:B:268:LEU:HB2	2.05	0.55
8:G:537:ILE:HG23	8:G:563:ILE:HD13	1.87	0.55
6:5:384:ILE:O	6:5:388:ILE:HG13	2.07	0.55
9:X:264:VAL:HG13	9:X:378:LYS:HZ1	1.71	0.55
4:3:408:VAL:HA	4:3:516:ALA:O	2.07	0.55
5:4:819:LEU:O	5:4:823:GLN:HG2	2.07	0.55
10:Z:135:PHE:HE1	10:Z:156:LYS:HB3	1.70	0.55
7:F:520:VAL:HG12	7:F:754:TYR:HE2	1.71	0.55
3:2:508:HIS:O	3:2:512:LYS:HG2	2.06	0.55
6:5:493:ILE:HG22	6:5:497:MET:HE3	1.88	0.55
9:X:278:LEU:O	9:X:282:ILE:HG12	2.07	0.55
11:Y:155:ILE:O	11:Y:158:GLN:HG3	2.06	0.55
7:F:301:ARG:NH2	7:F:618:GLY:HA3	2.21	0.55
7:6:486:ALA:O	7:6:490:ALA:HB3	2.07	0.55
7:6:808:GLU:O	7:6:812:ARG:HG3	2.06	0.55
9:X:411:GLU:HA	9:X:414:ILE:HG22	1.89	0.55
1:O:19:DT:H2"	1:O:20:DG:N7	2.22	0.55
5:D:443:PRO:HG3	5:D:457:TYR:CZ	2.42	0.55
6:5:625:ASN:HD21	6:5:681:ILE:HG12	1.72	0.55
8:7:527:ASP:HB3	8:7:586:LEU:HD21	1.88	0.55
9:X:188:LYS:O	9:X:192:ARG:HG3	2.07	0.55
3:B:363:PHE:HE1	3:B:368:LYS:HA	1.72	0.54
5:D:519:TYR:HD1	5:D:811:MET:SD	2.30	0.54
7:F:330:PRO:HG2	7:F:344:TRP:CE2	2.42	0.54
11:Y:178:ASN:HA	11:Y:181:ARG:HG2	1.89	0.54
8:G:615:HIS:O	8:G:619:VAL:HG23	2.08	0.54
4:3:537:ASP:HB3	8:7:572:GLY:HA3	1.89	0.54
6:5:625:ASN:ND2	6:5:681:ILE:HG12	2.22	0.54
8:7:182:ARG:HA	8:7:185:VAL:HG22	1.87	0.54
8:7:720:VAL:O	8:7:724:LYS:HG2	2.07	0.54
10:Z:48:LEU:HD11	10:Z:259:LEU:HD11	1.89	0.54
3:2:774:ILE:HG22	3:2:776:PRO:HD3	1.90	0.54
5:D:798:LEU:HA	5:D:801:MET:HE2	1.89	0.54
6:E:604:THR:O	6:E:608:LEU:HG	2.07	0.54
6:E:141:SER:HB3	6:E:161:ARG:HD2	1.88	0.54
8:G:495:ALA:HB3	8:G:557:LEU:HD21	1.90	0.54
3:2:528:ASN:HB2	3:2:530:LYS:HG3	1.89	0.54
7:6:550:GLN:HE21	7:6:571:ILE:HG12	1.72	0.54
3:B:317:LEU:HD11	3:B:427:THR:HG22	1.90	0.54
3:B:548:ALA:HA	12:B:1001:ADP:H5'2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:345:ALA:HB2	5:D:365:ILE:HD13	1.89	0.54
5:D:688:VAL:O	5:D:692:ILE:HG12	2.08	0.54
7:6:772:TYR:CE1	7:6:776:LYS:HE3	2.41	0.54
7:6:838:VAL:HG23	7:6:840:VAL:HG23	1.88	0.54
8:7:494:THR:HG22	8:7:546:ILE:HD13	1.90	0.54
3:B:498:ILE:HD13	3:B:513:THR:HG22	1.89	0.54
6:E:344:ASN:O	6:E:344:ASN:ND2	2.41	0.54
5:4:525:SER:HA	5:4:741:VAL:HG13	1.90	0.54
3:B:790:TYR:HB2	3:B:810:LEU:HD13	1.90	0.54
5:D:692:ILE:HG21	5:D:699:LEU:HD13	1.88	0.54
6:E:485:MET:HE3	6:E:490:ARG:HA	1.90	0.54
3:2:525:LYS:HD3	6:5:577:THR:HG23	1.90	0.54
5:4:401:GLU:HG2	5:4:403:PRO:HD3	1.90	0.54
5:4:417:LEU:HD13	5:4:463:VAL:HG11	1.90	0.54
8:7:262:CYS:HB3	8:7:265:CYS:SG	2.48	0.54
3:B:835:ASP:HA	3:B:838:ILE:HG12	1.89	0.54
7:F:296:ARG:HB3	7:F:624:GLU:OE1	2.08	0.54
6:5:90:PHE:CE2	6:5:94:ILE:HD11	2.43	0.54
7:6:583:GLN:HA	7:6:586:LYS:HG2	1.90	0.54
3:B:795:ARG:HE	3:B:796:GLU:CD	2.16	0.54
7:F:361:ILE:O	7:F:376:THR:HA	2.07	0.54
5:4:640:SER:HB2	7:6:601:LYS:HE2	1.89	0.54
6:5:464:LEU:HD22	6:5:513:LEU:HD13	1.90	0.54
3:B:388:VAL:HG23	3:B:408:VAL:HB	1.89	0.53
3:B:432:ASN:HA	3:B:449:THR:HA	1.90	0.53
3:B:511:ILE:HD12	3:B:541:LEU:HD22	1.89	0.53
3:B:760:GLN:O	3:B:764:MET:HG3	2.07	0.53
8:G:425:ASN:O	8:G:429:LYS:HD2	2.07	0.53
8:G:625:GLN:HG2	8:G:627:ASP:H	1.73	0.53
3:2:788:ARG:HH11	3:2:788:ARG:HA	1.72	0.53
3:B:570:GLY:HA3	7:F:650:VAL:HG21	1.90	0.53
4:3:562:SER:O	4:3:566:LEU:HG	2.08	0.53
5:4:203:TYR:CE2	5:4:207:LYS:HE3	2.43	0.53
9:X:502:PHE:O	9:X:506:GLU:HG2	2.09	0.53
3:B:402:LEU:HD13	7:F:629:MET:HE1	1.90	0.53
4:C:408:VAL:HA	4:C:516:ALA:O	2.08	0.53
6:5:134:THR:HG21	6:5:195:ASN:HB2	1.88	0.53
8:7:685:THR:HG22	8:7:687:ARG:N	2.23	0.53
4:C:576:TYR:CE1	4:C:582:VAL:HA	2.44	0.53
5:D:437:GLY:HA3	5:D:463:VAL:HA	1.89	0.53
5:D:794:THR:H	5:D:797:GLN:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:271:PHE:CE2	3:B:295:VAL:HG11	2.44	0.53
7:F:505:LEU:HA	7:F:508:LEU:HD13	1.91	0.53
8:G:214:ARG:HE	8:G:215:TYR:HE1	1.56	0.53
3:2:854:ARG:HD2	3:2:858:ARG:HH12	1.74	0.53
8:7:73:ARG:HH12	8:7:132:ILE:HG12	1.73	0.53
9:X:414:ILE:O	9:X:418:LYS:HG3	2.09	0.53
10:Z:435:GLY:HA3	10:Z:479:LEU:HD21	1.90	0.53
3:B:662:PRO:HG3	3:B:850:LYS:HZ1	1.73	0.53
7:F:584:PHE:O	7:F:588:VAL:HG23	2.09	0.53
4:3:418:LEU:O	4:3:422:VAL:HG23	2.09	0.53
6:5:393:MET:HE1	6:5:603:ILE:HG12	1.91	0.53
4:C:493:GLN:HB3	4:C:509:ARG:HA	1.91	0.53
8:7:82:LEU:HD12	8:7:206:PRO:HA	1.89	0.53
10:Z:3:TYR:CD1	10:Z:7:GLN:HB3	2.41	0.53
3:B:789:VAL:HG13	3:B:864:TYR:HE1	1.73	0.53
4:C:697:ILE:HG23	4:C:701:THR:OG1	2.07	0.53
5:4:202:LYS:HZ3	5:4:222:GLU:HA	1.73	0.53
9:X:277:LEU:O	9:X:281:ILE:HD12	2.09	0.53
10:Z:344:VAL:O	10:Z:348:LEU:HB2	2.09	0.53
4:C:344:ASP:O	4:C:348:ARG:HG2	2.08	0.53
3:2:794:ARG:NH1	6:5:560:HIS:CE1	2.77	0.53
10:Z:541:ASN:HD21	10:Z:544:THR:HG23	1.74	0.53
3:B:304:TYR:HE2	3:B:313:ASN:HD21	1.56	0.53
5:D:548:THR:OG1	5:D:760:PRO:HD2	2.07	0.53
3:2:556:VAL:HG11	3:2:605:LEU:HD21	1.91	0.53
3:2:703:HIS:HE2	7:6:801:GLU:HG2	1.74	0.53
5:4:314:MET:HE3	5:4:439:PHE:HE1	1.72	0.53
7:6:188:VAL:HA	7:6:191:LYS:HE3	1.91	0.53
10:Z:433:GLU:HG3	10:Z:543:LEU:HB2	1.90	0.53
4:C:367:LEU:HD11	4:C:382:LEU:HB2	1.91	0.52
8:7:502:VAL:HG23	8:7:503:THR:HG23	1.89	0.52
3:B:774:ILE:HG22	3:B:776:PRO:HD3	1.90	0.52
5:D:526:ILE:HG23	5:D:580:TYR:CE2	2.44	0.52
5:D:774:TYR:HD2	7:F:728:ALA:HB2	1.74	0.52
6:E:318:GLY:HA3	6:E:323:ILE:HG21	1.91	0.52
8:G:411:TYR:CZ	8:G:430:LYS:HD3	2.44	0.52
5:4:393:ASP:HB3	5:4:424:VAL:HG11	1.91	0.52
5:4:437:GLY:HA3	5:4:463:VAL:HA	1.89	0.52
9:X:215:ILE:HG23	9:X:349:ARG:HH12	1.74	0.52
9:X:261:ASP:O	9:X:265:VAL:HG23	2.09	0.52
9:X:303:LYS:HA	9:X:303:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:262:CYS:HB3	8:G:265:CYS:SG	2.49	0.52
5:4:339:ILE:HB	5:4:394:LYS:O	2.09	0.52
7:6:796:THR:HG23	7:6:798:ARG:H	1.74	0.52
8:7:669:GLN:O	8:7:672:LYS:HB2	2.08	0.52
3:B:502:ALA:HB3	3:B:512:LYS:NZ	2.25	0.52
5:D:178:ARG:HH12	9:X:534:SER:HB2	1.75	0.52
6:E:5:ARG:HG3	6:E:218:GLU:OE2	2.09	0.52
3:2:498:ILE:HD13	3:2:513:THR:HG22	1.92	0.52
3:2:797:SER:HB3	3:2:805:ILE:HG12	1.91	0.52
5:4:212:ARG:HG2	5:4:212:ARG:O	2.08	0.52
5:4:303:VAL:HG12	5:4:305:PRO:HD3	1.90	0.52
10:Z:468:ASN:O	10:Z:471:LYS:HG2	2.09	0.52
6:5:622:LEU:HD11	6:5:656:ILE:HG21	1.91	0.52
7:6:304:LEU:HA	7:6:353:PHE:HA	1.91	0.52
10:Z:426:GLU:HA	10:Z:429:THR:HG22	1.92	0.52
7:F:614:ARG:HH22	7:F:619:GLY:HA2	1.74	0.52
8:G:494:THR:HG22	8:G:546:ILE:HD13	1.91	0.52
3:2:335:LYS:HB3	3:2:381:VAL:HG13	1.91	0.52
3:2:404:ARG:NH1	7:6:299:GLU:HA	2.25	0.52
4:C:656:LEU:O	4:C:660:VAL:HG23	2.09	0.52
5:D:844:LYS:HA	5:D:844:LYS:HE3	1.92	0.52
7:F:750:GLN:HA	7:F:753:ARG:HG2	1.92	0.52
3:2:432:ASN:HA	3:2:449:THR:HA	1.91	0.52
3:2:601:LYS:HD3	3:2:643:ARG:HH21	1.74	0.52
3:2:662:PRO:HG3	3:2:850:LYS:NZ	2.24	0.52
3:2:782:ASP:O	3:2:785:LYS:HB3	2.09	0.52
4:3:683:TYR:CD2	4:3:702:LEU:HB2	2.43	0.52
3:2:854:ARG:HB2	3:2:858:ARG:NH1	2.24	0.52
8:7:85:ILE:O	8:7:89:GLN:HG3	2.08	0.52
8:7:457:CYS:HB3	8:7:597:LEU:HD12	1.91	0.52
10:Z:386:ARG:HD3	10:Z:386:ARG:N	2.25	0.52
8:G:440:VAL:HG22	8:G:697:GLN:OE1	2.10	0.52
6:5:436:ALA:HA	6:5:476:VAL:O	2.10	0.52
9:X:264:VAL:HG13	9:X:378:LYS:HZ3	1.75	0.52
9:X:295:GLU:HB3	9:X:299:LYS:HZ1	1.74	0.52
4:3:683:TYR:CZ	4:3:687:ARG:HD2	2.45	0.52
5:4:396:VAL:HG21	7:6:412:LEU:HD22	1.91	0.52
6:5:39:ARG:HH22	6:5:42:SER:HA	1.75	0.52
8:7:548:ILE:HG23	8:7:550:LYS:HG3	1.91	0.52
3:B:707:HIS:CE1	7:F:762:LYS:NZ	2.78	0.51
4:C:457:LEU:HD11	4:C:502:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:477:VAL:HG13	6:E:519:VAL:HG23	1.92	0.51
7:F:144:LYS:HE2	7:F:195:GLU:HG2	1.93	0.51
7:F:658:GLN:HB2	7:F:660:THR:HG22	1.92	0.51
5:4:564:ILE:HG12	5:4:704:LEU:HB2	1.91	0.51
7:6:748:ALA:HB1	7:6:752:ARG:NH1	2.24	0.51
7:6:751:LEU:O	7:6:755:ILE:HG12	2.09	0.51
8:7:138:VAL:HG21	8:7:303:ARG:NH1	2.26	0.51
10:Z:612:ILE:HG21	10:Z:644:LEU:HD21	1.93	0.51
3:2:486:LYS:HA	3:2:489:ARG:HD2	1.93	0.51
3:2:536:ASP:HB2	3:2:645:SER:HB3	1.91	0.51
4:3:483:ARG:O	4:3:486:ILE:HG22	2.11	0.51
6:5:92:THR:O	6:5:96:GLN:HG3	2.10	0.51
8:7:82:LEU:HD23	8:7:85:ILE:HD12	1.91	0.51
8:7:477:SER:HB3	8:7:520:ILE:HD12	1.91	0.51
3:B:203:VAL:O	3:B:207:ILE:HG12	2.10	0.51
5:D:209:LEU:HD22	5:D:250:ALA:HB2	1.93	0.51
3:2:195:SER:O	3:2:199:THR:HG23	2.11	0.51
8:7:580:PRO:O	8:7:584:ILE:HG12	2.10	0.51
3:B:854:ARG:HG3	3:B:858:ARG:NH1	2.25	0.51
5:D:342:MET:HE1	7:F:448:LEU:HD23	1.93	0.51
6:E:65:MET:HE3	6:E:79:LEU:HD23	1.92	0.51
7:F:601:LYS:HE2	7:F:601:LYS:HA	1.93	0.51
7:F:720:ASN:HB3	7:F:723:ILE:HG12	1.93	0.51
8:G:82:LEU:HD23	8:G:85:ILE:HD12	1.91	0.51
3:2:696:ALA:O	3:2:700:VAL:HG12	2.11	0.51
3:2:794:ARG:NH1	6:5:560:HIS:HE1	2.08	0.51
5:4:447:ASN:HB3	5:4:450:GLN:HB3	1.92	0.51
5:D:775:VAL:O	5:D:779:LYS:HG2	2.10	0.51
7:F:798:ARG:HG2	7:F:798:ARG:HH11	1.75	0.51
3:2:692:ASP:C	7:6:778:LYS:HZ2	2.18	0.51
6:5:90:PHE:O	6:5:94:ILE:HG13	2.09	0.51
8:7:457:CYS:HB2	8:7:594:PHE:CE1	2.45	0.51
10:Z:12:TYR:O	10:Z:16:LEU:HG	2.10	0.51
10:Z:324:TYR:CE1	10:Z:405:ILE:HG13	2.45	0.51
2:S:-33:DT:H2"	2:S:-32:DC:C5	2.45	0.51
6:E:178:TYR:HB3	6:E:249:LYS:HB2	1.93	0.51
4:3:32:LEU:HD13	4:3:132:LEU:HD23	1.93	0.51
6:5:415:LEU:O	6:5:555:ILE:HA	2.10	0.51
9:X:166:TYR:C	9:X:239:LYS:HZ1	2.19	0.51
9:X:169:LEU:HD13	9:X:273:LEU:HD23	1.92	0.51
4:C:347:ILE:O	4:C:351:ASN:ND2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:400:ARG:HH21	4:C:707:ARG:NH2	2.09	0.51
5:D:510:ARG:HD3	5:D:813:LEU:HD12	1.93	0.51
5:D:571:SER:HB3	8:G:686:PRO:HD2	1.93	0.51
6:E:183:CYS:HB3	6:E:186:CYS:O	2.10	0.51
8:G:432:LEU:HD23	8:G:473:ILE:CG1	2.41	0.51
3:2:690:GLU:OE2	3:2:694:ARG:HD3	2.11	0.51
7:6:368:ILE:HD11	7:6:374:PRO:HB3	1.91	0.51
10:Z:58:ILE:HD12	10:Z:477:PHE:HE2	1.75	0.51
3:B:708:PRO:HG2	3:B:709:GLU:OE2	2.11	0.51
3:B:814:LEU:HD21	6:E:573:ILE:HG13	1.93	0.51
4:C:103:LEU:HG	4:C:111:TRP:HB2	1.92	0.51
4:C:451:GLU:HG3	4:C:452:THR:HG23	1.93	0.51
4:C:621:VAL:HG23	4:C:622:PHE:HD1	1.76	0.51
5:D:487:GLN:HA	5:D:490:VAL:HG12	1.93	0.51
7:F:516:LEU:HD21	7:F:757:TYR:CD2	2.46	0.51
3:2:519:LEU:HD21	3:2:560:ALA:HB2	1.92	0.51
6:5:198:ASN:ND2	6:5:251:ILE:HD11	2.26	0.51
8:7:248:VAL:HG13	8:7:311:GLN:HE21	1.76	0.51
6:E:381:ASN:HB3	6:E:384:ILE:HB	1.92	0.51
7:F:751:LEU:O	7:F:755:ILE:HG12	2.10	0.51
3:2:793:LEU:HD11	3:2:842:VAL:HG12	1.91	0.51
10:Z:508:ASN:HA	10:Z:511:VAL:HG22	1.93	0.51
3:B:547:THR:HG21	3:B:683:VAL:HG21	1.93	0.51
4:C:184:GLY:HA2	4:C:261:MET:HG3	1.94	0.51
5:D:794:THR:HG22	5:D:795:THR:H	1.75	0.51
6:E:39:ARG:HD3	6:E:44:PHE:CE1	2.46	0.51
7:F:656:MET:HB3	7:F:708:ARG:HG2	1.93	0.51
3:2:551:GLN:HE22	12:2:1001:ADP:H5'1	1.74	0.51
7:6:707:SER:HB2	7:6:798:ARG:HH12	1.76	0.51
8:7:437:VAL:HG21	8:7:702:LEU:HD13	1.93	0.51
3:B:213:SER:HA	3:B:216:LEU:HG	1.93	0.50
5:D:603:ALA:HB2	7:F:373:MET:HE1	1.93	0.50
3:2:591:LEU:HD11	3:2:631:ILE:HG21	1.93	0.50
3:2:790:TYR:HB2	3:2:810:LEU:HD13	1.92	0.50
4:3:347:ILE:O	4:3:351:ASN:ND2	2.44	0.50
6:5:444:SER:HB3	6:5:447:ALA:HB3	1.92	0.50
8:7:693:ILE:O	8:7:697:GLN:HG3	2.12	0.50
4:C:537:ASP:OD1	4:C:696:PRO:HG3	2.12	0.50
7:F:820:THR:HG22	7:F:822:SER:H	1.77	0.50
3:2:690:GLU:O	3:2:694:ARG:HG2	2.11	0.50
9:X:228:LEU:HD21	9:X:263:CYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:331:HIS:CE1	10:Z:419:ILE:HD13	2.44	0.50
3:B:267:MET:HG3	3:B:268:LEU:H	1.77	0.50
3:B:508:HIS:O	3:B:512:LYS:HG2	2.10	0.50
5:D:527:ALA:HB1	5:D:530:ILE:HD12	1.93	0.50
6:E:189:THR:HG21	4:3:236:THR:HG22	1.93	0.50
4:3:341:MET:HG2	4:3:592:VAL:HG21	1.94	0.50
5:4:578:LEU:HD21	5:4:674:SER:HB2	1.93	0.50
6:5:31:PHE:CG	6:5:90:PHE:HD1	2.28	0.50
10:Z:121:TYR:HA	10:Z:141:GLN:HE21	1.76	0.50
1:O:37:DA:H5'	3:B:437:ASN:HD21	1.77	0.50
3:B:238:ASN:HD21	10:Z:369:PRO:HA	1.75	0.50
4:C:358:ASP:OD2	4:C:361:ASP:HB2	2.10	0.50
6:E:198:ASN:ND2	6:E:251:ILE:HD11	2.26	0.50
8:G:423:TYR:HB2	8:G:615:HIS:CD2	2.46	0.50
4:3:654:PRO:HA	4:3:657:ARG:HD3	1.93	0.50
5:4:203:TYR:HE2	5:4:207:LYS:HE3	1.77	0.50
6:5:462:PHE:CD2	6:5:509:ILE:HB	2.46	0.50
10:Z:524:ILE:HG21	10:Z:645:THR:HA	1.92	0.50
4:C:472:ILE:HG21	4:C:475:PHE:HD1	1.77	0.50
5:D:687:PRO:HG2	5:D:690:GLU:HG3	1.94	0.50
5:D:762:ILE:HB	7:F:736:MET:HG2	1.93	0.50
7:F:123:SER:HA	7:F:134:LYS:HA	1.93	0.50
7:6:304:LEU:HD12	7:6:307:ALA:HB2	1.92	0.50
7:6:748:ALA:HB1	7:6:752:ARG:HH12	1.76	0.50
10:Z:316:LEU:HD11	10:Z:411:ARG:HB2	1.93	0.50
4:C:97:ILE:CG2	4:C:158:LYS:HD3	2.42	0.50
6:E:39:ARG:HD3	6:E:44:PHE:HE1	1.77	0.50
7:F:838:VAL:HG23	7:F:840:VAL:HG23	1.94	0.50
2:S:-36:DC:H2''	2:S:-35:DA:C8	2.46	0.50
5:D:701:ARG:HH12	7:F:578:SER:HA	1.75	0.50
8:G:697:GLN:O	8:G:701:LYS:HG3	2.11	0.50
6:5:433:SER:HB3	6:5:436:ALA:HB2	1.94	0.50
7:6:161:ARG:HG3	7:6:162:GLU:HG2	1.94	0.50
4:C:421:PHE:HB2	6:E:404:MET:HE1	1.94	0.50
5:D:244:ASP:HB3	5:D:247:ASN:OD1	2.11	0.50
5:D:347:PHE:CZ	5:D:367:GLU:HB3	2.47	0.50
6:E:77:LYS:HZ1	10:Z:382:HIS:N	2.09	0.50
4:3:568:THR:HG23	6:5:400:LEU:HD21	1.94	0.50
4:3:656:LEU:O	4:3:660:VAL:HG23	2.11	0.50
5:4:581:VAL:HA	5:4:584:ILE:HG22	1.94	0.50
5:4:701:ARG:HG2	5:4:701:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:383:ASP:HA	6:5:386:LYS:HD3	1.92	0.50
6:5:455:ARG:HB3	6:5:460:ARG:HA	1.94	0.50
7:6:330:PRO:HG2	7:6:344:TRP:CE2	2.47	0.50
10:Z:570:ALA:HB1	10:Z:579:TYR:HD1	1.76	0.50
11:Y:188:LEU:HD12	11:Y:191:LEU:HD11	1.94	0.50
5:D:533:LEU:O	5:D:536:VAL:HG12	2.12	0.50
7:F:189:VAL:HG13	7:F:197:LEU:HD11	1.94	0.50
3:2:228:GLY:O	3:2:232:ARG:HG2	2.11	0.50
5:4:603:ALA:HB2	7:6:373:MET:HE1	1.93	0.50
2:S:-21:DT:H2"	2:S:-20:DC:C6	2.46	0.49
5:D:203:TYR:CE2	5:D:207:LYS:HE3	2.47	0.49
3:2:778:LEU:HD23	6:5:577:THR:OG1	2.12	0.49
5:4:315:ARG:NH2	5:4:413:HIS:HD2	2.10	0.49
2:S:-29:DT:H2"	2:S:-28:DC:C5	2.47	0.49
5:D:742:LEU:HD22	5:D:746:PHE:CD2	2.47	0.49
6:E:31:PHE:CG	6:E:90:PHE:HD1	2.30	0.49
7:F:550:GLN:HE22	7:F:679:LEU:HB2	1.76	0.49
6:5:456:ASP:OD1	6:5:457:PRO:HD2	2.11	0.49
9:X:227:LEU:HG	9:X:266:LEU:HD23	1.94	0.49
3:B:417:VAL:HG21	3:B:456:ILE:HG21	1.94	0.49
3:B:481:GLU:O	3:B:485:ARG:HG2	2.12	0.49
5:4:445:ARG:HH22	5:4:449:ARG:HA	1.77	0.49
7:6:112:ARG:HG2	7:6:112:ARG:HH11	1.78	0.49
8:7:220:ILE:HA	8:7:223:LYS:HE3	1.94	0.49
11:Y:176:HIS:HB3	11:Y:180:LYS:HZ1	1.76	0.49
3:B:789:VAL:HG13	3:B:864:TYR:CE1	2.48	0.49
4:C:329:LEU:HD13	4:C:588:LEU:HD13	1.94	0.49
8:G:418:ILE:O	8:G:429:LYS:HE2	2.12	0.49
4:3:537:ASP:OD1	4:3:696:PRO:HG3	2.12	0.49
8:7:591:LEU:HD21	8:7:681:PHE:HD1	1.77	0.49
10:Z:502:LEU:HB3	10:Z:547:ARG:NH2	2.27	0.49
5:D:228:LYS:HA	5:D:231:ASN:HD22	1.77	0.49
5:D:525:SER:HA	5:D:741:VAL:HG13	1.94	0.49
5:D:319:PRO:HB3	8:G:253:PRO:HB3	1.95	0.49
5:D:639:ASP:HB3	7:F:643:LYS:HE3	1.94	0.49
8:G:355:PHE:CE2	8:G:374:THR:HB	2.48	0.49
3:2:530:LYS:NZ	6:5:596:ILE:HG12	2.27	0.49
4:3:212:ARG:HD2	4:3:232:PRO:HG3	1.95	0.49
5:4:601:LEU:HD23	5:4:620:ALA:HB3	1.94	0.49
6:5:449:LEU:HD21	6:5:485:MET:HE2	1.95	0.49
7:6:777:TYR:CD2	7:6:800:LEU:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:231:HIS:CE1	10:Z:233:TYR:HB2	2.47	0.49
10:Z:366:MET:HE3	10:Z:366:MET:HA	1.93	0.49
10:Z:530:LEU:HD23	10:Z:569:LEU:HG	1.94	0.49
11:Y:183:GLN:O	11:Y:186:GLU:HG3	2.13	0.49
2:S:-23:DA:H2"	2:S:-22:DG:C8	2.48	0.49
3:B:283:TYR:CE1	10:Z:364:ALA:HB1	2.40	0.49
3:B:309:LEU:HD23	3:B:430:TYR:CE1	2.48	0.49
3:2:553:LEU:O	3:2:557:GLU:HG2	2.13	0.49
4:3:621:VAL:HG23	4:3:622:PHE:CD1	2.46	0.49
10:Z:343:TYR:HE1	10:Z:347:LYS:HE3	1.78	0.49
3:B:195:SER:O	3:B:199:THR:HG23	2.13	0.49
3:B:802:SER:HB3	3:B:853:VAL:HG11	1.94	0.49
5:D:565:LEU:HD13	5:D:702:PHE:CZ	2.47	0.49
5:D:785:ARG:HG2	5:D:785:ARG:HH11	1.76	0.49
6:E:437:VAL:HG13	6:E:477:VAL:HG23	1.95	0.49
8:G:117:PHE:HB3	8:G:202:LEU:HD11	1.95	0.49
8:G:574:TYR:HB3	8:G:601:LEU:HD11	1.94	0.49
6:5:88:PRO:O	6:5:92:THR:HG23	2.13	0.49
7:6:174:TYR:CE2	7:6:178:LEU:HD13	2.48	0.49
4:C:391:LYS:HB2	4:C:399:LEU:HB2	1.94	0.49
5:D:393:ASP:OD2	7:F:280:ARG:HD2	2.13	0.49
5:D:762:ILE:HD13	5:D:817:VAL:HG11	1.94	0.49
6:E:415:LEU:O	6:E:555:ILE:HA	2.12	0.49
3:2:442:ASN:HA	7:6:326:LYS:NZ	2.28	0.49
3:2:670:THR:HG23	3:2:672:PRO:HD2	1.94	0.49
4:3:472:ILE:HG21	4:3:475:PHE:HD1	1.76	0.49
3:B:228:GLY:O	3:B:232:ARG:HG2	2.13	0.49
4:C:654:PRO:HA	4:C:657:ARG:HD3	1.94	0.49
5:4:315:ARG:HE	5:4:413:HIS:CD2	2.31	0.49
7:6:311:CYS:HB2	7:6:340:ASN:ND2	2.28	0.49
10:Z:552:LEU:HA	10:Z:555:CYS:SG	2.53	0.49
5:D:440:ARG:HH11	5:D:440:ARG:HG3	1.78	0.48
7:F:656:MET:HE2	7:F:708:ARG:HB3	1.95	0.48
6:5:366:LEU:HA	6:5:369:ILE:HD13	1.95	0.48
6:E:436:ALA:HA	6:E:476:VAL:O	2.13	0.48
7:F:311:CYS:HB3	7:F:314:CYS:H	1.78	0.48
4:3:245:TYR:CD2	8:7:356:LEU:HD22	2.48	0.48
5:4:312:LYS:HB3	5:4:316:GLU:HB2	1.95	0.48
9:X:339:TYR:O	9:X:342:GLN:HB2	2.13	0.48
5:D:347:PHE:CE1	5:D:384:LEU:HB2	2.49	0.48
8:G:81:ASP:HA	8:G:205:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:700:ALA:HA	8:G:703:ARG:NH1	2.28	0.48
6:5:64:ASN:HB3	6:5:67:HIS:CD2	2.48	0.48
6:5:87:ILE:O	6:5:91:GLU:HG3	2.13	0.48
5:D:820:GLU:HA	5:D:823:GLN:HG2	1.96	0.48
7:F:520:VAL:HG23	11:Y:149:LYS:NZ	2.29	0.48
5:4:762:ILE:HD13	5:4:817:VAL:HG11	1.95	0.48
7:6:174:TYR:CE1	7:6:287:LEU:HD12	2.49	0.48
10:Z:522:LEU:HD23	10:Z:524:ILE:H	1.76	0.48
5:D:315:ARG:NH2	5:D:413:HIS:HD2	2.11	0.48
8:G:214:ARG:HG3	8:G:215:TYR:HD1	1.78	0.48
8:G:477:SER:HB3	8:G:520:ILE:HD12	1.95	0.48
3:2:279:THR:HG21	3:2:293:ILE:HD11	1.94	0.48
3:2:796:GLU:HG3	3:2:861:PHE:CE2	2.49	0.48
4:3:533:ILE:HG22	4:3:535:LEU:HB2	1.94	0.48
9:X:415:GLN:O	9:X:415:GLN:NE2	2.43	0.48
3:B:794:ARG:HG3	6:E:565:ASP:OD1	2.12	0.48
5:D:312:LYS:O	5:D:316:GLU:HB2	2.13	0.48
6:5:207:LEU:HD11	6:5:243:ILE:HD11	1.96	0.48
8:7:459:MET:HE1	8:7:584:ILE:HB	1.95	0.48
9:X:384:LYS:HD3	9:X:391:VAL:HG21	1.95	0.48
10:Z:135:PHE:CE1	10:Z:156:LYS:HB3	2.47	0.48
10:Z:637:LEU:O	10:Z:640:PHE:HB3	2.13	0.48
3:B:267:MET:HG3	3:B:268:LEU:N	2.28	0.48
5:D:340:PRO:HG3	7:F:452:ILE:HD11	1.93	0.48
5:4:418:CYS:SG	7:6:413:PRO:HB2	2.53	0.48
6:5:161:ARG:NH2	6:5:293:THR:HG21	2.29	0.48
6:5:453:VAL:HG12	6:5:464:LEU:HA	1.95	0.48
10:Z:500:GLN:HB3	10:Z:504:ARG:HH12	1.74	0.48
3:B:306:LEU:HB2	3:B:392:GLU:HG2	1.95	0.48
3:B:819:SER:O	3:B:823:MET:HG3	2.14	0.48
6:E:146:ILE:H	6:E:146:ILE:HD12	1.78	0.48
7:F:145:ILE:HG13	7:F:146:TYR:HD2	1.79	0.48
7:F:412:LEU:HG	7:F:413:PRO:HD2	1.94	0.48
3:2:190:LYS:HD3	3:2:197:TRP:CZ3	2.49	0.48
3:2:306:LEU:HD12	3:2:406:ARG:HG2	1.94	0.48
3:2:774:ILE:HG21	3:2:822:LYS:HA	1.95	0.48
4:3:400:ARG:HB3	4:3:707:ARG:NH1	2.29	0.48
8:7:179:ASP:HA	8:7:182:ARG:CZ	2.43	0.48
10:Z:68:ARG:NH1	10:Z:68:ARG:HA	2.29	0.48
6:E:161:ARG:NH2	6:E:293:THR:HG21	2.22	0.48
6:E:426:LEU:HD22	6:E:478:CYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:513:ALA:HB2	5:4:813:LEU:HD23	1.95	0.48
6:5:106:ARG:HH22	6:5:130:ASN:HD22	1.62	0.48
3:B:218:TYR:CZ	3:B:248:HIS:HB3	2.48	0.48
5:D:683:ASN:H	5:D:691:ASN:HD21	1.61	0.48
8:G:621:MET:HE3	8:G:622:HIS:CE1	2.49	0.48
4:3:26:ARG:O	4:3:30:GLU:HG3	2.14	0.48
4:3:495:VAL:HG12	4:3:497:ILE:HD11	1.95	0.48
8:7:485:GLY:H	8:7:525:GLU:HB2	1.77	0.48
10:Z:348:LEU:HD21	10:Z:401:LEU:HD11	1.96	0.48
10:Z:609:PHE:HA	10:Z:612:ILE:HG22	1.96	0.48
3:B:494:ILE:O	3:B:498:ILE:HG13	2.14	0.47
5:D:303:VAL:HG12	5:D:305:PRO:HD3	1.95	0.47
7:6:301:ARG:HH22	7:6:618:GLY:HA3	1.79	0.47
7:6:309:PHE:CE1	7:6:346:LEU:HD13	2.49	0.47
7:6:333:CYS:SG	7:6:338:CYS:HB2	2.54	0.47
8:7:423:TYR:HB2	8:7:615:HIS:CD2	2.49	0.47
9:X:352:ILE:HD13	10:Z:642:GLU:OE2	2.14	0.47
3:B:363:PHE:HE2	7:6:341:ARG:HB2	1.79	0.47
3:B:806:THR:HG23	6:E:419:GLY:HA3	1.95	0.47
6:E:464:LEU:HD21	6:E:470:VAL:HG21	1.95	0.47
6:E:597:GLU:CD	6:E:597:GLU:H	2.22	0.47
3:2:553:LEU:HG	3:2:605:LEU:HD22	1.96	0.47
10:Z:48:LEU:HD21	10:Z:259:LEU:HD21	1.96	0.47
10:Z:598:LYS:HZ1	10:Z:601:ILE:HG13	1.79	0.47
5:D:315:ARG:HH21	5:D:413:HIS:HD2	1.62	0.47
5:D:519:TYR:CE2	5:D:538:LYS:HD3	2.50	0.47
8:G:162:ARG:HH11	8:G:162:ARG:HG3	1.78	0.47
3:2:326:ARG:HG2	3:2:389:THR:HB	1.97	0.47
3:2:695:LEU:O	3:2:699:VAL:HG23	2.14	0.47
10:Z:319:ASN:HB3	10:Z:410:VAL:HG13	1.97	0.47
2:S:-52:DC:H2"	2:S:-51:DA:C8	2.49	0.47
3:B:569:GLN:HE22	3:B:611:LYS:HE2	1.79	0.47
3:B:785:LYS:O	3:B:789:VAL:HG23	2.14	0.47
7:F:696:ARG:NH1	7:F:706:MET:HE2	2.30	0.47
5:4:265:PRO:HB3	5:4:325:LEU:HB2	1.96	0.47
5:4:834:LYS:HE2	5:4:850:VAL:HG13	1.96	0.47
7:6:173:GLN:OE1	7:6:176:ARG:HD3	2.14	0.47
7:6:417:PRO:HB2	7:6:448:LEU:HB2	1.94	0.47
10:Z:634:ARG:HG3	10:Z:635:GLU:N	2.29	0.47
3:B:211:LEU:HD22	3:B:271:PHE:HE1	1.79	0.47
3:B:233:THR:HA	3:B:236:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:240:GLU:HB2	3:B:413:ASP:OD2	2.15	0.47
4:C:235:ASP:OD2	4:C:236:THR:N	2.48	0.47
4:C:331:ALA:HB3	4:C:334:THR:HG21	1.96	0.47
7:F:182:GLN:O	7:F:186:ARG:HG2	2.14	0.47
7:F:519:MET:O	7:F:525:ILE:HD12	2.14	0.47
4:3:330:HIS:CE1	4:3:338:ALA:HB2	2.50	0.47
6:5:631:LYS:HD2	6:5:631:LYS:C	2.40	0.47
1:O:15:DT:H2''	1:O:16:DG:C8	2.50	0.47
3:B:387:ARG:HD2	3:B:407:GLU:OE1	2.15	0.47
5:D:233:MET:HE2	5:D:301:TYR:CD1	2.50	0.47
4:3:687:ARG:HG2	4:3:697:ILE:HG21	1.97	0.47
5:4:272:MET:HA	5:4:275:THR:HG22	1.96	0.47
7:6:653:HIS:CE1	7:6:704:PRO:HB2	2.50	0.47
10:Z:578:THR:HG21	10:Z:619:LYS:NZ	2.30	0.47
3:B:554:LYS:O	3:B:558:LYS:HG3	2.14	0.47
5:D:438:THR:OG1	5:D:462:ASP:HB3	2.15	0.47
5:D:643:SER:HB2	7:F:640:GLU:OE1	2.14	0.47
5:D:820:GLU:HG2	5:D:821:ASP:N	2.29	0.47
4:3:245:TYR:HD2	8:7:356:LEU:HD22	1.80	0.47
4:3:576:TYR:CE1	4:3:582:VAL:HA	2.49	0.47
5:4:251:TYR:HB3	5:4:254:THR:CG2	2.43	0.47
5:4:314:MET:HE3	5:4:439:PHE:CE1	2.49	0.47
5:4:331:LEU:HD13	5:4:432:ARG:HG2	1.97	0.47
7:6:484:MET:O	7:6:488:LEU:HD23	2.15	0.47
8:7:435:LEU:HD12	8:7:456:VAL:HG23	1.97	0.47
8:7:575:ASN:HB3	8:7:583:ASN:ND2	2.29	0.47
9:X:160:TYR:O	9:X:164:LYS:HG2	2.14	0.47
7:F:134:LYS:HE2	7:F:137:ARG:HG3	1.97	0.47
3:2:806:THR:CG2	6:5:419:GLY:HA3	2.44	0.47
4:3:276:VAL:HG11	4:3:294:VAL:HG11	1.96	0.47
5:4:711:LYS:NZ	5:4:847:MET:HB3	2.30	0.47
5:4:835:ASP:HA	5:4:838:THR:HG22	1.97	0.47
6:5:208:PRO:HG2	6:5:241:TYR:CD2	2.50	0.47
6:5:650:ILE:H	6:5:650:ILE:HD12	1.80	0.47
10:Z:233:TYR:CZ	10:Z:237:LEU:HD21	2.50	0.47
3:B:548:ALA:HB2	12:B:1001:ADP:C8	2.50	0.47
3:B:629:ILE:HG23	6:E:445:SER:OG	2.15	0.47
4:C:572:LEU:HD12	4:C:573:PRO:HD2	1.97	0.47
6:E:594:ILE:HG23	6:E:598:LYS:HG3	1.97	0.47
5:4:530:ILE:HD13	5:4:577:ILE:HD13	1.96	0.47
8:7:262:CYS:SG	8:7:296:GLY:HA3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:295:GLU:HB3	9:X:299:LYS:NZ	2.30	0.47
10:Z:576:THR:HG23	10:Z:578:THR:H	1.80	0.47
4:C:653:ILE:O	4:C:657:ARG:HG3	2.15	0.47
6:E:77:LYS:NZ	10:Z:382:HIS:H	2.10	0.47
6:E:208:PRO:HG2	6:E:241:TYR:CD2	2.50	0.47
7:F:192:TYR:CE2	11:Y:182:LEU:HD22	2.50	0.47
8:G:17:LEU:HD22	8:G:102:LEU:HD13	1.97	0.47
8:G:578:LEU:HD23	8:G:579:SER:N	2.30	0.47
6:5:600:LYS:HE3	6:5:600:LYS:HB2	1.67	0.47
7:6:580:SER:HB2	7:6:583:GLN:HG3	1.96	0.47
8:7:234:PHE:HD1	8:7:239:ILE:HG21	1.80	0.47
8:7:669:GLN:O	8:7:673:ARG:HD2	2.15	0.47
9:X:207:MET:HA	9:X:210:LYS:NZ	2.29	0.47
10:Z:365:ARG:HG3	10:Z:399:TYR:HE2	1.81	0.47
3:B:802:SER:HB2	3:B:849:GLN:NE2	2.31	0.46
3:B:811:GLU:HA	3:B:811:GLU:OE2	2.15	0.46
6:E:251:ILE:HD12	6:E:280:ARG:HG3	1.97	0.46
4:3:35:PHE:CE2	4:3:102:ASP:HB3	2.50	0.46
5:4:594:LYS:HG2	8:7:532:SER:HA	1.97	0.46
7:6:137:ARG:HH22	7:6:192:TYR:CB	2.29	0.46
3:B:402:LEU:CD2	7:F:391:PRO:HG2	2.45	0.46
3:2:494:ILE:HG23	3:2:823:MET:HE2	1.97	0.46
6:5:341:SER:H	6:5:344:ASN:HB2	1.79	0.46
7:6:314:CYS:C	7:6:315:ARG:HE	2.22	0.46
10:Z:233:TYR:O	10:Z:237:LEU:HG	2.15	0.46
10:Z:524:ILE:HG23	10:Z:525:TYR:HD1	1.80	0.46
10:Z:550:ASN:HA	10:Z:553:ILE:HG12	1.96	0.46
1:O:28:DG:H2''	1:O:29:DA:C8	2.50	0.46
2:S:-23:DA:H2''	2:S:-22:DG:H8	1.80	0.46
3:B:758:ILE:H	3:B:758:ILE:HD12	1.80	0.46
4:C:389:VAL:HG23	4:C:710:THR:HG21	1.97	0.46
4:C:544:ASP:HB3	4:C:704:THR:HG23	1.98	0.46
5:D:314:MET:HE3	5:D:439:PHE:HE1	1.80	0.46
6:E:90:PHE:CE2	6:E:94:ILE:HD11	2.49	0.46
6:E:197:PHE:CZ	6:E:205:VAL:HG23	2.51	0.46
7:F:778:LYS:HB3	7:F:782:LYS:NZ	2.29	0.46
4:3:20:VAL:O	4:3:24:ARG:HG2	2.16	0.46
4:3:467:ARG:HD3	4:3:509:ARG:HH21	1.80	0.46
5:4:226:TYR:O	5:4:230:LEU:HD23	2.15	0.46
3:B:446:VAL:HG11	7:F:301:ARG:HE	1.81	0.46
3:B:520:PHE:CD1	3:B:823:MET:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:103:LEU:HD21	4:C:114:ILE:HD12	1.97	0.46
7:F:297:THR:HG23	7:F:391:PRO:HG3	1.97	0.46
7:F:580:SER:HB2	7:F:583:GLN:NE2	2.30	0.46
3:2:554:LYS:O	3:2:557:GLU:HB2	2.16	0.46
4:3:369:PRO:HB2	4:3:627:PRO:HG2	1.97	0.46
6:5:434:PRO:HA	6:5:600:LYS:HD3	1.96	0.46
9:X:407:PRO:HG2	9:X:408:HIS:HD2	1.81	0.46
10:Z:34:LEU:HD23	10:Z:34:LEU:H	1.81	0.46
10:Z:572:ILE:HG13	10:Z:579:TYR:CE2	2.51	0.46
5:D:521:LEU:HA	5:D:524:ARG:CZ	2.46	0.46
7:F:296:ARG:CZ	7:F:613:VAL:HG21	2.45	0.46
7:F:333:CYS:SG	7:F:338:CYS:HB2	2.55	0.46
7:F:550:GLN:NE2	7:F:679:LEU:HB2	2.30	0.46
8:G:400:ARG:HH11	8:G:400:ARG:HG3	1.81	0.46
10:Z:60:PRO:HG3	10:Z:477:PHE:CD2	2.51	0.46
10:Z:84:VAL:HA	10:Z:123:LEU:HB2	1.98	0.46
10:Z:330:ARG:O	10:Z:377:TRP:HB3	2.15	0.46
10:Z:375:GLU:HG3	10:Z:380:MET:HB3	1.97	0.46
3:B:361:ILE:HG13	3:B:373:PHE:HD2	1.80	0.46
6:E:197:PHE:HZ	6:E:205:VAL:HG23	1.81	0.46
8:G:360:TYR:HA	8:G:373:GLU:HG2	1.97	0.46
8:G:437:VAL:O	8:G:646:LYS:HE2	2.14	0.46
3:2:667:VAL:HG12	3:2:669:LEU:H	1.80	0.46
3:2:798:ILE:HG13	6:5:560:HIS:CE1	2.51	0.46
5:4:458:LYS:NZ	7:6:413:PRO:HG3	2.30	0.46
6:5:46:TYR:CZ	6:5:63:VAL:HG23	2.50	0.46
6:5:405:ARG:NH1	6:5:500:GLN:HB2	2.29	0.46
7:6:330:PRO:HG2	7:6:344:TRP:CZ2	2.50	0.46
7:6:791:SER:N	7:6:837:ARG:HA	2.30	0.46
8:7:248:VAL:CG1	8:7:311:GLN:HE21	2.28	0.46
10:Z:32:SER:HB3	10:Z:34:LEU:HD23	1.97	0.46
1:O:55:DT:H2''	1:O:56:DG:C8	2.51	0.46
4:C:700:ARG:HE	12:G:1001:ADP:H5'1	1.81	0.46
6:E:631:LYS:HD2	6:E:631:LYS:C	2.40	0.46
7:F:297:THR:HG22	7:F:359:VAL:HG23	1.97	0.46
7:F:653:HIS:HB2	7:F:705:ILE:HD11	1.98	0.46
8:G:247:ARG:NH1	8:G:247:ARG:HB3	2.30	0.46
8:G:539:GLU:HG3	8:G:543:GLN:NE2	2.30	0.46
3:2:218:TYR:CZ	3:2:248:HIS:HB3	2.51	0.46
3:2:638:THR:HG21	6:5:165:ILE:HD11	1.98	0.46
5:4:654:ILE:HG22	5:4:656:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:604:THR:O	6:5:608:LEU:HG	2.16	0.46
10:Z:385:LYS:HA	10:Z:388:LEU:CD2	2.46	0.46
2:S:-35:DA:H2''	2:S:-34:DG:C8	2.50	0.46
3:B:591:LEU:HD12	3:B:636:ILE:HG21	1.97	0.46
4:C:369:PRO:HB2	4:C:627:PRO:HG2	1.98	0.46
5:D:180:ILE:HA	9:X:532:GLN:HA	1.98	0.46
5:D:265:PRO:O	5:D:269:ILE:HG12	2.16	0.46
6:E:500:GLN:HB3	6:E:516:ARG:HA	1.97	0.46
8:G:589:ALA:HB1	8:G:593:ARG:NH1	2.30	0.46
3:2:777:LYS:HB3	6:5:577:THR:HB	1.98	0.46
4:3:462:MET:HE1	4:3:486:ILE:HD11	1.97	0.46
5:4:207:LYS:HG3	5:4:216:ILE:HG12	1.98	0.46
5:4:621:LEU:HD13	5:4:648:VAL:HG21	1.96	0.46
5:4:782:ASP:OD2	7:6:719:CYS:HB2	2.15	0.46
6:5:605:TYR:CE2	6:5:609:LYS:HE3	2.51	0.46
8:7:637:LYS:HA	8:7:640:GLU:HG2	1.98	0.46
9:X:273:LEU:O	9:X:276:LEU:HB3	2.16	0.46
9:X:408:HIS:HA	9:X:411:GLU:HG3	1.98	0.46
1:O:25:DA:H2''	1:O:26:DC:H5'	1.98	0.46
5:D:308:VAL:HG11	5:D:325:LEU:HG	1.98	0.46
7:F:513:ILE:HG22	11:Y:153:ILE:HD12	1.98	0.46
4:3:359:ILE:HA	4:3:362:ILE:HG22	1.97	0.46
4:3:653:ILE:O	4:3:657:ARG:HG3	2.16	0.46
8:7:247:ARG:NH1	8:7:247:ARG:HB3	2.31	0.46
9:X:271:ILE:O	9:X:275:ILE:HD12	2.16	0.46
10:Z:122:VAL:O	10:Z:123:LEU:HD23	2.16	0.46
10:Z:345:ASN:OD1	10:Z:350:LEU:HB2	2.16	0.46
10:Z:493:ASN:HA	10:Z:496:ILE:HD12	1.98	0.46
11:Y:159:GLN:HA	11:Y:162:GLN:CD	2.41	0.46
7:F:168:MET:HG3	7:F:172:GLU:OE1	2.16	0.46
7:F:301:ARG:HH22	7:F:618:GLY:HA3	1.81	0.46
7:F:612:VAL:HG22	7:F:623:ILE:HG22	1.98	0.46
5:4:486:MET:O	5:4:490:VAL:HG23	2.16	0.46
5:4:717:ASP:OD1	8:7:668:ARG:HG3	2.16	0.46
6:5:293:THR:HB	6:5:334:GLN:HB2	1.96	0.46
7:6:591:PHE:CZ	7:6:751:LEU:HD22	2.50	0.46
8:7:409:ASP:OD2	8:7:412:ASN:HB2	2.16	0.46
9:X:230:PRO:HB3	9:X:237:ASP:HA	1.98	0.46
3:B:362:SER:O	3:B:370:LYS:HG3	2.17	0.45
3:B:821:ALA:HB2	3:B:829:VAL:HG12	1.96	0.45
5:D:256:ASP:O	5:D:260:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:570:PRO:HD2	5:D:680:SER:O	2.16	0.45
5:D:616:LEU:HD11	5:D:661:ILE:HD13	1.97	0.45
7:F:145:ILE:HG13	7:F:146:TYR:CD2	2.51	0.45
7:F:517:LYS:HE3	11:Y:150:GLU:HA	1.98	0.45
7:F:608:LEU:HD23	7:F:627:ALA:HB3	1.98	0.45
8:G:138:VAL:HG21	8:G:303:ARG:HH12	1.81	0.45
5:4:510:ARG:HH11	5:4:510:ARG:HG3	1.81	0.45
6:5:426:LEU:HD22	6:5:478:CYS:HB3	1.98	0.45
7:6:191:LYS:HD2	7:6:192:TYR:CD2	2.51	0.45
8:7:152:ARG:HB3	8:7:152:ARG:NH1	2.31	0.45
8:7:444:VAL:HG12	8:7:446:ASP:H	1.82	0.45
9:X:240:ARG:HA	9:X:243:CYS:SG	2.56	0.45
10:Z:116:PHE:CE2	10:Z:139:ILE:HD13	2.51	0.45
10:Z:580:LEU:HD21	10:Z:629:ILE:HD11	1.98	0.45
3:B:191:ALA:HB3	3:B:197:TRP:HB2	1.98	0.45
3:B:361:ILE:HG13	3:B:373:PHE:CD2	2.51	0.45
3:B:616:ASP:O	3:B:620:ILE:HG12	2.17	0.45
3:B:662:PRO:HG3	3:B:850:LYS:NZ	2.31	0.45
4:C:26:ARG:O	4:C:30:GLU:HG3	2.16	0.45
5:D:335:SER:HB2	5:D:395:GLN:HE21	1.82	0.45
5:D:393:ASP:HB3	5:D:424:VAL:HG21	1.97	0.45
5:D:769:GLU:HB3	5:D:822:VAL:HG11	1.98	0.45
6:E:386:LYS:NZ	6:E:682:ARG:HH22	2.13	0.45
7:F:143:MET:HA	7:F:148:LEU:HB2	1.97	0.45
8:G:64:MET:HE2	8:G:64:MET:HA	1.98	0.45
4:3:43:ARG:O	4:3:43:ARG:HD3	2.17	0.45
5:4:758:ILE:HG22	5:4:760:PRO:HD3	1.97	0.45
9:X:525:MET:O	9:X:529:GLN:HG2	2.16	0.45
10:Z:511:VAL:O	10:Z:515:GLU:HG2	2.16	0.45
3:B:483:GLU:O	3:B:487:ILE:HG12	2.15	0.45
3:B:853:VAL:O	3:B:857:LEU:HD23	2.17	0.45
5:D:715:LYS:HB3	5:D:715:LYS:HE2	1.73	0.45
3:2:505:ILE:HD11	3:2:551:GLN:HB2	1.99	0.45
5:4:550:LYS:HG2	7:6:738:ARG:HH21	1.81	0.45
6:5:391:LEU:HD12	6:5:412:VAL:HG23	1.99	0.45
7:6:311:CYS:HB3	7:6:344:TRP:CZ3	2.51	0.45
7:6:377:LEU:HD21	7:6:454:PHE:HB2	1.98	0.45
8:7:162:ARG:HE	8:7:181:LEU:CD2	2.28	0.45
8:7:181:LEU:HD12	8:7:181:LEU:HA	1.72	0.45
10:Z:48:LEU:O	10:Z:51:LYS:HG3	2.15	0.45
10:Z:161:LYS:HD2	10:Z:161:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:226:GLU:O	11:Y:230:ILE:HG12	2.16	0.45
4:C:621:VAL:HG23	4:C:622:PHE:CD1	2.52	0.45
5:D:830:ARG:HG2	5:D:830:ARG:HH11	1.81	0.45
3:2:501:MET:HG2	3:2:555:TYR:CE2	2.52	0.45
5:4:240:ASN:ND2	5:4:302:LYS:HB2	2.30	0.45
9:X:276:LEU:HB2	9:X:393:PHE:CZ	2.52	0.45
10:Z:329:LEU:HD12	10:Z:330:ARG:HG3	1.97	0.45
11:Y:164:LYS:HA	11:Y:164:LYS:HD2	1.64	0.45
11:Y:169:THR:HA	11:Y:172:TYR:CE1	2.52	0.45
3:B:531:HIS:NE2	3:B:533:ILE:HD11	2.30	0.45
3:B:791:ALA:O	3:B:794:ARG:HB2	2.16	0.45
4:C:687:ARG:HG2	4:C:697:ILE:HG21	1.98	0.45
5:D:703:ASP:HA	5:D:800:SER:OG	2.17	0.45
5:D:745:GLU:H	5:D:745:GLU:CD	2.25	0.45
7:F:711:LEU:HD11	7:F:806:LEU:HD21	1.98	0.45
8:G:181:LEU:O	8:G:185:VAL:HG13	2.16	0.45
3:2:361:ILE:HG13	3:2:373:PHE:CD1	2.51	0.45
3:2:553:LEU:HD23	3:2:565:PHE:HE1	1.82	0.45
3:2:578:ALA:HA	3:2:592:GLU:O	2.16	0.45
4:3:294:VAL:HG22	4:3:326:VAL:HG22	1.99	0.45
5:4:224:LEU:O	5:4:228:LYS:HG2	2.16	0.45
5:4:407:PRO:HD2	5:4:410:GLN:OE1	2.17	0.45
6:5:489:ASP:O	6:5:493:ILE:HG12	2.16	0.45
7:6:486:ALA:O	7:6:490:ALA:CB	2.65	0.45
