



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:58 PM UTC

PDB ID : 8KG8 / pdb_00008kg8
EMDB ID : EMD-37213
Title : Yeast replisome in state II
Authors : Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on : 2023-08-17
Resolution : 4.23 Å(reported)
Based on initial model : 6SKL

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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 EMD 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) : 2.49

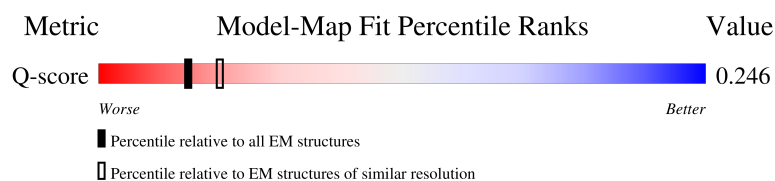
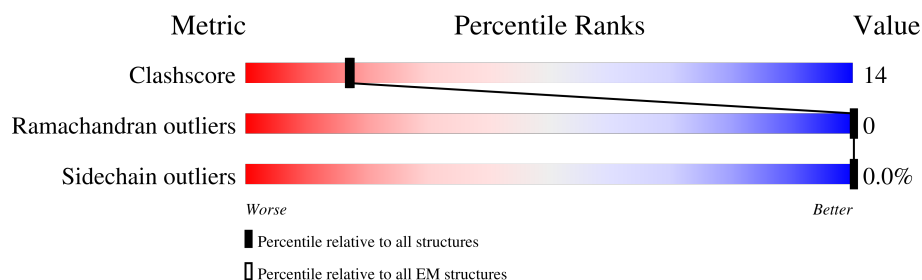
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

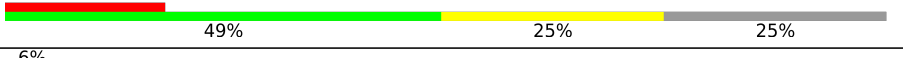
The reported resolution of this entry is 4.23 Å.

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	4685 (3.74 - 4.73)

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	2	868	
2	3	971	
3	4	933	
4	5	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	J	61	
15	M	2222	
16	N	689	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 63829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	662	Total	C	N	O	S	0	0
			5245	3292	942	992	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	645	Total	C	N	O	S	0	0
			5005	3148	888	956	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	697	Total	C	N	O	S	0	0
			5503	3452	950	1070	31		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	677	Total	C	N	O	S	0	0
			5334	3345	928	1037	24		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	619	Total	C	N	O	S	0	0
			4880	3085	854	916	25		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	647	Total	C	N	O	S	0	0
			5023	3169	877	950	27		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	200	Total	C	N	O	S	0	0
			1625	1021	280	316	8		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	195	Total	C	N	O	S	0	0
			1630	1046	289	290	5		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	173	Total	C	N	O	S	0	0
			1394	907	224	256	7		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4591	2930	774	873	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	433	Total	C	N	O	S	0	0
			3467	2223	577	651	16		
12	G	421	Total	C	N	O	S	0	0
			3362	2162	555	629	16		
12	H	421	Total	C	N	O	S	0	0
			3358	2159	553	631	15		

- Molecule 13 is a DNA chain called DNA (71-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	20	Total	C	N	O	P	0	0
			406	200	49	137	20		

- Molecule 14 is a DNA chain called DNA (61-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	5	Total	C	N	O	P	0	0
			99	47	19	28	5		

- Molecule 15 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	813	Total	C	N	O	S	0	0
			6490	4202	1060	1193	35		

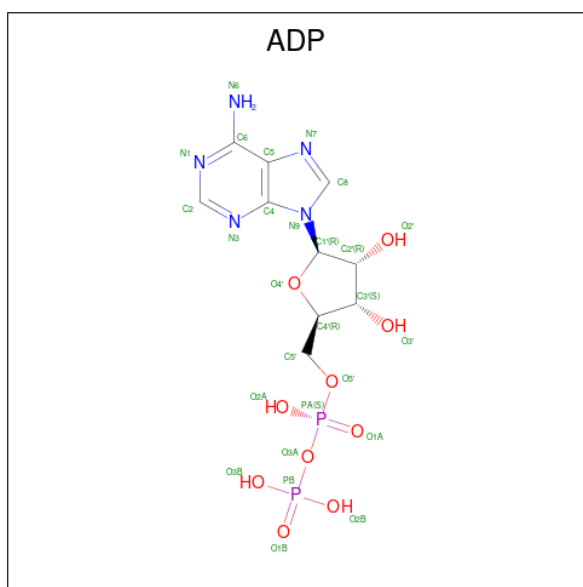
- Molecule 16 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	536	Total	C	N	O	S	0	0
			4254	2726	725	786	17		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	5	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	
17	M	2	Total	Zn	0
			2	2	

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

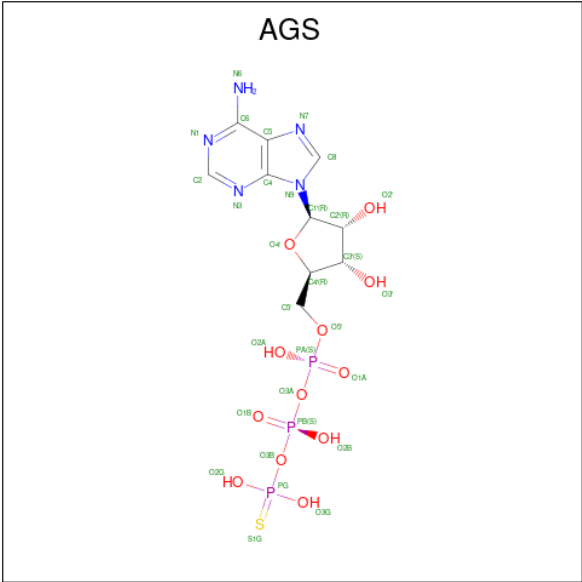


Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

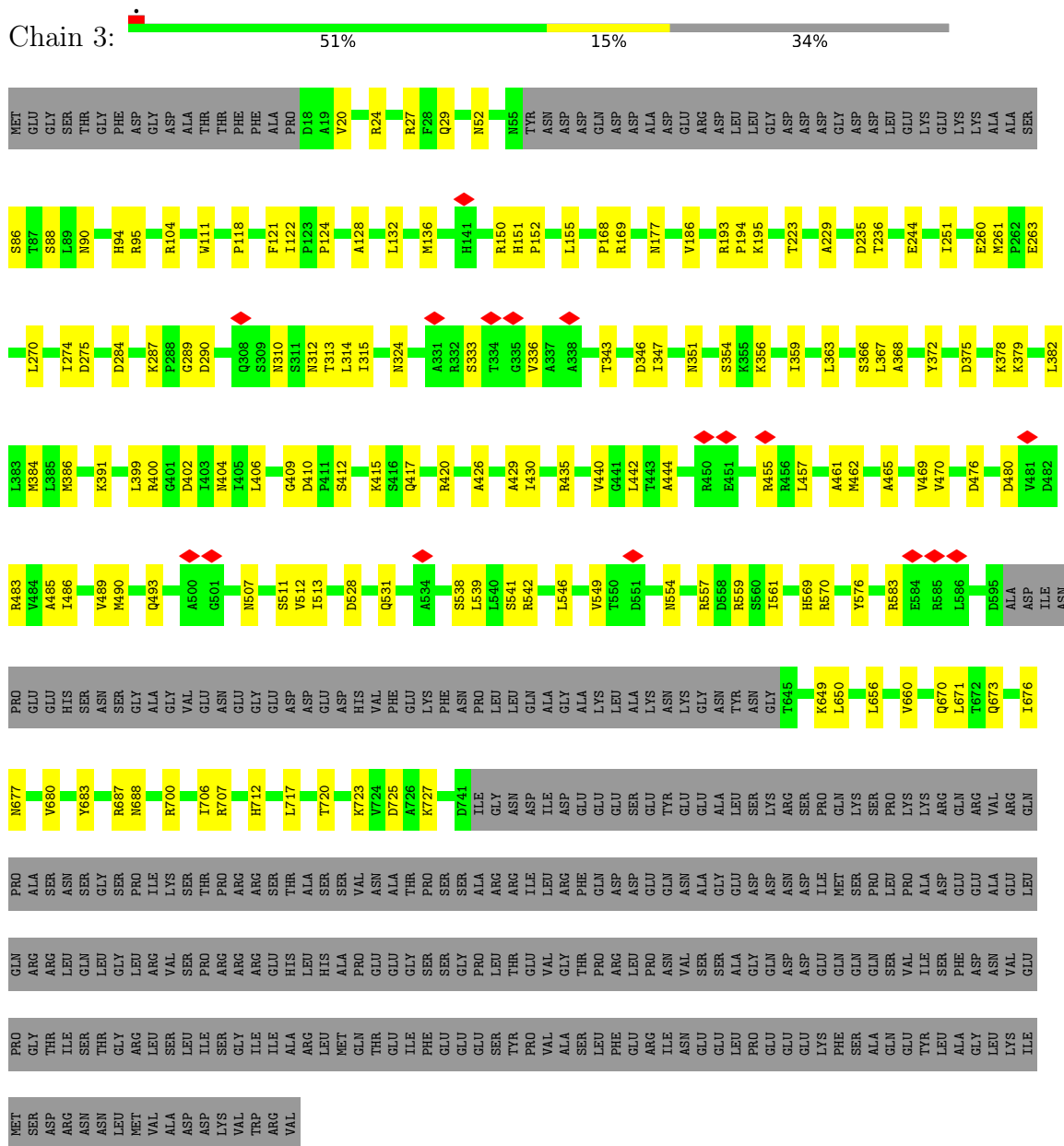
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	2	1	Total	Mg	0
			1	1	
19	3	1	Total	Mg	0
			1	1	
19	5	1	Total	Mg	0
			1	1	
19	6	1	Total	Mg	0
			1	1	
19	7	1	Total	Mg	0
			1	1	

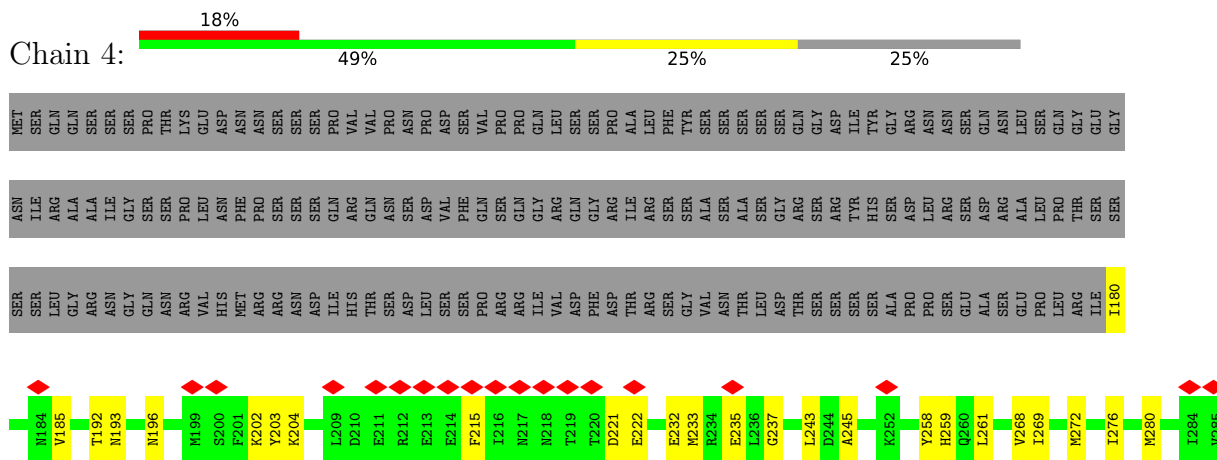
- Molecule 20 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

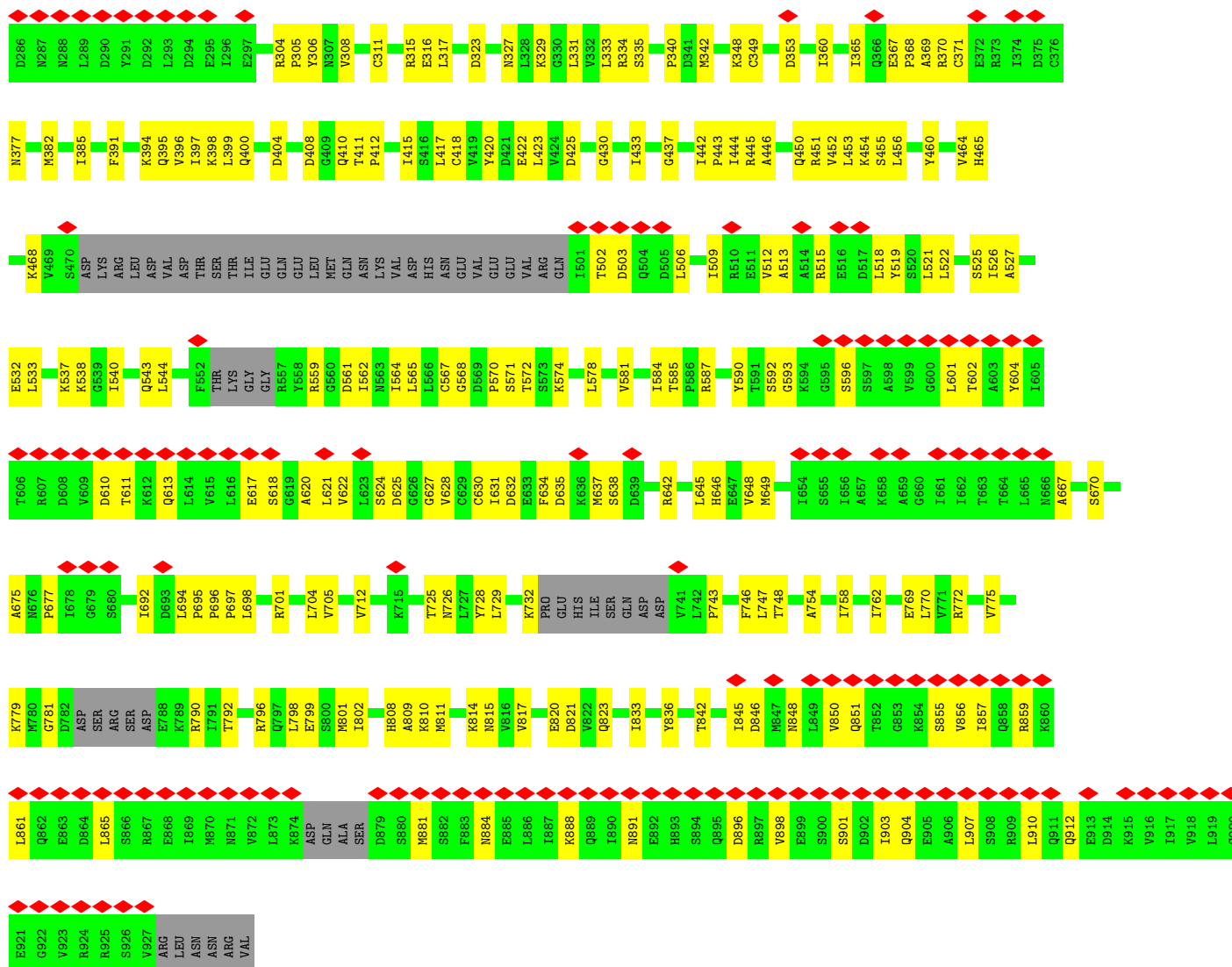


Mol	Chain	Residues	Atoms						AltConf
20	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
20	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
20	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

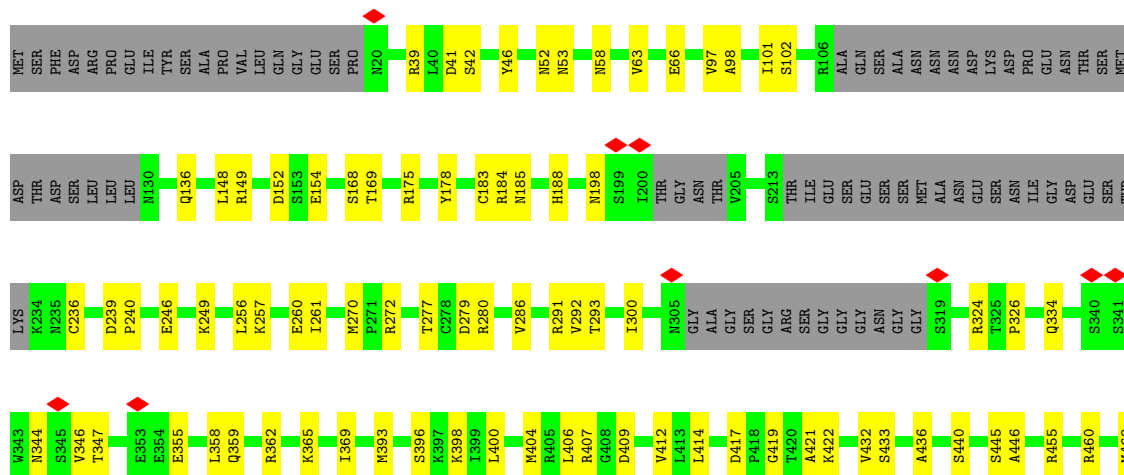


- Molecule 3: DNA replication licensing factor MCM4





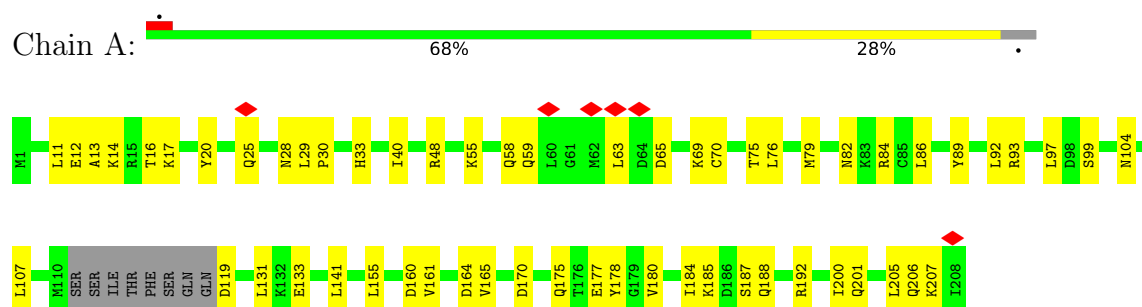
• Molecule 4: Minichromosome maintenance protein 5



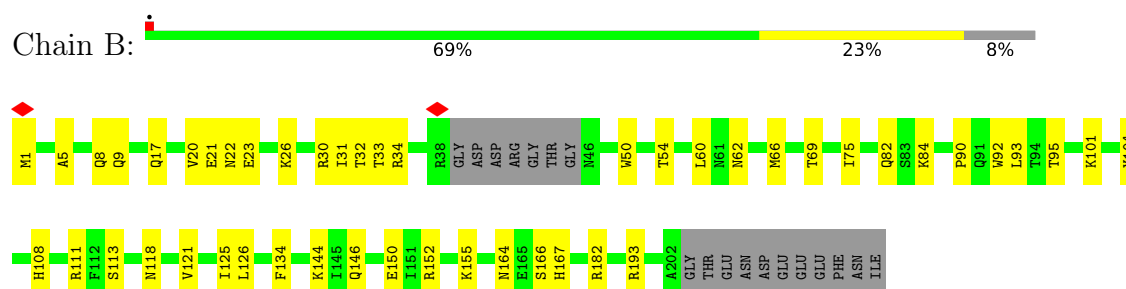




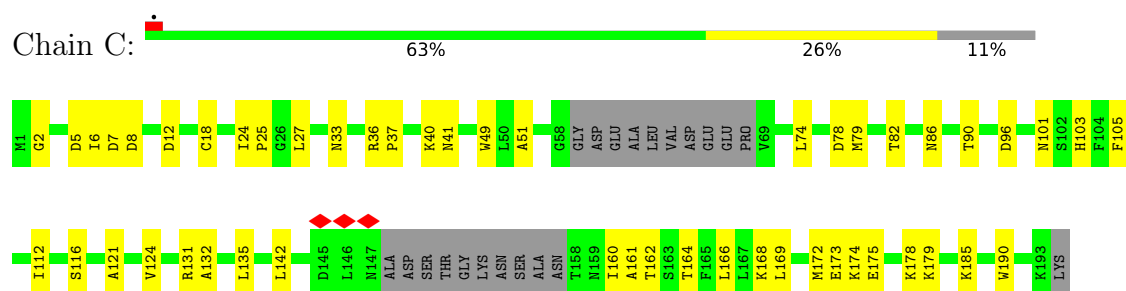
- Molecule 7: DNA replication complex GINS protein PSF1



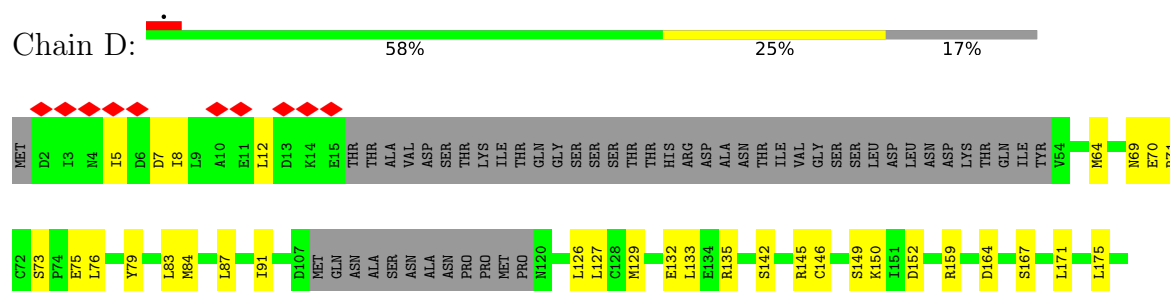
- Molecule 8: DNA replication complex GINS protein PSF2