7:6:517:LYS:O	7:6:521:LYS:HG2	2.17	0.45
9:X:416:LYS:HA	9:X:416:LYS:HD3	1.76	0.45
10:Z:509:THR:O	10:Z:513:ILE:HG13	2.15	0.45
1:O:38:DC:H1'	5:D:449:ARG:NH2	2.32	0.45
2:S:-38:DG:C8	2:S:-37:DT:H72	2.52	0.45
4:3:450:ARG:HD2	4:3:450:ARG:HA	1.82	0.45
5:4:571:SER:HA	8:7:687:ARG:HD2	1.98	0.45
6:5:594:ILE:HG23	6:5:598:LYS:HG3	1.98	0.45
1:O:38:DC:H2''	1:O:39:DT:H5''	1.98	0.45
4:C:688:ASN:HD21	8:G:605:SER:C	2.25	0.45
7:F:614:ARG:HD2	7:F:614:ARG:HA	1.77	0.45
7:F:778:LYS:HB3	7:F:782:LYS:HZ3	1.81	0.45
8:G:31:ASP:C	8:G:62:LYS:HD2	2.42	0.45
3:2:497:ILE:HD11	3:2:823:MET:HE3	1.99	0.45
3:2:543:GLY:HA3	3:2:549:LYS:HD3	1.99	0.45
4:3:256:ILE:HG13	4:3:276:VAL:HB	1.99	0.45
7:6:486:ALA:HA	7:6:489:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:360:TYR:HA	8:7:373:GLU:HG2	1.99	0.45
10:Z:4:GLY:N	10:Z:7:GLN:HB2	2.32	0.45
5:D:689:THR:HG21	5:D:696:PRO:HG3	1.98	0.45
6:E:77:LYS:NZ	10:Z:382:HIS:HB2	2.32	0.45
6:E:207:LEU:HD11	6:E:243:ILE:HD11	1.99	0.45
6:E:355:GLU:O	6:E:359:GLN:HG2	2.16	0.45
7:F:108:GLY:HA2	7:F:111:VAL:HG12	1.99	0.45
3:2:459:ARG:HH11	3:2:459:ARG:HG3	1.82	0.45
3:2:676:ARG:HH11	3:2:808:ARG:HH21	1.65	0.45
6:5:5:ARG:HG2	6:5:5:ARG:HH11	1.81	0.45
9:X:186:ARG:HD2	9:X:187:LEU:HD22	1.98	0.45
3:B:276:MET:HE3	3:B:292:GLU:HA	1.99	0.45
4:C:374:HIS:O	4:C:378:LYS:HG3	2.16	0.45
5:D:795:THR:HG23	7:F:731:ILE:HD13	1.99	0.45
8:G:464:VAL:HG23	8:G:466:LYS:HG3	1.99	0.45
3:2:793:LEU:HB3	3:2:805:ILE:HG13	1.98	0.45
3:2:821:ALA:HB2	3:2:829:VAL:HG23	1.99	0.45
5:4:194:PHE:HE1	5:4:248:LEU:HD21	1.81	0.45
5:4:293:LEU:O	5:4:297:GLU:HG2	2.17	0.45
5:4:772:ARG:HD2	5:4:772:ARG:C	2.42	0.45
7:6:540:HIS:O	7:6:544:LYS:HG2	2.16	0.45
8:7:117:PHE:HB3	8:7:202:LEU:HD11	1.99	0.45
8:7:606:ARG:HA	8:7:606:ARG:HD3	1.81	0.45
10:Z:127:ARG:NH2	10:Z:147:THR:HB	2.31	0.45
10:Z:621:ARG:HA	10:Z:621:ARG:NH1	2.31	0.45
3:B:279:THR:O	3:B:283:TYR:HB2	2.17	0.45
4:C:200:VAL:HG12	4:C:244:GLU:HB2	1.99	0.45
6:E:540:ILE:HD13	6:E:547:LEU:HD11	1.98	0.45
6:5:411:ASN:HA	6:5:519:VAL:O	2.17	0.45
8:7:574:TYR:HB3	8:7:601:LEU:HD11	1.97	0.45
10:Z:11:ALA:HA	10:Z:14:LYS:NZ	2.32	0.45
11:Y:188:LEU:O	11:Y:192:ILE:HG12	2.16	0.45
3:B:519:LEU:HD21	3:B:556:VAL:HG13	1.99	0.44
5:D:534:GLU:O	5:D:538:LYS:HG3	2.17	0.44
5:D:794:THR:HG22	5:D:795:THR:N	2.32	0.44
4:3:394:GLU:H	4:3:394:GLU:CD	2.25	0.44
6:5:584:GLN:O	6:5:588:GLU:HB2	2.17	0.44
7:6:767:LYS:O	7:6:770:ARG:HG2	2.17	0.44
10:Z:26:GLN:HG2	10:Z:27:LEU:HD22	1.98	0.44
10:Z:340:TYR:CD2	10:Z:503:GLN:HB3	2.52	0.44
10:Z:353:GLU:HA	10:Z:356:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:152:SER:O	11:Y:156:ILE:HG12	2.17	0.44
3:2:414:LEU:HD22	3:2:456:ILE:HG12	1.99	0.44
6:5:184:ARG:HG3	6:5:240:PRO:O	2.18	0.44
9:X:186:ARG:NH1	9:X:190:THR:HG21	2.32	0.44
11:Y:179:ASP:O	11:Y:182:LEU:HG	2.18	0.44
3:B:690:GLU:O	3:B:693:GLU:HB2	2.17	0.44
4:C:495:VAL:HG12	4:C:497:ILE:HG12	2.00	0.44
3:2:276:MET:HE2	3:2:280:GLU:HG3	1.99	0.44
4:3:489:VAL:HG22	4:3:495:VAL:HG22	1.99	0.44
4:3:490:MET:HG3	4:3:542:ARG:HG2	1.99	0.44
6:5:106:ARG:HH21	6:5:130:ASN:HB3	1.83	0.44
7:6:628:LEU:HD11	7:6:652:ILE:HG12	2.00	0.44
7:6:797:VAL:O	7:6:800:LEU:HB3	2.17	0.44
8:7:434:LEU:HD11	8:7:699:LEU:HD21	1.99	0.44
3:B:810:LEU:HA	3:B:813:ILE:HD12	1.98	0.44
5:D:243:LEU:O	5:D:305:PRO:HA	2.18	0.44
5:D:314:MET:SD	5:D:415:ILE:HG21	2.57	0.44
5:D:728:TYR:OH	8:G:450:ILE:HG21	2.17	0.44
8:G:409:ASP:OD2	8:G:412:ASN:HB2	2.18	0.44
3:2:785:LYS:O	3:2:789:VAL:HG23	2.18	0.44
6:5:167:ILE:HD11	6:5:257:LYS:HG2	1.99	0.44
8:7:450:ILE:HG22	8:7:694:ARG:HH12	1.82	0.44
10:Z:131:LEU:HA	10:Z:134:ILE:HG12	2.00	0.44
11:Y:239:SER:HB3	11:Y:242:SER:OG	2.17	0.44
4:C:330:HIS:CE1	4:C:338:ALA:HB2	2.53	0.44
5:D:335:SER:HB2	5:D:395:GLN:NE2	2.32	0.44
7:F:533:ILE:HD12	7:F:551:MET:HE1	2.00	0.44
7:F:772:TYR:CZ	7:F:776:LYS:HE3	2.53	0.44
8:G:103:VAL:O	8:G:107:GLN:HG3	2.16	0.44
3:2:701:ASP:HA	3:2:704:VAL:HG12	1.99	0.44
10:Z:325:TYR:CE1	10:Z:343:TYR:HB2	2.53	0.44
1:O:12:DG:H2''	1:O:13:DA:C8	2.53	0.44
5:D:447:ASN:ND2	5:D:450:GLN:HG3	2.32	0.44
5:D:510:ARG:HH11	5:D:510:ARG:HG3	1.81	0.44
5:D:581:VAL:HA	5:D:584:ILE:HG22	2.00	0.44
5:D:681:ARG:HH12	5:D:683:ASN:HB2	1.83	0.44
5:D:699:LEU:HD23	5:D:791:ILE:HD11	1.98	0.44
6:E:391:LEU:HD12	6:E:412:VAL:HG23	1.99	0.44
8:G:226:SER:O	8:G:230:ILE:HG12	2.17	0.44
8:G:575:ASN:OD1	8:G:577:ARG:HD3	2.17	0.44
3:2:211:LEU:HB3	3:2:274:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:33:ASN:HB2	6:5:37:GLU:OE2	2.17	0.44
6:5:41:ASP:O	6:5:43:GLN:HG2	2.17	0.44
8:7:537:ILE:O	8:7:541:MET:HG3	2.17	0.44
8:7:656:VAL:O	8:7:660:VAL:HG23	2.17	0.44
9:X:346:TYR:O	9:X:349:ARG:HG2	2.18	0.44
10:Z:43:LYS:HE2	10:Z:484:LEU:HD23	1.99	0.44
10:Z:127:ARG:HH21	10:Z:147:THR:HB	1.83	0.44
1:O:27:DT:H2"	1:O:28:DG:N7	2.32	0.44
5:D:194:PHE:HB3	5:D:275:THR:HG21	2.00	0.44
6:5:365:LYS:O	6:5:369:ILE:HD12	2.17	0.44
7:6:571:ILE:HG22	7:6:711:LEU:HB2	1.98	0.44
8:7:710:ILE:HG22	8:7:714:GLU:OE1	2.18	0.44
9:X:177:ALA:HA	9:X:180:VAL:HG22	2.00	0.44
9:X:278:LEU:HA	9:X:281:ILE:HD13	2.00	0.44
9:X:343:LEU:HA	9:X:346:TYR:HB2	2.00	0.44
10:Z:513:ILE:HA	10:Z:518:LEU:HD13	2.00	0.44
3:B:242:LEU:HD21	3:B:275:ALA:HB1	2.00	0.44
4:C:686:LEU:HB3	4:C:697:ILE:HD13	2.00	0.44
6:E:12:PRO:HG2	8:7:153:MET:HE2	2.00	0.44
7:F:144:LYS:HE3	7:F:193:ALA:HB1	2.00	0.44
7:F:341:ARG:HB2	3:2:363:PHE:CE1	2.53	0.44
3:2:627:GLN:OE1	3:2:643:ARG:HA	2.18	0.44
4:3:384:MET:HE3	4:3:469:VAL:HG21	1.99	0.44
9:X:302:LEU:HD23	9:X:305:ARG:NH2	2.32	0.44
10:Z:321:GLN:NE2	10:Z:323:ASP:HB3	2.33	0.44
10:Z:609:PHE:O	10:Z:613:THR:HG22	2.18	0.44
4:C:97:ILE:HD13	4:C:156:SER:OG	2.18	0.44
6:E:648:ILE:HA	6:E:652:GLN:HG3	2.00	0.44
7:F:507:SER:C	7:F:508:LEU:HD12	2.43	0.44
7:F:773:LEU:HD12	7:F:803:MET:HE2	1.99	0.44
8:G:586:LEU:HD22	8:G:590:LEU:HD21	1.99	0.44
3:2:189:VAL:HG23	3:2:197:TRP:CG	2.53	0.44
3:2:853:VAL:O	3:2:857:LEU:HD23	2.17	0.44
5:4:728:TYR:OH	8:7:450:ILE:HG21	2.17	0.44
7:6:108:GLY:HA2	7:6:111:VAL:HG12	2.00	0.44
8:7:104:SER:O	8:7:108:GLN:HG2	2.17	0.44
9:X:168:ALA:HB2	9:X:179:PHE:HD2	1.83	0.44
10:Z:66:GLU:O	10:Z:69:ARG:HG3	2.18	0.44
10:Z:290:ARG:HG3	10:Z:291:LEU:HD22	2.00	0.44
10:Z:549:GLY:O	10:Z:552:LEU:HG	2.18	0.44
10:Z:564:LEU:HB3	10:Z:600:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:336:TYR:HB2	3:B:381:VAL:HG12	2.00	0.43
3:B:364:CYS:HB3	3:B:373:PHE:CZ	2.53	0.43
5:D:802:ILE:HG21	7:F:735:HIS:ND1	2.32	0.43
6:E:498:GLU:HA	6:E:498:GLU:OE1	2.17	0.43
7:F:765:LEU:HD23	7:F:819:ILE:HD12	2.00	0.43
3:2:344:CYS:HB3	3:2:367:CYS:SG	2.56	0.43
3:2:856:GLN:HA	3:2:859:ARG:HB2	2.00	0.43
5:4:774:TYR:HD2	7:6:728:ALA:HB2	1.83	0.43
7:6:309:PHE:CD2	7:6:330:PRO:HD3	2.53	0.43
7:6:601:LYS:HA	7:6:601:LYS:HD2	1.81	0.43
9:X:158:LYS:HZ1	9:X:210:LYS:HZ3	1.66	0.43
9:X:204:TYR:CZ	9:X:208:LEU:HD23	2.53	0.43
11:Y:162:GLN:NE2	11:Y:163:ARG:HH12	2.16	0.43
1:O:30:DC:H2''	1:O:31:DT:C6	2.53	0.43
1:O:51:DT:H2''	1:O:52:DG:C8	2.53	0.43
4:C:683:TYR:CD2	4:C:702:LEU:HB2	2.53	0.43
7:F:732:VAL:HG12	7:F:736:MET:HE3	1.99	0.43
3:2:206:THR:HG22	3:2:209:ARG:HH22	1.83	0.43
3:2:569:GLN:NE2	7:6:646:ILE:HD11	2.33	0.43
3:2:704:VAL:HG21	7:6:770:ARG:NH2	2.33	0.43
4:3:367:LEU:HD12	4:3:378:LYS:HB3	2.00	0.43
5:4:412:PRO:HD2	8:7:557:LEU:HG	2.00	0.43
7:6:798:ARG:HH11	7:6:798:ARG:HG3	1.82	0.43
9:X:191:CYS:SG	9:X:204:TYR:HB2	2.58	0.43
10:Z:607:MET:O	10:Z:610:GLN:HG3	2.19	0.43
1:O:43:DT:H2''	1:O:44:DG:N7	2.32	0.43
5:D:202:LYS:HZ3	5:D:222:GLU:HA	1.83	0.43
5:D:314:MET:HE3	5:D:439:PHE:CE1	2.54	0.43
5:D:399:LEU:HD13	5:D:417:LEU:HD11	2.00	0.43
7:F:591:PHE:CZ	7:F:751:LEU:HD22	2.48	0.43
4:3:333:SER:O	6:5:510:THR:HG22	2.19	0.43
4:3:374:HIS:O	4:3:378:LYS:HG3	2.18	0.43
5:4:344:VAL:HB	5:4:390:SER:HB3	1.99	0.43
6:5:626:PHE:CD1	6:5:653:LEU:HD22	2.54	0.43
7:6:308:SER:OG	7:6:347:ASN:HB2	2.17	0.43
9:X:270:GLU:O	9:X:273:LEU:HG	2.18	0.43
3:B:576:LEU:HD13	3:B:595:ALA:HB3	1.99	0.43
4:C:400:ARG:HH21	4:C:707:ARG:CZ	2.31	0.43
5:D:420:TYR:HE2	5:D:462:ASP:OD1	2.01	0.43
6:E:455:ARG:HB2	6:E:460:ARG:HH21	1.84	0.43
6:E:462:PHE:CD2	6:E:509:ILE:HB	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:143:MET:HE2	7:F:143:MET:HB3	1.85	0.43
8:G:485:GLY:HA2	8:G:529:MET:HE3	1.99	0.43
5:4:228:LYS:HE2	5:4:231:ASN:HD22	1.83	0.43
5:4:637:MET:HG2	5:4:642:ARG:HB2	2.00	0.43
5:4:763:THR:HG23	5:4:766:ALA:H	1.82	0.43
6:5:582:ALA:O	6:5:586:GLN:HG2	2.18	0.43
8:7:520:ILE:HA	8:7:562:SER:O	2.17	0.43
9:X:234:PRO:O	9:X:237:ASP:HB3	2.18	0.43
9:X:243:CYS:HA	9:X:246:LYS:HG3	2.00	0.43
10:Z:61:ILE:HD11	10:Z:86:PHE:HZ	1.82	0.43
10:Z:353:GLU:HG2	10:Z:357:LYS:NZ	2.33	0.43
10:Z:621:ARG:HH12	10:Z:630:ILE:HG23	1.83	0.43
2:S:-29:DT:C5'	6:E:209:ARG:HH12	2.31	0.43
4:C:519:VAL:HG23	4:C:520:PHE:CD2	2.53	0.43
5:D:469:VAL:HG21	5:D:499:ARG:HB3	1.99	0.43
6:E:106:ARG:NH2	6:E:107:ALA:HA	2.34	0.43
6:E:649:THR:H	6:E:652:GLN:HG2	1.84	0.43
7:F:112:ARG:HG2	7:F:112:ARG:HH11	1.83	0.43
7:F:191:LYS:HD2	7:F:192:TYR:CD2	2.54	0.43
7:F:490:ALA:HB1	7:F:495:GLN:HE22	1.83	0.43
7:F:521:LYS:HB3	11:Y:149:LYS:NZ	2.32	0.43
3:2:267:MET:C	3:2:269:LYS:H	2.26	0.43
4:3:110:PHE:HE2	4:3:114:ILE:HD11	1.83	0.43
5:4:208:ILE:HA	5:4:213:GLU:HG3	2.00	0.43
5:4:682:TYR:CE1	5:4:707:LEU:HD11	2.52	0.43
5:4:706:TYR:OH	5:4:828:LEU:HD11	2.19	0.43
6:5:430:GLU:HG2	6:5:438:TYR:HB2	2.01	0.43
6:5:458:MET:HE2	6:5:458:MET:HB3	1.91	0.43
10:Z:470:ARG:CZ	10:Z:470:ARG:HA	2.49	0.43
3:B:273:LEU:O	3:B:277:GLU:HG3	2.18	0.43
4:C:32:LEU:HD13	4:C:132:LEU:HD23	2.01	0.43
4:C:45:ILE:HG23	4:C:92:LEU:HB2	2.00	0.43
6:E:571:HIS:CE1	6:E:575:ILE:HD11	2.54	0.43
3:2:341:CYS:HB3	3:2:373:PHE:CE2	2.54	0.43
4:3:398:HIS:HE1	4:3:493:GLN:HE21	1.66	0.43
4:3:586:LEU:HG	4:3:588:LEU:HD21	2.00	0.43
6:5:423:SER:HB3	6:5:427:LYS:NZ	2.34	0.43
6:5:464:LEU:HD21	6:5:470:VAL:HG21	2.01	0.43
8:7:335:VAL:HG13	8:7:339:LEU:HB3	1.99	0.43
3:B:221:GLU:OE1	3:B:222:THR:HG23	2.18	0.43
3:B:268:LEU:HA	3:B:271:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:363:PHE:CE2	7:6:341:ARG:HB2	2.52	0.43
5:D:578:LEU:HB3	5:D:590:TYR:HE2	1.82	0.43
5:D:764:GLU:O	5:D:767:LYS:HB3	2.18	0.43
6:E:33:ASN:HA	6:E:36:LEU:HD12	2.01	0.43
6:E:449:LEU:HD21	6:E:493:ILE:HD11	2.01	0.43
7:F:313:MET:HE3	7:F:338:CYS:HB3	2.00	0.43
7:F:771:SER:O	7:F:775:GLU:HG2	2.18	0.43
8:G:448:MET:HE3	8:G:448:MET:HB3	1.90	0.43
3:2:213:SER:O	3:2:217:GLU:HG3	2.18	0.43
4:3:569:HIS:ND1	6:5:657:ILE:HG21	2.34	0.43
5:4:509:ILE:HG23	5:4:750:TYR:CD2	2.53	0.43
6:5:397:LYS:HE3	6:5:405:ARG:HH21	1.83	0.43
7:6:568:ASP:HB2	7:6:677:SER:OG	2.18	0.43
7:6:766:THR:H	7:6:769:ALA:HB3	1.83	0.43
7:6:784:ASP:OD2	7:6:785:ALA:N	2.51	0.43
9:X:276:LEU:HD22	9:X:393:PHE:HZ	1.84	0.43
9:X:279:LEU:HD12	9:X:282:ILE:HB	2.00	0.43
10:Z:69:ARG:HD2	10:Z:70:HIS:N	2.34	0.43
10:Z:377:TRP:NE1	10:Z:385:LYS:HE3	2.33	0.43
10:Z:384:ILE:O	10:Z:388:LEU:HB3	2.19	0.43
2:S:-29:DT:H5'	6:E:209:ARG:HH12	1.83	0.43
4:C:330:HIS:ND1	4:C:338:ALA:HB2	2.34	0.43
7:F:110:LYS:O	7:F:113:GLU:HG3	2.19	0.43
8:G:589:ALA:O	8:G:593:ARG:HG2	2.19	0.43
4:3:493:GLN:HB3	4:3:509:ARG:HA	2.00	0.43
5:4:202:LYS:HE3	5:4:224:LEU:HD12	2.01	0.43
5:4:207:LYS:HA	5:4:207:LYS:HD3	1.75	0.43
5:4:604:TYR:CE2	5:4:617:GLU:HB3	2.54	0.43
6:5:62:THR:HA	6:5:138:ILE:O	2.19	0.43
7:6:270:LEU:HD22	7:6:289:SER:HB3	2.01	0.43
10:Z:576:THR:HG21	10:Z:631:GLU:OE2	2.18	0.43
3:B:246:TYR:CZ	3:B:257:ALA:HB1	2.54	0.43
4:C:216:ASP:OD2	4:C:219:THR:HG23	2.19	0.43
6:E:493:ILE:CG2	6:E:497:MET:HE3	2.49	0.43
7:F:139:GLN:O	7:F:143:MET:HG3	2.19	0.43
7:F:182:GLN:HE22	7:F:264:GLN:HA	1.83	0.43
7:F:798:ARG:HG2	7:F:798:ARG:NH1	2.32	0.43
3:2:424:VAL:HG22	3:2:425:GLU:N	2.32	0.43
3:2:629:ILE:HG23	6:5:445:SER:OG	2.19	0.43
7:6:588:VAL:HG11	7:6:635:ILE:HG21	2.01	0.43
10:Z:397:ASP:HA	10:Z:402:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:474:PHE:HB3	3:B:768:HIS:ND1	2.34	0.43
3:B:562:ARG:O	3:B:602:GLY:HA3	2.19	0.43
4:C:268:GLY:HA2	6:E:465:GLU:O	2.19	0.43
8:G:634:GLU:OE1	8:G:637:LYS:HB2	2.17	0.43
5:4:315:ARG:NE	5:4:413:HIS:CD2	2.87	0.43
6:5:435:ILE:HG22	6:5:475:GLY:HA3	2.01	0.43
8:7:471:LYS:HG2	8:7:475:LYS:NZ	2.34	0.43
10:Z:36:ILE:HD12	10:Z:36:ILE:H	1.84	0.43
10:Z:280:LEU:HB3	10:Z:287:VAL:CG2	2.49	0.43
10:Z:513:ILE:HD11	10:Z:530:LEU:HD11	2.01	0.43
11:Y:153:ILE:HA	11:Y:156:ILE:HG12	2.01	0.43
4:C:27:ARG:HD2	4:C:27:ARG:HA	1.88	0.42
4:C:703:GLU:O	4:C:707:ARG:HG3	2.19	0.42
5:D:631:ILE:HD12	5:D:671:ILE:HG23	2.01	0.42
8:G:605:SER:O	8:G:609:ASP:HB2	2.19	0.42
3:2:205:ARG:HG3	3:2:205:ARG:HH11	1.84	0.42
6:5:420:THR:O	6:5:420:THR:HG22	2.19	0.42
10:Z:349:SER:O	10:Z:355:GLY:HA3	2.19	0.42
1:O:12:DG:H2"	1:O:13:DA:H8	1.84	0.42
4:C:459:ALA:HB2	8:G:327:ILE:HD11	2.01	0.42
6:E:31:PHE:HE1	6:E:75:ILE:HD12	1.84	0.42
6:E:34:PHE:HD2	6:E:71:TYR:CG	2.38	0.42
3:2:442:ASN:HA	7:6:326:LYS:HZ3	1.83	0.42
3:2:548:ALA:HB2	12:2:1001:ADP:C8	2.54	0.42
4:3:97:ILE:HD13	4:3:156:SER:OG	2.20	0.42
4:3:519:VAL:HG11	4:3:534:ALA:HB3	2.01	0.42
4:3:566:LEU:HD13	6:5:619:ALA:HB1	2.01	0.42
6:5:39:ARG:HH22	6:5:42:SER:CA	2.32	0.42
6:5:182:MET:HG3	6:5:189:THR:HG22	2.01	0.42
9:X:170:PHE:HZ	9:X:231:PHE:CE1	2.35	0.42
10:Z:385:LYS:HA	10:Z:388:LEU:HG	2.01	0.42
2:S:-14:DG:C8	2:S:-13:DT:H72	2.55	0.42
5:D:235:GLU:OE1	5:D:235:GLU:HA	2.19	0.42
6:E:276:MET:HE3	6:E:330:ILE:HD11	2.01	0.42
7:F:429:THR:HG21	3:2:340:ASN:HD22	1.84	0.42
8:G:198:ARG:HG2	8:G:200:TYR:CE1	2.54	0.42
8:G:605:SER:OG	8:G:608:ASP:HB2	2.20	0.42
5:4:235:GLU:OE1	5:4:235:GLU:HA	2.19	0.42
5:4:289:LEU:HD23	5:4:291:TYR:H	1.84	0.42
5:4:589:VAL:HG22	5:4:624:SER:OG	2.19	0.42
6:5:427:LYS:O	6:5:430:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:462:PHE:HE2	6:5:508:GLY:HA3	1.83	0.42
7:6:777:TYR:CE2	7:6:800:LEU:HB2	2.54	0.42
11:Y:155:ILE:O	11:Y:159:GLN:OE1	2.37	0.42
2:S:-58:DG:H2''	2:S:-57:DT:H5'	2.00	0.42
3:B:854:ARG:HA	3:B:857:LEU:HB2	2.01	0.42
4:C:263:GLU:CD	4:C:263:GLU:H	2.28	0.42
4:C:687:ARG:HD3	8:G:609:ASP:OD1	2.19	0.42
4:C:688:ASN:HD22	8:G:606:ARG:HD2	1.84	0.42
5:D:522:LEU:HD22	5:D:747:LEU:HD13	2.00	0.42
5:D:527:ALA:HB3	5:D:537:LYS:HE2	2.00	0.42
5:D:559:ARG:HD2	5:D:559:ARG:HA	1.74	0.42
5:D:663:THR:HG21	7:F:374:PRO:HG3	2.00	0.42
7:F:339:GLU:HB3	7:F:341:ARG:HH21	1.84	0.42
3:2:221:GLU:OE1	3:2:222:THR:HG23	2.19	0.42
3:2:620:ILE:O	3:2:624:MET:HG3	2.19	0.42
5:4:348:LYS:HB2	5:4:348:LYS:HE3	1.83	0.42
5:4:366:GLN:OE1	5:4:366:GLN:HA	2.19	0.42
5:4:532:GLU:H	5:4:537:LYS:NZ	2.17	0.42
8:7:88:TYR:O	8:7:91:GLU:HG2	2.19	0.42
8:7:154:LEU:HD21	8:7:191:LEU:HD11	2.01	0.42
9:X:243:CYS:O	9:X:246:LYS:HG3	2.19	0.42
10:Z:39:LEU:O	10:Z:42:THR:HG22	2.19	0.42
10:Z:296:GLN:HA	10:Z:299:VAL:HG22	2.01	0.42
10:Z:550:ASN:O	10:Z:551:TRP:C	2.63	0.42
4:C:734:ARG:HA	4:C:734:ARG:HD2	1.88	0.42
6:E:637:GLU:OE1	6:E:643:ARG:HA	2.19	0.42
8:G:500:ASP:OD1	8:G:502:VAL:HG22	2.20	0.42
3:2:337:VAL:HG13	3:2:375:VAL:HG13	2.00	0.42
4:3:189:THR:HB	4:3:254:GLN:NE2	2.35	0.42
6:5:584:GLN:NE2	6:5:588:GLU:HG3	2.34	0.42
6:5:599:MET:HE3	6:5:599:MET:HB2	1.84	0.42
7:6:556:HIS:HB3	7:6:564:LYS:NZ	2.34	0.42
8:7:118:CYS:HB3	8:7:198:ARG:HH11	1.84	0.42
8:7:355:PHE:CE2	8:7:374:THR:HB	2.55	0.42
8:7:596:ILE:HD12	8:7:598:PHE:CE2	2.52	0.42
2:S:-44:DC:H2''	2:S:-43:DA:N7	2.35	0.42
3:B:808:ARG:O	3:B:811:GLU:HB2	2.18	0.42
4:C:20:VAL:O	4:C:24:ARG:HG3	2.19	0.42
4:C:230:ILE:HA	6:5:225:SER:HB3	2.01	0.42
4:C:333:SER:O	6:E:510:THR:HG22	2.20	0.42
4:C:686:LEU:HD23	4:C:686:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:789:LYS:HG3	5:D:790:ARG:HG3	2.01	0.42
6:E:95:THR:HA	6:E:135:PHE:CD2	2.54	0.42
6:E:534:LYS:HA	6:E:534:LYS:HD3	1.90	0.42
6:E:695:ASP:OD1	6:E:696:PRO:HD2	2.20	0.42
8:G:596:ILE:HD12	8:G:598:PHE:HE1	1.85	0.42
3:2:789:VAL:HG13	3:2:864:TYR:CE2	2.47	0.42
4:3:303:ALA:HA	6:5:243:ILE:HD13	2.01	0.42
4:3:368:ALA:HB3	4:3:378:LYS:NZ	2.34	0.42
5:4:696:PRO:N	5:4:697:PRO:HD2	2.33	0.42
7:6:557:LYS:HB2	7:6:565:LEU:HD11	2.02	0.42
7:6:606:ALA:HB1	7:6:611:ALA:HB2	2.01	0.42
10:Z:133:ASN:OD1	10:Z:134:ILE:HG23	2.20	0.42
1:O:43:DT:H2''	1:O:44:DG:C8	2.55	0.42
5:D:274:GLN:HB2	9:X:525:MET:HE3	2.01	0.42
6:E:682:ARG:HE	6:E:682:ARG:HB3	1.68	0.42
8:G:17:LEU:HD23	8:G:17:LEU:HA	1.78	0.42
8:G:157:ARG:HD3	8:G:157:ARG:HA	1.80	0.42
3:2:623:ALA:HB2	3:2:629:ILE:HD11	2.02	0.42
5:4:773:ALA:O	5:4:777:MET:HG3	2.20	0.42
6:5:45:ILE:HG13	6:5:46:TYR:N	2.35	0.42
6:5:212:LEU:HD23	6:5:215:ILE:HG13	2.01	0.42
8:7:628:LEU:HD12	8:7:628:LEU:HA	1.89	0.42
9:X:161:ILE:HB	9:X:187:LEU:HG	2.00	0.42
10:Z:281:ASP:HB2	10:Z:288:TYR:CD2	2.54	0.42
10:Z:299:VAL:O	10:Z:303:THR:HB	2.19	0.42
5:D:294:ASP:O	5:D:298:THR:HG23	2.20	0.42
5:D:631:ILE:HD13	5:D:645:LEU:HD11	2.02	0.42
6:E:456:ASP:OD2	6:E:458:MET:HG2	2.19	0.42
8:G:718:ARG:HH11	8:G:718:ARG:HG2	1.84	0.42
4:3:103:LEU:HD21	4:3:114:ILE:HD12	2.01	0.42
4:3:483:ARG:HA	4:3:486:ILE:HG22	2.02	0.42
4:3:483:ARG:HB3	4:3:539:LEU:HD11	2.01	0.42
5:4:683:ASN:H	5:4:691:ASN:ND2	2.17	0.42
5:4:693:ASP:O	5:4:693:ASP:OD2	2.37	0.42
6:5:83:PRO:O	6:5:87:ILE:HG12	2.19	0.42
8:7:247:ARG:HB3	8:7:247:ARG:CZ	2.50	0.42
10:Z:92:LEU:HD12	10:Z:96:LEU:HD13	2.01	0.42
11:Y:155:ILE:HA	11:Y:158:GLN:HG3	2.01	0.42
2:S:-43:DA:H5''	7:F:666:ALA:HB2	2.01	0.42
3:B:205:ARG:HG3	3:B:205:ARG:HH11	1.85	0.42
5:D:760:PRO:HA	5:D:815:ASN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:132:LEU:HD23	6:E:135:PHE:HZ	1.84	0.42
6:E:551:ASP:HB3	6:E:655:ALA:HB1	2.01	0.42
3:2:555:TYR:CD1	3:2:558:LYS:HE2	2.52	0.42
3:2:756:SER:HB3	3:2:757:PRO:HD3	2.02	0.42
5:4:548:THR:H	5:4:806:GLU:CD	2.27	0.42
6:5:19:PRO:HB3	6:5:26:GLU:OE1	2.20	0.42
6:5:413:LEU:HD12	6:5:414:LEU:N	2.34	0.42
6:5:562:GLU:O	6:5:566:ILE:HG12	2.19	0.42
3:B:505:ILE:HG21	3:B:552:ILE:HD11	2.02	0.42
5:D:178:ARG:NH1	9:X:534:SER:HB2	2.35	0.42
8:G:18:PHE:CE2	8:G:119:ARG:HD2	2.55	0.42
8:G:85:ILE:O	8:G:89:GLN:HG3	2.20	0.42
8:G:656:VAL:O	8:G:660:VAL:HG23	2.19	0.42
3:2:530:LYS:HB3	6:5:428:PHE:HE1	1.85	0.42
3:2:693:GLU:CD	7:6:778:LYS:HE3	2.44	0.42
4:3:374:HIS:ND1	4:3:377:ILE:HD12	2.35	0.42
4:3:570:ARG:HB2	6:5:613:ARG:HH21	1.85	0.42
7:6:307:ALA:HA	7:6:351:SER:OG	2.20	0.42
7:6:586:LYS:HE2	7:6:586:LYS:HB2	1.78	0.42
8:7:276:ARG:HE	8:7:277:THR:HG23	1.85	0.42
8:7:590:LEU:O	8:7:594:PHE:HB2	2.20	0.42
9:X:352:ILE:O	9:X:356:LEU:HD23	2.20	0.42
10:Z:434:VAL:HG22	10:Z:472:ARG:NH2	2.34	0.42
3:B:207:ILE:HD11	3:B:270:ILE:HD11	2.02	0.41
3:B:851:VAL:HA	3:B:854:ARG:HG2	2.02	0.41
6:E:192:ILE:HD11	6:E:208:PRO:HD3	2.02	0.41
6:E:420:THR:HG21	6:E:556:VAL:HG21	2.01	0.41
7:F:341:ARG:HA	7:F:341:ARG:HD3	1.90	0.41
7:F:803:MET:HB3	7:F:831:LEU:HD12	2.01	0.41
8:G:428:VAL:O	8:G:432:LEU:HD13	2.20	0.41
8:G:581:LEU:HD23	8:G:584:ILE:HD11	2.02	0.41
3:2:519:LEU:HD23	3:2:519:LEU:HA	1.92	0.41
3:2:667:VAL:HG12	3:2:669:LEU:HG	2.01	0.41
5:4:187:ILE:H	5:4:187:ILE:HD12	1.85	0.41
5:4:578:LEU:HD13	5:4:672:LEU:HG	2.02	0.41
7:6:720:ASN:HB3	7:6:723:ILE:HB	2.02	0.41
3:B:202:ASN:O	3:B:206:THR:HG23	2.20	0.41
4:C:394:GLU:H	4:C:394:GLU:CD	2.27	0.41
4:C:410:ASP:HB2	4:C:411:PRO:HD2	2.02	0.41
7:F:595:SER:HA	7:F:635:ILE:O	2.20	0.41
8:G:247:ARG:HB3	8:G:247:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:189:THR:HG22	4:3:256:ILE:HG22	2.03	0.41
5:4:788:GLU:OE1	5:4:788:GLU:N	2.53	0.41
8:7:485:GLY:C	8:7:487:GLY:H	2.29	0.41
10:Z:382:HIS:O	10:Z:385:LYS:HB2	2.20	0.41
10:Z:413:LEU:HB3	10:Z:416:ARG:CZ	2.50	0.41
10:Z:642:GLU:O	10:Z:646:LEU:HG	2.21	0.41
2:S:-36:DC:H2"	2:S:-35:DA:H8	1.85	0.41
4:C:537:ASP:HB3	8:G:572:GLY:HA3	2.03	0.41
5:D:646:HIS:NE2	7:F:577:PRO:HB3	2.36	0.41
6:E:151:LEU:HD11	6:E:162:LEU:HD13	2.02	0.41
3:2:472:ASP:HB3	3:2:473:VAL:H	1.67	0.41
3:2:616:ASP:O	3:2:620:ILE:HG12	2.20	0.41
4:3:346:ASP:O	4:3:350:ILE:HG13	2.19	0.41
5:4:657:ALA:O	7:6:607:GLY:HA3	2.20	0.41
6:5:623:SER:O	6:5:627:VAL:HG23	2.20	0.41
7:6:770:ARG:O	7:6:774:VAL:HG23	2.20	0.41
8:7:437:VAL:O	8:7:646:LYS:HE2	2.20	0.41
8:7:605:SER:O	8:7:609:ASP:HB2	2.20	0.41
9:X:407:PRO:HA	9:X:410:VAL:HG22	2.02	0.41
10:Z:82:LEU:HD23	10:Z:121:TYR:HB2	2.02	0.41
10:Z:126:HIS:CG	10:Z:245:THR:HB	2.56	0.41
10:Z:370:LEU:O	10:Z:374:GLN:HG2	2.20	0.41
3:B:806:THR:HG21	3:B:808:ARG:NE	2.29	0.41
5:D:387:ASN:N	5:D:387:ASN:HD22	2.18	0.41
6:E:656:ILE:HD11	6:E:684:PHE:CD2	2.55	0.41
8:G:206:PRO:HG3	8:G:352:THR:HG21	2.03	0.41
8:G:664:TYR:CD1	8:G:689:LEU:HB2	2.56	0.41
8:G:685:THR:HG22	8:G:687:ARG:N	2.27	0.41
3:2:327:ARG:HG2	3:2:388:VAL:HG12	2.02	0.41
3:2:606:ILE:HG21	3:2:609:PHE:HD1	1.85	0.41
4:3:118:PRO:HB2	4:3:122:ILE:HD12	2.02	0.41
4:3:369:PRO:HB3	4:3:650:LEU:HD21	2.02	0.41
5:4:709:LEU:HD23	5:4:834:LYS:NZ	2.35	0.41
6:5:571:HIS:CE1	6:5:575:ILE:HD11	2.55	0.41
8:7:351:VAL:HG22	8:7:381:VAL:HG13	2.02	0.41
9:X:268:SER:HA	9:X:271:ILE:HG12	2.03	0.41
10:Z:341:SER:O	10:Z:345:ASN:HB2	2.20	0.41
1:O:48:DG:H2"	1:O:49:DA:C8	2.56	0.41
4:C:232:PRO:HB3	8:G:5:LEU:HD11	2.03	0.41
4:C:478:MET:HG2	4:C:482:ASP:HB2	2.01	0.41
4:C:530:HIS:C	4:C:530:HIS:HD1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:701:ARG:HA	5:D:796:ARG:HG2	2.02	0.41
6:E:64:ASN:HB3	6:E:67:HIS:ND1	2.35	0.41
6:E:183:CYS:SG	6:E:240:PRO:HB2	2.60	0.41
6:E:421:ALA:HB2	12:E:1001:ADP:C8	2.55	0.41
3:2:502:ALA:HB3	3:2:512:LYS:HZ1	1.85	0.41
4:3:172:THR:OG1	4:3:174:GLN:HG2	2.21	0.41
5:4:209:LEU:HD22	5:4:250:ALA:HB2	2.03	0.41
5:4:233:MET:SD	5:4:241:LEU:HB2	2.61	0.41
5:4:348:LYS:HB3	5:4:355:THR:HG22	2.03	0.41
6:5:87:ILE:HD12	6:5:137:LEU:HD23	2.02	0.41
6:5:360:LEU:O	6:5:366:LEU:HD12	2.20	0.41
6:5:635:ILE:HD13	6:5:635:ILE:HA	1.93	0.41
7:6:270:LEU:HD21	7:6:287:LEU:HD23	2.02	0.41
7:6:523:GLU:HG2	7:6:524:HIS:ND1	2.35	0.41
7:6:529:LEU:HD11	7:6:754:TYR:CE2	2.56	0.41
7:6:799:GLN:HA	7:6:802:SER:HB3	2.02	0.41
9:X:303:LYS:NZ	10:Z:601:ILE:HG23	2.35	0.41
10:Z:324:TYR:HD1	10:Z:404:ILE:HG22	1.85	0.41
3:B:345:GLY:O	7:6:428:LYS:HD3	2.20	0.41
5:D:681:ARG:O	5:D:681:ARG:HG3	2.20	0.41
5:D:779:LYS:HE2	7:F:721:GLU:OE2	2.20	0.41
6:E:39:ARG:CG	10:Z:313:PRO:HG3	2.48	0.41
3:2:214:PHE:HD2	3:2:215:LEU:HD22	1.86	0.41
6:5:552:MET:HE3	6:5:552:MET:HB2	1.89	0.41
7:6:299:GLU:O	7:6:301:ARG:HD2	2.20	0.41
7:6:695:LEU:HB2	7:6:792:SER:HB2	2.03	0.41
1:O:26:DC:H2"	1:O:27:DT:C6	2.56	0.41
2:S:-44:DC:H2"	2:S:-43:DA:C8	2.56	0.41
3:B:304:TYR:O	3:B:320:VAL:HA	2.20	0.41
5:D:226:TYR:O	5:D:230:LEU:HD23	2.20	0.41
5:D:334:ARG:HE	5:D:398:LYS:HD2	1.83	0.41
7:F:428:LYS:NZ	3:2:346:SER:HB3	2.36	0.41
8:G:61:PRO:HB2	8:G:64:MET:HB2	2.03	0.41
8:G:281:LEU:HD23	8:G:281:LEU:H	1.85	0.41
3:2:485:ARG:HB3	3:2:489:ARG:HH12	1.86	0.41
3:2:705:ARG:C	3:2:710:ASN:HD21	2.29	0.41
3:2:768:HIS:O	3:2:772:THR:HG23	2.20	0.41
4:3:569:HIS:O	6:5:398:LYS:HE2	2.20	0.41
5:4:319:PRO:HB3	8:7:253:PRO:HB3	2.03	0.41
10:Z:26:GLN:HE21	10:Z:79:ASN:HB3	1.85	0.41
10:Z:71:TYR:O	10:Z:74:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:95:PHE:HD2	10:Z:96:LEU:HD12	1.85	0.41
10:Z:330:ARG:HA	10:Z:377:TRP:CD2	2.55	0.41
3:B:238:ASN:HB2	10:Z:370:LEU:HD23	2.03	0.41
3:B:625:GLU:HG2	3:B:676:ARG:HD2	2.03	0.41
4:C:104:ARG:HB2	4:C:111:TRP:CD1	2.55	0.41
4:C:110:PHE:HE2	4:C:114:ILE:HD11	1.85	0.41
4:C:171:LEU:HD23	4:C:171:LEU:HA	1.87	0.41
5:D:603:ALA:HA	5:D:617:GLU:O	2.20	0.41
6:E:31:PHE:CE1	6:E:75:ILE:HD12	2.56	0.41
7:F:385:SER:O	7:F:388:ARG:HG3	2.21	0.41
7:F:403:VAL:HB	7:F:450:TYR:HB3	2.02	0.41
7:F:516:LEU:O	7:F:519:MET:HB2	2.21	0.41
7:F:644:MET:HG2	7:F:649:GLN:HG2	2.03	0.41
8:G:265:CYS:HB3	8:G:289:CYS:SG	2.61	0.41
8:G:459:MET:HE2	8:G:586:LEU:HD12	2.02	0.41
3:2:319:ARG:HG3	3:2:425:GLU:OE1	2.20	0.41
4:3:345:PHE:HD2	4:3:348:ARG:HH22	1.68	0.41
5:4:212:ARG:HG2	5:4:215:PHE:HB2	2.02	0.41
6:5:24:ASN:O	6:5:28:ILE:HG13	2.21	0.41
6:5:65:MET:SD	6:5:139:LEU:HD13	2.60	0.41
6:5:351:GLU:HA	6:5:354:GLU:OE1	2.20	0.41
6:5:561:ASN:OD1	6:5:564:ARG:HG2	2.20	0.41
6:5:610:CYS:HB3	6:5:665:LYS:HG3	2.02	0.41
7:6:315:ARG:HE	7:6:315:ARG:N	2.18	0.41
7:6:772:TYR:CD2	7:6:821:PRO:HB2	2.56	0.41
8:7:500:ASP:OD2	8:7:502:VAL:HG22	2.21	0.41
8:7:541:MET:HE1	8:7:594:PHE:CZ	2.56	0.41
9:X:296:LYS:HA	9:X:299:LYS:HE2	2.03	0.41
10:Z:12:TYR:HA	10:Z:15:ILE:HG12	2.03	0.41
10:Z:387:GLU:O	10:Z:391:ILE:HG12	2.21	0.41
1:O:5:DA:C8	1:O:5:DA:H5'	2.56	0.41
1:O:32:DG:H2''	1:O:33:DA:C8	2.55	0.41
3:B:423:GLU:HG2	3:B:459:ARG:HG3	2.02	0.41
3:B:530:LYS:NZ	6:E:596:ILE:HG12	2.35	0.41
3:B:809:HIS:O	3:B:813:ILE:HG13	2.21	0.41
3:B:822:LYS:HB2	3:B:822:LYS:HE3	1.87	0.41
4:C:172:THR:OG1	4:C:174:GLN:HG2	2.21	0.41
4:C:576:TYR:HE1	4:C:582:VAL:HA	1.85	0.41
5:D:349:CYS:HB3	5:D:352:CYS:HB2	2.02	0.41
5:D:605:ILE:HG21	5:D:614:LEU:HD13	2.03	0.41
5:D:659:ALA:HB2	7:F:606:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:701:ARG:NH1	7:F:578:SER:HA	2.36	0.41
6:E:184:ARG:HG3	6:E:240:PRO:O	2.21	0.41
6:E:449:LEU:CD2	6:E:493:ILE:HD11	2.51	0.41
6:E:490:ARG:HG2	6:E:494:HIS:HE1	1.86	0.41
7:F:795:ILE:HD12	7:F:799:GLN:HG2	2.03	0.41
4:3:389:VAL:HG23	4:3:710:THR:HG21	2.03	0.41
4:3:622:PHE:CD2	4:3:649:LYS:HE2	2.55	0.41
5:4:762:ILE:HA	5:4:817:VAL:HG12	2.02	0.41
5:4:765:ALA:O	5:4:769:GLU:HG2	2.21	0.41
6:5:494:HIS:CE1	6:5:546:ILE:HG12	2.56	0.41
6:5:634:LEU:HD12	6:5:638:LEU:HD23	2.02	0.41
7:6:360:ARG:NE	7:6:376:THR:HG21	2.32	0.41
7:6:379:VAL:HG11	7:6:397:PHE:CD1	2.56	0.41
8:7:174:PRO:HB2	8:7:175:SER:H	1.65	0.41
8:7:295:LYS:HA	8:7:295:LYS:HD3	1.95	0.41
8:7:536:ALA:O	8:7:540:VAL:HG23	2.21	0.41
9:X:169:LEU:CD1	9:X:269:ARG:HB3	2.50	0.41
9:X:411:GLU:O	9:X:414:ILE:HG22	2.21	0.41
10:Z:297:ASP:O	10:Z:300:LYS:HG2	2.20	0.41
11:Y:159:GLN:HA	11:Y:162:GLN:NE2	2.36	0.41
3:B:214:PHE:HB2	3:B:253:LYS:HE3	2.03	0.41
3:B:238:ASN:ND2	10:Z:369:PRO:HA	2.36	0.41
3:B:532:SER:O	3:B:533:ILE:HD13	2.21	0.41
6:E:39:ARG:NH1	6:E:42:SER:H	2.19	0.41
6:E:552:MET:HB3	6:E:687:SER:HB2	2.03	0.41
3:2:446:VAL:CG1	7:6:301:ARG:HG3	2.51	0.41
3:2:521:GLY:O	3:2:822:LYS:HD2	2.21	0.41
5:4:578:LEU:HD12	5:4:630:CYS:HB3	2.02	0.41
5:4:791:ILE:HD13	5:4:833:ILE:HD11	2.03	0.41
7:6:642:ASP:CG	7:6:683:ASN:HB2	2.46	0.41
7:6:692:LYS:HA	7:6:839:ASP:HB3	2.03	0.41
10:Z:14:LYS:HA	10:Z:17:ARG:NH1	2.36	0.41
6:E:74:ASP:O	6:E:78:LYS:HG2	2.21	0.40
6:E:220:SER:HB3	8:7:359:PRO:HG3	2.02	0.40
8:G:394:THR:O	8:G:398:GLU:HB2	2.21	0.40
3:2:780:GLN:O	3:2:783:MET:HB3	2.21	0.40
3:2:854:ARG:HG3	3:2:858:ARG:HH22	1.85	0.40
4:3:155:LEU:HD23	4:3:155:LEU:HA	1.82	0.40
4:3:211:TYR:HD1	8:7:8:ILE:HB	1.87	0.40
4:3:280:ASP:HB3	4:3:281:ASP:H	1.71	0.40
5:4:337:PRO:HB3	7:6:375:ARG:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:373:ARG:HG2	5:4:375:ASP:H	1.86	0.40
6:5:61:LEU:HB3	6:5:94:ILE:HD13	2.04	0.40
6:5:486:ARG:NH1	6:5:486:ARG:HG3	2.36	0.40
7:6:547:ILE:HD11	7:6:584:PHE:HB3	2.02	0.40
8:7:157:ARG:HG3	8:7:185:VAL:HG12	2.02	0.40
8:7:596:ILE:HG21	8:7:695:LEU:HD11	2.03	0.40
10:Z:382:HIS:HA	10:Z:385:LYS:HD3	2.03	0.40
10:Z:502:LEU:O	10:Z:506:ILE:HG12	2.20	0.40
3:B:494:ILE:HA	3:B:497:ILE:HG12	2.02	0.40
3:B:569:GLN:O	3:B:569:GLN:HG2	2.20	0.40
4:C:118:PRO:HB2	4:C:122:ILE:HD12	2.02	0.40
6:E:572:VAL:HA	6:E:575:ILE:HD13	2.03	0.40
7:F:186:ARG:HA	7:F:189:VAL:HG12	2.02	0.40
8:G:242:ARG:HB2	8:G:350:ASP:OD1	2.21	0.40
3:2:512:LYS:HG2	3:2:512:LYS:H	1.67	0.40
5:4:183:THR:HG22	5:4:264:TYR:CD1	2.56	0.40
5:4:526:ILE:HG23	5:4:580:TYR:CE2	2.57	0.40
8:7:610:GLU:O	8:7:614:GLU:HG2	2.21	0.40
9:X:373:THR:O	9:X:376:GLU:HG3	2.21	0.40
10:Z:570:ALA:HB1	10:Z:579:TYR:CD1	2.56	0.40
10:Z:607:MET:HA	10:Z:610:GLN:HG3	2.03	0.40
10:Z:621:ARG:HA	10:Z:621:ARG:CZ	2.52	0.40
3:B:479:GLU:HG2	3:B:480:GLU:N	2.36	0.40
3:B:806:THR:O	3:B:809:HIS:HB2	2.22	0.40
5:D:327:ASN:HA	5:D:435:VAL:O	2.22	0.40
5:D:374:ILE:H	5:D:374:ILE:HD12	1.86	0.40
5:D:525:SER:HB3	5:D:747:LEU:HD22	2.03	0.40
5:D:565:LEU:HB2	5:D:702:PHE:CE2	2.57	0.40
5:D:770:LEU:HD13	5:D:802:ILE:HG12	2.03	0.40
6:E:13:VAL:HG21	8:7:268:GLU:CD	2.47	0.40
6:E:366:LEU:HA	6:E:369:ILE:HD13	2.02	0.40
6:E:462:PHE:HE2	6:E:508:GLY:HA3	1.86	0.40
3:2:551:GLN:NE2	12:2:1001:ADP:H5'1	2.36	0.40
3:2:853:VAL:O	3:2:856:GLN:HG2	2.21	0.40
4:3:132:LEU:O	4:3:136:MET:HG3	2.21	0.40
4:3:376:HIS:HA	4:3:379:LYS:HD2	2.03	0.40
4:3:671:LEU:HD23	4:3:671:LEU:HA	1.89	0.40
6:5:183:CYS:SG	6:5:240:PRO:HB2	2.61	0.40
6:5:679:GLU:HA	6:5:679:GLU:OE2	2.21	0.40
8:7:674:GLU:HG2	8:7:679:PHE:CE1	2.56	0.40
9:X:159:GLU:O	9:X:162:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:DT:H2''	1:O:8:DG:C8	2.57	0.40
3:B:296:ARG:HA	3:B:296:ARG:HD3	1.96	0.40
3:B:596:LEU:HD11	3:B:620:ILE:HD13	2.03	0.40
4:C:467:ARG:N	4:C:467:ARG:HD2	2.36	0.40
5:D:211:GLU:HG2	5:D:211:GLU:O	2.22	0.40
5:D:248:LEU:HD22	5:D:254:THR:HG21	2.02	0.40
5:D:334:ARG:HD3	5:D:617:GLU:OE2	2.21	0.40
5:D:493:ASN:O	5:D:494:GLU:HG2	2.22	0.40
5:D:657:ALA:O	7:F:607:GLY:HA3	2.22	0.40
7:F:126:SER:HB2	7:F:129:THR:OG1	2.21	0.40
3:2:190:LYS:N	3:2:190:LYS:HD2	2.36	0.40
3:2:551:GLN:NE2	12:2:1001:ADP:H3'	2.36	0.40
5:4:175:GLU:HA	5:4:176:PRO:HD3	1.99	0.40
5:4:542:LEU:HA	5:4:542:LEU:HD23	1.87	0.40
5:4:644:VAL:O	5:4:648:VAL:HG23	2.20	0.40
6:5:63:VAL:O	6:5:139:LEU:HA	2.21	0.40
6:5:82:GLU:O	6:5:86:ILE:HG12	2.22	0.40
6:5:584:GLN:O	6:5:588:GLU:CB	2.69	0.40
7:6:172:GLU:HG3	7:6:173:GLN:HG2	2.02	0.40
8:7:223:LYS:HA	8:7:224:PRO:HD3	1.92	0.40
9:X:309:LEU:HD11	10:Z:604:ASN:ND2	2.37	0.40
3:B:496:LYS:HE3	3:B:758:ILE:HD11	2.04	0.40
5:D:565:LEU:HD13	5:D:702:PHE:CE2	2.57	0.40
5:D:655:SER:HA	5:D:664:THR:HA	2.04	0.40
7:F:503:VAL:HA	7:F:506:ASN:ND2	2.36	0.40
7:F:794:ARG:HD3	7:F:795:ILE:N	2.37	0.40
8:G:309:ALA:O	8:G:336:ASN:HA	2.21	0.40
6:5:166:ILE:HD13	6:5:286:VAL:HG21	2.04	0.40
7:6:392:GLY:HA3	7:6:630:LEU:HD22	2.03	0.40
8:7:207:LEU:HD13	8:7:212:ALA:HB2	2.04	0.40
11:Y:224:ARG:HH22	11:Y:228:LYS:HD3	1.87	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	
3	2	624/868 (72%)	604 (97%)	20 (3%)	0	100	100
3	B	624/868 (72%)	603 (97%)	21 (3%)	0	100	100
4	3	627/971 (65%)	613 (98%)	14 (2%)	0	100	100
4	C	627/971 (65%)	608 (97%)	19 (3%)	0	100	100
5	4	669/933 (72%)	649 (97%)	20 (3%)	0	100	100
5	D	669/933 (72%)	642 (96%)	27 (4%)	0	100	100
6	5	657/775 (85%)	635 (97%)	22 (3%)	0	100	100
6	E	657/775 (85%)	634 (96%)	22 (3%)	1 (0%)	43	72
7	6	642/1017 (63%)	621 (97%)	21 (3%)	0	100	100
7	F	642/1017 (63%)	615 (96%)	27 (4%)	0	100	100
8	7	687/845 (81%)	663 (96%)	24 (4%)	0	100	100
8	G	687/845 (81%)	667 (97%)	20 (3%)	0	100	100
9	X	248/668 (37%)	237 (96%)	11 (4%)	0	100	100
10	Z	545/650 (84%)	520 (95%)	24 (4%)	1 (0%)	43	72
11	Y	70/257 (27%)	66 (94%)	4 (6%)	0	100	100
All	All	8675/12393 (70%)	8377 (97%)	296 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	382	GLU
10	Z	537	ASP