- Molecule 9: DNA replication complex GINS protein PSF3

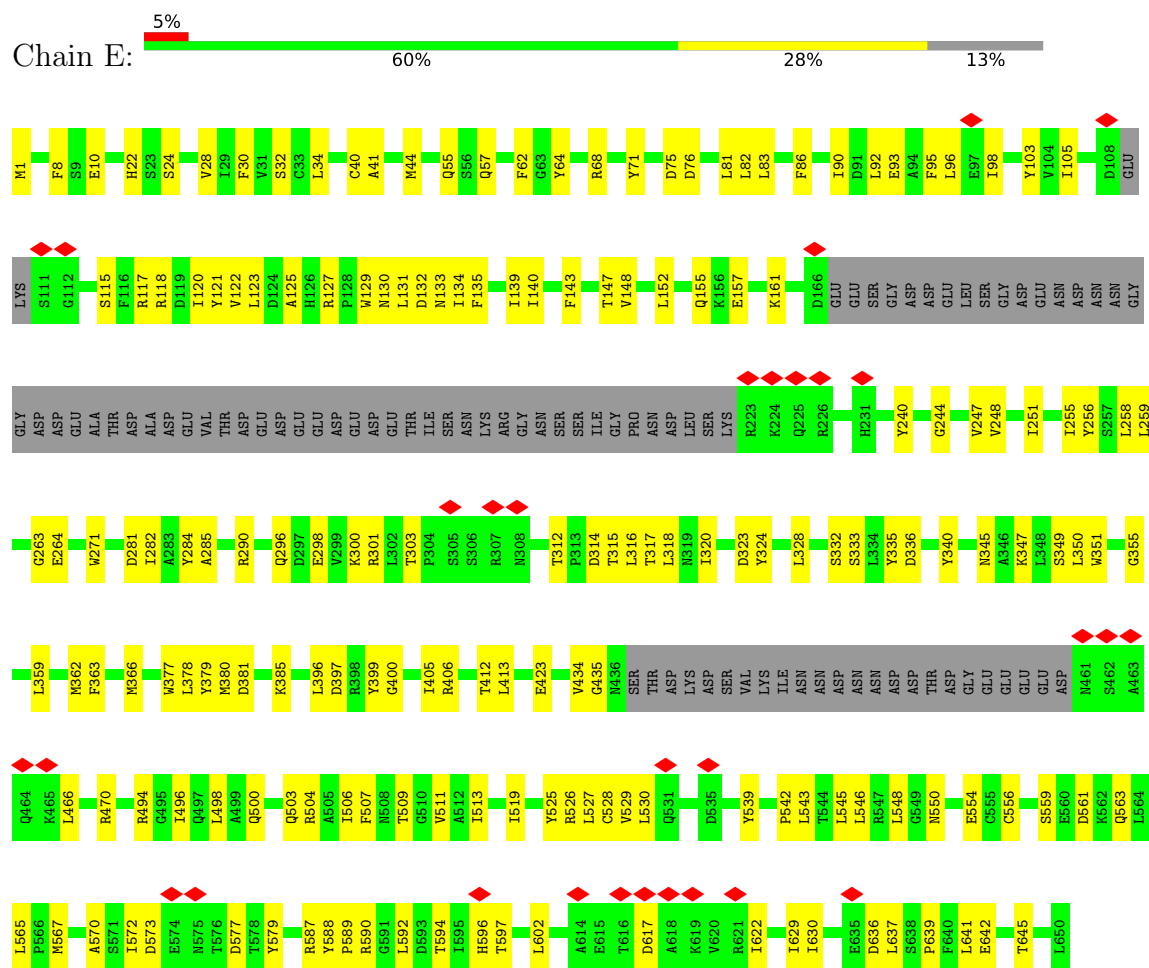


- Molecule 10: DNA replication complex GINS protein SLD5

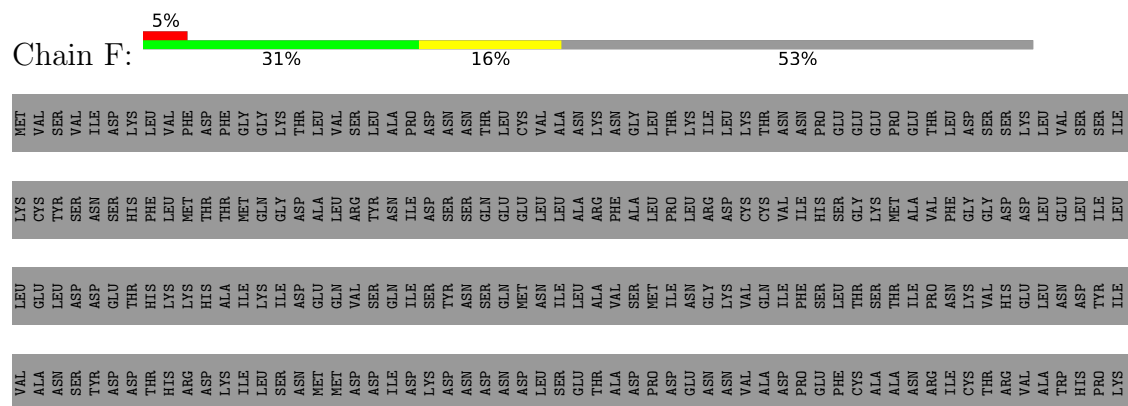


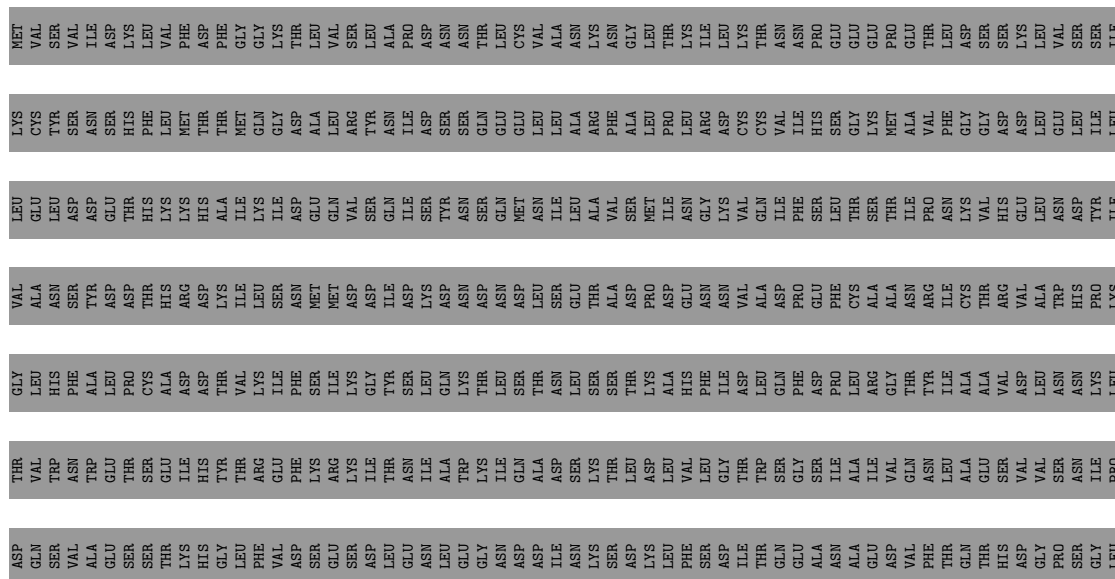


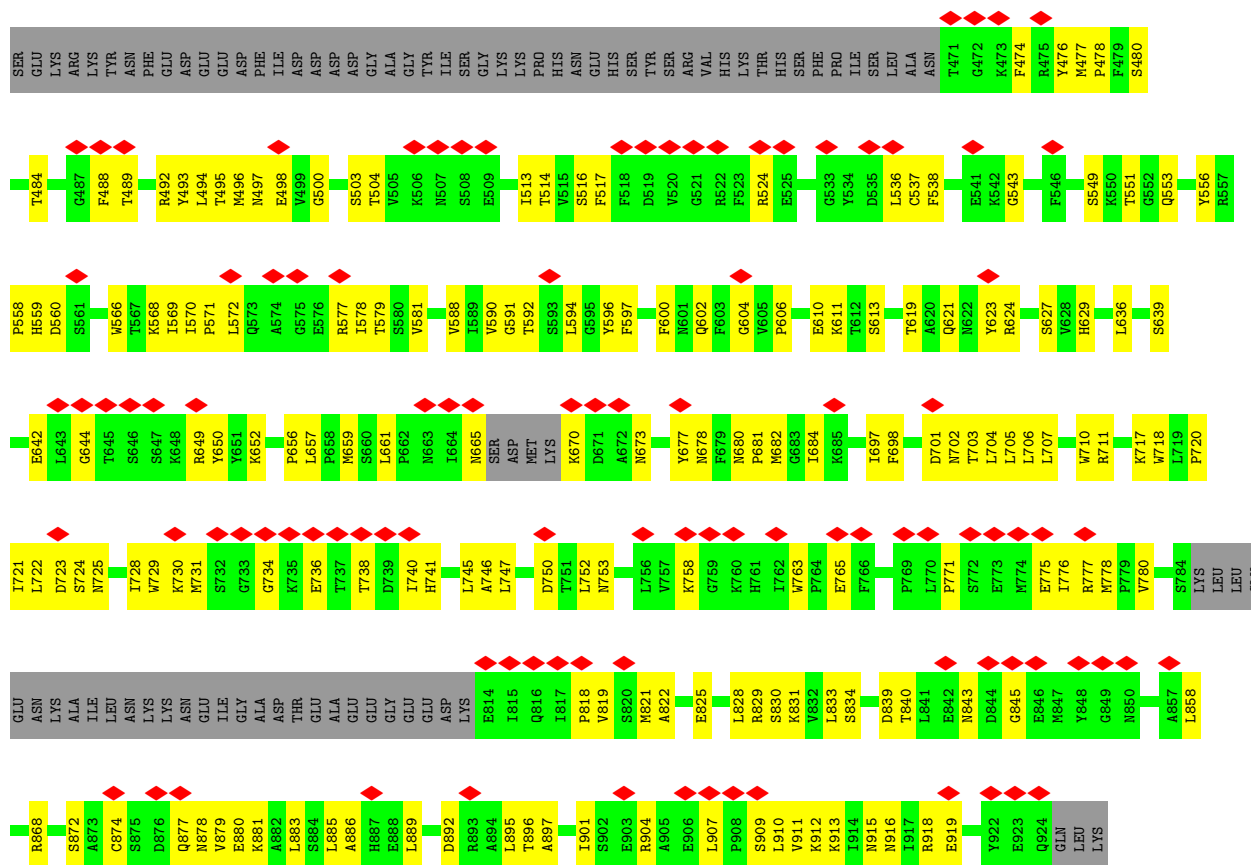
• Molecule 11: Cell division control protein 45



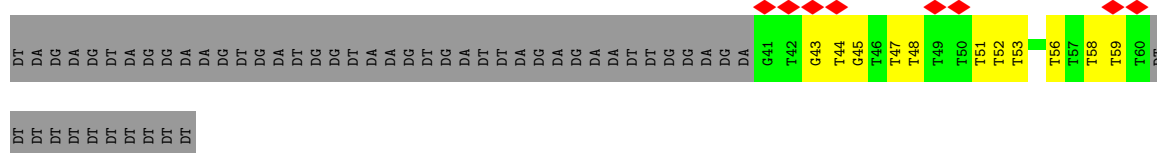
• Molecule 12: DNA polymerase alpha-binding protein



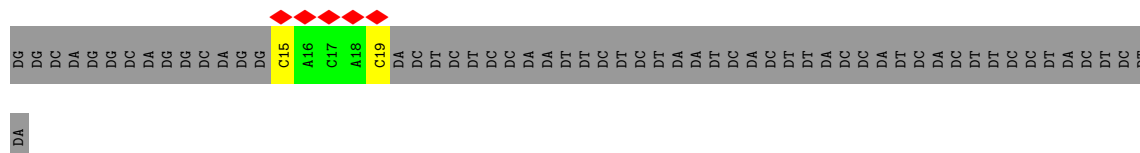




• Molecule 13: DNA (71-mer)



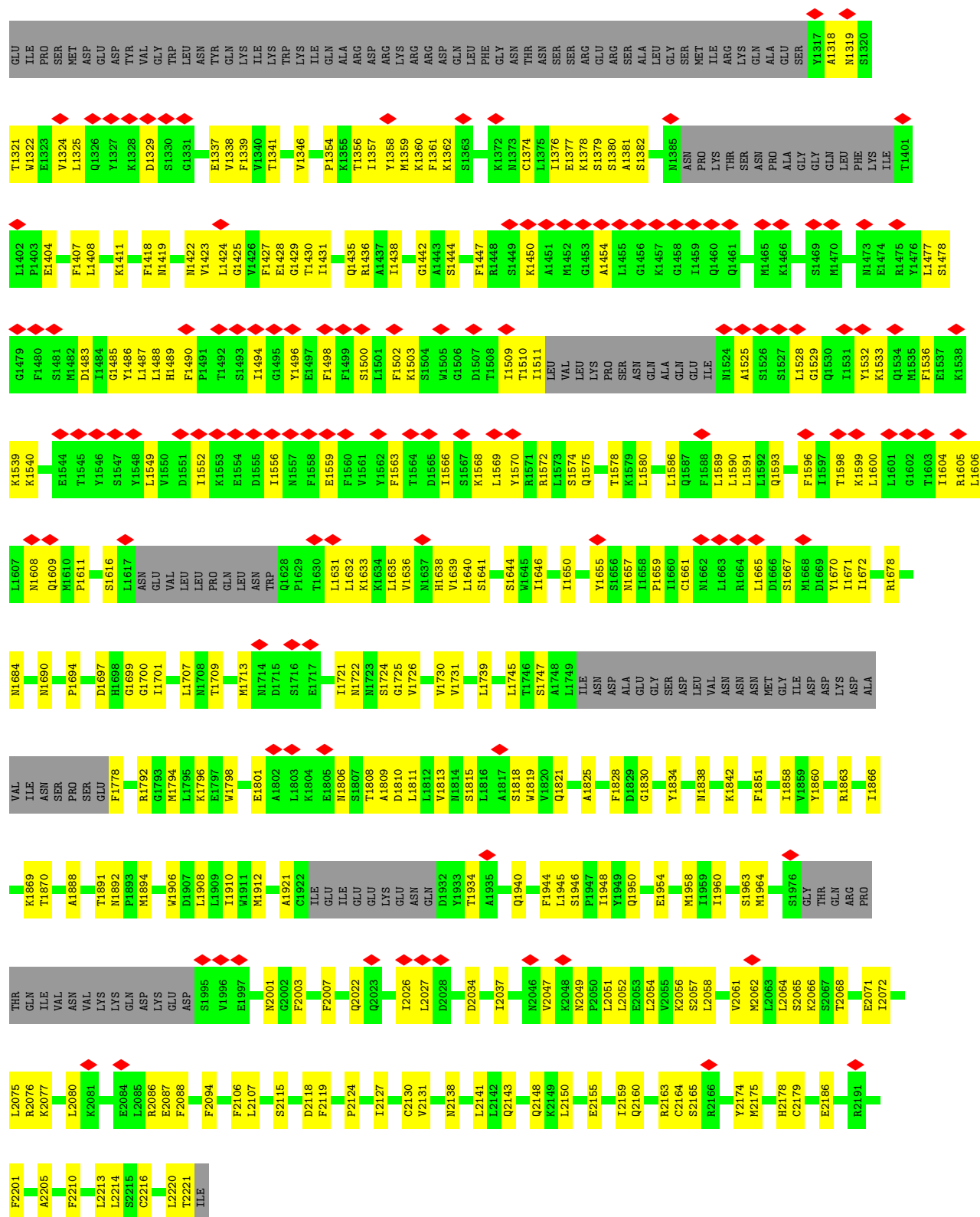
• Molecule 14: DNA (61-mer)



• Molecule 15: DNA polymerase epsilon catalytic subunit A

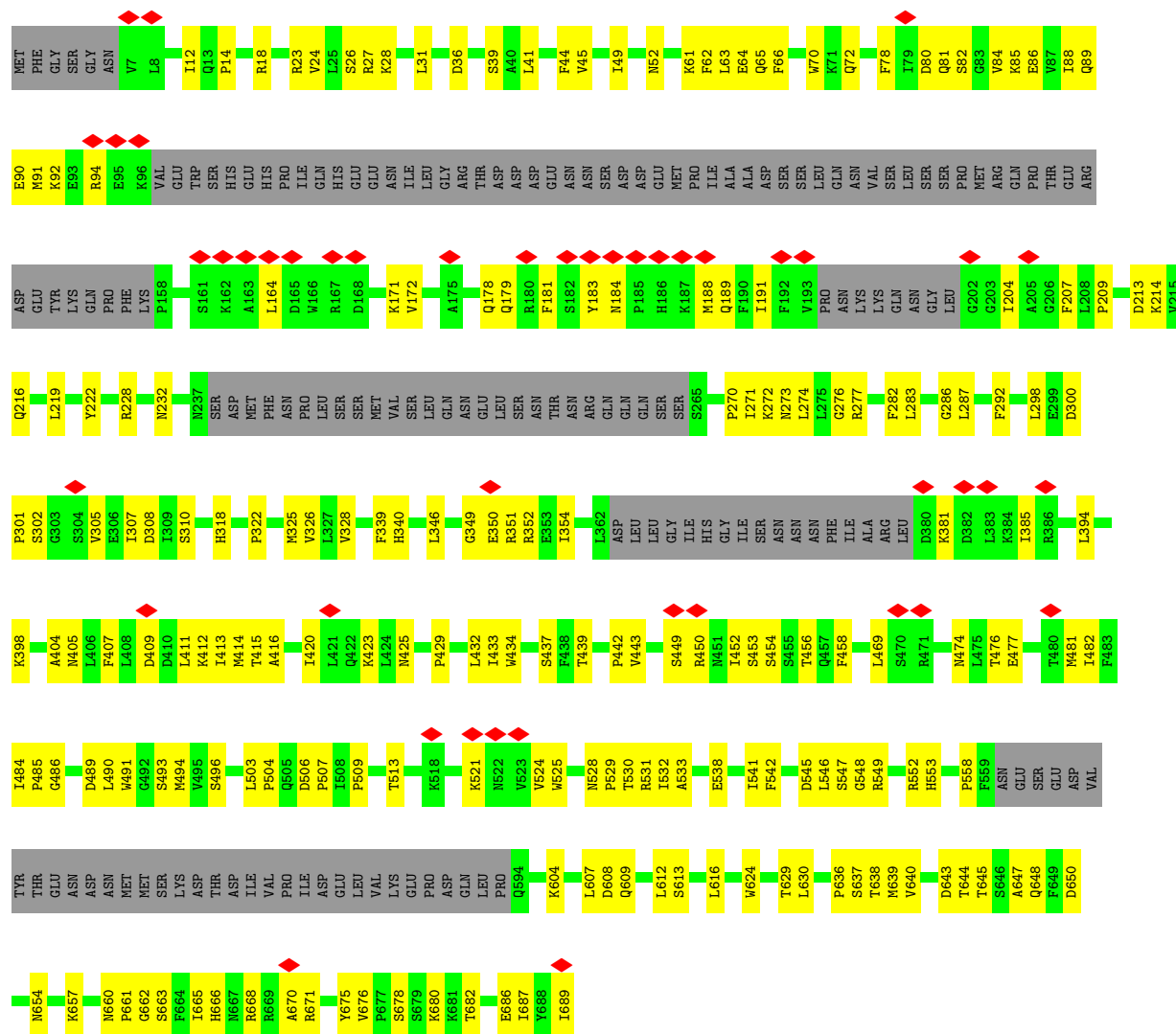






• Molecule 16: DNA polymerase epsilon subunit B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.082	Depositor
Minimum map value	-0.182	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	572.39996, 572.39996, 572.39996	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.11	0/5334	0.32	0/7203
2	3	0.12	0/5091	0.34	0/6914
3	4	0.11	0/5575	0.34	0/7531
4	5	0.11	0/5407	0.32	0/7302
5	6	0.12	0/4957	0.33	0/6684
6	7	0.13	0/5097	0.35	0/6896
7	A	0.13	0/1645	0.32	0/2215
8	B	0.12	0/1663	0.34	0/2249
9	C	0.11	0/1426	0.32	0/1929
10	D	0.13	0/2040	0.34	0/2755
11	E	0.11	0/4677	0.31	0/6335
12	F	0.12	0/3553	0.35	0/4811
12	G	0.12	0/3448	0.33	0/4675
12	H	0.12	0/3443	0.34	0/4668
13	I	0.16	0/448	0.44	0/691
14	J	0.14	0/110	0.21	0/166
15	M	0.12	0/6632	0.33	0/8976
16	N	0.13	0/4345	0.35	0/5884
All	All	0.12	0/64891	0.33	0/87884

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2	5245	0	5290	120	0
2	3	5005	0	5043	103	0
3	4	5503	0	5537	177	0
4	5	5334	0	5383	126	0
5	6	4880	0	4914	177	0
6	7	5023	0	5042	178	0
7	A	1625	0	1621	47	0
8	B	1630	0	1685	38	0
9	C	1394	0	1405	40	0
10	D	2004	0	2001	58	0
11	E	4591	0	4567	121	0
12	F	3467	0	3410	113	0
12	G	3362	0	3299	125	0
12	H	3358	0	3283	122	0
13	I	406	0	238	9	0
14	J	99	0	56	3	0
15	M	6490	0	6446	189	0
16	N	4254	0	4256	153	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
17	M	2	0	0	0	0
18	2	27	0	12	3	0
18	3	27	0	12	3	0
19	2	1	0	0	0	0
19	3	1	0	0	0	0
19	5	1	0	0	0	0
19	6	1	0	0	0	0
19	7	1	0	0	0	0
20	5	31	0	12	5	0
20	6	31	0	12	6	0
20	7	31	0	12	1	0
All	All	63829	0	63536	1754	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 14.