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	
3	2	554/770 (72%)	554 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	554/770 (72%)	554 (100%)	0	100	100
4	3	553/835 (66%)	553 (100%)	0	100	100
4	C	553/835 (66%)	553 (100%)	0	100	100
5	4	611/848 (72%)	610 (100%)	1 (0%)	87	96
5	D	611/848 (72%)	611 (100%)	0	100	100
6	5	595/688 (86%)	595 (100%)	0	100	100
6	E	595/688 (86%)	595 (100%)	0	100	100
7	6	571/886 (64%)	571 (100%)	0	100	100
7	F	571/886 (64%)	571 (100%)	0	100	100
8	7	612/753 (81%)	612 (100%)	0	100	100
8	G	612/753 (81%)	611 (100%)	1 (0%)	87	96
9	X	246/628 (39%)	246 (100%)	0	100	100
10	Z	499/586 (85%)	497 (100%)	2 (0%)	84	94
11	Y	70/234 (30%)	70 (100%)	0	100	100
All	All	7807/11008 (71%)	7803 (100%)	4 (0%)	87	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	87	GLN
5	4	666	ASN
10	Z	52	GLN
10	Z	55	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	238	ASN
3	B	290	HIS
3	B	366	ASN
3	B	437	ASN
3	B	526	ASN
3	B	551	GLN
3	B	849	GLN
4	C	307	ASN
4	C	308	GLN