All (1754) 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)
5:6:734:LEU:HD21	5:6:742:ILE:CD1	1.66	1.25
5:6:734:LEU:CD2	5:6:742:ILE:CD1	2.21	1.18
5:6:734:LEU:HD21	5:6:742:ILE:HD11	1.27	1.11
5:6:734:LEU:HD21	5:6:742:ILE:CG1	1.83	1.07
5:6:734:LEU:CD2	5:6:742:ILE:HG13	1.86	1.06
5:6:535:PRO:HB2	5:6:742:ILE:HG21	1.36	1.02
5:6:535:PRO:O	5:6:742:ILE:HD13	1.64	0.98
5:6:734:LEU:CD2	5:6:742:ILE:CG1	2.41	0.97
6:7:284:CYS:HB3	6:7:289:CYS:SG	2.14	0.87
5:6:734:LEU:HD23	5:6:742:ILE:HG13	1.54	0.86
5:6:734:LEU:CD2	5:6:742:ILE:HD11	1.96	0.86
15:M:1908:LEU:HD21	15:M:1964:MET:HG3	1.57	0.86
5:6:734:LEU:HD22	5:6:742:ILE:HD12	1.58	0.84
5:6:536:ALA:HA	5:6:742:ILE:CD1	2.08	0.83
5:6:535:PRO:HB2	5:6:742:ILE:CG2	2.08	0.83
12:F:702:ASN:HB3	12:F:724:SER:HB3	1.61	0.83
2:3:671:LEU:HB3	6:7:621:MET:HE1	1.62	0.81
5:6:734:LEU:HD22	5:6:742:ILE:CD1	2.07	0.81
12:F:661:LEU:HD11	12:F:682:MET:HB2	1.63	0.81
5:6:734:LEU:CD2	5:6:742:ILE:HD12	2.10	0.81
12:G:544:THR:HG1	12:G:559:HIS:HE2	1.27	0.80
11:E:120:ILE:HD11	11:E:140:ILE:HG13	1.64	0.80
15:M:1657:ASN:O	15:M:1678:ARG:NH2	2.16	0.79
16:N:352:ARG:HH12	16:N:538:GLU:H	1.32	0.78
11:E:526:ARG:HB2	11:E:567:MET:HG3	1.66	0.78
15:M:1954:GLU:HG3	15:M:1958:MET:HE1	1.67	0.76
16:N:666:HIS:HB2	16:N:671:ARG:HE	1.48	0.76
1:2:502:ALA:HB3	1:2:512:LYS:HE2	1.68	0.76
9:C:33:ASN:HB2	9:C:36:ARG:HB3	1.66	0.76
6:7:668:ARG:HG3	6:7:683:GLN:HE22	1.49	0.76
15:M:1533:LYS:HA	15:M:1536:PHE:HB3	1.68	0.76
2:3:52:ASN:ND2	2:3:90:ASN:O	2.19	0.75
12:H:879:VAL:O	12:H:913:LYS:NZ	2.19	0.75
10:D:195:ASN:HA	10:D:199:LEU:HB2	1.67	0.75
6:7:316:GLN:HE21	6:7:328:PRO:HB2	1.51	0.74
5:6:641:PHE:HB3	5:6:682:ALA:HB2	1.68	0.74
16:N:449:SER:OG	16:N:450:ARG:NH1	2.19	0.74
2:3:442:LEU:HB3	2:3:462:MET:HE1	1.68	0.74
3:4:565:LEU:HB3	3:4:705:VAL:HG12	1.69	0.74
6:7:498:MET:HG3	6:7:499:LYS:HG3	1.69	0.74
6:7:664:TYR:HB2	6:7:689:LEU:HD21	1.70	0.74
6:7:264:GLN:HE21	6:7:294:THR:HB	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:40:ILE:HG21	7:A:86:LEU:HD21	1.69	0.73
12:F:592:THR:HB	12:F:596:TYR:H	1.53	0.73
8:B:20:VAL:HG21	8:B:121:VAL:HG21	1.70	0.73
11:E:155:GLN:HE21	11:E:240:TYR:HB2	1.53	0.73
4:5:393:MET:HG3	4:5:666:LEU:HB3	1.68	0.73
5:6:734:LEU:HD21	5:6:742:ILE:HG13	1.53	0.73
1:2:494:ILE:HD11	1:2:824:ARG:HD3	1.70	0.73
15:M:1488:LEU:HA	15:M:1593:GLN:HB3	1.72	0.72
15:M:1745:LEU:O	15:M:1796:LYS:NZ	2.23	0.72
2:3:310:ASN:HB3	2:3:313:THR:HB	1.72	0.72
4:5:183:CYS:HB3	4:5:188:HIS:H	1.55	0.71
15:M:1589:LEU:HG	15:M:1611:PRO:HB2	1.72	0.71
4:5:575:ILE:HA	4:5:580:ALA:HB2	1.72	0.71
5:6:338:CYS:SG	5:6:340:ASN:ND2	2.62	0.71
5:6:535:PRO:C	5:6:742:ILE:HD13	2.14	0.71
12:G:839:ASP:O	12:G:843:ASN:HB3	1.91	0.71
9:C:131:ARG:NH2	9:C:168:LYS:O	2.23	0.71
5:6:143:MET:HE1	5:6:151:ILE:HA	1.72	0.71
3:4:694:LEU:HD12	3:4:695:PRO:HD2	1.73	0.71
4:5:52:ASN:ND2	9:C:142:LEU:O	2.23	0.70
1:2:502:ALA:HB1	1:2:505:ILE:HB	1.74	0.70
15:M:1700:GLY:O	16:N:552:ARG:NH1	2.24	0.70
12:G:705:LEU:HD11	12:H:611:LYS:HD3	1.74	0.70
6:7:351:VAL:HG22	6:7:381:VAL:HG22	1.73	0.70
6:7:645:ALA:HB3	6:7:701:LYS:HG3	1.72	0.70
15:M:1324:VAL:HA	15:M:1661:CYS:HB3	1.74	0.70
11:E:303:THR:O	12:F:491:ARG:NH2	2.25	0.70
12:F:585:PRO:O	12:F:602:GLN:NE2	2.22	0.70
18:3:1001:ADP:O1A	4:5:651:ARG:NH2	2.24	0.69
12:G:629:HIS:O	12:G:636:LEU:HA	1.92	0.69
12:H:697:ILE:HB	12:H:705:LEU:HB2	1.72	0.69
3:4:456:LEU:HD12	6:7:252:LYS:HD3	1.72	0.69
4:5:455:ARG:HD3	4:5:460:ARG:HE	1.57	0.69
12:G:879:VAL:O	12:G:913:LYS:NZ	2.26	0.69
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.74	0.69
12:H:659:MET:HG3	12:H:684:ILE:HD11	1.75	0.69
16:N:541:ILE:HA	16:N:640:VAL:HB	1.74	0.69
2:3:700:ARG:NH2	20:7:903:AGS:O2A	2.24	0.69
12:H:753:ASN:HB2	12:H:771:PRO:HB2	1.74	0.69
1:2:609:PHE:HA	1:2:612:MET:HE1	1.73	0.69
6:7:311:GLN:HB2	6:7:340:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:597:PHE:HB3	12:F:610:GLU:HB3	1.73	0.69
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.75	0.69
12:H:670:LYS:HB3	12:H:673:ASN:HB2	1.73	0.69
7:A:165:VAL:HA	7:A:207:LYS:HB3	1.75	0.68
10:D:210:ASN:HB2	10:D:219:ILE:HD11	1.76	0.68
5:6:641:PHE:HA	5:6:644:MET:HE3	1.74	0.68
7:A:84:ARG:NH1	9:C:12:ASP:OD2	2.26	0.68
15:M:1731:VAL:HG12	15:M:1869:LYS:HA	1.74	0.68
12:H:895:LEU:HD21	12:H:918:ARG:HA	1.74	0.68
6:7:670:ASP:HA	6:7:673:ARG:HG2	1.76	0.68
1:2:468:GLU:HG2	1:2:473:VAL:HG13	1.75	0.68
7:A:84:ARG:NH2	9:C:8:ASP:OD2	2.25	0.68
9:C:12:ASP:HB3	9:C:49:TRP:HB3	1.74	0.68
5:6:140:ILE:HG22	5:6:144:LYS:HE2	1.75	0.68
5:6:307:ALA:HB3	5:6:321:VAL:HB	1.75	0.68
11:E:509:THR:OG1	11:E:539:TYR:OH	2.12	0.68
16:N:636:PRO:HG2	16:N:639:MET:HE1	1.75	0.68
12:G:659:MET:HE2	12:G:684:ILE:HD11	1.76	0.67
5:6:340:ASN:O	5:6:341:ARG:NH1	2.27	0.67
11:E:248:VAL:O	11:E:290:ARG:NH2	2.27	0.67
12:F:566:TRP:NE1	12:F:602:GLN:O	2.26	0.67
6:7:206:PRO:HB3	6:7:352:THR:HG21	1.76	0.67
3:4:506:LEU:HA	3:4:509:ILE:HD12	1.77	0.67
11:E:8:PHE:HB3	11:E:258:LEU:HD13	1.76	0.67
12:G:775:GLU:HG3	12:G:829:ARG:HH12	1.60	0.67
12:F:548:GLN:HB3	12:F:552:GLY:HA2	1.76	0.67
15:M:1529:GLY:HA2	15:M:1636:VAL:HG21	1.76	0.67
12:G:493:TYR:HA	12:G:503:SER:HA	1.77	0.67
12:H:597:PHE:HB3	12:H:610:GLU:HB3	1.77	0.67
12:H:551:THR:H	12:H:572:LEU:HD22	1.59	0.67
16:N:484:ILE:HG23	16:N:528:ASN:HA	1.77	0.67
11:E:435:GLY:O	11:E:494:ARG:NH2	2.27	0.66
12:H:704:LEU:HB2	12:H:721:ILE:HB	1.76	0.66
4:5:369:ILE:HD12	4:5:592:SER:HA	1.78	0.66
4:5:526:ILE:HD11	4:5:541:ASP:HB3	1.77	0.66
11:E:328:LEU:HD12	11:E:500:GLN:HG3	1.76	0.66
16:N:325:MET:O	16:N:609:GLN:NE2	2.26	0.66
16:N:661:PRO:O	16:N:671:ARG:NH1	2.27	0.66
10:D:75:GLU:O	10:D:150:LYS:NZ	2.22	0.66
4:5:482:PHE:HB3	4:5:523:ALA:HB2	1.75	0.66
11:E:434:VAL:HG23	11:E:498:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:722:LEU:HD12	12:G:776:ILE:HA	1.77	0.66
10:D:73:SER:OG	10:D:150:LYS:NZ	2.28	0.66
2:3:195:LYS:HB3	6:7:371:LEU:HD12	1.78	0.66
11:E:377:TRP:HA	11:E:380:MET:HE2	1.77	0.66
4:5:552:MET:HE1	4:5:684:PHE:HD1	1.61	0.66
6:7:545:THR:HG23	6:7:558:ASN:HA	1.77	0.66
7:A:99:SER:OG	8:B:1:MET:N	2.28	0.66
11:E:148:VAL:HA	11:E:152:LEU:HD13	1.78	0.66
1:2:630:SER:HB2	4:5:440:SER:HB3	1.77	0.66
15:M:2022:GLN:NE2	15:M:2049:ASN:OD1	2.28	0.65
1:2:690:GLU:HB3	1:2:694:ARG:HH12	1.61	0.65
3:4:701:ARG:NH2	20:6:1103:AGS:S1G	2.59	0.65
3:4:559:ARG:HH22	3:4:796:ARG:HH21	1.42	0.65
13:I:47:DT:H2''	13:I:48:DT:H5'	1.79	0.65
1:2:424:VAL:HG12	1:2:458:ARG:HA	1.79	0.65
4:5:535:SER:HA	4:5:696:PRO:HG3	1.79	0.65
7:A:79:MET:HB3	10:D:202:MET:HE1	1.79	0.65
15:M:1566:ILE:HA	15:M:1569:LEU:HB2	1.78	0.65
11:E:281:ASP:OD2	11:E:406:ARG:NH1	2.29	0.65
6:7:289:CYS:SG	6:7:294:THR:OG1	2.55	0.65
2:3:104:ARG:NH1	9:C:90:THR:OG1	2.29	0.64
2:3:670:GLN:H	2:3:720:THR:HA	1.60	0.64
11:E:123:LEU:HD13	11:E:143:PHE:HB2	1.78	0.64
16:N:70:TRP:HD1	16:N:72:GLN:HE22	1.45	0.64
16:N:407:PHE:HB2	16:N:413:ILE:HD12	1.80	0.64
1:2:621:HIS:HA	1:2:624:MET:HE2	1.80	0.64
5:6:149:ASN:ND2	5:6:262:VAL:O	2.28	0.64
12:H:728:ILE:HD11	12:H:740:ILE:HB	1.78	0.64
4:5:169:THR:HG22	4:5:256:LEU:HD22	1.80	0.64
5:6:379:VAL:HG13	5:6:454:PHE:HB3	1.78	0.64
3:4:635:ASP:O	3:4:642:ARG:NH2	2.30	0.64
11:E:526:ARG:NH2	11:E:563:GLN:O	2.31	0.64
11:E:301:ARG:O	12:F:491:ARG:NH2	2.31	0.64
12:F:692:TYR:HB3	12:F:840:THR:HG21	1.80	0.64
3:4:637:MET:HE3	3:4:642:ARG:HG2	1.81	0.63
4:5:724:ILE:HA	4:5:772:ARG:HG2	1.80	0.63
12:H:819:VAL:HG13	12:H:868:ARG:HH21	1.63	0.63
2:3:402:ASP:OD2	2:3:493:GLN:NE2	2.31	0.63
4:5:412:VAL:HG22	4:5:552:MET:HB2	1.80	0.63
6:7:228:ARG:NH2	6:7:327:ILE:O	2.31	0.63
11:E:349:SER:OG	11:E:351:TRP:NE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:315:ARG:NH2	3:4:411:THR:O	2.31	0.63
4:5:419:GLY:HA2	20:5:802:AGS:H5'2	1.81	0.63
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.81	0.63
9:C:96:ASP:HA	9:C:168:LYS:HB3	1.79	0.63
15:M:1486:TYR:HA	15:M:1591:LEU:HB3	1.79	0.63
6:7:260:TYR:HB3	6:7:298:LEU:HB3	1.81	0.63
8:B:22:ASN:OD1	10:D:135:ARG:NH2	2.31	0.63
12:F:610:GLU:OE2	12:F:653:ARG:NH2	2.32	0.63
12:H:636:LEU:HD21	12:H:659:MET:HE3	1.81	0.63
6:7:399:GLU:HA	6:7:402:MET:HE2	1.80	0.63
7:A:161:VAL:HG11	10:D:127:LEU:HD11	1.80	0.63
11:E:594:THR:H	11:E:597:THR:HB	1.63	0.63
12:G:493:TYR:HB3	12:G:496:MET:HE1	1.80	0.63
15:M:1486:TYR:HH	15:M:1638:HIS:HD1	1.47	0.63
3:4:513:ALA:HA	3:4:518:LEU:HD22	1.81	0.63
9:C:82:THR:O	9:C:86:ASN:ND2	2.31	0.63
6:7:349:VAL:HG12	6:7:383:GLN:HA	1.80	0.63
12:H:729:TRP:NE1	12:H:736:GLU:OE1	2.30	0.63
1:2:472:ASP:HB3	1:2:475:SER:HB3	1.80	0.62
5:6:701:MET:SD	5:6:706:MET:HB3	2.39	0.62
12:G:581:VAL:HG12	12:G:590:VAL:HG23	1.81	0.62
16:N:503:LEU:HD23	16:N:630:LEU:HD13	1.81	0.62
5:6:536:ALA:HA	5:6:742:ILE:HD13	1.81	0.62
12:G:680:ASN:ND2	12:G:682:MET:SD	2.72	0.62
15:M:1963:SER:OG	15:M:2003:PHE:O	2.17	0.62
16:N:482:ILE:HG12	16:N:524:VAL:HB	1.82	0.62
16:N:643:ASP:OD1	16:N:644:THR:N	2.32	0.62
8:B:90:PRO:HD2	8:B:93:LEU:HD12	1.79	0.62
12:H:476:TYR:H	12:H:577:ARG:HH21	1.47	0.62
5:6:696:ARG:HD3	5:6:794:ARG:HD3	1.81	0.62
11:E:24:SER:O	11:E:55:GLN:NE2	2.33	0.62
5:6:310:THR:HG22	5:6:317:ILE:HG12	1.82	0.62
5:6:360:ARG:HE	5:6:376:THR:HB	1.64	0.62
2:3:29:GLN:HG3	2:3:128:ALA:HB1	1.81	0.62
4:5:561:ASN:ND2	4:5:563:GLU:OE2	2.33	0.62
4:5:358:LEU:HB3	4:5:362:ARG:HH12	1.64	0.62
16:N:477:GLU:OE1	16:N:521:LYS:NZ	2.30	0.62
6:7:618:TYR:HB3	6:7:626:PRO:HG3	1.81	0.62
12:H:568:LYS:NZ	12:H:604:GLY:O	2.33	0.62
5:6:275:ARG:NH1	5:6:367:GLU:OE1	2.33	0.62
6:7:498:MET:HE1	6:7:507:ILE:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:509:GLU:HG2	12:F:510:GLN:HG3	1.82	0.62
15:M:1360:LYS:HG3	15:M:1362:LYS:HG3	1.82	0.62
16:N:425:ASN:O	16:N:474:ASN:ND2	2.33	0.61
1:2:230:ARG:NH1	1:2:243:GLU:O	2.33	0.61
2:3:86:SER:N	6:7:215:TYR:O	2.33	0.61
6:7:89:GLN:OE1	6:7:102:LEU:N	2.33	0.61
16:N:648:GLN:HA	16:N:660:ASN:O	2.00	0.61
1:2:340:ASN:OD1	1:2:374:ARG:NH1	2.33	0.61
1:2:425:GLU:OE2	1:2:459:ARG:NH1	2.34	0.61
1:2:534:ARG:NH2	1:2:678:ASP:OD1	2.34	0.61
15:M:1616:SER:O	16:N:450:ARG:NE	2.25	0.61
3:4:798:LEU:HA	3:4:801:MET:HE3	1.83	0.61
4:5:184:ARG:NH1	4:5:239:ASP:O	2.34	0.61
5:6:706:MET:HE1	5:6:794:ARG:CZ	2.31	0.61
11:E:340:TYR:OH	11:E:504:ARG:NH1	2.33	0.61
12:G:553:GLN:HG3	12:G:569:ILE:HD13	1.82	0.61
4:5:344:ASN:HD22	9:C:160:ILE:HD11	1.65	0.61
12:G:819:VAL:HG13	12:G:868:ARG:HH21	1.66	0.61
3:4:335:SER:OG	3:4:395:GLN:NE2	2.33	0.61
3:4:645:LEU:O	3:4:649:MET:HG2	2.00	0.61
7:A:155:LEU:HD21	10:D:145:ARG:HD3	1.81	0.61
10:D:12:LEU:O	12:F:893:ARG:NH1	2.33	0.61
15:M:1731:VAL:HG22	15:M:1906:TRP:HB2	1.83	0.61
6:7:462:PRO:HD3	6:7:569:PRO:HD2	1.82	0.61
10:D:8:ILE:HD13	12:F:901:ILE:HG12	1.83	0.61
12:F:533:GLY:O	12:F:548:GLN:NE2	2.33	0.61
15:M:1821:GLN:HE21	15:M:2107:LEU:HD12	1.65	0.61
16:N:411:LEU:HA	16:N:414:MET:HE2	1.82	0.61
6:7:405:ILE:HG12	6:7:703:ARG:HH22	1.65	0.61
12:F:712:SER:HB3	12:F:715:GLU:HB2	1.83	0.61
2:3:313:THR:HG22	2:3:315:ILE:HG12	1.83	0.61
13:I:43:DG:H2"	13:I:44:DT:H5"	1.83	0.61
3:4:399:LEU:HB3	3:4:415:ILE:HG22	1.82	0.60
3:4:593:GLY:N	3:4:632:ASP:O	2.29	0.60
5:6:566:ARG:NH1	5:6:568:ASP:O	2.34	0.60
7:A:200:ILE:HG12	7:A:205:LEU:HB2	1.82	0.60
12:G:638:TYR:HB3	12:G:657:LEU:HB3	1.83	0.60
12:H:728:ILE:HA	12:H:731:MET:HE2	1.82	0.60
15:M:1528:LEU:HD21	15:M:1633:LYS:HG3	1.83	0.60
12:G:662:PRO:HB3	12:G:665:ASN:HD22	1.66	0.60
5:6:117:GLN:HA	5:6:120:GLU:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:833:GLN:O	5:6:837:ARG:NH1	2.34	0.60
10:D:71:ARG:NH2	10:D:142:SER:OG	2.33	0.60
12:G:776:ILE:O	12:G:829:ARG:NH1	2.34	0.60
12:H:549:SER:HA	12:H:578:ILE:HB	1.82	0.60
6:7:410:VAL:HA	6:7:414:LEU:HD23	1.82	0.60
12:F:597:PHE:N	12:F:610:GLU:O	2.31	0.60
15:M:1356:THR:O	15:M:1430:THR:OG1	2.19	0.60
2:3:122:ILE:HG23	2:3:155:LEU:HD12	1.82	0.60
11:E:121:TYR:HB3	11:E:143:PHE:HE1	1.65	0.60
12:H:680:ASN:ND2	12:H:682:MET:SD	2.75	0.60
3:4:587:ARG:NH2	3:4:625:ASP:OD1	2.35	0.60
7:A:165:VAL:HG21	7:A:205:LEU:HD13	1.84	0.60
11:E:328:LEU:HA	11:E:423:GLU:HG2	1.83	0.60
15:M:1818:SER:HB2	15:M:2107:LEU:HD11	1.84	0.60
4:5:184:ARG:N	4:5:240:PRO:O	2.33	0.60
5:6:140:ILE:HA	5:6:143:MET:HG3	1.84	0.60
6:7:576:PRO:HB2	6:7:577:ARG:HH21	1.67	0.60
11:E:10:GLU:OE1	11:E:10:GLU:N	2.35	0.60
12:F:778:MET:HE1	12:F:829:ARG:HG2	1.83	0.60
3:4:634:PHE:HB3	3:4:675:ALA:HB2	1.83	0.60
12:H:840:THR:O	12:H:845:GLY:N	2.35	0.60
16:N:547:SER:HB3	16:N:645:THR:HG23	1.83	0.60
5:6:609:THR:HB	5:6:661:ILE:HD13	1.84	0.59
11:E:317:THR:HG1	11:E:412:THR:HG1	1.48	0.59
12:G:682:MET:HG2	12:G:684:ILE:H	1.67	0.59
15:M:1486:TYR:OH	15:M:1638:HIS:ND1	2.35	0.59
15:M:1510:THR:HA	15:M:1559:GLU:HB2	1.84	0.59
2:3:683:TYR:OH	2:3:687:ARG:NH1	2.35	0.59
3:4:848:ASN:ND2	5:6:686:GLY:O	2.36	0.59
11:E:41:ALA:HB1	11:E:255:ILE:HD12	1.83	0.59
3:4:202:LYS:HD2	3:4:222:GLU:HA	1.84	0.59
9:C:40:LYS:HD3	9:C:41:ASN:HB2	1.84	0.59
12:G:639:SER:HB3	12:G:654:GLU:H	1.67	0.59
15:M:2130:CYS:SG	15:M:2131:VAL:N	2.76	0.59
2:3:347:ILE:O	2:3:351:ASN:ND2	2.32	0.59
5:6:522:ASP:HB3	5:6:525:ILE:HB	1.83	0.59
16:N:662:GLY:HA3	16:N:671:ARG:HH22	1.68	0.59
2:3:420:ARG:NH2	4:5:501:THR:OG1	2.35	0.59
4:5:729:SER:O	4:5:732:THR:OG1	2.17	0.59
9:C:131:ARG:NH2	9:C:173:GLU:OE1	2.32	0.59
10:D:209:ILE:C	10:D:218:MET:HE1	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:485:PRO:O	16:N:528:ASN:ND2	2.35	0.59
5:6:326:LYS:HG2	5:6:327:TYR:H	1.67	0.59
10:D:232:VAL:HA	10:D:291:VAL:HG12	1.85	0.59
12:G:502:VAL:HG22	12:G:515:VAL:HG22	1.85	0.59
16:N:171:LYS:HG2	16:N:533:ALA:HB3	1.85	0.59
16:N:490:LEU:HB3	16:N:491:TRP:HE3	1.65	0.59
1:2:503:PRO:HB2	1:2:755:ILE:HD12	1.85	0.59
12:G:704:LEU:HD12	12:G:722:LEU:HB3	1.84	0.59
5:6:529:LEU:HD22	5:6:751:LEU:HD13	1.85	0.59
15:M:2022:GLN:O	15:M:2026:ILE:N	2.36	0.59
4:5:524:ASN:ND2	20:5:802:AGS:S1G	2.75	0.59
7:A:97:LEU:HD11	7:A:131:LEU:HB2	1.85	0.59
15:M:1806:ASN:OD1	15:M:1808:THR:OG1	2.19	0.59
15:M:1948:ILE:HB	15:M:2034:ASP:HB3	1.83	0.59
16:N:213:ASP:HA	16:N:216:GLN:HE21	1.68	0.59
3:4:443:PRO:HB2	3:4:453:LEU:HD22	1.85	0.58
3:4:532:GLU:CD	3:4:533:LEU:H	2.10	0.58
2:3:490:MET:HE3	2:3:542:ARG:HD3	1.86	0.58
3:4:601:LEU:HD12	3:4:620:ALA:HB3	1.85	0.58
3:4:646:HIS:HA	3:4:649:MET:HE2	1.84	0.58
12:H:581:VAL:HG12	12:H:590:VAL:HG23	1.83	0.58
15:M:1379:SER:O	15:M:1684:ASN:ND2	2.36	0.58
15:M:1713:MET:HE1	15:M:1830:GLY:HA3	1.85	0.58
16:N:81:GLN:HG2	16:N:85:LYS:HZ3	1.66	0.58
1:2:288:ARG:NH2	11:E:366:MET:O	2.37	0.58
3:4:519:TYR:HD1	3:4:811:MET:HE3	1.67	0.58
6:7:451:ARG:NH2	6:7:542:GLU:O	2.36	0.58
12:G:597:PHE:HB3	12:G:610:GLU:HB3	1.84	0.58
2:3:24:ARG:HD2	2:3:27:ARG:HH21	1.68	0.58
4:5:355:GLU:OE2	4:5:359:GLN:NE2	2.31	0.58
11:E:81:LEU:HB3	11:E:120:ILE:HG22	1.85	0.58
12:H:494:LEU:HD13	12:H:537:CYS:HB2	1.85	0.58
2:3:673:GLN:OE1	2:3:677:ASN:ND2	2.36	0.58
3:4:370:ARG:HD3	3:4:377:ASN:HB2	1.85	0.58
6:7:494:THR:HG22	6:7:512:ALA:HB3	1.86	0.58
15:M:2065:SER:OG	15:M:2068:THR:OG1	2.20	0.58
1:2:307:ARG:NH2	1:2:402:LEU:O	2.35	0.58
4:5:185:ASN:HB2	4:5:236:CYS:SG	2.44	0.58
4:5:398:LYS:HB2	4:5:406:LEU:HB2	1.84	0.58
12:G:504:THR:HB	12:G:511:TYR:HB3	1.84	0.58
12:H:492:ARG:HH12	12:H:494:LEU:HD23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:496:MET:SD	12:H:745:LEU:HD13	2.44	0.58
15:M:1600:LEU:HA	15:M:1604:ILE:HB	1.84	0.58
1:2:625:GLU:HG2	1:2:808:ARG:HH21	1.69	0.58
10:D:126:LEU:HA	10:D:129:MET:HE2	1.85	0.58
12:G:730:LYS:HA	12:G:734:GLY:HA2	1.84	0.58
15:M:2138:ASN:HB2	15:M:2141:LEU:HB2	1.86	0.58
12:F:704:LEU:HD11	12:F:752:LEU:HD22	1.85	0.58
15:M:1444:SER:HB2	15:M:1477:LEU:HD11	1.85	0.58
15:M:1533:LYS:HD2	15:M:1536:PHE:HD2	1.67	0.58
2:3:480:ASP:OD1	2:3:483:ARG:NH1	2.37	0.58
5:6:683:ASN:OD1	20:6:1103:AGS:O3G	2.21	0.58
12:F:737:THR:OG1	12:F:739:ASP:OD1	2.22	0.58
12:G:755:ILE:HG23	12:G:769:PRO:HD2	1.86	0.58
15:M:1435:GLN:H	15:M:1438:ILE:HD13	1.69	0.58
16:N:612:LEU:HD12	16:N:630:LEU:HA	1.85	0.58
1:2:794:ARG:NH1	1:2:805:ILE:O	2.37	0.58
6:7:426:LEU:HD13	6:7:429:LYS:HD2	1.86	0.58
12:F:721:ILE:HG22	12:F:776:ILE:HB	1.86	0.58
12:G:638:TYR:N	12:G:655:CYS:O	2.35	0.58
2:3:169:ARG:NH2	2:3:270:LEU:O	2.37	0.57
5:6:801:GLU:HB3	5:6:805:ARG:HH12	1.69	0.57
6:7:405:ILE:HG23	6:7:703:ARG:HH12	1.68	0.57
7:A:92:LEU:HD12	9:C:6:ILE:HD11	1.85	0.57
15:M:1337:GLU:OE2	15:M:1609:GLN:NE2	2.37	0.57
15:M:1490:PHE:HB3	15:M:1498:PHE:HD2	1.69	0.57
15:M:1725:GLY:HA2	15:M:2064:LEU:HB3	1.86	0.57
2:3:312:ASN:O	4:5:198:ASN:ND2	2.37	0.57
3:4:645:LEU:HA	3:4:648:VAL:HG12	1.85	0.57
6:7:453:ASP:O	6:7:694:ARG:NH1	2.37	0.57
6:7:569:PRO:HG2	6:7:574:TYR:HB2	1.87	0.57
12:G:676:TYR:O	12:G:680:ASN:N	2.35	0.57
12:H:623:TYR:HB3	12:H:644:GLY:HA2	1.85	0.57
3:4:233:MET:HE1	3:4:280:MET:HG2	1.86	0.57
6:7:81:ASP:HA	6:7:205:LYS:HB3	1.86	0.57
12:G:610:GLU:OE2	12:G:653:ARG:NH2	2.37	0.57
1:2:791:ALA:HB1	4:5:562:GLU:HG3	1.86	0.57
4:5:407:ARG:NH1	4:5:409:ASP:O	2.37	0.57
8:B:95:THR:HG23	8:B:144:LYS:HE3	1.86	0.57
12:G:495:THR:C	12:G:496:MET:HE2	2.28	0.57
12:G:883:LEU:HG	12:G:887:HIS:HE1	1.69	0.57
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:762:ILE:HA	3:4:817:VAL:HB	1.87	0.57
4:5:469:MET:HE1	4:5:502:ILE:HD11	1.85	0.57
5:6:640:GLU:HB3	5:6:643:LYS:HB2	1.85	0.57
4:5:620:GLU:HB3	16:N:273:ASN:HD21	1.69	0.57
7:A:58:GLN:HG2	7:A:63:LEU:HB2	1.87	0.57
12:F:636:LEU:O	12:G:634:HIS:NE2	2.37	0.57
1:2:609:PHE:HZ	1:2:673:ILE:HD11	1.69	0.57
3:4:382:MET:HE2	5:6:441:ARG:HH12	1.68	0.57
5:6:535:PRO:O	5:6:742:ILE:CD1	2.47	0.57
10:D:152:ASP:OD2	10:D:182:TYR:OH	2.12	0.57
5:6:535:PRO:CB	5:6:742:ILE:HG21	2.24	0.57
11:E:347:LYS:NZ	11:E:400:GLY:O	2.38	0.57
1:2:397:VAL:HG21	1:2:403:PRO:HB3	1.86	0.56
2:3:343:THR:OG1	2:3:346:ASP:OD2	2.22	0.56
5:6:112:ARG:NH1	5:6:116:GLU:OE2	2.38	0.56
15:M:1358:TYR:HB2	15:M:1429:GLY:HA2	1.87	0.56
1:2:527:VAL:HG21	4:5:575:ILE:HG23	1.87	0.56
5:6:283:LYS:O	5:6:286:SER:OG	2.21	0.56
5:6:638:ILE:HD12	5:6:678:ILE:HG23	1.87	0.56
12:H:702:ASN:OD1	12:H:725:ASN:ND2	2.35	0.56
16:N:81:GLN:HE21	16:N:85:LYS:HZ2	1.53	0.56
1:2:534:ARG:O	1:2:815:ARG:NH1	2.35	0.56
2:3:528:ASP:OD1	2:3:531:GLN:NE2	2.38	0.56
2:3:570:ARG:NH1	4:5:614:LEU:O	2.34	0.56
5:6:147:ASP:OD1	5:6:261:ARG:NH2	2.37	0.56
6:7:284:CYS:SG	6:7:289:CYS:CB	2.93	0.56
12:F:624:ARG:HA	12:F:642:GLU:HA	1.87	0.56
12:G:510:GLN:NE2	12:G:529:GLU:OE2	2.38	0.56
12:G:572:LEU:HG	12:G:576:GLU:HB3	1.87	0.56
15:M:1428:GLU:H	15:M:1699:GLY:HA2	1.70	0.56
16:N:88:ILE:HG22	16:N:92:LYS:HE2	1.85	0.56
3:4:446:ALA:HB3	3:4:452:VAL:HG23	1.88	0.56
11:E:316:LEU:HD12	11:E:413:LEU:HD13	1.87	0.56
16:N:443:VAL:HG23	16:N:454:SER:HB3	1.87	0.56
6:7:137:ASP:HB2	6:7:140:ASP:HB2	1.86	0.56
6:7:479:ARG:NH2	6:7:515:LEU:O	2.38	0.56
10:D:257:THR:OG1	10:D:268:GLU:OE1	2.18	0.56
12:G:763:TRP:NE1	12:G:765:GLU:OE1	2.30	0.56
12:H:707:LEU:HB3	12:H:710:TRP:HB3	1.86	0.56
15:M:2163:ARG:NH1	15:M:2186:GLU:OE2	2.39	0.56
16:N:271:ILE:HD13	16:N:305:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:293:THR:HA	5:6:394:ARG:HA	1.88	0.56
6:7:414:LEU:HA	6:7:417:SER:HB3	1.86	0.56
9:C:2:GLY:N	9:C:5:ASP:OD1	2.38	0.56
11:E:131:LEU:HA	11:E:134:ILE:HG22	1.87	0.56
11:E:76:ASP:O	11:E:117:ARG:NH1	2.38	0.56
11:E:359:LEU:HA	11:E:362:MET:HE2	1.87	0.56
12:F:720:PRO:HG3	12:G:611:LYS:HB2	1.87	0.56
12:H:492:ARG:O	12:H:504:THR:N	2.34	0.56
15:M:1641:SER:O	15:M:1644:SER:OG	2.23	0.56
8:B:9:GLN:OE1	10:D:226:LYS:NZ	2.29	0.56
9:C:7:ASP:OD1	9:C:103:HIS:ND1	2.39	0.56
11:E:282:ILE:O	11:E:590:ARG:NH2	2.37	0.56
16:N:14:PRO:HG3	16:N:39:SER:HA	1.87	0.56
16:N:404:ALA:HB3	16:N:663:SER:HA	1.86	0.56
4:5:500:GLN:HG2	4:5:516:ARG:HA	1.86	0.56
12:G:883:LEU:HD13	12:G:913:LYS:HD2	1.88	0.56
12:H:740:ILE:HG12	12:H:758:LYS:HZ3	1.70	0.56
1:2:473:VAL:O	1:2:765:LYS:NZ	2.39	0.56
3:4:833:ILE:HA	3:4:836:TYR:CE1	2.42	0.56
6:7:524:ASP:HA	6:7:566:ALA:HB3	1.88	0.56
12:F:777:ARG:NH1	12:F:826:GLU:OE2	2.39	0.56
2:3:688:ASN:ND2	6:7:605:SER:O	2.32	0.55
11:E:105:ILE:O	11:E:115:SER:OG	2.20	0.55
11:E:362:MET:HB3	11:E:366:MET:HE1	1.88	0.55
2:3:363:LEU:HD22	2:3:656:LEU:HD13	1.88	0.55
2:3:386:MET:HB3	2:3:660:VAL:HG13	1.89	0.55
5:6:571:ILE:HD12	5:6:711:LEU:HB2	1.88	0.55
5:6:720:ASN:HB3	5:6:723:ILE:HB	1.88	0.55
12:H:649:ARG:NH1	12:H:650:TYR:O	2.39	0.55
15:M:1361:PHE:HB2	15:M:1377:GLU:H	1.71	0.55
15:M:1540:LYS:HE3	15:M:1552:ILE:HG22	1.86	0.55
15:M:1604:ILE:O	15:M:1608:ASN:ND2	2.40	0.55
3:4:180:ILE:N	3:4:185:VAL:O	2.39	0.55
16:N:351:ARG:HB2	16:N:354:ILE:HG13	1.87	0.55
1:2:792:ASP:OD2	1:2:864:TYR:OH	2.20	0.55
12:F:485:PRO:HB3	12:F:679:PHE:HB2	1.87	0.55
13:I:58:DT:H2"	13:I:59:DT:H5"	1.88	0.55
15:M:1834:TYR:O	15:M:1838:ASN:ND2	2.39	0.55
6:7:683:GLN:NE2	6:7:684:ALA:O	2.35	0.55
11:E:92:LEU:H	11:E:133:ASN:HD21	1.55	0.55
1:2:577:THR:HG22	1:2:596:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:576:TYR:OH	2:3:583:ARG:O	2.25	0.55
3:4:323:ASP:OD2	6:7:302:THR:OG1	2.24	0.55
4:5:579:ASN:HB3	4:5:583:MET:HE2	1.89	0.55
12:G:621:GLN:HG3	12:G:622:ASN:H	1.71	0.55
4:5:486:ARG:NE	4:5:488:GLU:OE2	2.32	0.55
5:6:311:CYS:HB2	5:6:340:ASN:HD22	1.72	0.55
7:A:175:GLN:HA	7:A:180:VAL:HG23	1.89	0.55
11:E:127:ARG:NH1	11:E:147:THR:OG1	2.39	0.55
12:G:910:LEU:HD12	12:G:913:LYS:HE2	1.89	0.55
3:4:370:ARG:NH1	3:4:377:ASN:O	2.39	0.55
5:6:577:PRO:O	20:6:1103:AGS:O2B	2.25	0.55
9:C:79:MET:HE1	9:C:101:ASN:HD22	1.71	0.55
15:M:1478:SER:HB3	15:M:1650:ILE:HD12	1.88	0.55
15:M:2205:ALA:HB2	15:M:2213:LEU:HD23	1.88	0.55
16:N:232:ASN:ND2	16:N:349:GLY:O	2.39	0.55
16:N:671:ARG:HG2	16:N:686:GLU:HG2	1.89	0.55
6:7:104:SER:OG	6:7:214:ARG:NH2	2.39	0.55
12:G:683:GLY:O	12:G:700:SER:N	2.40	0.55
12:H:706:LEU:HD13	12:H:721:ILE:HG13	1.89	0.55
3:4:261:LEU:HB2	3:4:268:VAL:HG11	1.89	0.54
4:5:724:ILE:HG23	15:M:1842:LYS:HE2	1.88	0.54
12:H:747:LEU:HD13	12:H:752:LEU:HB2	1.89	0.54
16:N:434:TRP:HE1	16:N:481:MET:HB3	1.72	0.54
3:4:418:CYS:HB3	3:4:420:TYR:HE1	1.72	0.54
9:C:25:PRO:HA	9:C:37:PRO:HB3	1.88	0.54
12:F:634:HIS:CD2	12:H:656:PRO:HB3	2.42	0.54
15:M:1709:THR:O	15:M:1713:MET:HG2	2.07	0.54
15:M:1810:ASP:OD1	15:M:1811:LEU:N	2.40	0.54
6:7:68:GLN:NE2	6:7:72:ASN:OD1	2.41	0.54
12:H:566:TRP:NE1	12:H:602:GLN:O	2.40	0.54
4:5:763:LEU:HG	4:5:770:ILE:HG12	1.90	0.54
5:6:581:LYS:HB3	5:6:681:ALA:HB1	1.90	0.54
5:6:581:LYS:NZ	5:6:683:ASN:OD1	2.38	0.54
6:7:658:ASP:O	6:7:661:VAL:HG12	2.08	0.54
12:G:587:ARG:NH2	12:G:645:THR:O	2.40	0.54
12:H:493:TYR:HA	12:H:503:SER:HA	1.89	0.54
15:M:1665:LEU:HD13	16:N:450:ARG:HG2	1.90	0.54
3:4:272:MET:O	3:4:276:ILE:HG12	2.08	0.54
4:5:419:GLY:O	20:5:802:AGS:H8	2.07	0.54
6:7:441:ASP:O	6:7:450:ILE:N	2.40	0.54
11:E:83:LEU:HD12	11:E:122:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:588:VAL:HG13	12:H:600:PHE:HB2	1.88	0.54
16:N:214:LYS:HB2	16:N:624:TRP:CD2	2.43	0.54
2:3:333:SER:HB3	2:3:336:VAL:HG22	1.90	0.54
3:4:779:LYS:HD3	5:6:721:GLU:HG2	1.89	0.54
11:E:527:LEU:HD11	11:E:641:LEU:HD13	1.89	0.54
12:F:505:VAL:O	12:F:511:TYR:HA	2.07	0.54
3:4:444:ILE:HG13	3:4:454:LYS:HB2	1.90	0.54
5:6:759:ARG:O	5:6:812:ARG:NH2	2.40	0.54
7:A:133:GLU:CD	10:D:189:ILE:HG12	2.33	0.54
12:H:778:MET:HE2	12:H:828:LEU:HG	1.90	0.54
12:H:874:CYS:O	12:H:877:GLN:NE2	2.40	0.54
6:7:500:ASP:HB2	6:7:501:PRO:HD3	1.89	0.54
11:E:120:ILE:HG12	11:E:139:ILE:HG22	1.89	0.54
12:F:491:ARG:HD3	12:F:505:VAL:HB	1.90	0.54
5:6:141:GLU:HA	5:6:144:LYS:HD2	1.89	0.54
6:7:541:MET:HE1	6:7:593:ARG:HB3	1.90	0.54
11:E:68:ARG:NH1	11:E:95:PHE:O	2.41	0.54
5:6:312:ASP:O	5:6:315:ARG:NH1	2.32	0.54
11:E:130:ASN:ND2	11:E:132:ASP:OD1	2.41	0.54
12:F:586:VAL:HG11	12:F:645:THR:HA	1.90	0.54
8:B:164:ASN:ND2	8:B:167:HIS:O	2.38	0.53
11:E:296:GLN:HG3	11:E:320:ILE:HD13	1.90	0.53
12:H:911:VAL:O	12:H:915:ASN:ND2	2.38	0.53
13:I:44:DT:H2''	13:I:45:DG:H5'	1.91	0.53