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Mol	Chain	Res	Type
4	C	376	HIS
4	C	404	ASN
4	C	507	ASN
4	C	531	GLN
4	C	673	GLN
4	C	688	ASN
5	D	288	ASN
5	D	366	GLN
5	D	377	ASN
5	D	387	ASN
5	D	413	HIS
5	D	483	GLN
5	D	797	GLN
5	D	823	GLN
6	E	185	ASN
6	E	196	ASN
6	E	245	HIS
6	E	344	ASN
6	E	411	ASN
6	E	424	GLN
6	E	514	ASN
7	F	335	ASN
7	F	362	GLN
7	F	497	ASN
7	F	540	HIS
7	F	570	ASN
8	G	68	GLN
8	G	72	ASN
8	G	144	ASN
8	G	326	HIS
8	G	425	ASN
8	G	583	ASN
3	2	454	ASN
3	2	551	GLN
3	2	653	ASN
4	3	94	HIS
4	3	269	GLN
4	3	365	GLN
4	3	493	GLN
4	3	503	HIS
4	3	507	ASN
4	3	531	GLN

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Mol	Chain	Res	Type
4	3	673	GLN
4	3	688	ASN
5	4	196	ASN
5	4	240	ASN
5	4	318	ASN
5	4	320	ASN
5	4	413	HIS
5	4	579	GLN
5	4	691	ASN
5	4	823	GLN
6	5	67	HIS
6	5	185	ASN
6	5	424	GLN
6	5	560	HIS
6	5	625	ASN
6	5	636	ASN
7	6	335	ASN
7	6	550	GLN
7	6	649	GLN
7	6	653	HIS
8	7	68	GLN
8	7	178	ASN
8	7	321	GLN
8	7	334	HIS
9	X	209	GLN
9	X	408	HIS
10	Z	141	GLN
10	Z	360	HIS
10	Z	374	GLN
10	Z	497	GLN
10	Z	575	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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
12	ADP	3	1001	-	27,29,29	1.35	4 (14%)	42,45,45	2.01	12 (28%)
12	ADP	2	1001	-	27,29,29	1.36	4 (14%)	42,45,45	1.96	9 (21%)
12	ADP	B	1001	-	27,29,29	1.36	4 (14%)	42,45,45	2.08	9 (21%)
12	ADP	C	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	11 (26%)
12	ADP	G	1001	-	27,29,29	1.35	4 (14%)	42,45,45	1.97	11 (26%)
12	ADP	5	1001	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
12	ADP	E	1001	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
12	ADP	7	1001	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	11 (26%)