1:2:530:LYS:HG2	4:5:596:ILE:HD11	1.89	0.53
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.89	0.53
4:5:715:GLU:HG2	4:5:755:LEU:HD11	1.90	0.53
10:D:164:ASP:HB3	10:D:167:SER:HB3	1.90	0.53
15:M:1739:LEU:HD23	15:M:1863:ARG:HG2	1.88	0.53
15:M:2160:GLN:O	16:N:214:LYS:NZ	2.30	0.53
11:E:333:SER:OG	11:E:336:ASP:OD2	2.26	0.53
12:F:570:ILE:HG21	12:F:578:ILE:HD11	1.89	0.53
15:M:2068:THR:O	15:M:2072:ILE:HG12	2.08	0.53
1:2:434:TYR:HB2	1:2:447:PHE:CE1	2.44	0.53
3:4:769:GLU:OE2	3:4:772:ARG:NH2	2.37	0.53
4:5:446:ALA:HB2	4:5:489:ASP:HA	1.89	0.53
6:7:251:VAL:HG13	6:7:340:VAL:HG11	1.90	0.53
7:A:28:ASN:OD1	7:A:29:LEU:N	2.42	0.53
12:F:545:LEU:HD11	12:F:554:ILE:HB	1.90	0.53
1:2:573:ALA:HB2	1:2:616:ASP:HA	1.89	0.53
4:5:136:GLN:NE2	4:5:279:ASP:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:28:VAL:HG22	11:E:57:GLN:HB3	1.90	0.53
12:F:743:TRP:HE1	12:F:762:ILE:HG22	1.73	0.53
12:G:672:ALA:HB2	12:G:760:LYS:HE3	1.91	0.53
3:4:315:ARG:O	6:7:341:ARG:NH1	2.41	0.53
3:4:442:ILE:HG12	3:4:460:TYR:HE1	1.74	0.53
4:5:614:LEU:HD11	4:5:657:ILE:HG23	1.90	0.53
2:3:354:SER:HB3	2:3:717:LEU:HD12	1.91	0.53
3:4:394:LYS:NZ	5:6:435:SER:OG	2.40	0.53
3:4:437:GLY:HA2	3:4:464:VAL:HG22	1.88	0.53
8:B:182:ARG:NH1	10:D:294:ILE:O	2.34	0.53
15:M:1436:ARG:NH1	15:M:1670:TYR:OH	2.42	0.53
16:N:486:GLY:N	16:N:489:ASP:OD2	2.41	0.53
3:4:571:SER:HB3	3:4:574:LYS:HG3	1.91	0.53
4:5:561:ASN:HB3	4:5:564:ARG:HB3	1.91	0.53
7:A:75:THR:HG22	7:A:79:MET:HE1	1.91	0.53
11:E:123:LEU:HG	11:E:251:ILE:HG23	1.91	0.53
15:M:1724:SER:O	15:M:2066:LYS:NZ	2.38	0.53
11:E:90:ILE:O	11:E:133:ASN:ND2	2.42	0.53
12:F:605:VAL:HG13	12:H:881:LYS:HE2	1.91	0.53
12:G:910:LEU:HA	12:G:913:LYS:HE2	1.90	0.53
2:3:168:PRO:HD2	2:3:260:GLU:HB3	1.90	0.53
2:3:351:ASN:O	2:3:354:SER:OG	2.27	0.53
8:B:146:GLN:NE2	8:B:150:GLU:OE2	2.34	0.53
12:H:703:THR:HA	12:H:722:LEU:O	2.09	0.53
15:M:1318:ALA:HA	15:M:1447:PHE:HD1	1.74	0.53
15:M:1359:MET:HE2	15:M:1424:LEU:H	1.73	0.53
1:2:707:HIS:HB3	1:2:710:ASN:HB2	1.90	0.52
3:4:781:GLY:HA3	3:4:792:THR:HG21	1.91	0.52
3:4:790:ARG:HD2	3:4:842:THR:HG23	1.91	0.52
7:A:170:ASP:HB2	7:A:185:LYS:HB2	1.91	0.52
11:E:32:SER:HB3	11:E:86:PHE:HD1	1.73	0.52
11:E:259:LEU:O	11:E:263:GLY:N	2.41	0.52
12:H:570:ILE:HG21	12:H:578:ILE:HD11	1.92	0.52
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.91	0.52
3:4:694:LEU:HD11	3:4:698:LEU:HD23	1.90	0.52
5:6:539:GLY:O	5:6:544:LYS:NZ	2.41	0.52
5:6:596:VAL:HG22	5:6:631:ALA:HB2	1.91	0.52
8:B:22:ASN:ND2	10:D:64:MET:HE1	2.23	0.52
8:B:166:SER:HB3	10:D:263:LEU:HD22	1.92	0.52
15:M:2118:ASP:OD1	15:M:2119:PHE:N	2.42	0.52
16:N:549:ARG:HG2	16:N:552:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:342:MET:HE1	3:4:360:ILE:HG13	1.91	0.52
5:6:311:CYS:SG	5:6:316:ALA:N	2.81	0.52
7:A:12:GLU:OE2	7:A:33:HIS:NE2	2.43	0.52
8:B:193:ARG:HD2	10:D:225:ASN:HB3	1.91	0.52
12:G:548:GLN:HB2	12:G:552:GLY:HA2	1.92	0.52
1:2:353:GLN:HG3	1:2:355:SER:H	1.75	0.52
5:6:275:ARG:H	5:6:278:ASP:HB2	1.74	0.52
5:6:365:ALA:HA	5:6:368:ILE:HD12	1.92	0.52
11:E:554:GLU:HB2	11:E:587:ARG:HH21	1.72	0.52
12:F:634:HIS:NE2	12:H:636:LEU:HB2	2.24	0.52
3:4:845:ILE:HD13	3:4:851:GLN:HB2	1.92	0.52
6:7:409:ASP:OD1	6:7:409:ASP:N	2.42	0.52
7:A:65:ASP:O	7:A:69:LYS:HB3	2.09	0.52
12:F:621:GLN:HB2	12:F:689:PHE:CD2	2.44	0.52
15:M:1483:ASP:OD1	15:M:1503:LYS:NZ	2.43	0.52
6:7:141:VAL:HA	6:7:144:ASN:HD21	1.73	0.52
11:E:506:ILE:HD12	11:E:548:LEU:HB2	1.91	0.52
15:M:1486:TYR:HB3	15:M:1502:PHE:HB3	1.92	0.52
16:N:183:TYR:HA	16:N:189:GLN:HA	1.90	0.52
4:5:393:MET:HA	4:5:393:MET:HE3	1.90	0.52
12:H:478:PRO:HB2	12:H:536:LEU:HD21	1.91	0.52
16:N:394:LEU:O	16:N:678:SER:OG	2.26	0.52
1:2:738:LEU:N	1:2:742:GLN:HE21	2.08	0.52
3:4:311:CYS:HB3	3:4:329:LYS:HD2	1.91	0.52
6:7:397:VAL:HG12	6:7:400:ARG:HH12	1.74	0.52
1:2:355:SER:HB3	1:2:383:ARG:HH21	1.75	0.52
6:7:679:PHE:H	6:7:728:TYR:HE2	1.58	0.52
7:A:192:ARG:NH2	11:E:22:HIS:O	2.42	0.52
12:F:886:ALA:HA	12:F:889:LEU:HD23	1.92	0.52
15:M:1532:TYR:HD2	15:M:1640:LEU:HD12	1.75	0.52
1:2:459:ARG:NH2	1:2:466:GLU:OE2	2.41	0.52
2:3:356:LYS:HB2	2:3:359:ILE:HB	1.92	0.52
4:5:768:GLN:HG2	16:N:292:PHE:HA	1.92	0.52
5:6:382:ARG:O	5:6:385:SER:OG	2.27	0.52
6:7:284:CYS:SG	6:7:286:SER:OG	2.67	0.52
12:H:738:THR:O	12:H:741:HIS:NE2	2.43	0.52
15:M:1570:TYR:O	15:M:1574:SER:N	2.38	0.52
15:M:1825:ALA:HB3	15:M:1828:PHE:HB2	1.91	0.52
15:M:1888:ALA:O	15:M:1891:THR:OG1	2.28	0.52
3:4:522:LEU:O	3:4:526:ILE:HG12	2.10	0.51
6:7:282:SER:HA	6:7:298:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:397:ASP:OD1	11:E:397:ASP:N	2.43	0.51
12:G:476:TYR:OH	12:G:630:TYR:O	2.24	0.51
12:H:746:ALA:O	12:H:752:LEU:HA	2.09	0.51
16:N:530:THR:HG22	16:N:541:ILE:HB	1.92	0.51
1:2:782:ASP:HB3	15:M:2086:ARG:HG2	1.92	0.51
6:7:494:THR:OG1	6:7:495:ALA:N	2.43	0.51
7:A:11:LEU:O	7:A:14:LYS:HG3	2.09	0.51
15:M:1726:VAL:HG22	15:M:1910:ILE:HG23	1.92	0.51
15:M:2076:ARG:NH2	15:M:2087:GLU:O	2.43	0.51
1:2:488:SER:HB3	1:2:825:LEU:HD12	1.92	0.51
1:2:553:LEU:HB3	1:2:565:PHE:HE2	1.76	0.51
6:7:263:ASP:HB3	6:7:299:PHE:CE2	2.46	0.51
11:E:466:LEU:O	11:E:470:ARG:HG2	2.10	0.51
12:G:711:ARG:HH21	12:G:839:ASP:HA	1.75	0.51
12:G:902:SER:HA	12:G:910:LEU:HD23	1.92	0.51
12:H:504:THR:HG22	12:H:513:ILE:HD12	1.92	0.51
15:M:1563:PHE:HD1	15:M:1568:LYS:HG2	1.76	0.51
2:3:263:GLU:HA	4:5:514:ASN:OD1	2.11	0.51
5:6:136:TYR:O	5:6:140:ILE:HG13	2.10	0.51
5:6:773:LEU:HB2	5:6:824:ILE:HD13	1.93	0.51
11:E:247:VAL:HB	11:E:284:TYR:CE2	2.46	0.51
4:5:407:ARG:HB2	4:5:500:GLN:NE2	2.25	0.51
7:A:164:ASP:HB2	7:A:188:GLN:HE21	1.74	0.51
12:H:494:LEU:HB3	12:H:537:CYS:HB3	1.93	0.51
1:2:424:VAL:HB	1:2:456:ILE:HD11	1.93	0.51
6:7:520:ILE:HG12	6:7:562:SER:HB2	1.93	0.51
15:M:1450:LYS:HB3	15:M:1454:ALA:HB3	1.93	0.51
15:M:1858:ILE:HD12	15:M:1866:ILE:HD11	1.91	0.51
15:M:2221:THR:OG1	16:N:204:ILE:O	2.23	0.51
1:2:408:VAL:HG22	1:2:451:ILE:HB	1.92	0.51
3:4:590:TYR:HA	3:4:630:CYS:HB2	1.93	0.51
6:7:459:MET:SD	6:7:460:GLY:N	2.83	0.51
11:E:34:LEU:HB3	11:E:543:LEU:HG	1.92	0.51
1:2:785:LYS:HE2	1:2:838:ILE:HD13	1.92	0.51
15:M:1322:TRP:HB3	15:M:1338:VAL:HG13	1.92	0.51
15:M:1815:SER:O	15:M:1819:TRP:CB	2.59	0.51
2:3:261:MET:HB3	2:3:263:GLU:CD	2.36	0.51
3:4:454:LYS:HE2	3:4:456:LEU:HD23	1.93	0.51
5:6:612:VAL:HG12	5:6:623:ILE:HD13	1.92	0.51
10:D:171:LEU:HB3	10:D:180:ILE:HD11	1.91	0.51
12:F:638:TYR:N	12:F:655:CYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:883:LEU:HG	12:G:887:HIS:CE1	2.46	0.51
12:H:474:PHE:O	12:H:577:ARG:NH2	2.44	0.51
1:2:268:LEU:HD11	1:2:429:ILE:HD11	1.92	0.50
1:2:625:GLU:OE1	1:2:808:ARG:NE	2.44	0.50
9:C:132:ALA:HA	9:C:135:LEU:HG	1.93	0.50
12:H:819:VAL:HA	12:H:822:ALA:HB3	1.93	0.50
12:H:831:LYS:O	12:H:834:SER:OG	2.23	0.50
3:4:543:GLN:NE2	3:4:562:ILE:O	2.44	0.50
5:6:514:ASN:O	5:6:518:GLU:HG2	2.10	0.50
11:E:71:TYR:CE1	11:E:98:ILE:HD11	2.46	0.50
16:N:26:SER:HA	16:N:31:LEU:H	1.76	0.50
1:2:508:HIS:HB3	1:2:511:ILE:HD12	1.94	0.50
18:2:902:ADP:O2A	5:6:798:ARG:NH2	2.37	0.50
2:3:538:SER:O	2:3:541:SER:OG	2.29	0.50
3:4:808:HIS:ND1	3:4:821:ASP:OD1	2.43	0.50
5:6:118:PHE:HD1	5:6:161:ARG:HD3	1.77	0.50
5:6:276:ILE:HB	5:6:363:GLU:HG3	1.93	0.50
6:7:450:ILE:HG22	6:7:451:ARG:HG3	1.93	0.50
12:G:711:ARG:NE	12:G:839:ASP:OD1	2.39	0.50
12:G:831:LYS:O	12:G:834:SER:OG	2.27	0.50
15:M:2026:ILE:HG23	15:M:2027:LEU:HG	1.94	0.50
15:M:2068:THR:HB	15:M:2071:GLU:HG2	1.94	0.50
16:N:491:TRP:CE3	16:N:509:PRO:HG3	2.45	0.50
16:N:513:THR:HB	16:N:525:TRP:CZ2	2.46	0.50
2:3:570:ARG:O	4:5:613:ARG:NH1	2.44	0.50
7:A:55:LYS:O	7:A:59:GLN:HG2	2.11	0.50
11:E:507:PHE:O	11:E:511:VAL:HG13	2.12	0.50
11:E:550:ASN:O	11:E:587:ARG:NH2	2.44	0.50
12:F:631:SER:OG	12:F:634:HIS:ND1	2.28	0.50
12:G:711:ARG:HH22	12:G:843:ASN:HB2	1.76	0.50
12:G:782:VAL:HG22	12:H:571:PRO:HG3	1.93	0.50
3:4:848:ASN:ND2	3:4:850:VAL:O	2.44	0.50
5:6:151:ILE:HG22	5:6:153:ILE:HG13	1.93	0.50
5:6:600:GLY:HA2	5:6:644:MET:HE2	1.93	0.50
12:H:778:MET:HG2	12:H:780:VAL:HG23	1.94	0.50
2:3:404:ASN:HA	2:3:512:VAL:O	2.12	0.50
3:4:192:THR:O	3:4:196:ASN:ND2	2.45	0.50
3:4:896:ASP:OD1	3:4:896:ASP:N	2.45	0.50
6:7:459:MET:HE2	6:7:584:ILE:HD11	1.94	0.50
6:7:484:THR:OG1	6:7:486:LYS:O	2.30	0.50
16:N:181:PHE:HD1	16:N:189:GLN:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:315:ILE:O	4:5:175:ARG:NH1	2.44	0.50
2:3:406:LEU:O	2:3:546:LEU:HA	2.11	0.50
4:5:759:GLU:O	4:5:773:SER:OG	2.29	0.50
6:7:521:CYS:HB2	6:7:561:THR:HG21	1.92	0.50
12:G:639:SER:HA	12:G:652:LYS:O	2.11	0.50
12:H:484:THR:HG23	12:H:763:TRP:HB2	1.93	0.50
15:M:1357:ILE:HB	15:M:1404:GLU:HB2	1.94	0.50
15:M:1801:GLU:HB3	15:M:1806:ASN:HD22	1.76	0.50
15:M:2001:ASN:HA	15:M:2068:THR:HG22	1.93	0.50
1:2:344:CYS:SG	1:2:366:ASN:HB3	2.52	0.50
8:B:1:MET:HE2	10:D:149:SER:HA	1.93	0.50
12:F:707:LEU:HB3	12:F:710:TRP:HB3	1.92	0.50
5:6:312:ASP:OD1	5:6:340:ASN:ND2	2.39	0.50
12:F:491:ARG:HD2	12:F:766:PHE:CZ	2.47	0.50
12:F:910:LEU:O	12:F:914:ILE:HG12	2.11	0.50
12:G:534:TYR:CG	12:G:546:PHE:HB3	2.47	0.50
12:G:708:SER:HA	12:G:836:LEU:HD21	1.93	0.50
15:M:1354:PRO:HB3	15:M:1407:PHE:CD1	2.47	0.50
16:N:12:ILE:HG21	16:N:52:ASN:HB3	1.93	0.50
1:2:222:THR:HG23	1:2:224:ARG:HG2	1.95	0.49
6:7:89:GLN:HE22	6:7:103:VAL:HG22	1.77	0.49
8:B:21:GLU:OE1	10:D:135:ARG:NH1	2.36	0.49
8:B:34:ARG:HH11	12:F:848:TYR:HB3	1.76	0.49
10:D:199:LEU:O	10:D:207:GLN:NE2	2.45	0.49
12:F:918:ARG:NE	12:F:922:TYR:OH	2.45	0.49
12:G:578:ILE:HD13	12:G:592:THR:HG22	1.94	0.49
12:H:489:THR:OG1	12:H:765:GLU:OE1	2.26	0.49
15:M:1360:LYS:HD3	15:M:1382:SER:HB2	1.93	0.49
15:M:2216:CYS:SG	16:N:491:TRP:NE1	2.84	0.49
16:N:178:GLN:HE22	16:N:531:ARG:HH11	1.59	0.49
5:6:296:ARG:O	5:6:360:ARG:N	2.38	0.49
6:7:538:HIS:O	6:7:541:MET:HG3	2.12	0.49
7:A:14:LYS:HB3	9:C:6:ILE:HG21	1.94	0.49
10:D:193:LEU:O	10:D:197:SER:HB2	2.12	0.49
11:E:323:ASP:N	11:E:406:ARG:O	2.45	0.49
12:G:883:LEU:O	12:G:887:HIS:ND1	2.45	0.49
12:H:636:LEU:HB3	12:H:657:LEU:HD23	1.94	0.49
12:H:907:LEU:O	12:H:911:VAL:HG23	2.11	0.49
1:2:596:LEU:HD21	1:2:646:ILE:HD11	1.93	0.49
6:7:498:MET:HG2	6:7:550:LYS:HE2	1.93	0.49
6:7:685:THR:O	6:7:688:THR:OG1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:692:TYR:HE2	12:F:749:TYR:HB2	1.76	0.49
12:F:885:LEU:HD21	12:G:605:VAL:HG11	1.94	0.49
12:G:702:ASN:HB3	12:G:724:SER:HB3	1.94	0.49
3:4:203:TYR:HB3	3:4:221:ASP:HA	1.93	0.49
4:5:39:ARG:NH2	11:E:314:ASP:OD2	2.40	0.49
5:6:260:GLU:OE1	5:6:352:ARG:NH1	2.46	0.49
6:7:244:ILE:HB	6:7:348:ILE:HG12	1.94	0.49
11:E:125:ALA:HB3	11:E:247:VAL:HG13	1.93	0.49
11:E:525:TYR:HE2	11:E:527:LEU:HD12	1.78	0.49
12:G:576:GLU:HG3	12:G:594:LEU:HD23	1.95	0.49
15:M:1809:ALA:O	15:M:1813:VAL:HG13	2.13	0.49
2:3:430:ILE:HG13	2:3:465:ALA:HB2	1.93	0.49
5:6:360:ARG:HD2	5:6:377:LEU:O	2.12	0.49
6:7:140:ASP:O	6:7:144:ASN:ND2	2.45	0.49
5:6:568:ASP:OD2	5:6:659:GLN:NE2	2.46	0.49
7:A:13:ALA:HB1	7:A:92:LEU:HD13	1.93	0.49
9:C:161:ALA:HA	9:C:164:THR:HG22	1.95	0.49
12:G:518:PHE:HZ	12:G:768:LEU:HD11	1.76	0.49
16:N:308:ASP:HB3	16:N:340:HIS:HA	1.95	0.49
16:N:666:HIS:HB2	16:N:671:ARG:NE	2.23	0.49
8:B:30:ARG:HB2	8:B:84:LYS:C	2.38	0.49
10:D:277:MET:HA	10:D:277:MET:HE3	1.94	0.49
11:E:93:GLU:HA	11:E:98:ILE:HB	1.94	0.49
12:H:730:LYS:HA	12:H:734:GLY:HA2	1.95	0.49
15:M:1722:ASN:ND2	15:M:1912:MET:O	2.36	0.49
2:3:671:LEU:HB3	6:7:621:MET:CE	2.38	0.49
3:4:638:SER:O	3:4:642:ARG:HG3	2.13	0.49
5:6:155:TYR:CD2	5:6:271:PRO:HD3	2.48	0.49
6:7:460:GLY:HA3	6:7:466:LYS:HD3	1.95	0.49
6:7:540:VAL:O	6:7:544:GLN:N	2.39	0.49
12:G:587:ARG:HE	12:G:643:LEU:HB3	1.77	0.49
12:H:613:SER:HB3	12:H:629:HIS:HB3	1.95	0.49
15:M:2062:MET:HE1	15:M:2075:LEU:HD13	1.93	0.49
15:M:2175:MET:HB3	16:N:301:PRO:HA	1.93	0.49
16:N:432:LEU:HB3	16:N:481:MET:HG3	1.94	0.49
16:N:549:ARG:HG2	16:N:552:ARG:NH2	2.27	0.49
1:2:562:ARG:NH2	1:2:598:LEU:O	2.46	0.49
1:2:669:LEU:HB3	1:2:673:ILE:HG21	1.94	0.49
2:3:111:TRP:HZ2	9:C:90:THR:HG23	1.77	0.49
6:7:718:ARG:HG2	6:7:721:ARG:HH22	1.77	0.49
12:H:503:SER:OG	12:H:514:THR:OG1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:2056:LYS:HB3	15:M:2094:PHE:HD1	1.78	0.49
1:2:629:ILE:O	1:2:640:LEU:N	2.40	0.49
6:7:700:ALA:HA	6:7:707:MET:HE3	1.95	0.49
8:B:104:TYR:OH	8:B:111:ARG:NH1	2.46	0.49
9:C:142:LEU:HD21	9:C:185:LYS:HA	1.94	0.49
12:G:624:ARG:HA	12:G:642:GLU:HA	1.95	0.49
15:M:1357:ILE:HD12	15:M:1427:PHE:HE1	1.78	0.49
15:M:1838:ASN:O	15:M:1842:LYS:HG2	2.12	0.49
3:4:396:VAL:HA	3:4:417:LEU:O	2.12	0.48
3:4:726:ASN:HA	3:4:729:LEU:HD12	1.94	0.48
4:5:46:TYR:HE1	4:5:63:VAL:HA	1.77	0.48
4:5:286:VAL:HG11	4:5:292:VAL:HG11	1.94	0.48
7:A:12:GLU:O	7:A:16:THR:HG23	2.13	0.48
12:G:698:PHE:CG	12:G:744:PRO:HG3	2.49	0.48
16:N:65:GLN:HB3	16:N:84:VAL:HG13	1.94	0.48
16:N:209:PRO:HB2	16:N:624:TRP:CE3	2.48	0.48
1:2:485:ARG:NH2	1:2:769:TYR:OH	2.42	0.48
2:3:314:LEU:HD22	4:5:277:THR:HG21	1.95	0.48
2:3:455:ARG:HH22	13:I:51:DT:H1'	1.78	0.48
2:3:723:LYS:HG2	2:3:727:LYS:HE2	1.94	0.48
3:4:400:GLN:HE21	3:4:412:PRO:HG2	1.77	0.48
3:4:846:ASP:N	3:4:846:ASP:OD1	2.46	0.48
5:6:794:ARG:NH2	5:6:835:ILE:HG22	2.28	0.48
6:7:366:LEU:HD22	14:J:15:DC:H2''	1.95	0.48
12:H:560:ASP:OD1	12:H:560:ASP:N	2.46	0.48
15:M:1694:PRO:HD2	16:N:442:PRO:HD2	1.95	0.48
5:6:532:SER:HB2	5:6:745:PRO:HG2	1.94	0.48
6:7:93:PHE:HA	6:7:97:THR:HA	1.94	0.48
12:F:895:LEU:HD21	12:F:918:ARG:HA	1.95	0.48
15:M:1892:ASN:HB3	15:M:1894:MET:SD	2.54	0.48
1:2:376:ASN:O	1:2:380:THR:OG1	2.30	0.48
6:7:224:PRO:HA	6:7:240:THR:HG23	1.95	0.48
6:7:546:ILE:O	6:7:556:THR:OG1	2.19	0.48
8:B:113:SER:OG	8:B:152:ARG:NH1	2.46	0.48
12:G:685:LYS:HE3	12:G:743:TRP:CE3	2.49	0.48
16:N:179:GLN:HB3	16:N:191:ILE:HD11	1.95	0.48
16:N:214:LYS:HD2	16:N:624:TRP:CE2	2.49	0.48
16:N:228:ARG:NH1	16:N:608:ASP:O	2.46	0.48
16:N:503:LEU:HB3	16:N:504:PRO:HD3	1.96	0.48
1:2:342:LEU:HD12	1:2:372:PRO:HB2	1.94	0.48
1:2:604:CYS:HB3	1:2:646:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:137:ARG:O	5:6:141:GLU:HG2	2.13	0.48
6:7:679:PHE:O	6:7:728:TYR:OH	2.31	0.48
12:G:573:GLN:OE1	12:G:596:TYR:OH	2.24	0.48
15:M:1339:PHE:HE2	15:M:1586:LEU:HD11	1.78	0.48
15:M:2058:LEU:O	15:M:2062:MET:HG2	2.13	0.48
1:2:813:ILE:HG12	1:2:841:VAL:HG21	1.96	0.48
2:3:367:LEU:HD11	2:3:382:LEU:HB2	1.96	0.48
6:7:273:VAL:HG21	6:7:278:PHE:HB3	1.95	0.48
10:D:204:GLU:HA	10:D:207:GLN:HB2	1.95	0.48
12:F:637:SER:HA	12:F:656:PRO:HA	1.93	0.48
12:G:711:ARG:NH2	12:G:843:ASN:HB2	2.29	0.48
12:H:910:LEU:HD12	12:H:913:LYS:HE2	1.95	0.48
15:M:1485:GLY:N	15:M:1589:LEU:O	2.47	0.48
15:M:1486:TYR:HE2	15:M:1639:VAL:HA	1.78	0.48
1:2:438:LEU:HD22	1:2:448:ALA:HB2	1.95	0.48
3:4:568:GLY:O	3:4:677:PRO:HD3	2.14	0.48
4:5:149:ARG:NH2	4:5:270:MET:O	2.47	0.48
6:7:153:MET:HE1	6:7:267:TYR:OH	2.13	0.48
12:G:534:TYR:HA	12:G:548:GLN:HG3	1.95	0.48
12:H:524:ARG:NH2	12:H:559:HIS:O	2.46	0.48
15:M:1428:GLU:H	15:M:1699:GLY:CA	2.27	0.48
2:3:229:ALA:HB2	6:7:370:LEU:HD23	1.96	0.48
2:3:687:ARG:HG3	6:7:604:PRO:HB3	1.96	0.48
3:4:769:GLU:O	3:4:772:ARG:HG3	2.14	0.48
5:6:528:LYS:HG2	5:6:531:ARG:HH21	1.79	0.48
6:7:358:ALA:HB2	6:7:375:TYR:CD1	2.49	0.48
7:A:165:VAL:HB	7:A:205:LEU:HB3	1.95	0.48
10:D:260:ILE:O	10:D:264:LYS:N	2.46	0.48
12:F:743:TRP:NE1	12:F:762:ILE:HG22	2.29	0.48
12:F:782:VAL:HB	12:F:785:LYS:HG2	1.95	0.48
12:G:839:ASP:O	12:G:843:ASN:CB	2.60	0.48
12:H:886:ALA:HA	12:H:889:LEU:HD23	1.96	0.48
15:M:1636:VAL:HA	15:M:1639:VAL:HG22	1.95	0.48
3:4:712:VAL:HG23	6:7:668:ARG:HG2	1.96	0.48
3:4:798:LEU:O	3:4:801:MET:HG2	2.14	0.48
4:5:152:ASP:OD1	4:5:154:GLU:HG2	2.14	0.48
12:F:596:TYR:HE1	12:H:720:PRO:HG2	1.78	0.48
12:G:597:PHE:N	12:G:610:GLU:O	2.29	0.48
15:M:1341:THR:HA	15:M:1346:VAL:HG12	1.96	0.48
15:M:1418:PHE:HB2	15:M:1423:VAL:HG23	1.96	0.48
16:N:482:ILE:HA	16:N:524:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:542:PHE:HE2	16:N:546:LEU:HD11	1.79	0.48
1:2:687:VAL:N	5:6:790:ARG:O	2.46	0.48
1:2:792:ASP:O	1:2:796:GLU:HG2	2.14	0.48
2:3:444:ALA:HB1	2:3:457:LEU:HD22	1.96	0.48
2:3:688:ASN:ND2	6:7:606:ARG:HD2	2.29	0.48
3:4:701:ARG:O	3:4:796:ARG:NH2	2.47	0.48
11:E:340:TYR:HB3	11:E:503:GLN:HG2	1.96	0.48
12:G:721:ILE:HA	12:G:778:MET:HE1	1.94	0.48
15:M:1690:ASN:HB2	15:M:1697:ASP:HB2	1.96	0.48
1:2:215:LEU:O	1:2:227:TYR:HB2	2.14	0.47
1:2:564:VAL:HB	1:2:599:ALA:HB2	1.96	0.47
3:4:397:ILE:HB	3:4:417:LEU:HD12	1.96	0.47
12:G:503:SER:OG	12:G:514:THR:OG1	2.20	0.47
12:H:775:GLU:OE2	12:H:777:ARG:NH2	2.47	0.47
15:M:1536:PHE:HA	15:M:1539:LYS:HB3	1.96	0.47
15:M:1596:PHE:HD2	15:M:1598:THR:HG22	1.77	0.47
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.96	0.47
5:6:513:ILE:HG22	5:6:517:LYS:HE2	1.96	0.47
5:6:663:ILE:O	5:6:669:HIS:HA	2.14	0.47
15:M:2062:MET:HE2	15:M:2072:ILE:HG23	1.96	0.47
8:B:126:LEU:HB3	8:B:134:PHE:HZ	1.79	0.47
11:E:296:GLN:HG2	11:E:300:LYS:HZ2	1.80	0.47
12:G:501:TYR:CE1	12:G:516:SER:HB2	2.49	0.47
15:M:1604:ILE:HG22	15:M:1608:ASN:ND2	2.30	0.47
16:N:506:ASP:N	16:N:506:ASP:OD1	2.47	0.47
5:6:752:ARG:HG2	5:6:756:LYS:HE3	1.96	0.47
12:F:768:LEU:HD12	12:F:769:PRO:HD2	1.96	0.47
12:H:711:ARG:NH2	12:H:839:ASP:O	2.48	0.47
2:3:485:ALA:O	2:3:489:VAL:HG23	2.15	0.47
5:6:656:MET:HE3	5:6:656:MET:HB2	1.84	0.47
5:6:771:SER:O	5:6:775:GLU:HG2	2.15	0.47
7:A:48:ARG:HD3	10:D:203:PRO:HD3	1.96	0.47
9:C:36:ARG:HG2	9:C:37:PRO:HD2	1.97	0.47
9:C:121:ALA:HA	9:C:124:VAL:HG12	1.95	0.47
12:H:780:VAL:HB	12:H:825:GLU:HG2	1.96	0.47
15:M:2077:LYS:HB2	15:M:2087:GLU:HG3	1.96	0.47
15:M:2174:TYR:CZ	16:N:616:LEU:HD22	2.50	0.47
16:N:298:LEU:HD13	16:N:307:ILE:HG21	1.97	0.47
16:N:433:ILE:HG21	16:N:541:ILE:HD13	1.97	0.47
3:4:369:ALA:O	5:6:441:ARG:NH2	2.44	0.47
10:D:211:ASP:H	10:D:218:MET:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:573:ASP:O	11:E:577:ASP:N	2.48	0.47
12:F:621:GLN:HB3	12:F:624:ARG:HG2	1.97	0.47
12:H:478:PRO:HA	12:H:579:THR:HA	1.96	0.47
12:H:543:GLY:HA2	12:H:558:PRO:HA	1.97	0.47
12:H:705:LEU:HB3	12:H:718:TRP:CE3	2.49	0.47
15:M:1361:PHE:H	15:M:1377:GLU:H	1.63	0.47
15:M:2037:ILE:HG13	15:M:2047:VAL:HB	1.96	0.47
3:4:397:ILE:HB	3:4:417:LEU:HB2	1.96	0.47
3:4:418:CYS:HB3	3:4:420:TYR:CE1	2.49	0.47
3:4:758:ILE:HG21	3:4:810:LYS:HA	1.97	0.47
3:4:857:ILE:O	3:4:861:LEU:HD23	2.15	0.47
6:7:149:ARG:HA	6:7:152:ARG:HD3	1.96	0.47
6:7:353:GLY:HA3	6:7:378:ALA:HA	1.96	0.47
11:E:345:ASN:HA	11:E:350:LEU:HG	1.96	0.47
12:F:595:GLY:HA2	12:F:614:PRO:HA	1.95	0.47
12:H:661:LEU:HD12	12:H:682:MET:HA	1.95	0.47
12:H:698:PHE:HD1	12:H:704:LEU:HD23	1.78	0.47
15:M:1794:MET:HE3	15:M:1798:TRP:NE1	2.30	0.47
3:4:304:ARG:HB3	3:4:465:HIS:HB2	1.95	0.47
4:5:432:VAL:HA	4:5:596:ILE:HG23	1.97	0.47
5:6:136:TYR:HE1	5:6:153:ILE:HA	1.79	0.47
5:6:536:ALA:HA	5:6:742:ILE:HD11	1.94	0.47
5:6:776:LYS:HD3	5:6:776:LYS:HA	1.59	0.47
6:7:418:ILE:HD12	6:7:476:ILE:HD12	1.96	0.47
8:B:31:ILE:HD11	8:B:84:LYS:HB3	1.96	0.47
11:E:98:ILE:HD12	11:E:103:TYR:CE2	2.50	0.47
11:E:328:LEU:O	11:E:332:SER:OG	2.21	0.47
11:E:381:ASP:N	11:E:381:ASP:OD1	2.47	0.47
12:H:750:ASP:OD1	12:H:776:ILE:HG12	2.14	0.47
16:N:647:ALA:O	16:N:660:ASN:ND2	2.47	0.47
4:5:97:VAL:O	4:5:101:ILE:HG12	2.14	0.47
4:5:574:ASN:HB3	4:5:583:MET:HE1	1.97	0.47
11:E:98:ILE:HD12	11:E:103:TYR:HE2	1.80	0.47
11:E:350:LEU:HA	11:E:355:GLY:HA3	1.97	0.47
16:N:23:ARG:HA	16:N:27:ARG:HD2	1.97	0.47
16:N:469:LEU:HD21	16:N:476:THR:HG21	1.96	0.47
1:2:538:ASN:HA	1:2:646:ILE:O	2.15	0.47
2:3:409:GLY:HA3	2:3:549:VAL:HB	1.96	0.47
2:3:507:ASN:ND2	6:7:319:SER:OG	2.27	0.47
4:5:545:THR:O	4:5:548:SER:OG	2.32	0.47
4:5:571:HIS:O	4:5:575:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:629:ILE:HG22	4:5:648:ILE:HG21	1.97	0.47
5:6:395:CYS:HA	5:6:461:SER:HA	1.97	0.47
5:6:702:THR:HG23	5:6:704:PRO:HD2	1.97	0.47
6:7:690:LEU:HG	6:7:694:ARG:HH21	1.79	0.47
12:F:592:THR:HG22	12:F:594:LEU:H	1.79	0.47
12:H:665:ASN:ND2	12:H:677:TYR:OH	2.48	0.47
15:M:1354:PRO:HB3	15:M:1407:PHE:HD1	1.80	0.47
2:3:559:ARG:HB2	16:N:276:GLY:HA3	1.96	0.46
5:6:197:LEU:HA	5:6:260:GLU:HA	1.98	0.46
11:E:75:ASP:O	11:E:118:ARG:NH2	2.47	0.46
11:E:157:GLU:O	11:E:161:LYS:HG2	2.16	0.46
12:F:652:LYS:HD3	12:F:652:LYS:HA	1.67	0.46
12:G:592:THR:HG1	12:G:596:TYR:H	1.61	0.46
4:5:436:ALA:HA	4:5:476:VAL:O	2.15	0.46
6:7:86:LEU:HD13	6:7:103:VAL:HG21	1.96	0.46
8:B:26:LYS:HA	8:B:69:THR:O	2.15	0.46
10:D:202:MET:SD	10:D:203:PRO:HD2	2.55	0.46
11:E:519:ILE:HG22	11:E:528:CYS:HB2	1.97	0.46
12:F:614:PRO:HD2	12:F:631:SER:HB3	1.96	0.46
12:F:776:ILE:HG13	12:F:829:ARG:HD2	1.97	0.46
16:N:443:VAL:O	16:N:494:MET:HA	2.14	0.46
1:2:808:ARG:NH2	20:5:802:AGS:O3A	2.48	0.46
3:4:809:ALA:HB2	3:4:817:VAL:HA	1.97	0.46
3:4:891:ASN:ND2	3:4:898:VAL:O	2.47	0.46
5:6:730:HIS:NE2	5:6:734:LEU:HD11	2.30	0.46
6:7:498:MET:HG2	6:7:550:LYS:HG3	1.97	0.46
6:7:672:LYS:O	6:7:672:LYS:HD3	2.16	0.46
12:G:526:TYR:HE2	12:G:557:ARG:HH21	1.64	0.46
15:M:1960:ILE:HG22	15:M:1964:MET:CE	2.44	0.46
16:N:88:ILE:HA	16:N:91:MET:HG3	1.98	0.46
4:5:684:PHE:CE2	4:5:689:MET:HE3	2.50	0.46
6:7:420:PRO:HB2	6:7:625:GLN:HG2	1.97	0.46
10:D:76:LEU:HD21	10:D:175:LEU:HD21	1.97	0.46
11:E:529:VAL:HG22	11:E:570:ALA:HB3	1.96	0.46
16:N:184:ASN:N	16:N:188:MET:O	2.47	0.46
2:3:412:SER:HB3	4:5:651:ARG:NH1	2.30	0.46
3:4:306:TYR:HB3	3:4:465:HIS:CD2	2.51	0.46
3:4:308:VAL:HG12	3:4:327:ASN:HB2	1.98	0.46
3:4:525:SER:HB3	3:4:743:PRO:HD2	1.97	0.46
4:5:414:LEU:HD23	4:5:554:PHE:HB2	1.96	0.46
5:6:583:GLN:N	20:6:1103:AGS:O2A	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:13:ALA:HB2	7:A:89:TYR:HD1	1.81	0.46
8:B:90:PRO:HB2	8:B:92:TRP:CD1	2.50	0.46
11:E:617:ASP:N	11:E:617:ASP:OD1	2.49	0.46
12:F:556:TYR:HB3	12:F:566:TRP:CE2	2.50	0.46
15:M:1362:LYS:HB2	15:M:1422:ASN:HB2	1.98	0.46
2:3:186:VAL:O	2:3:289:GLY:N	2.36	0.46
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.47	0.46
3:4:775:VAL:HG11	5:6:725:THR:HG22	1.97	0.46
11:E:1:MET:N	11:E:135:PHE:HE1	2.13	0.46
11:E:282:ILE:H	11:E:282:ILE:HD12	1.80	0.46
12:G:490:ASP:HA	12:G:506:LYS:HE2	1.96	0.46
1:2:259:PHE:C	1:2:267:MET:HE1	2.40	0.46
1:2:600:ASP:OD2	1:2:643:ARG:NH2	2.36	0.46
3:4:561:ASP:OD1	3:4:562:ILE:N	2.45	0.46
4:5:421:ALA:N	20:5:802:AGS:O2B	2.48	0.46
5:6:533:ILE:HG13	5:6:548:LEU:HB2	1.96	0.46
7:A:76:LEU:HA	7:A:79:MET:HE2	1.97	0.46
16:N:453:SER:O	16:N:456:THR:N	2.49	0.46
2:3:415:LYS:NZ	18:3:1001:ADP:O3B	2.25	0.46
2:3:417:GLN:HG3	18:3:1001:ADP:H3'	1.97	0.46
3:4:604:TYR:O	3:4:617:GLU:HG3	2.16	0.46
5:6:149:ASN:HB2	5:6:263:PHE:HA	1.96	0.46
6:7:18:PHE:HE1	6:7:120:ALA:HB2	1.81	0.46
6:7:146:ARG:HD3	6:7:192:PHE:CE1	2.51	0.46
8:B:34:ARG:NH2	8:B:62:ASN:HB3	2.31	0.46
12:F:489:THR:HG23	12:F:491:ARG:H	1.81	0.46
12:F:711:ARG:HH21	12:F:843:ASN:HB3	1.79	0.46
12:G:486:PHE:CG	12:G:492:ARG:HD3	2.51	0.46
12:H:592:THR:HG23	12:H:594:LEU:H	1.80	0.46
1:2:446:VAL:HA	5:6:303:GLU:HA	1.96	0.46
1:2:506:TYR:HH	1:2:694:ARG:HE	1.63	0.46
1:2:685:ASP:OD1	5:6:781:ARG:NH2	2.48	0.46
2:3:223:THR:OG1	4:5:246:GLU:OE1	2.32	0.46
5:6:600:GLY:H	5:6:640:GLU:HB2	1.81	0.46
5:6:645:ASP:OD1	5:6:646:ILE:N	2.49	0.46
6:7:335:VAL:HG12	6:7:378:ALA:HB3	1.97	0.46
12:F:820:SER:HA	12:F:868:ARG:NH1	2.30	0.46
12:F:883:LEU:HD12	12:F:917:ILE:HD11	1.98	0.46
12:H:498:GLU:N	12:H:745:LEU:HD11	2.30	0.46
15:M:1359:MET:HE2	15:M:1424:LEU:N	2.30	0.46
2:3:673:GLN:HA	2:3:676:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:409:ASP:OD2	4:5:500:GLN:NE2	2.48	0.46
5:6:775:GLU:O	5:6:779:GLU:HG2	2.16	0.46
6:7:82:LEU:HD21	6:7:106:ILE:HD11	1.98	0.46
7:A:133:GLU:OE2	10:D:189:ILE:HG12	2.16	0.46
8:B:31:ILE:HG22	8:B:32:THR:H	1.81	0.46
9:C:51:ALA:HB1	9:C:74:LEU:HD21	1.98	0.46
10:D:70:GLU:OE2	10:D:150:LYS:HD2	2.15	0.46
10:D:262:ASP:OD2	10:D:278:ARG:NH1	2.49	0.46
12:H:480:SER:HG	12:H:495:THR:HG1	1.64	0.46