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
12	ADP	3	1001	-	-	3/16/32/32	0/3/3/3
12	ADP	2	1001	-	-	5/16/32/32	0/3/3/3
12	ADP	B	1001	-	-	3/16/32/32	0/3/3/3
12	ADP	C	1001	-	-	3/16/32/32	0/3/3/3
12	ADP	G	1001	-	-	3/16/32/32	0/3/3/3
12	ADP	5	1001	-	-	2/16/32/32	0/3/3/3
12	ADP	E	1001	-	-	2/16/32/32	0/3/3/3
12	ADP	7	1001	-	-	3/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1001	ADP	C5-C4	4.61	1.47	1.39
12	2	1001	ADP	C5-C4	4.53	1.47	1.39
12	5	1001	ADP	C5-C4	4.50	1.47	1.39
12	G	1001	ADP	C5-C4	4.48	1.47	1.39
12	7	1001	ADP	C5-C4	4.47	1.47	1.39
12	E	1001	ADP	C5-C4	4.43	1.47	1.39
12	3	1001	ADP	C5-C4	4.39	1.47	1.39
12	C	1001	ADP	C5-C4	4.37	1.47	1.39
12	3	1001	ADP	C5-C6	2.65	1.48	1.41
12	G	1001	ADP	C5-C6	2.63	1.48	1.41
12	5	1001	ADP	C5-C6	2.63	1.48	1.41
12	2	1001	ADP	C5-C6	2.62	1.48	1.41
12	E	1001	ADP	C5-C6	2.62	1.48	1.41
12	B	1001	ADP	C5-C6	2.61	1.48	1.41
12	7	1001	ADP	C5-C6	2.61	1.48	1.41
12	C	1001	ADP	C5-C6	2.60	1.48	1.41
12	5	1001	ADP	C8-N7	2.45	1.36	1.31
12	3	1001	ADP	C8-N7	2.44	1.36	1.31
12	C	1001	ADP	C8-N7	2.40	1.36	1.31
12	E	1001	ADP	C8-N7	2.39	1.36	1.31
12	G	1001	ADP	C8-N7	2.39	1.36	1.31
12	7	1001	ADP	C8-N7	2.37	1.36	1.31
12	B	1001	ADP	C5-N7	-2.33	1.34	1.39
12	2	1001	ADP	C8-N7	2.32	1.36	1.31
12	E	1001	ADP	C5-N7	-2.26	1.34	1.39
12	2	1001	ADP	C5-N7	-2.25	1.34	1.39
12	5	1001	ADP	C5-N7	-2.24	1.34	1.39
12	B	1001	ADP	C8-N7	2.23	1.35	1.31
12	7	1001	ADP	C5-N7	-2.22	1.34	1.39
12	G	1001	ADP	C5-N7	-2.21	1.34	1.39
12	3	1001	ADP	C5-N7	-2.21	1.34	1.39
12	C	1001	ADP	C5-N7	-2.17	1.34	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1001	ADP	C5-C4-N3	-6.98	117.64	126.75
12	2	1001	ADP	C5-C4-N3	-6.32	118.51	126.75
12	7	1001	ADP	C5-C4-N3	-6.25	118.59	126.75
12	E	1001	ADP	C5-C4-N3	-6.21	118.64	126.75
12	5	1001	ADP	C5-C4-N3	-6.20	118.66	126.75
12	G	1001	ADP	C5-C4-N3	-6.15	118.72	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	1001	ADP	C5-C4-N3	-5.99	118.93	126.75
12	C	1001	ADP	C5-C4-N3	-5.93	119.01	126.75
12	B	1001	ADP	N3-C4-N9	5.62	136.34	127.08
12	2	1001	ADP	N3-C4-N9	5.02	135.36	127.08
12	7	1001	ADP	N3-C4-N9	4.95	135.24	127.08
12	E	1001	ADP	N3-C4-N9	4.93	135.20	127.08
12	5	1001	ADP	N3-C4-N9	4.86	135.08	127.08
12	G	1001	ADP	N3-C4-N9	4.80	134.99	127.08
12	C	1001	ADP	N3-C4-N9	4.66	134.77	127.08
12	3	1001	ADP	N3-C4-N9	4.65	134.75	127.08
12	B	1001	ADP	C2-N3-C4	4.15	121.54	111.75
12	2	1001	ADP	C2-N3-C4	3.87	120.89	111.75
12	7	1001	ADP	C2-N3-C4	3.86	120.87	111.75
12	3	1001	ADP	C2-N3-C4	3.86	120.86	111.75
12	G	1001	ADP	C2-N3-C4	3.85	120.85	111.75
12	5	1001	ADP	C2-N3-C4	3.85	120.84	111.75
12	E	1001	ADP	C2-N3-C4	3.84	120.81	111.75
12	5	1001	ADP	PA-O3A-PB	-3.83	119.70	132.83
12	C	1001	ADP	C2-N3-C4	3.82	120.78	111.75
12	B	1001	ADP	PA-O3A-PB	-3.82	119.70	132.83
12	3	1001	ADP	PA-O3A-PB	-3.78	119.86	132.83
12	E	1001	ADP	PA-O3A-PB	-3.61	120.44	132.83
12	G	1001	ADP	PA-O3A-PB	-3.55	120.63	132.83
12	C	1001	ADP	PA-O3A-PB	-3.45	120.99	132.83
12	C	1001	ADP	N3-C2-N1	-3.33	123.40	128.60
12	G	1001	ADP	C4-C5-N7	-3.28	106.62	110.62
12	3	1001	ADP	C4-C5-N7	-3.28	106.63	110.62
12	2	1001	ADP	PA-O3A-PB	-3.28	121.58	132.83
12	3	1001	ADP	N3-C2-N1	-3.27	123.49	128.60
12	C	1001	ADP	C4-C5-N7	-3.24	106.67	110.62
12	5	1001	ADP	C4-C5-N7	-3.23	106.68	110.62
12	7	1001	ADP	C4-C5-N7	-3.20	106.72	110.62
12	G	1001	ADP	N3-C2-N1	-3.17	123.64	128.60
12	7	1001	ADP	PA-O3A-PB	-3.17	121.95	132.83
12	E	1001	ADP	C4-C5-N7	-3.17	106.76	110.62
12	B	1001	ADP	N3-C2-N1	-3.15	123.68	128.60
12	2	1001	ADP	N3-C2-N1	-3.13	123.71	128.60
12	7	1001	ADP	N3-C2-N1	-3.13	123.71	128.60
12	5	1001	ADP	N3-C2-N1	-3.10	123.75	128.60
12	E	1001	ADP	N3-C2-N1	-3.10	123.76	128.60
12	2	1001	ADP	C4-C5-N7	-3.08	106.86	110.62
12	B	1001	ADP	C4-C5-N7	-2.98	106.99	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1001	ADP	C4-N9-C8	2.81	108.77	105.73
12	3	1001	ADP	C5-N7-C8	2.78	107.46	103.51
12	G	1001	ADP	C5-N7-C8	2.77	107.44	103.51
12	C	1001	ADP	C5-N7-C8	2.74	107.40	103.51
12	7	1001	ADP	C5-N7-C8	2.72	107.38	103.51
12	5	1001	ADP	C5-N7-C8	2.72	107.38	103.51
12	3	1001	ADP	C4-N9-C8	2.70	108.66	105.73
12	E	1001	ADP	C5-N7-C8	2.70	107.34	103.51
12	E	1001	ADP	C4-N9-C8	2.65	108.60	105.73
12	7	1001	ADP	C4-N9-C8	2.64	108.59	105.73
12	5	1001	ADP	C4-N9-C8	2.62	108.57	105.73
12	2	1001	ADP	C5-N7-C8	2.61	107.21	103.51
12	G	1001	ADP	C4-N9-C8	2.58	108.53	105.73
12	B	1001	ADP	C5-N7-C8	2.57	107.16	103.51
12	2	1001	ADP	C4-N9-C8	2.42	108.35	105.73
12	2	1001	ADP	C3'-C2'-C1'	2.32	105.83	101.43
12	3	1001	ADP	C6-C5-N7	2.30	136.30	132.02
12	B	1001	ADP	C3'-C2'-C1'	2.29	105.77	101.43
12	3	1001	ADP	C3'-C2'-C1'	2.27	105.75	101.43
12	C	1001	ADP	C6-C5-N7	2.26	136.24	132.02
12	G	1001	ADP	C6-C5-N7	2.20	136.12	132.02
12	7	1001	ADP	C3'-C2'-C1'	2.18	105.58	101.43
12	C	1001	ADP	N9-C8-N7	-2.18	110.94	113.91
12	3	1001	ADP	N9-C8-N7	-2.18	110.94	113.91
12	5	1001	ADP	C6-C5-N7	2.13	135.99	132.02
12	B	1001	ADP	C4-N9-C8	2.13	108.03	105.73
12	G	1001	ADP	C3'-C2'-C1'	2.11	105.44	101.43
12	7	1001	ADP	C6-C5-N7	2.09	135.92	132.02
12	5	1001	ADP	C3'-C2'-C1'	2.08	105.38	101.43
12	5	1001	ADP	N9-C8-N7	-2.04	111.12	113.91
12	G	1001	ADP	N9-C8-N7	-2.04	111.13	113.91
12	E	1001	ADP	C6-C5-N7	2.03	135.81	132.02
12	7	1001	ADP	N9-C8-N7	-2.02	111.15	113.91
12	E	1001	ADP	N9-C8-N7	-2.02	111.15	113.91
12	3	1001	ADP	C2'-C1'-N9	-2.02	108.18	113.30
12	C	1001	ADP	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1001	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
12	C	1001	ADP	C5'-O5'-PA-O1A
12	C	1001	ADP	C5'-O5'-PA-O2A
12	E	1001	ADP	C5'-O5'-PA-O3A
12	G	1001	ADP	C5'-O5'-PA-O1A
12	G	1001	ADP	C5'-O5'-PA-O2A
12	2	1001	ADP	C5'-O5'-PA-O1A
12	2	1001	ADP	C5'-O5'-PA-O2A
12	3	1001	ADP	C5'-O5'-PA-O1A
12	3	1001	ADP	C5'-O5'-PA-O2A
12	5	1001	ADP	C5'-O5'-PA-O3A
12	7	1001	ADP	C5'-O5'-PA-O1A
12	7	1001	ADP	C5'-O5'-PA-O2A
12	2	1001	ADP	O4'-C4'-C5'-O5'
12	2	1001	ADP	C3'-C4'-C5'-O5'
12	B	1001	ADP	C2'-C1'-N9-C4
12	B	1001	ADP	C2'-C1'-N9-C8
12	E	1001	ADP	C5'-O5'-PA-O1A
12	5	1001	ADP	C5'-O5'-PA-O1A
12	C	1001	ADP	C5'-O5'-PA-O3A
12	G	1001	ADP	C5'-O5'-PA-O3A
12	2	1001	ADP	C5'-O5'-PA-O3A
12	3	1001	ADP	C5'-O5'-PA-O3A
12	7	1001	ADP	C5'-O5'-PA-O3A