16:N:287:LEU:HA	16:N:325:MET:HA	1.97	0.46
1:2:578:ALA:HB1	1:2:591:LEU:HD11	1.98	0.45
4:5:53:ASN:HB3	4:5:58:ASN:O	2.16	0.45
4:5:261:ILE:HG23	4:5:291:ARG:HH21	1.80	0.45
11:E:32:SER:HB3	11:E:86:PHE:CD1	2.50	0.45
12:F:640:LEU:H	12:F:652:LYS:HB3	1.82	0.45
12:G:782:VAL:HB	12:G:785:LYS:HB2	1.97	0.45
15:M:1438:ILE:O	15:M:1442:GLY:N	2.46	0.45
15:M:1494:ILE:HD12	15:M:1496:TYR:HE1	1.81	0.45
15:M:1604:ILE:HG22	15:M:1608:ASN:HD22	1.81	0.45
15:M:1921:ALA:O	15:M:1934:THR:OG1	2.32	0.45
16:N:270:PRO:HG2	16:N:273:ASN:HB2	1.99	0.45
2:3:20:VAL:O	2:3:24:ARG:HD3	2.16	0.45
3:4:451:ARG:HB2	14:J:19:DC:OP1	2.16	0.45
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.81	0.45
4:5:760:THR:OG1	4:5:775:VAL:O	2.32	0.45
5:6:171:SER:O	5:6:286:SER:HB2	2.16	0.45
6:7:291:GLN:NE2	6:7:292:ASN:OD1	2.50	0.45
6:7:397:VAL:O	6:7:401:VAL:HG13	2.16	0.45
11:E:96:LEU:HB2	11:E:98:ILE:HG12	1.98	0.45
15:M:1319:ASN:H	15:M:1447:PHE:HB2	1.81	0.45
3:4:570:PRO:HD3	3:4:677:PRO:HD2	1.98	0.45
4:5:630:ARG:NH1	4:5:648:ILE:O	2.44	0.45
5:6:304:LEU:HD11	5:6:307:ALA:HA	1.98	0.45
5:6:832:ARG:HA	5:6:835:ILE:HG12	1.98	0.45
6:7:524:ASP:OD1	6:7:525:GLU:N	2.49	0.45
9:C:175:GLU:HG3	9:C:179:LYS:HE2	1.98	0.45
12:F:551:THR:H	12:F:572:LEU:HD22	1.81	0.45
12:F:581:VAL:HG12	12:F:590:VAL:HG23	1.98	0.45
12:G:696:CYS:SG	12:G:704:LEU:HD22	2.57	0.45
12:H:818:PRO:HG2	12:H:821:MET:HG3	1.98	0.45
15:M:2057:SER:O	15:M:2061:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:62:PHE:CE2	16:N:81:GLN:HA	2.52	0.45
3:4:340:PRO:HG3	5:6:452:ILE:HG13	1.97	0.45
3:4:762:ILE:HG23	5:6:736:MET:HE1	1.98	0.45
6:7:275:SER:OG	6:7:277:THR:O	2.28	0.45
7:A:55:LYS:HA	7:A:55:LYS:HD2	1.78	0.45
10:D:7:ASP:N	10:D:7:ASP:OD1	2.50	0.45
11:E:513:ILE:HD11	11:E:530:LEU:HD21	1.99	0.45
11:E:579:TYR:CG	11:E:637:LEU:HD22	2.50	0.45
12:G:642:GLU:HB3	12:G:649:ARG:HB2	1.99	0.45
3:4:712:VAL:HG11	6:7:672:LYS:HB2	1.99	0.45
4:5:594:ILE:HB	4:5:599:MET:HE3	1.99	0.45
5:6:557:LYS:NZ	5:6:808:GLU:OE2	2.48	0.45
5:6:795:ILE:HD12	5:6:799:GLN:HG2	1.99	0.45
6:7:617:THR:O	6:7:621:MET:HG2	2.16	0.45
8:B:17:GLN:HG3	8:B:125:ILE:HD11	1.98	0.45
11:E:312:THR:OG1	11:E:315:THR:HG23	2.17	0.45
12:F:698:PHE:HD2	12:F:704:LEU:HD23	1.82	0.45
12:H:500:GLY:HA3	12:H:517:PHE:HA	1.98	0.45
16:N:423:LYS:HE3	16:N:687:ILE:HG21	1.99	0.45
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.52	0.45
1:2:364:CYS:HB3	1:2:367:CYS:O	2.16	0.45
6:7:410:VAL:HG13	6:7:411:TYR:HD1	1.82	0.45
10:D:126:LEU:HD23	11:E:22:HIS:HE2	1.82	0.45
12:G:637:SER:C	12:G:657:LEU:HD23	2.41	0.45
12:G:697:ILE:HD13	12:G:718:TRP:HZ3	1.80	0.45
12:H:701:ASP:OD1	12:H:701:ASP:N	2.47	0.45
15:M:1487:LEU:HD23	15:M:1487:LEU:O	2.17	0.45
2:3:400:ARG:O	2:3:707:ARG:NH1	2.48	0.45
2:3:569:HIS:CE1	4:5:406:LEU:HD13	2.52	0.45
4:5:41:ASP:N	4:5:41:ASP:OD1	2.49	0.45
4:5:396:SER:HB2	4:5:611:ALA:HB1	1.99	0.45
5:6:293:THR:HG22	5:6:394:ARG:HB2	1.98	0.45
6:7:255:VAL:HG21	6:7:258:ILE:HG13	1.98	0.45
6:7:471:LYS:O	6:7:475:LYS:HG2	2.16	0.45
11:E:259:LEU:HD11	11:E:264:GLU:HB2	1.99	0.45
16:N:222:TYR:HA	16:N:325:MET:HE1	1.99	0.45
16:N:350:GLU:N	16:N:654:ASN:HD21	2.15	0.45
3:4:422:GLU:HG3	3:4:423:LEU:H	1.81	0.45
3:4:578:LEU:HD22	3:4:630:CYS:HB3	1.97	0.45
4:5:445:SER:OG	13:I:56:DT:OP1	2.32	0.45
5:6:816:VAL:HG22	5:6:818:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:82:LEU:HD12	6:7:206:PRO:HA	1.98	0.45
6:7:414:LEU:O	6:7:418:ILE:HG12	2.16	0.45
8:B:5:ALA:HA	8:B:8:GLN:HG2	1.98	0.45
10:D:5:ILE:HD11	12:F:868:ARG:HG2	1.98	0.45
12:F:490:ASP:HB3	12:F:506:LYS:HB2	1.99	0.45
12:G:541:GLU:HG3	12:G:542:LYS:HG3	1.98	0.45
12:G:626:PHE:CE1	12:G:638:TYR:HB2	2.51	0.45
15:M:1408:LEU:O	15:M:1411:LYS:NZ	2.38	0.45
2:3:88:SER:O	6:7:223:LYS:NZ	2.50	0.45
2:3:384:MET:SD	2:3:513:ILE:HB	2.57	0.45
3:4:512:VAL:HA	3:4:515:ARG:HD3	1.99	0.45
3:4:572:THR:OG1	6:7:687:ARG:NH1	2.50	0.45
4:5:473:ASP:HA	4:5:517:THR:HG22	1.98	0.45
4:5:646:ILE:HD13	4:5:692:ALA:HA	1.97	0.45
4:5:760:THR:HG23	4:5:761:ILE:HG23	1.99	0.45
5:6:545:LYS:NZ	5:6:826:GLU:OE2	2.39	0.45
7:A:141:LEU:HD21	10:D:182:TYR:HB2	1.99	0.45
12:F:657:LEU:HD12	12:F:659:MET:H	1.82	0.45
12:G:824:GLU:HB2	12:G:869:LEU:HD21	1.99	0.45
15:M:1600:LEU:O	15:M:1605:ARG:N	2.40	0.45
3:4:204:LYS:HE3	3:4:215:PHE:HB2	1.98	0.45
3:4:404:ASP:OD1	3:4:404:ASP:N	2.48	0.45
3:4:743:PRO:O	3:4:747:LEU:HD22	2.17	0.45
3:4:799:GLU:OE2	20:6:1103:AGS:O3'	2.32	0.45
4:5:400:LEU:HD12	4:5:404:MET:SD	2.56	0.45
4:5:422:LYS:HE2	4:5:422:LYS:HB2	1.78	0.45
15:M:1329:ASP:N	15:M:1329:ASP:OD1	2.50	0.45
15:M:1815:SER:O	15:M:1819:TRP:HB3	2.17	0.45
1:2:353:GLN:HA	1:2:359:ILE:HD11	1.99	0.44
3:4:445:ARG:NH2	3:4:450:GLN:O	2.50	0.44
4:5:300:ILE:HG23	4:5:324:ARG:HB3	1.99	0.44
6:7:653:SER:HB3	6:7:656:VAL:HG23	1.99	0.44
6:7:671:SER:HB3	6:7:683:GLN:HA	1.98	0.44
12:F:513:ILE:HB	12:F:528:PHE:CE1	2.52	0.44
12:F:582:ALA:HB2	12:F:618:LEU:HB3	1.99	0.44
12:G:482:ALA:HB3	12:G:496:MET:H	1.82	0.44
12:G:554:ILE:N	12:G:568:LYS:O	2.45	0.44
12:H:477:MET:HE2	12:H:678:ASN:O	2.17	0.44
1:2:525:LYS:HB2	1:2:533:ILE:HB	1.99	0.44
2:3:462:MET:HE3	2:3:486:ILE:HG22	1.99	0.44
3:4:527:ALA:HB3	3:4:537:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.98	0.44
12:F:662:PRO:HG3	12:F:700:SER:HB2	1.98	0.44
12:G:704:LEU:HD23	12:G:704:LEU:HA	1.84	0.44
3:4:592:SER:O	3:4:596:SER:N	2.49	0.44
3:4:729:LEU:O	3:4:732:LYS:NZ	2.46	0.44
7:A:16:THR:HG22	7:A:30:PRO:HG2	1.99	0.44
7:A:89:TYR:CZ	7:A:93:ARG:HD2	2.53	0.44
8:B:34:ARG:HH21	8:B:62:ASN:HB3	1.82	0.44
11:E:256:TYR:OH	11:E:298:GLU:OE1	2.30	0.44
11:E:285:ALA:HB2	11:E:590:ARG:HH21	1.82	0.44
12:H:723:ASP:OD1	12:H:723:ASP:N	2.50	0.44
15:M:2205:ALA:HB1	15:M:2214:LEU:HG	2.00	0.44
1:2:608:GLU:HB3	1:2:611:LYS:HD2	1.99	0.44
3:4:334:ARG:NH2	3:4:398:LYS:HE3	2.32	0.44
4:5:633:LEU:HD22	4:5:648:ILE:HB	1.99	0.44
4:5:666:LEU:HD12	4:5:667:GLU:HG3	1.99	0.44
9:C:36:ARG:HD3	9:C:37:PRO:O	2.18	0.44
12:F:522:ARG:HH21	12:F:523:PHE:HZ	1.66	0.44
12:G:714:GLU:HG3	12:H:650:TYR:HB2	1.98	0.44
12:G:739:ASP:OD1	12:G:739:ASP:N	2.48	0.44
16:N:665:ILE:HD13	16:N:670:ALA:HA	2.00	0.44
1:2:300:PHE:HB3	1:2:319:ARG:HB2	1.99	0.44
3:4:317:LEU:HD23	3:4:317:LEU:HA	1.88	0.44
3:4:408:ASP:OD1	3:4:408:ASP:N	2.49	0.44
3:4:775:VAL:O	3:4:779:LYS:HG2	2.17	0.44
5:6:373:MET:SD	5:6:374:PRO:HD2	2.57	0.44
6:7:504:ASP:OD1	6:7:505:GLU:N	2.50	0.44
11:E:546:LEU:HD21	11:E:629:ILE:HD11	1.99	0.44
11:E:572:ILE:HB	11:E:579:TYR:CE1	2.53	0.44
12:F:478:PRO:HD3	12:F:577:ARG:HD3	1.98	0.44
12:F:726:MET:HE2	12:F:781:PHE:HB3	2.00	0.44
12:H:916:ASN:O	12:H:919:GLU:HG2	2.18	0.44
2:3:118:PRO:HD2	2:3:177:ASN:O	2.17	0.44
3:4:567:CYS:SG	3:4:568:GLY:N	2.91	0.44
3:4:732:LYS:HD3	6:7:651:VAL:HG23	1.99	0.44
4:5:765:HIS:CE1	15:M:1707:LEU:HB3	2.53	0.44
5:6:732:VAL:HG12	5:6:736:MET:HE3	2.00	0.44
7:A:70:CYS:HB3	9:C:24:ILE:HD11	1.99	0.44
7:A:160:ASP:OD1	7:A:160:ASP:N	2.50	0.44
11:E:589:PRO:HD2	11:E:592:LEU:HD22	2.00	0.44
12:G:690:SER:N	12:G:694:ASP:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:727:GLU:HA	12:G:730:LYS:HG2	1.99	0.44
16:N:52:ASN:O	16:N:52:ASN:ND2	2.51	0.44
16:N:650:ASP:OD1	16:N:657:LYS:HE3	2.18	0.44
1:2:547:THR:OG1	18:2:902:ADP:O1B	2.35	0.44
1:2:562:ARG:HB2	1:2:602:GLY:HA3	2.00	0.44
1:2:817:ALA:HB1	1:2:829:VAL:HG11	2.00	0.44
2:3:121:PHE:C	2:3:124:PRO:HD2	2.43	0.44
6:7:485:GLY:N	6:7:524:ASP:O	2.51	0.44
9:C:24:ILE:HG21	9:C:27:LEU:HD12	1.99	0.44
10:D:285:LEU:HD22	10:D:290:LYS:HD2	2.00	0.44
11:E:335:TYR:HA	11:E:363:PHE:CZ	2.53	0.44
12:H:909:SER:HA	12:H:912:LYS:HG2	1.99	0.44
15:M:1374:CYS:HA	15:M:1404:GLU:H	1.83	0.44
15:M:2049:ASN:HB3	15:M:2052:LEU:HB3	1.99	0.44
16:N:44:PHE:CE1	16:N:85:LYS:HD2	2.53	0.44
2:3:244:GLU:OE1	6:7:14:TYR:OH	2.34	0.44
3:4:269:ILE:HD11	3:4:305:PRO:HG3	1.99	0.44
3:4:848:ASN:HD21	3:4:850:VAL:HB	1.83	0.44
3:4:912:GLN:HB3	5:6:697:GLY:HA2	2.00	0.44
4:5:365:LYS:O	4:5:369:ILE:HG12	2.18	0.44
5:6:706:MET:HA	5:6:709:PHE:HD2	1.83	0.44
6:7:78:VAL:HG11	6:7:121:ILE:HD11	1.99	0.44
6:7:539:GLU:O	6:7:543:GLN:CB	2.66	0.44
7:A:20:TYR:HA	7:A:25:GLN:HE22	1.83	0.44
11:E:40:CYS:O	11:E:44:MET:HG3	2.18	0.44
12:F:685:LYS:HD2	12:F:698:PHE:CE1	2.52	0.44
12:G:874:CYS:HB3	12:G:905:ALA:HB1	1.98	0.44
15:M:2124:PRO:HA	15:M:2127:ILE:HG12	1.98	0.44
15:M:2148:GLN:HA	16:N:494:MET:HE1	2.00	0.44
16:N:81:GLN:HG2	16:N:85:LYS:NZ	2.32	0.44
16:N:493:SER:HA	16:N:496:SER:OG	2.18	0.44
16:N:528:ASN:HB3	16:N:529:PRO:HD3	1.98	0.44
16:N:548:GLY:H	16:N:645:THR:HG21	1.83	0.44
2:3:442:LEU:O	2:3:461:ALA:N	2.51	0.44
3:4:193:ASN:HA	3:4:196:ASN:HD21	1.82	0.44
3:4:410:GLN:OE1	3:4:410:GLN:N	2.51	0.44
4:5:417:ASP:O	4:5:422:LYS:NZ	2.49	0.44
6:7:204:PHE:H	6:7:379:GLN:HB3	1.82	0.44
7:A:28:ASN:ND2	7:A:119:ASP:O	2.50	0.44
8:B:121:VAL:HG12	9:C:190:TRP:CH2	2.53	0.44
11:E:64:TYR:HB3	11:E:95:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:507:ASN:OD1	12:G:510:GLN:NE2	2.51	0.44
15:M:1380:SER:OG	15:M:1381:ALA:N	2.51	0.44
15:M:2106:PHE:N	15:M:2115:SER:O	2.49	0.44
3:4:333:LEU:HG	3:4:400:GLN:HB2	2.00	0.43
3:4:425:ASP:OD2	5:6:375:ARG:NH1	2.51	0.43
3:4:856:VAL:HA	3:4:859:ARG:HE	1.83	0.43
4:5:455:ARG:NH2	13:I:52:DT:O2	2.45	0.43
5:6:443:LEU:HD11	5:6:448:LEU:HB2	2.00	0.43
6:7:398:GLU:OE1	6:7:402:MET:HE1	2.16	0.43
8:B:54:THR:HG23	10:D:132:GLU:OE2	2.18	0.43
2:3:193:ARG:HD3	2:3:193:ARG:HA	1.85	0.43
3:4:245:ALA:HB1	3:4:258:TYR:HE1	1.83	0.43
3:4:758:ILE:HD12	3:4:815:ASN:HB3	2.00	0.43
4:5:605:TYR:O	4:5:609:LYS:HB2	2.18	0.43
4:5:652:GLN:O	4:5:656:ILE:HG13	2.18	0.43
6:7:508:LEU:HD11	6:7:557:LEU:HD11	2.00	0.43
6:7:534:ARG:NH1	6:7:586:LEU:HD13	2.32	0.43
6:7:600:MET:O	6:7:600:MET:HG2	2.18	0.43
8:B:60:LEU:HD11	8:B:75:ILE:HD13	1.98	0.43
12:F:621:GLN:HB2	12:F:689:PHE:HD2	1.83	0.43
15:M:1500:SER:HB3	15:M:1511:ILE:HG12	2.00	0.43
15:M:1572:ARG:O	15:M:1575:GLN:HG3	2.17	0.43
16:N:282:PHE:HB2	16:N:339:PHE:CE1	2.53	0.43
16:N:458:PHE:CD2	16:N:490:LEU:HD23	2.53	0.43
2:3:435:ARG:HD2	2:3:435:ARG:HA	1.77	0.43
3:4:754:ALA:O	3:4:758:ILE:HB	2.18	0.43
4:5:300:ILE:HD13	4:5:326:PRO:HA	1.99	0.43
4:5:671:ILE:HG23	4:5:673:GLN:OE1	2.17	0.43
5:6:557:LYS:HB2	5:6:565:LEU:HD12	2.00	0.43
7:A:107:LEU:HD12	7:A:201:GLN:HG2	2.00	0.43
11:E:526:ARG:HG3	11:E:565:LEU:HD23	2.00	0.43
12:F:598:ARG:HA	12:F:609:VAL:HA	2.00	0.43
12:F:818:PRO:HG2	12:F:821:MET:SD	2.59	0.43
15:M:1511:ILE:HD13	15:M:1635:LEU:HD13	2.01	0.43
1:2:339:PHE:CD2	1:2:373:PHE:HB3	2.53	0.43
2:3:287:LYS:HG2	2:3:290:ASP:OD2	2.19	0.43
2:3:410:ASP:O	2:3:415:LYS:NZ	2.51	0.43
2:3:554:ASN:HB3	2:3:557:ARG:HB3	2.01	0.43
4:5:136:GLN:HG3	4:5:280:ARG:HH21	1.83	0.43
6:7:263:ASP:OD1	6:7:263:ASP:N	2.48	0.43
6:7:514:VAL:HG12	6:7:559:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:517:ASP:OD1	6:7:560:ARG:HG2	2.18	0.43
6:7:642:ILE:O	6:7:701:LYS:NZ	2.51	0.43
11:E:636:ASP:C	11:E:639:PRO:HD2	2.43	0.43
12:F:605:VAL:HG11	12:H:885:LEU:HD21	2.00	0.43
12:F:900:LYS:HA	12:F:903:GLU:HG2	2.00	0.43
12:H:497:ASN:C	12:H:745:LEU:HD11	2.44	0.43
12:H:627:SER:OG	12:H:639:SER:HB2	2.18	0.43
15:M:1376:ILE:C	15:M:1378:LYS:H	2.27	0.43
15:M:1486:TYR:CE1	15:M:1488:LEU:HB3	2.52	0.43
15:M:1701:ILE:HA	16:N:552:ARG:HH11	1.84	0.43
2:3:94:HIS:ND1	2:3:151:HIS:HB2	2.33	0.43
2:3:706:ILE:HG21	6:7:620:HIS:CE1	2.53	0.43
3:4:269:ILE:HA	3:4:272:MET:HB2	1.99	0.43
4:5:551:ASP:O	4:5:552:MET:HE2	2.17	0.43
5:6:105:ASP:OD2	5:6:108:GLY:N	2.51	0.43
5:6:309:PHE:N	5:6:318:VAL:O	2.49	0.43
10:D:91:ILE:HG23	10:D:133:LEU:HD11	2.01	0.43
10:D:202:MET:HE2	10:D:206:LEU:HB2	2.00	0.43
10:D:249:ASN:HB2	10:D:255:CYS:SG	2.58	0.43
12:F:638:TYR:N	12:F:657:LEU:HD23	2.32	0.43
12:F:639:SER:HB3	12:F:654:GLU:H	1.82	0.43
12:G:518:PHE:CZ	12:G:768:LEU:HD11	2.53	0.43
15:M:1503:LYS:HD3	15:M:1580:LEU:HD12	2.00	0.43
15:M:1731:VAL:CG2	15:M:1906:TRP:HB2	2.46	0.43