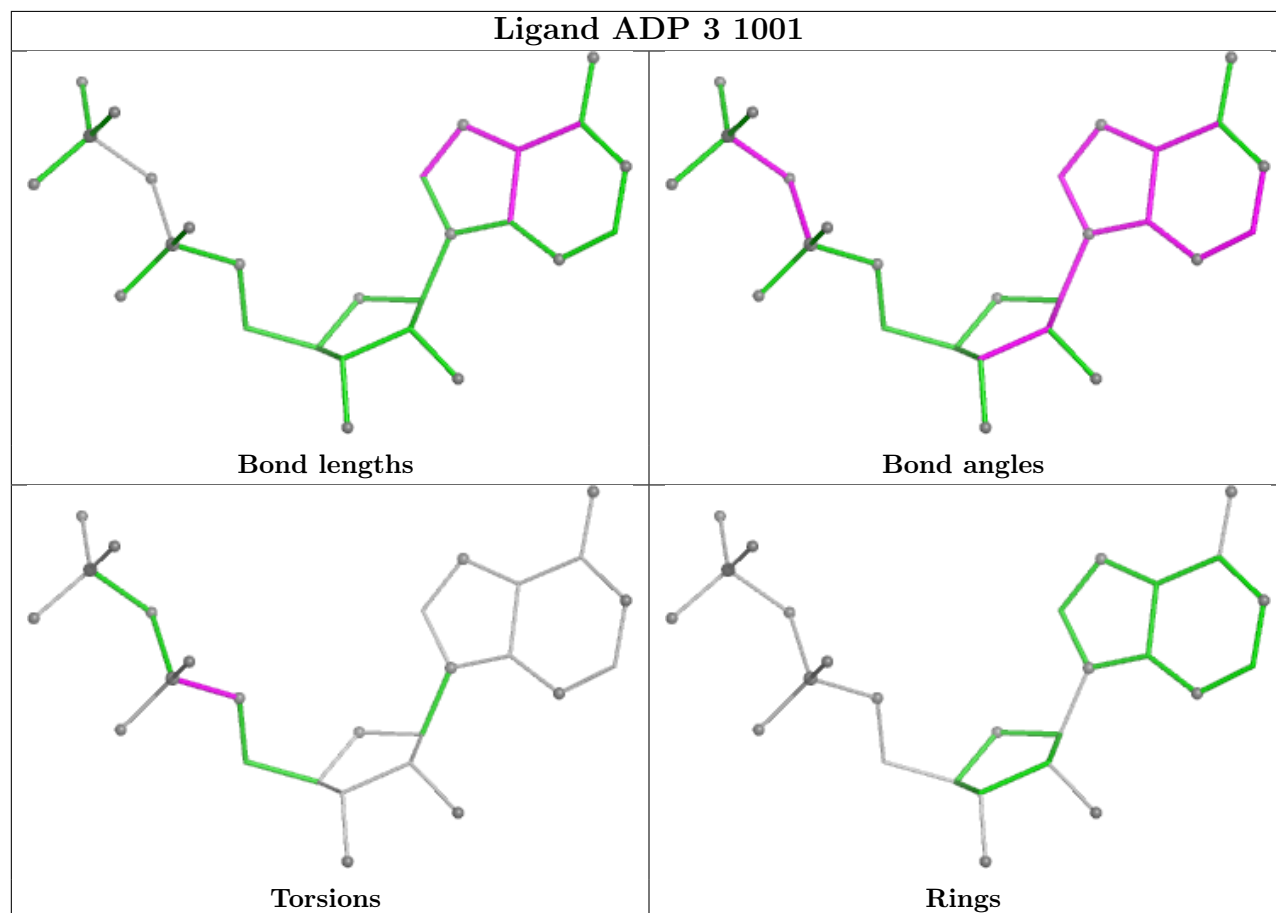
There are no ring outliers.

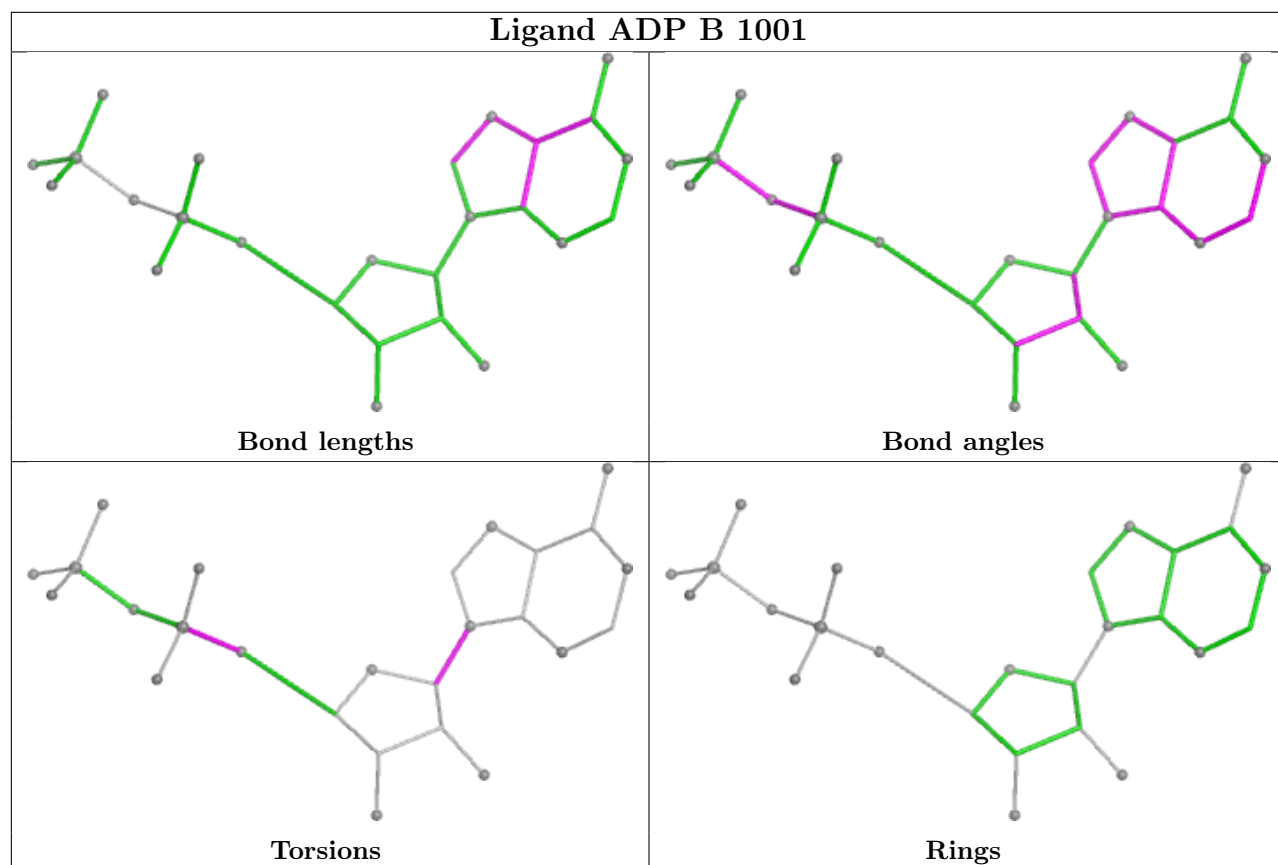
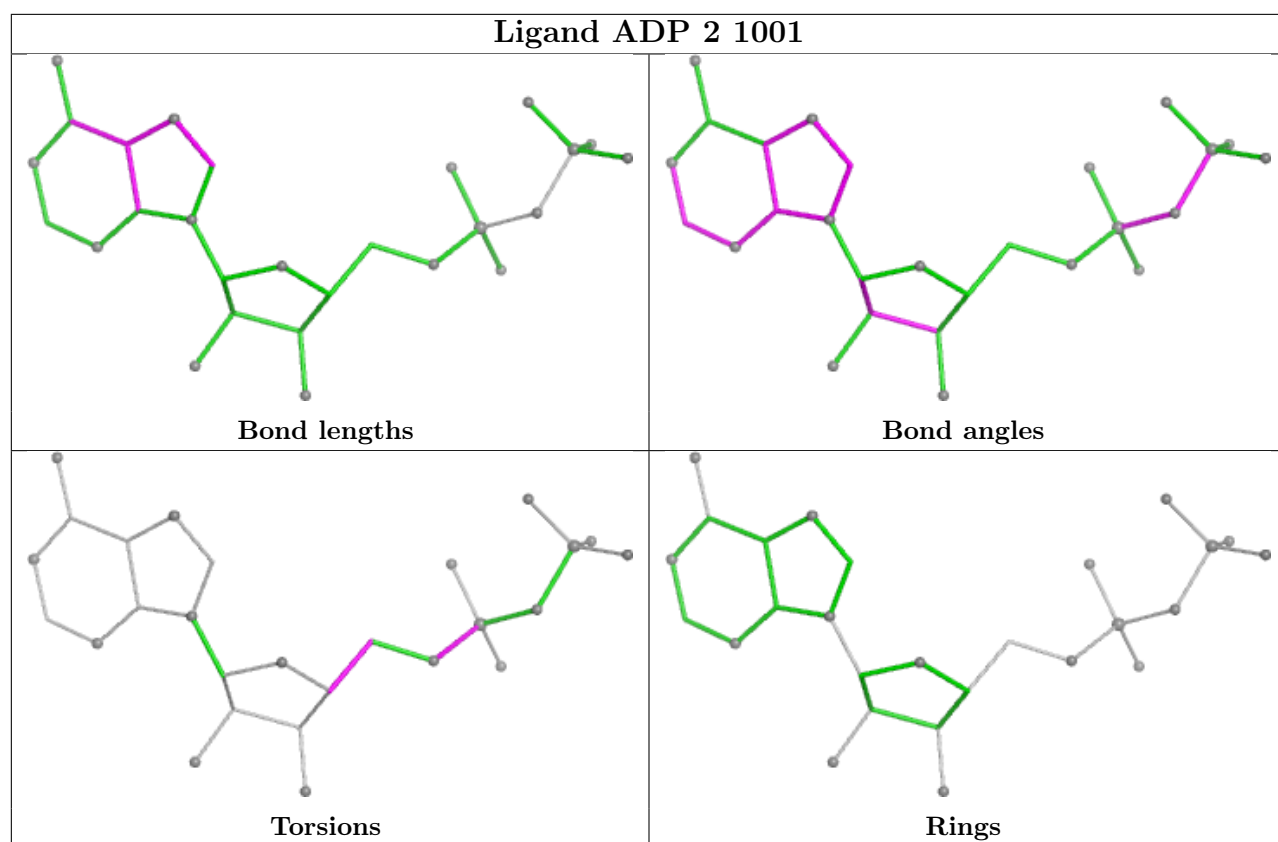
4 monomers are involved in 8 short contacts:

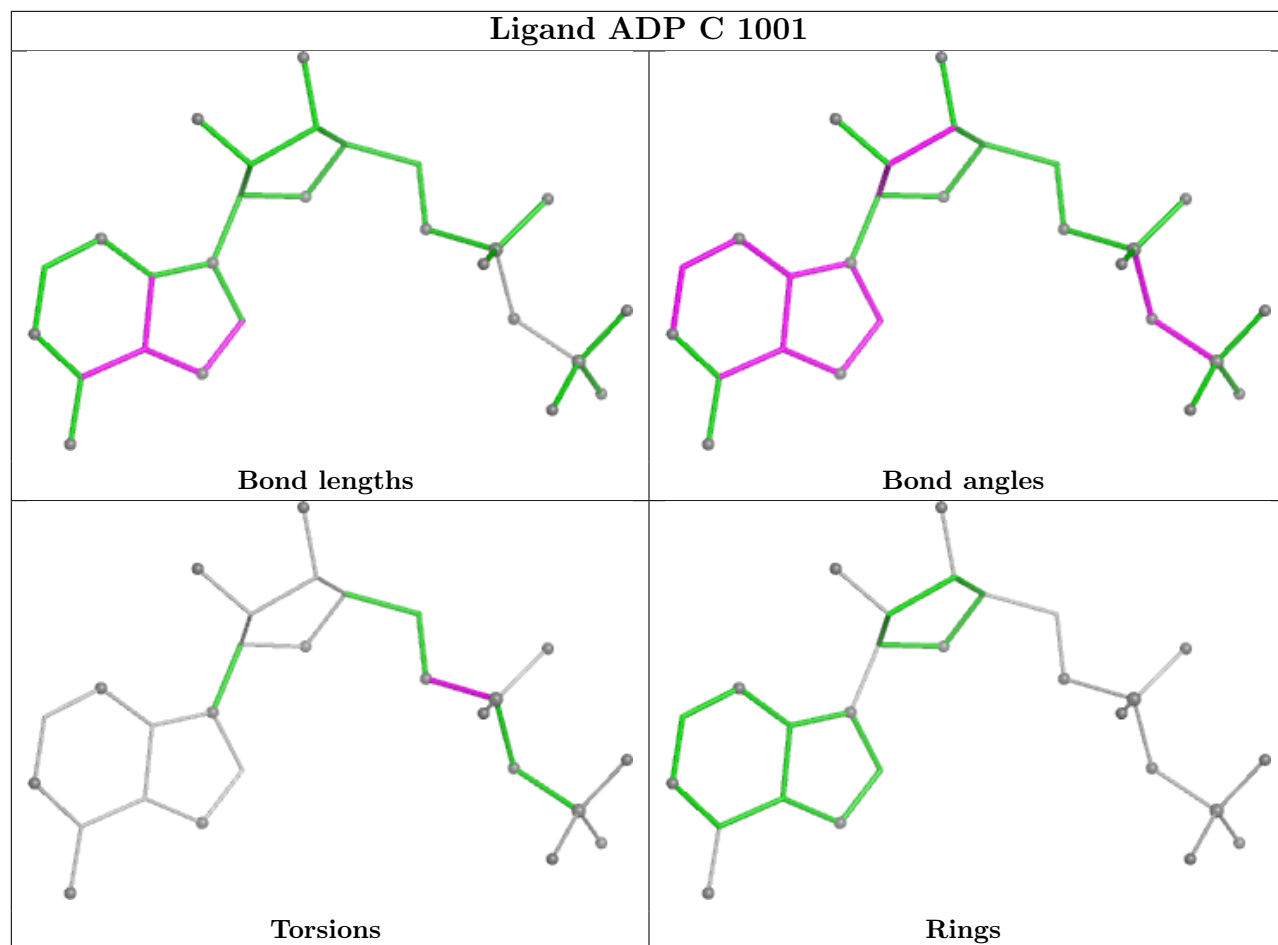
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	2	1001	ADP	4	0
12	B	1001	ADP	2	0
12	G	1001	ADP	1	0
12	E	1001	ADP	1	0

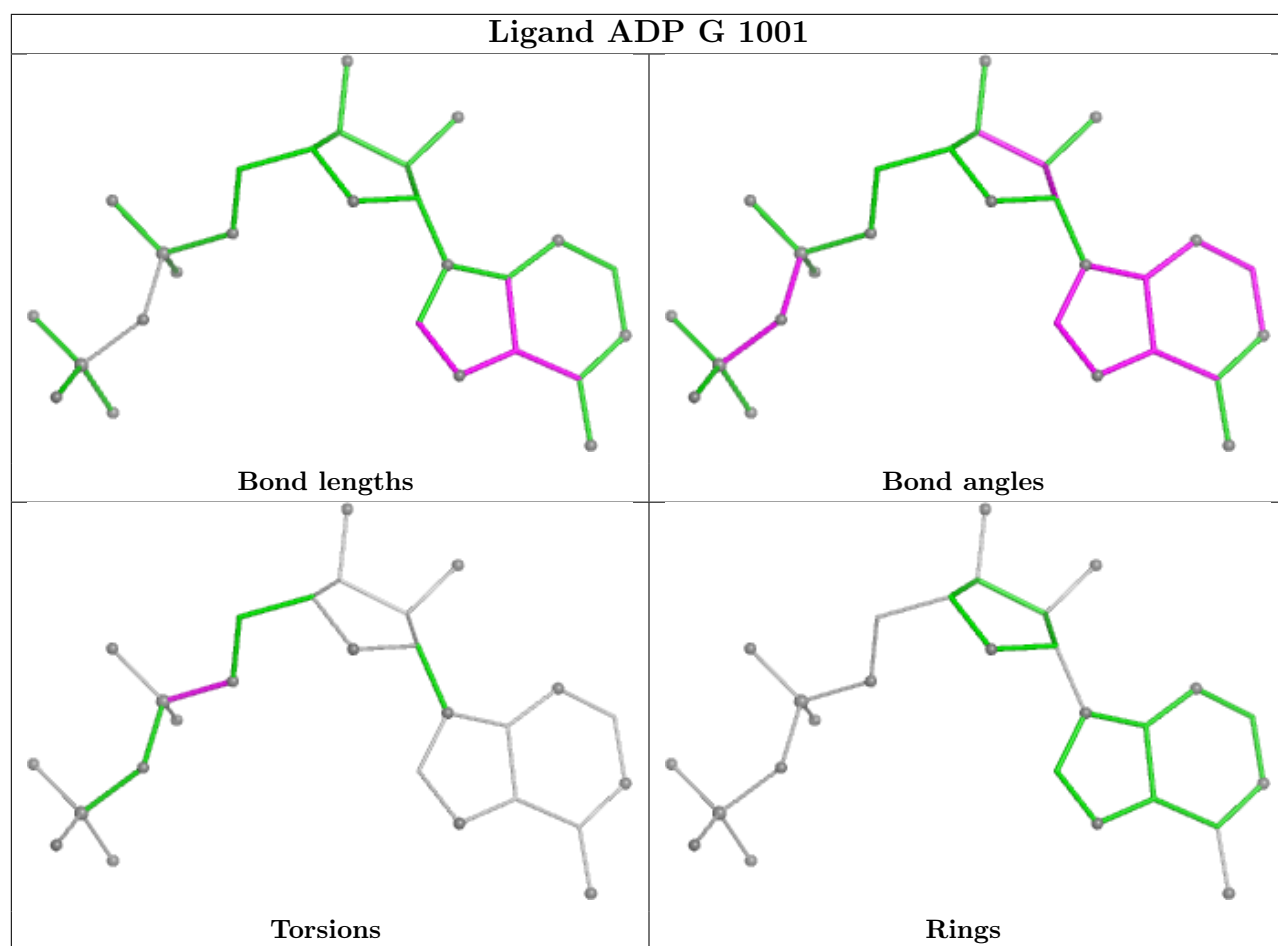
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

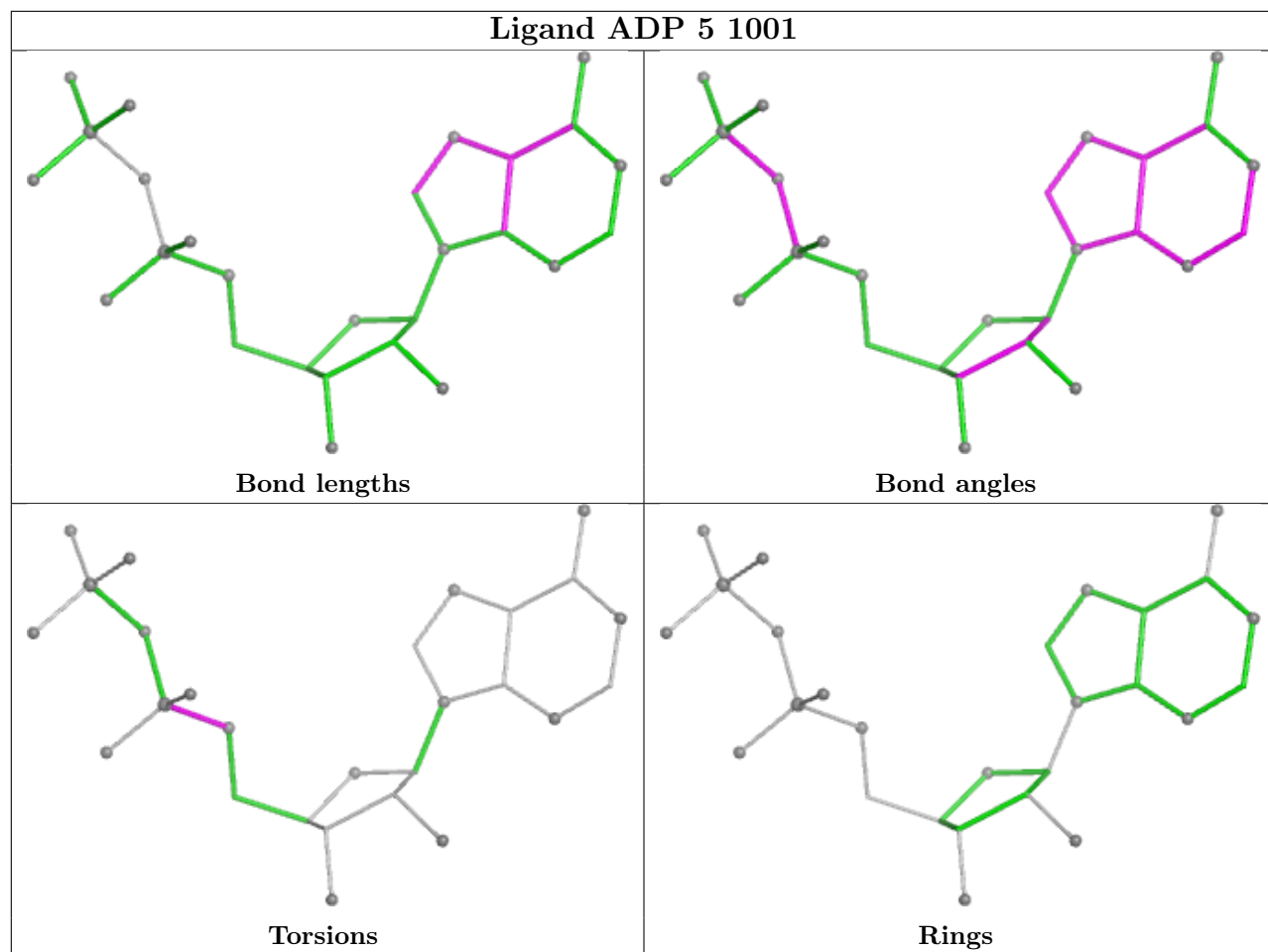
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

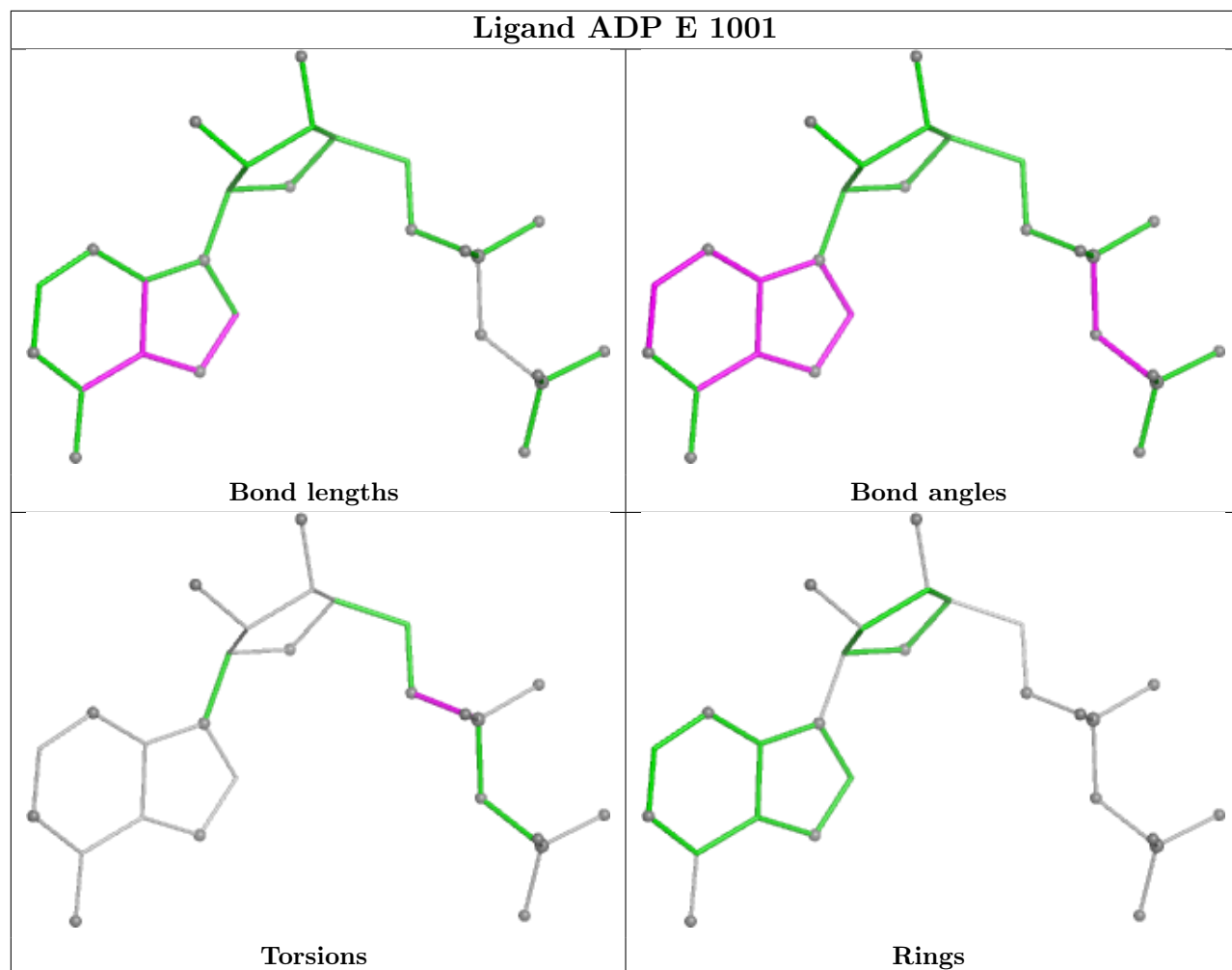


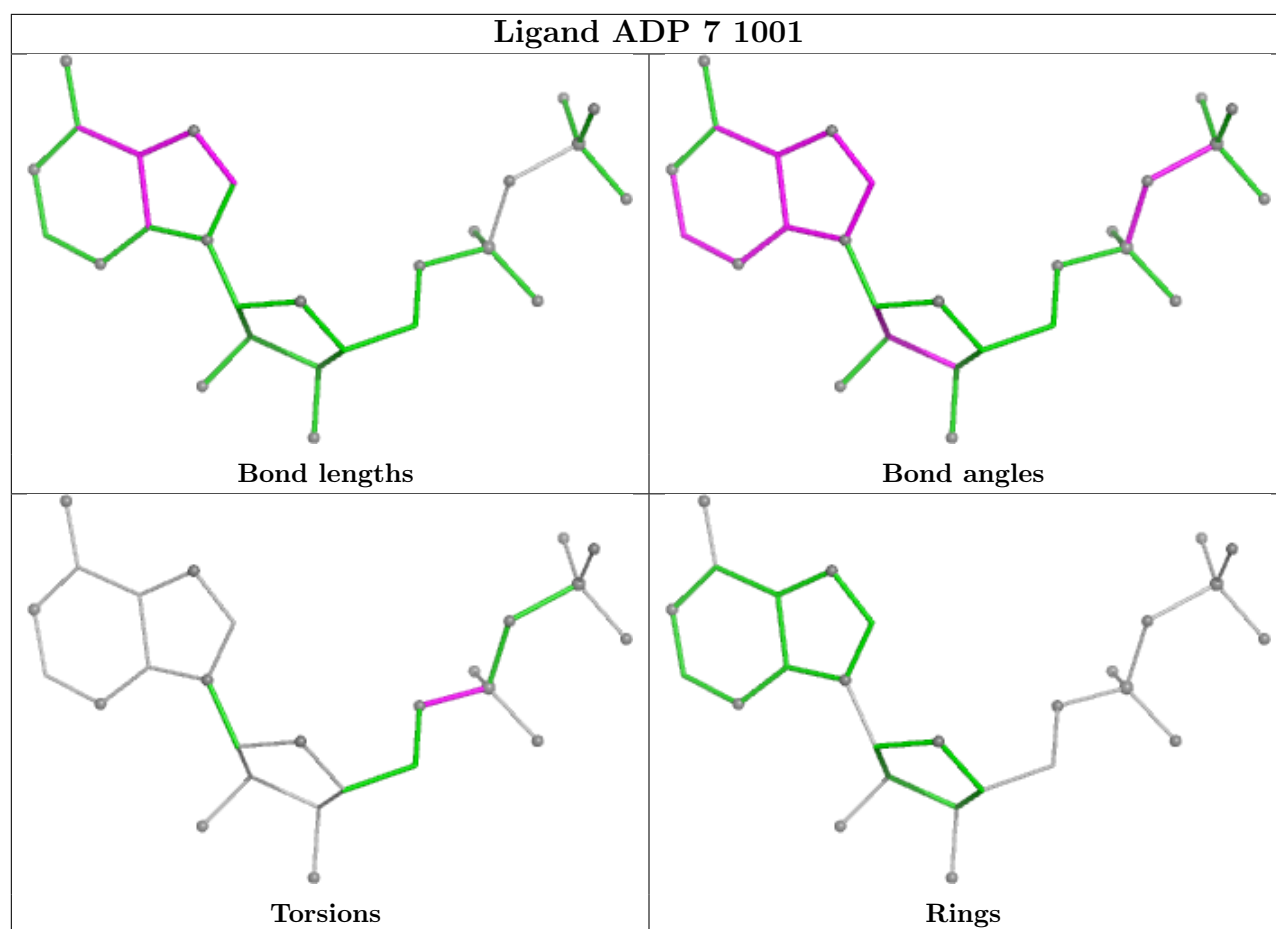












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

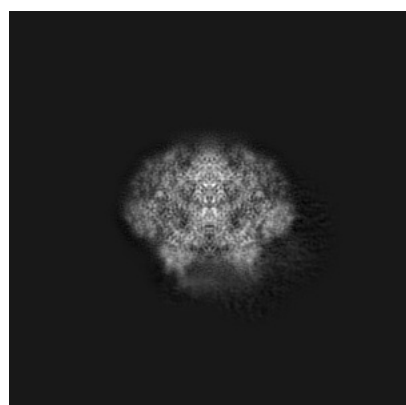
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55918. These allow visual inspection of the internal detail of the map and identification of artifacts.

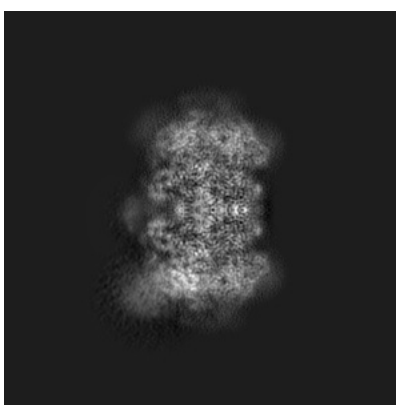
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

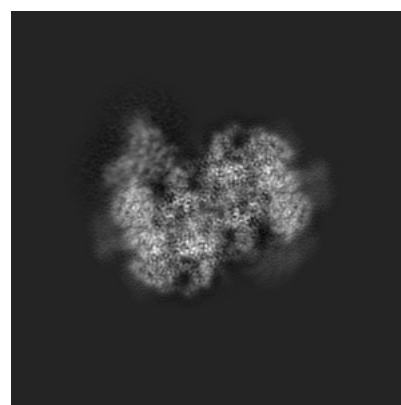
6.1.1 Primary map



X



Y

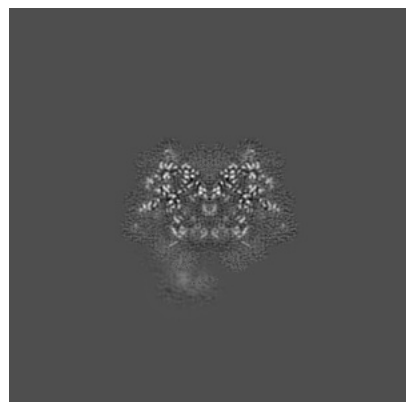


Z

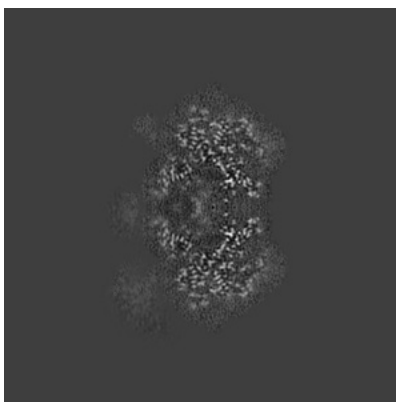
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

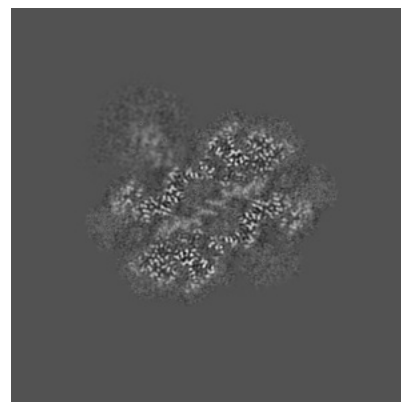
6.2.1 Primary map



X Index: 188



Y Index: 188

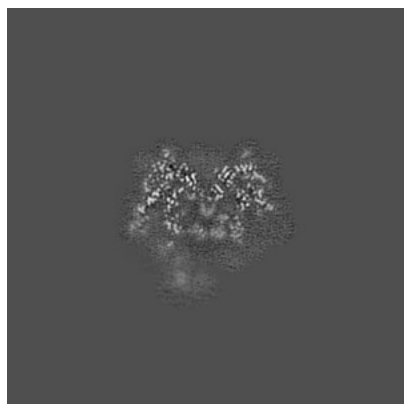


Z Index: 188

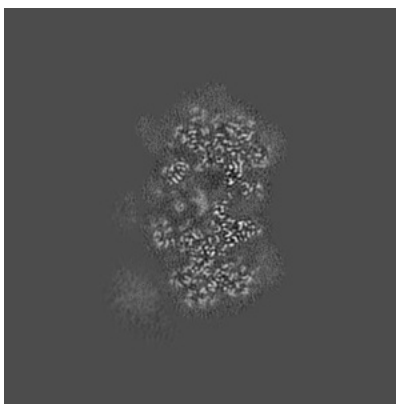
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

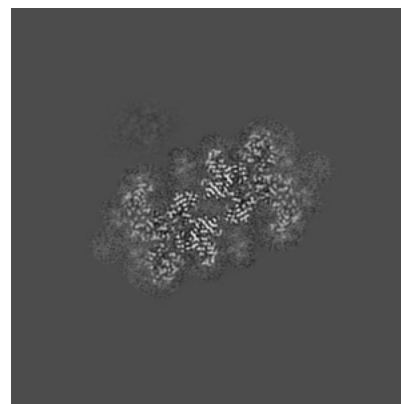
6.3.1 Primary map



X Index: 186



Y Index: 193

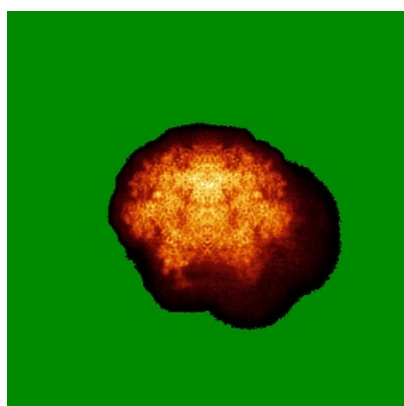


Z Index: 217

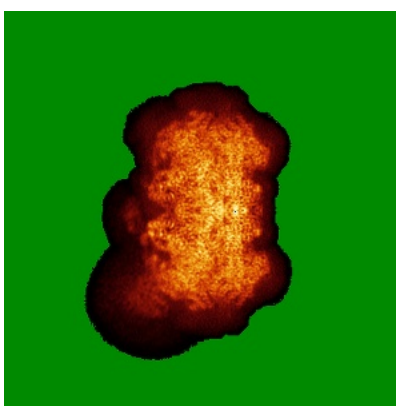
The images above show the largest variance slices of the map in three orthogonal directions.

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

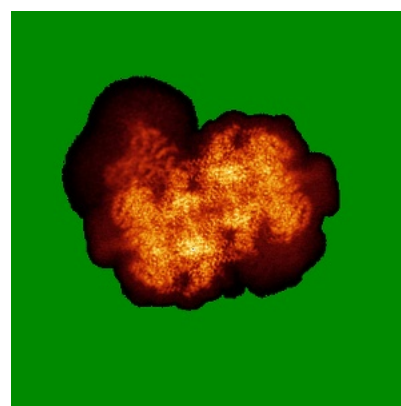
6.4.1 Primary map



X



Y

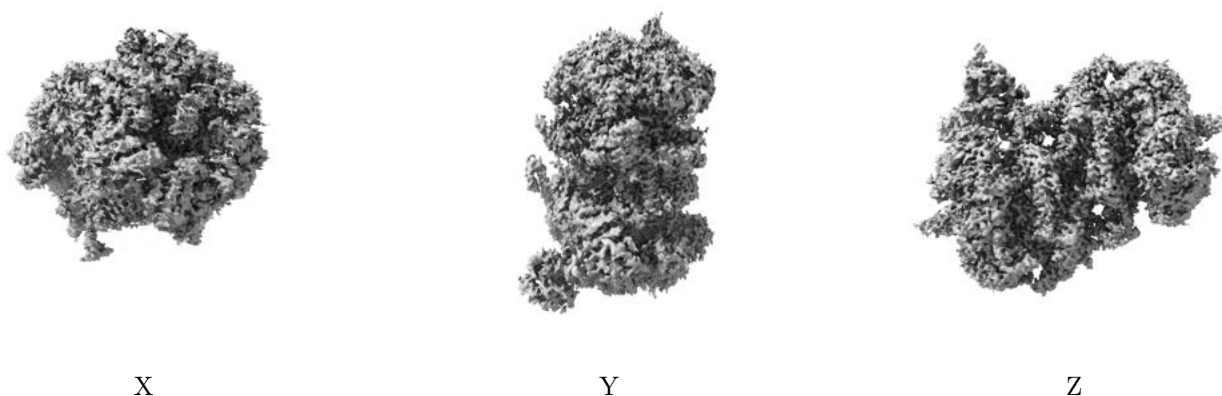


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.61. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

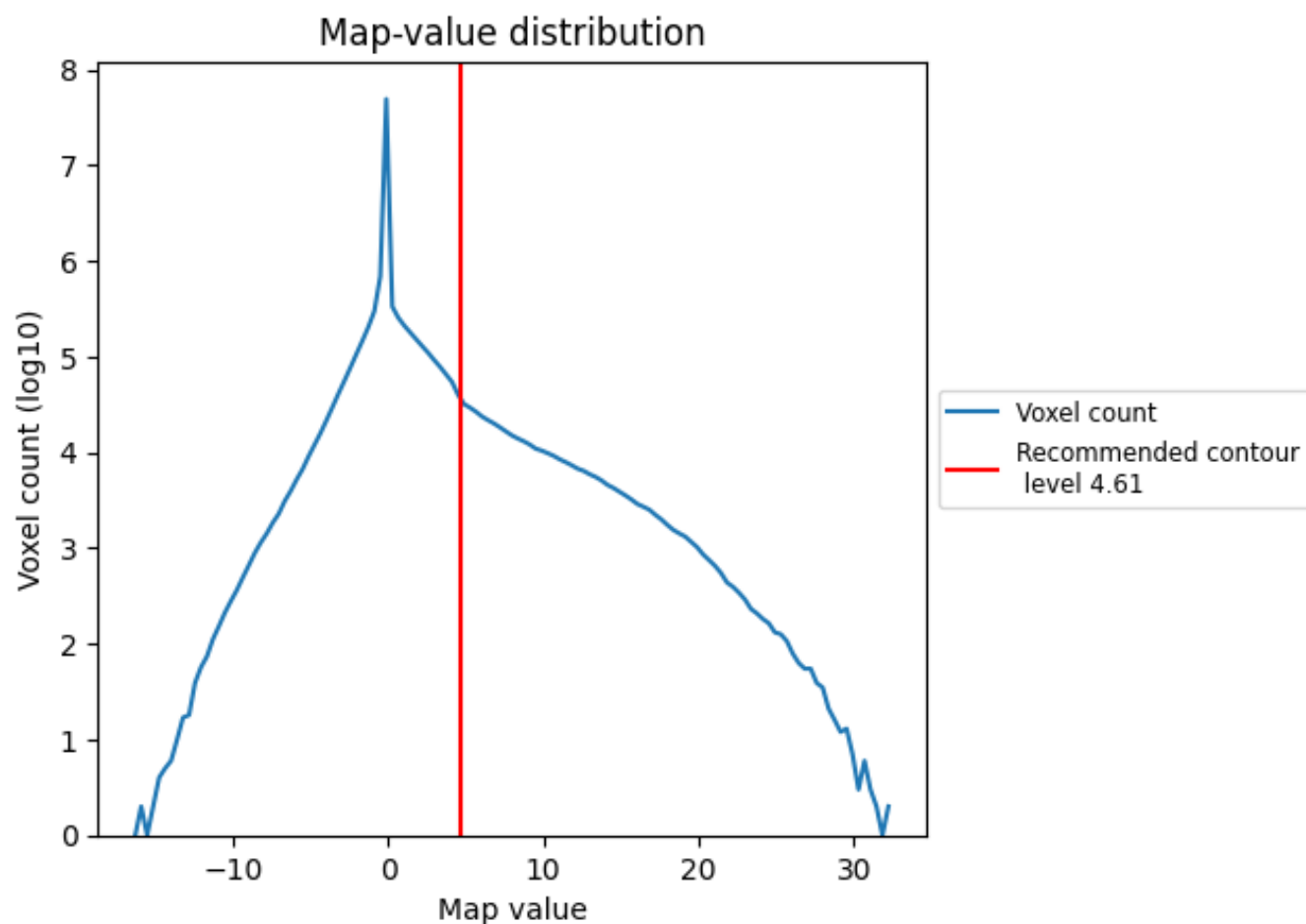
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

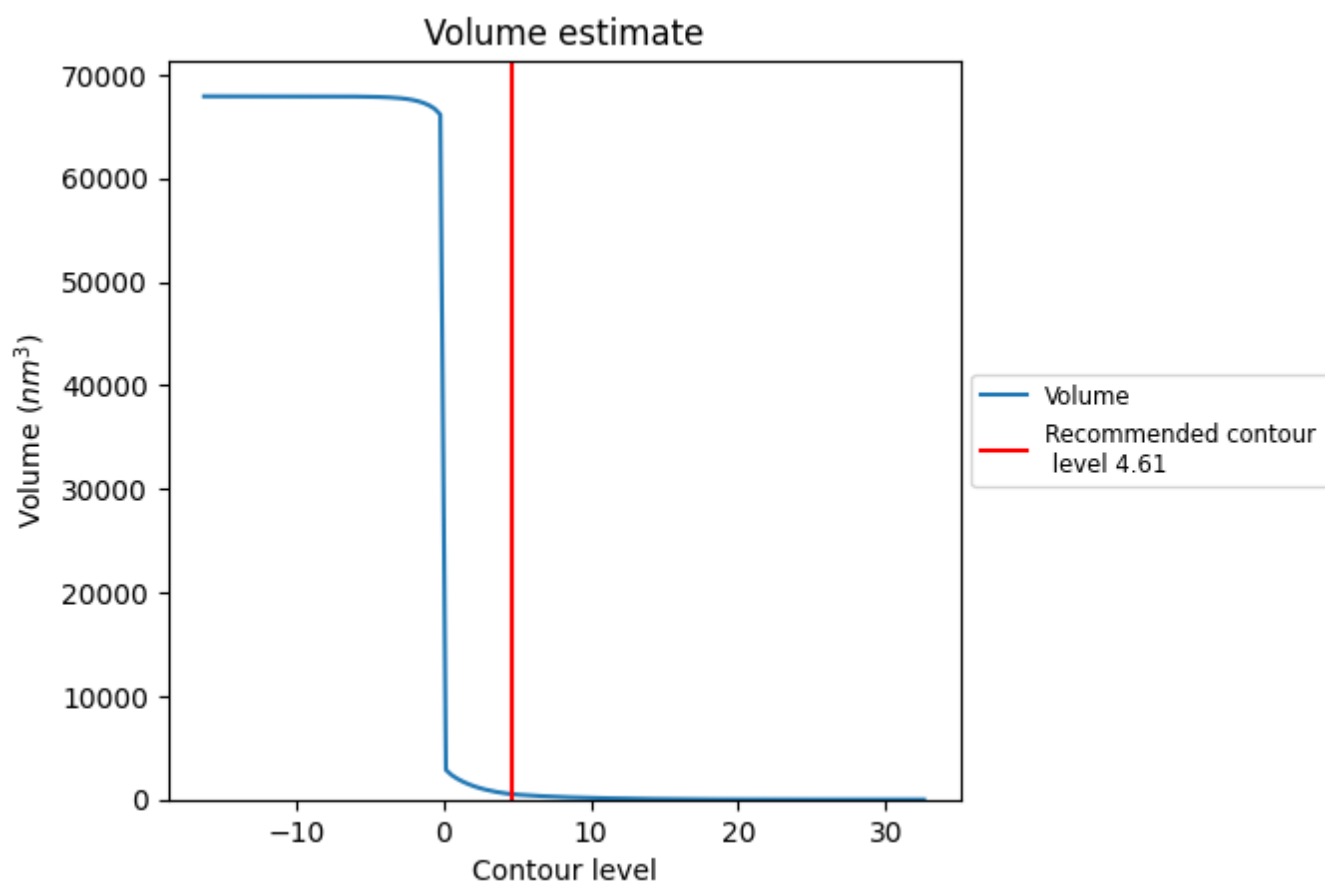
This section contains the results of statistical analysis of the map.

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.

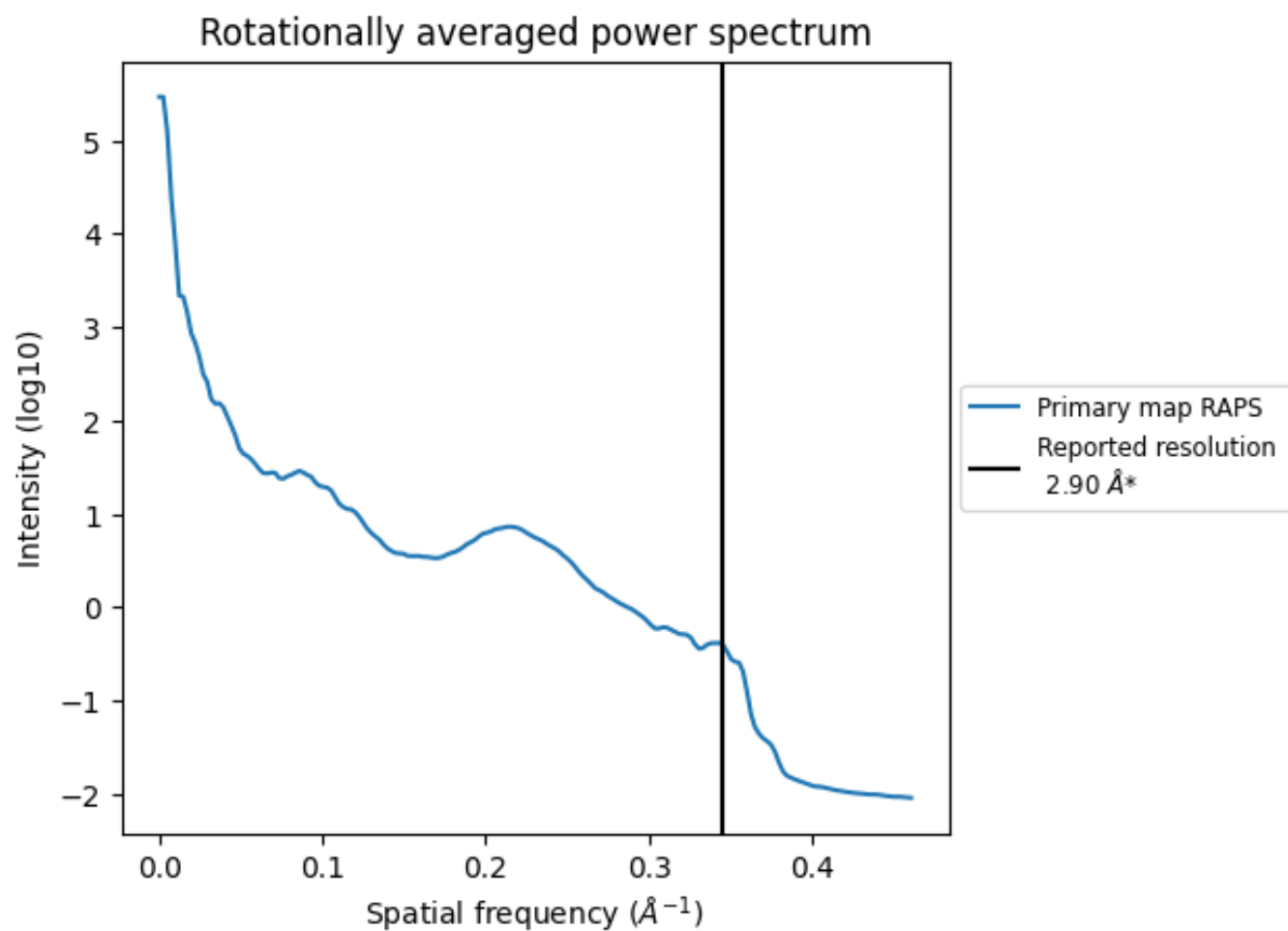
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm^3 ; this corresponds to an approximate mass of 475 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 0.345 Å⁻¹

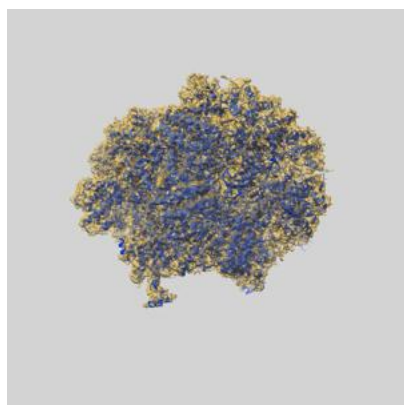
8 Fourier-Shell correlation ⓘ

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

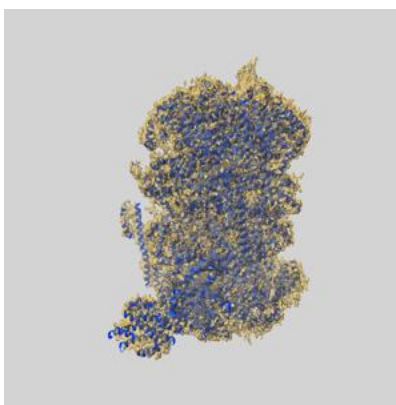
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55918 and PDB model 9TH8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

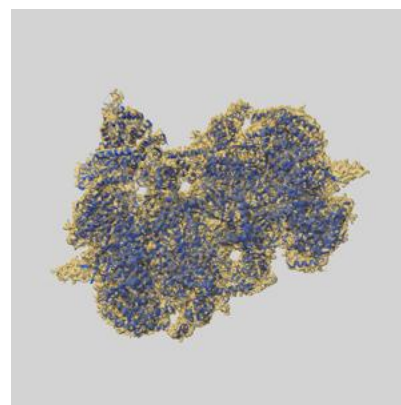
9.1 Map-model overlay [i](#)



X



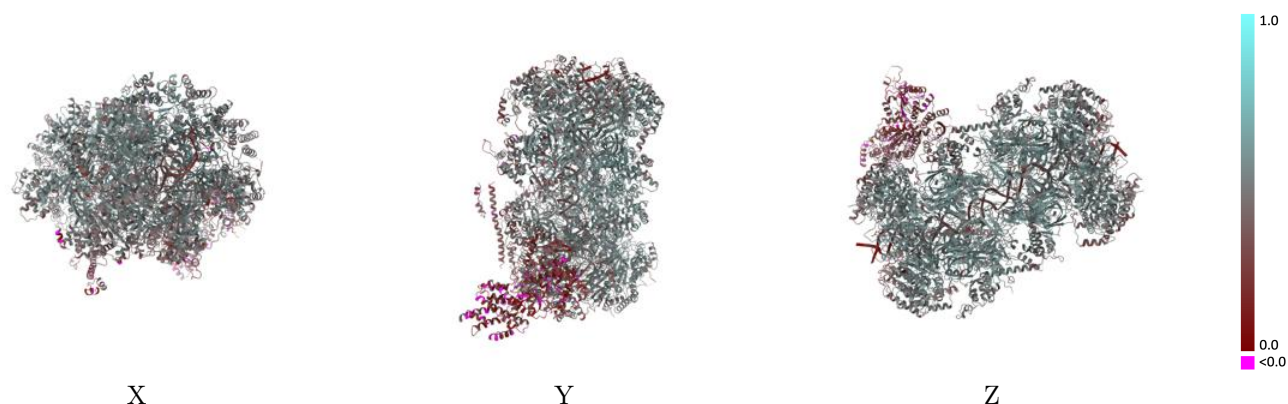
Y



Z

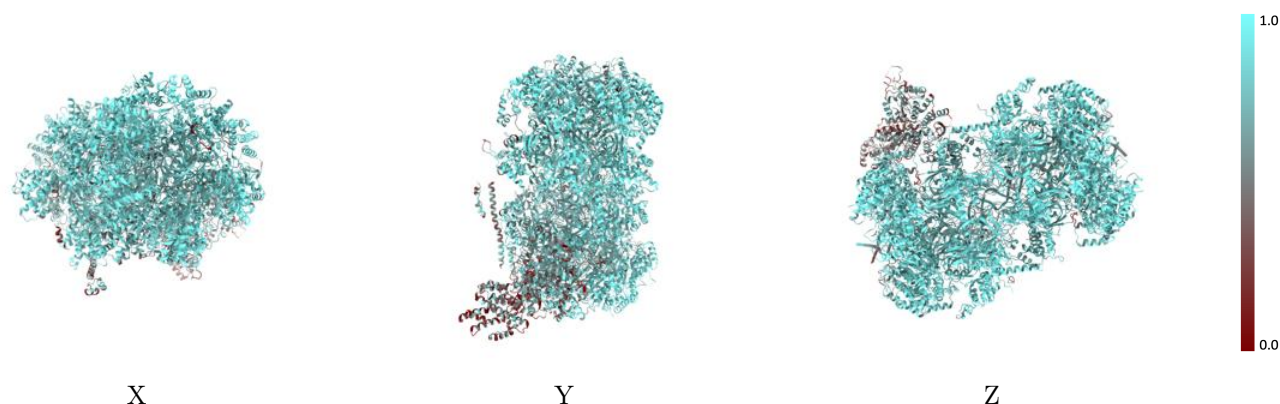
The images above show the 3D surface view of the map at the recommended contour level 4.61 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



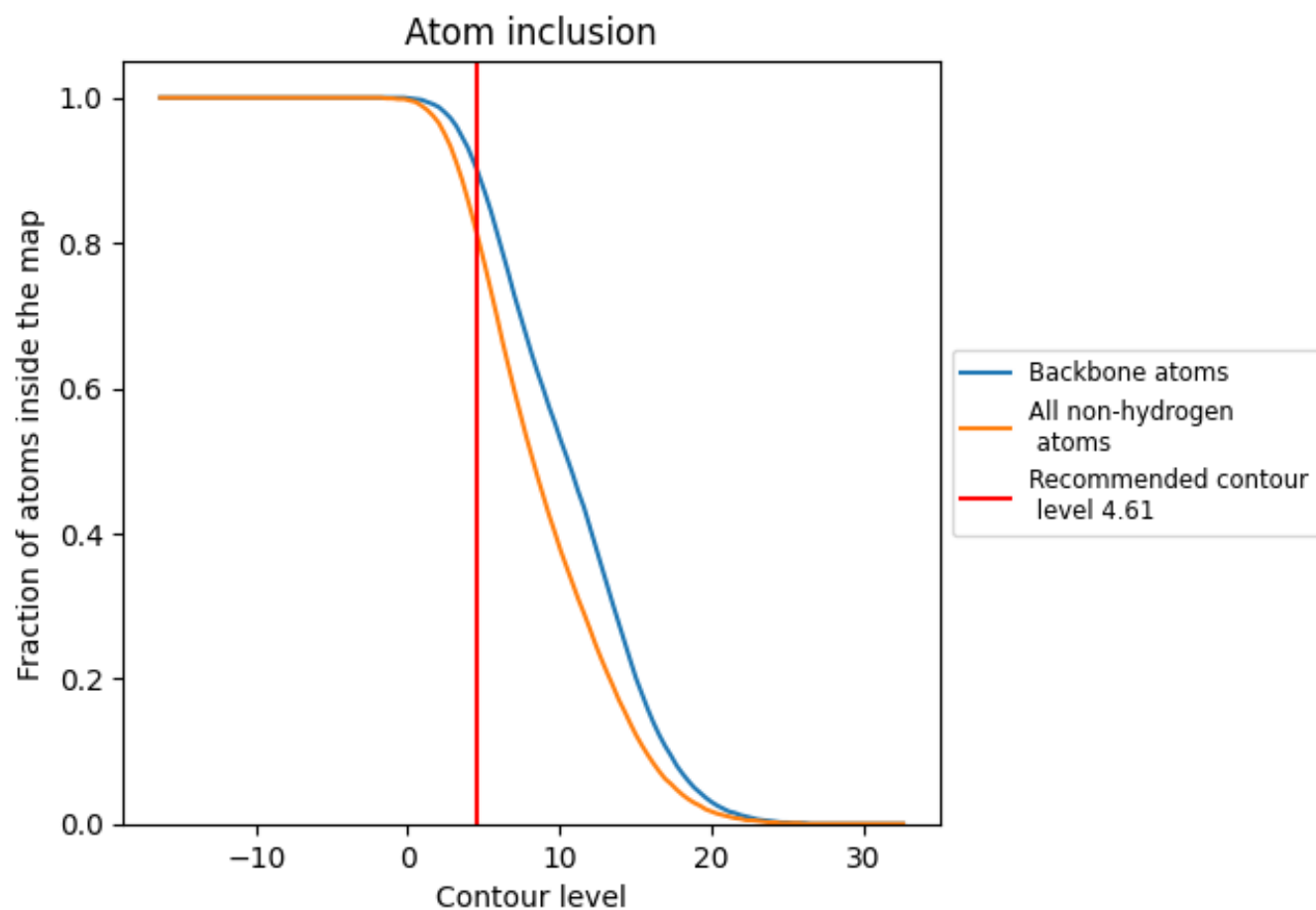
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.61).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (4.61) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4680
2	0.8230	0.4760
3	0.8940	0.5380
4	0.8650	0.5020
5	0.8360	0.5030
6	0.8200	0.4730
7	0.8690	0.5160
B	0.8050	0.4750
C	0.8960	0.5450
D	0.8600	0.5080
E	0.8330	0.5010
F	0.8420	0.4670
G	0.8660	0.5220
O	0.7560	0.3270
S	0.7760	0.3220
X	0.3810	0.1900
Y	0.5140	0.2320
Z	0.4890	0.2290

1.0

0.0

<0.0