15:M:1851:PHE:HB3	15:M:1858:ILE:HD11	1.99	0.43
16:N:416:ALA:HB2	16:N:689:ILE:HD13	2.00	0.43
16:N:648:GLN:HG3	16:N:661:PRO:HA	1.99	0.43
1:2:356:ASN:OD1	1:2:433:ASN:ND2	2.51	0.43
3:4:233:MET:O	3:4:237:GLY:N	2.47	0.43
3:4:316:GLU:N	3:4:316:GLU:OE1	2.52	0.43
4:5:605:TYR:CZ	4:5:609:LYS:HG3	2.54	0.43
6:7:398:GLU:CD	6:7:402:MET:HE1	2.43	0.43
6:7:538:HIS:HA	6:7:541:MET:HG3	2.00	0.43
7:A:178:TYR:O	16:N:18:ARG:NE	2.51	0.43
12:F:682:MET:HG3	12:F:684:ILE:HG12	2.00	0.43
12:G:743:TRP:CE3	12:G:764:PRO:HD3	2.54	0.43
12:H:642:GLU:N	12:H:649:ARG:O	2.52	0.43
15:M:1667:SER:O	15:M:1671:ILE:HG12	2.19	0.43
16:N:273:ASN:O	16:N:277:ARG:NH1	2.51	0.43
16:N:613:SER:O	16:N:613:SER:OG	2.31	0.43
1:2:364:CYS:HB2	1:2:373:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:490:MET:HE1	2:3:539:LEU:O	2.18	0.43
6:7:284:CYS:SG	6:7:289:CYS:HB2	2.58	0.43
10:D:8:ILE:HG21	12:F:901:ILE:HD11	2.00	0.43
12:F:755:ILE:HG23	12:F:769:PRO:HB2	2.01	0.43
12:G:486:PHE:CD1	12:G:492:ARG:HD3	2.54	0.43
12:G:669:LYS:HD3	12:G:669:LYS:HA	1.83	0.43
12:H:843:ASN:C	12:H:843:ASN:HD22	2.26	0.43
15:M:1374:CYS:SG	15:M:1404:GLU:HG3	2.59	0.43
16:N:222:TYR:OH	16:N:300:ASP:OD2	2.24	0.43
1:2:211:LEU:HD13	1:2:271:PHE:CD1	2.54	0.43
5:6:311:CYS:HB2	5:6:340:ASN:ND2	2.33	0.43
6:7:531:GLU:HA	6:7:534:ARG:HB2	2.00	0.43
9:C:112:ILE:HG21	9:C:121:ALA:HB2	2.00	0.43
10:D:194:VAL:HG22	10:D:199:LEU:HG	2.01	0.43
12:F:491:ARG:HB3	12:F:766:PHE:CE2	2.53	0.43
12:F:750:ASP:OD1	12:F:776:ILE:HG12	2.19	0.43
12:G:642:GLU:HB2	12:G:651:TYR:HE2	1.84	0.43
12:G:731:MET:SD	12:G:732:SER:N	2.91	0.43
12:G:741:HIS:HB3	12:G:762:ILE:HG23	2.01	0.43
12:H:704:LEU:HD12	12:H:721:ILE:HB	2.00	0.43
15:M:1509:ILE:HD13	15:M:1556:ILE:HG23	2.01	0.43
15:M:2175:MET:SD	16:N:219:LEU:HD23	2.59	0.43
16:N:607:LEU:HD23	16:N:607:LEU:HA	1.87	0.43
3:4:353:ASP:HB2	5:6:102:LYS:HG3	2.01	0.43
3:4:808:HIS:O	3:4:814:LYS:NZ	2.52	0.43
3:4:901:SER:O	3:4:904:GLN:NE2	2.37	0.43
5:6:551:MET:HE1	5:6:593:PRO:HD2	2.01	0.43
6:7:255:VAL:HA	6:7:307:PHE:HD1	1.84	0.43
6:7:344:SER:N	6:7:347:ASP:OD2	2.43	0.43
6:7:366:LEU:HB3	14:J:15:DC:C6	2.54	0.43
11:E:82:LEU:HD23	11:E:121:TYR:HB2	2.01	0.43
12:F:690:SER:HA	12:F:747:LEU:O	2.18	0.43
15:M:2220:LEU:HB3	16:N:207:PHE:CE1	2.54	0.43
16:N:271:ILE:HA	16:N:274:LEU:HG	2.00	0.43
16:N:490:LEU:HB3	16:N:491:TRP:CE3	2.49	0.43
16:N:675:TYR:HD1	16:N:682:THR:HG22	1.83	0.43
3:4:433:ILE:HG22	3:4:468:LYS:HA	2.01	0.43
4:5:178:TYR:HB3	4:5:249:LYS:HB2	1.99	0.43
10:D:69:ASN:HA	10:D:293:LEU:HD12	2.01	0.43
12:F:636:LEU:O	12:F:657:LEU:HG	2.18	0.43
12:G:485:PRO:HB3	12:G:679:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:592:THR:OG1	12:G:596:TYR:N	2.42	0.43
12:H:498:GLU:HA	12:H:745:LEU:HD21	2.01	0.43
12:H:868:ARG:NH1	12:H:872:SER:HB2	2.34	0.43
12:H:892:ASP:O	12:H:896:THR:HG23	2.18	0.43
15:M:1322:TRP:HE1	15:M:1659:PRO:HG3	1.84	0.43
15:M:1747:SER:OG	15:M:1792:ARG:NH2	2.50	0.43
1:2:311:GLU:HB3	5:6:302:PRO:HB3	2.01	0.42
2:3:462:MET:HG3	2:3:470:VAL:HG21	2.00	0.42
3:4:602:THR:HG23	3:4:604:TYR:HD1	1.84	0.42
3:4:613:GLN:HG3	5:6:360:ARG:NH2	2.33	0.42
3:4:851:GLN:O	3:4:855:SER:N	2.42	0.42
4:5:714:PHE:O	4:5:717:GLU:HG3	2.18	0.42
5:6:516:LEU:HD11	5:6:757:TYR:CD2	2.54	0.42
8:B:31:ILE:HD11	8:B:84:LYS:HD3	2.00	0.42
11:E:519:ILE:HG13	11:E:519:ILE:O	2.18	0.42
12:F:757:VAL:HG11	12:F:762:ILE:O	2.19	0.42
12:H:883:LEU:HB2	12:H:913:LYS:NZ	2.34	0.42
16:N:94:ARG:HB3	16:N:164:LEU:HD11	2.01	0.42
16:N:405:ASN:OD1	16:N:437:SER:OG	2.30	0.42
1:2:337:VAL:HG23	1:2:351:PHE:HD2	1.84	0.42
1:2:790:TYR:CD1	1:2:810:LEU:HB2	2.53	0.42
3:4:368:PRO:HG2	3:4:382:MET:HE3	2.01	0.42
3:4:696:PRO:N	3:4:697:PRO:HD2	2.34	0.42
5:6:522:ASP:OD2	5:6:528:LYS:NZ	2.38	0.42
5:6:643:LYS:HD3	5:6:643:LYS:HA	1.92	0.42
11:E:545:LEU:HD12	11:E:545:LEU:HA	1.85	0.42
11:E:556:CYS:O	11:E:559:SER:OG	2.32	0.42
12:H:553:GLN:HG2	12:H:569:ILE:HD12	2.00	0.42
12:H:901:ILE:HD12	12:H:904:ARG:HH21	1.82	0.42
15:M:1419:ASN:OD1	15:M:1425:GLY:HA2	2.19	0.42
16:N:638:THR:O	16:N:639:MET:HE2	2.18	0.42
3:4:259:HIS:HB3	6:7:135:LYS:HD2	2.01	0.42
3:4:349:CYS:SG	3:4:371:CYS:HB2	2.58	0.42
3:4:770:LEU:HD22	3:4:801:MET:HG3	2.00	0.42
5:6:340:ASN:OD1	5:6:343:PHE:HB2	2.19	0.42
6:7:396:ASP:OD1	6:7:396:ASP:N	2.52	0.42
8:B:33:THR:HG21	8:B:50:TRP:HH2	1.84	0.42
9:C:5:ASP:HB2	9:C:8:ASP:HB3	2.00	0.42
10:D:159:ARG:HH22	10:D:184:ASP:HA	1.84	0.42
12:F:725:ASN:OD1	12:F:726:MET:N	2.51	0.42
12:H:556:TYR:CE2	12:H:558:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:591:GLY:HA2	12:H:596:TYR:O	2.18	0.42
12:H:897:ALA:O	12:H:901:ILE:HG12	2.19	0.42
15:M:1960:ILE:HG12	15:M:2007:PHE:CZ	2.54	0.42
16:N:398:LYS:HE3	16:N:429:PRO:HB3	1.99	0.42
1:2:707:HIS:ND1	1:2:708:PRO:HD2	2.34	0.42
1:2:785:LYS:HB2	15:M:2088:PHE:HB2	2.00	0.42
4:5:642:GLU:OE2	4:5:643:ARG:N	2.53	0.42
5:6:652:ILE:O	5:6:656:MET:HG2	2.20	0.42
6:7:103:VAL:HG23	6:7:214:ARG:HH21	1.84	0.42
6:7:130:LYS:O	6:7:132:ILE:HD12	2.19	0.42
6:7:288:GLU:O	6:7:291:GLN:HG3	2.20	0.42
8:B:93:LEU:HD23	8:B:93:LEU:HA	1.92	0.42
11:E:34:LEU:HA	11:E:543:LEU:HD11	2.01	0.42
12:G:588:VAL:HG13	12:G:600:PHE:HB2	2.01	0.42
15:M:1606:LEU:HA	15:M:1609:GLN:OE1	2.19	0.42
15:M:1655:TYR:OH	15:M:1801:GLU:OE1	2.31	0.42
16:N:283:LEU:HD12	16:N:328:VAL:O	2.19	0.42
1:2:629:ILE:HB	1:2:640:LEU:HB2	2.01	0.42
1:2:634:ALA:HB2	13:I:56:DT:H5'	2.01	0.42
5:6:319:ASP:OD1	5:6:320:ASN:N	2.48	0.42
6:7:353:GLY:HA2	6:7:379:GLN:HG2	2.01	0.42
6:7:474:CYS:SG	6:7:475:LYS:NZ	2.93	0.42
9:C:162:THR:O	9:C:166:LEU:HG	2.19	0.42
12:F:843:ASN:C	12:F:843:ASN:HD22	2.27	0.42
12:H:600:PHE:CD1	12:H:606:PRO:HA	2.54	0.42
15:M:1431:ILE:HG21	15:M:1690:ASN:HA	2.01	0.42
15:M:1549:LEU:HB2	15:M:1646:ILE:HD12	2.02	0.42
16:N:41:LEU:HA	16:N:41:LEU:HD23	1.86	0.42
1:2:196:GLU:O	1:2:199:THR:OG1	2.35	0.42
1:2:393:ALA:O	1:2:397:VAL:HG23	2.20	0.42
1:2:520:PHE:CE1	1:2:823:MET:HA	2.54	0.42
1:2:686:LEU:HA	5:6:791:SER:HA	2.01	0.42
2:3:274:ILE:HG13	2:3:275:ASP:N	2.34	0.42
2:3:366:SER:HA	2:3:650:LEU:HD22	2.00	0.42
4:5:98:ALA:O	4:5:102:SER:HB3	2.20	0.42
4:5:148:LEU:HD22	4:5:260:GLU:HB3	2.02	0.42
4:5:494:HIS:CD2	4:5:546:ILE:HD13	2.54	0.42
6:7:398:GLU:O	6:7:401:VAL:HG22	2.20	0.42
11:E:127:ARG:O	11:E:129:TRP:N	2.49	0.42
11:E:328:LEU:HD13	11:E:496:ILE:HG23	2.01	0.42
11:E:588:TYR:CE2	11:E:597:THR:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:484:THR:HG22	12:G:764:PRO:HD2	2.02	0.42
12:G:642:GLU:N	12:G:649:ARG:O	2.51	0.42
12:G:723:ASP:OD1	12:G:723:ASP:N	2.49	0.42
12:G:826:GLU:CD	12:G:829:ARG:HH21	2.27	0.42
12:G:907:LEU:HB3	12:G:910:LEU:HB2	2.01	0.42
12:G:910:LEU:HD12	12:G:913:LYS:CE	2.49	0.42
12:H:621:GLN:N	12:H:624:ARG:O	2.50	0.42
15:M:1503:LYS:HA	15:M:1503:LYS:HD2	1.79	0.42
16:N:61:LYS:HA	16:N:64:GLU:HG2	2.01	0.42
1:2:505:ILE:HG23	18:2:902:ADP:C6	2.55	0.42
2:3:274:ILE:HG13	2:3:275:ASP:H	1.85	0.42
2:3:375:ASP:O	2:3:379:LYS:HG3	2.19	0.42
3:4:725:THR:HG21	6:7:661:VAL:HB	2.01	0.42
4:5:564:ARG:O	4:5:568:ILE:HG13	2.20	0.42
6:7:66:MET:O	6:7:70:VAL:HG23	2.20	0.42
6:7:264:GLN:O	6:7:265:CYS:HB3	2.20	0.42
7:A:17:LYS:HD3	9:C:6:ILE:HD12	2.01	0.42
7:A:184:ILE:O	7:A:187:SER:OG	2.35	0.42
11:E:362:MET:HG3	11:E:399:TYR:CE1	2.55	0.42
11:E:378:LEU:O	11:E:385:LYS:NZ	2.51	0.42
12:F:480:SER:OG	12:F:494:LEU:O	2.25	0.42
12:F:887:HIS:O	12:F:921:ARG:NH2	2.53	0.42
12:G:763:TRP:CD1	12:G:765:GLU:HB2	2.54	0.42
12:G:883:LEU:HB2	12:G:913:LYS:HD2	2.02	0.42
16:N:70:TRP:HD1	16:N:72:GLN:NE2	2.14	0.42
3:4:581:VAL:O	3:4:585:THR:HG22	2.19	0.42
3:4:631:ILE:HG21	3:4:634:PHE:HD1	1.85	0.42
3:4:865:LEU:HD11	3:4:903:ILE:HG23	2.02	0.42
5:6:113:GLU:O	5:6:116:GLU:HB2	2.20	0.42
5:6:122:PHE:CZ	5:6:157:HIS:HB3	2.55	0.42
5:6:309:PHE:CZ	5:6:346:LEU:HD12	2.55	0.42
5:6:555:VAL:N	5:6:808:GLU:OE1	2.46	0.42
12:G:689:PHE:CE2	12:G:695:PRO:HG3	2.55	0.42
12:G:910:LEU:O	12:G:914:ILE:HG12	2.20	0.42
12:H:538:PHE:CE1	12:H:619:THR:HG23	2.54	0.42
12:H:697:ILE:HG22	12:H:705:LEU:HD13	2.02	0.42
15:M:1940:GLN:HE22	15:M:1944:PHE:HE1	1.65	0.42
16:N:172:VAL:HG23	16:N:532:ILE:HG12	2.01	0.42
16:N:286:GLY:C	16:N:325:MET:HG3	2.45	0.42
1:2:339:PHE:HA	1:2:375:VAL:HA	2.02	0.42
3:4:365:ILE:N	5:6:438:THR:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:725:THR:HA	3:4:728:TYR:HD2	1.85	0.42
6:7:589:ALA:O	6:7:593:ARG:HG3	2.19	0.42
11:E:642:GLU:O	11:E:645:THR:OG1	2.30	0.42
12:F:506:LYS:HG2	12:F:511:TYR:CE1	2.55	0.42
12:F:659:MET:HE1	12:F:701:ASP:OD1	2.20	0.42
15:M:1322:TRP:CD1	15:M:1325:LEU:HD13	2.55	0.42
15:M:1532:TYR:CD2	15:M:1640:LEU:HD12	2.54	0.42
1:2:527:VAL:HB	1:2:531:HIS:HB3	2.02	0.42
3:4:521:LEU:HD11	3:4:743:PRO:HD3	2.02	0.42
3:4:692:ILE:HD12	3:4:692:ILE:HA	1.93	0.42
3:4:881:MET:N	3:4:881:MET:SD	2.92	0.42
5:6:508:LEU:HD23	5:6:513:ILE:HD13	2.01	0.42
5:6:528:LYS:HG2	5:6:531:ARG:NH2	2.35	0.42
5:6:690:ASN:O	5:6:698:ASN:ND2	2.49	0.42
6:7:531:GLU:HA	6:7:534:ARG:HD2	2.01	0.42
9:C:174:LYS:O	9:C:178:LYS:HG2	2.19	0.42
11:E:324:TYR:HD1	11:E:405:ILE:HA	1.85	0.42
12:G:502:VAL:HG23	12:G:539:LEU:HD11	2.00	0.42
12:H:600:PHE:HD1	12:H:606:PRO:HA	1.85	0.42
15:M:1721:ILE:O	15:M:1860:TYR:HA	2.19	0.42
16:N:82:SER:O	16:N:86:GLU:HG2	2.19	0.42
16:N:318:HIS:CD2	16:N:346:LEU:HD12	2.55	0.42
16:N:531:ARG:NH1	16:N:629:THR:O	2.35	0.42
1:2:631:ILE:O	1:2:637:VAL:HA	2.20	0.41
3:4:540:ILE:O	3:4:544:LEU:HD23	2.20	0.41
4:5:455:ARG:NH1	4:5:460:ARG:O	2.53	0.41
4:5:729:SER:HG	4:5:732:THR:HG23	1.84	0.41
5:6:321:VAL:HG11	5:6:330:PRO:HD3	2.02	0.41
5:6:323:GLN:NE2	5:6:328:THR:O	2.42	0.41
9:C:78:ASP:N	9:C:78:ASP:OD1	2.53	0.41
10:D:202:MET:HE3	10:D:203:PRO:HG2	2.02	0.41
10:D:203:PRO:HB2	10:D:205:GLU:OE1	2.20	0.41
12:G:689:PHE:HA	12:G:695:PRO:HA	2.02	0.41
12:G:698:PHE:CZ	12:G:702:ASN:HA	2.54	0.41
12:G:701:ASP:N	12:G:701:ASP:OD1	2.52	0.41
12:H:833:LEU:HB2	12:H:858:LEU:HD21	2.01	0.41
15:M:1322:TRP:CE2	15:M:1325:LEU:HD13	2.55	0.41
15:M:1485:GLY:O	15:M:1590:LEU:HD12	2.20	0.41
15:M:2178:HIS:ND1	15:M:2179:CYS:O	2.37	0.41
16:N:668:ARG:HD2	16:N:668:ARG:HA	1.91	0.41
1:2:820:PHE:O	1:2:824:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:294:VAL:HG21	5:6:389:ALA:HB1	2.02	0.41
7:A:104:ASN:HA	7:A:107:LEU:HB3	2.02	0.41
12:F:770:LEU:O	12:F:772:SER:N	2.52	0.41
12:H:707:LEU:HD13	12:H:717:LYS:O	2.20	0.41
15:M:1946:SER:O	15:M:1950:GLN:HG3	2.20	0.41
16:N:45:VAL:O	16:N:49:ILE:HG22	2.21	0.41
16:N:352:ARG:HH11	16:N:637:SER:H	1.68	0.41
2:3:676:ILE:HD11	6:7:621:MET:HE3	2.00	0.41
6:7:454:ILE:HD13	6:7:695:LEU:HD23	2.02	0.41
6:7:461:ASP:O	6:7:466:LYS:NZ	2.53	0.41
7:A:177:GLU:OE1	16:N:27:ARG:NH2	2.54	0.41
8:B:66:MET:HE2	8:B:66:MET:HA	2.01	0.41
10:D:253:LYS:HD2	10:D:253:LYS:HA	1.76	0.41
12:G:648:LYS:HE3	12:G:648:LYS:HB3	1.75	0.41
12:H:516:SER:OG	12:H:517:PHE:N	2.53	0.41
12:H:697:ILE:HD13	12:H:697:ILE:HA	1.93	0.41
15:M:2054:LEU:O	15:M:2058:LEU:HD23	2.20	0.41
1:2:242:LEU:HG	1:2:244:VAL:HG23	2.01	0.41
1:2:259:PHE:HB3	1:2:267:MET:HE1	2.02	0.41
2:3:95:ARG:NH1	2:3:324:ASN:O	2.53	0.41
3:4:348:LYS:HB3	3:4:385:ILE:HD11	2.02	0.41
3:4:455:SER:O	3:4:455:SER:OG	2.38	0.41
3:4:503:ASP:OD1	3:4:503:ASP:N	2.54	0.41
3:4:770:LEU:HD13	3:4:802:ILE:HG12	2.02	0.41
5:6:143:MET:HA	5:6:148:LEU:HD23	2.02	0.41
5:6:144:LYS:HB3	5:6:195:GLU:OE2	2.20	0.41
5:6:733:ASP:HA	5:6:736:MET:HG2	2.03	0.41
6:7:72:ASN:HA	6:7:132:ILE:HD11	2.02	0.41
8:B:108:HIS:O	8:B:155:LYS:NZ	2.46	0.41
10:D:70:GLU:HG3	10:D:146:CYS:SG	2.60	0.41
11:E:396:LEU:HA	11:E:396:LEU:HD23	1.86	0.41
12:F:491:ARG:HB3	12:F:766:PHE:CZ	2.56	0.41
12:H:480:SER:HB2	12:H:536:LEU:HD22	2.02	0.41
12:H:778:MET:HE1	12:H:829:ARG:HA	2.02	0.41
15:M:1575:GLN:HA	15:M:1578:THR:HG22	2.00	0.41
16:N:310:SER:HA	16:N:558:PRO:HG2	2.01	0.41
1:2:790:TYR:CZ	1:2:794:ARG:HD2	2.56	0.41
3:4:232:GLU:HA	3:4:235:GLU:HG2	2.02	0.41
3:4:331:LEU:HD21	3:4:430:GLY:HA2	2.02	0.41
5:6:119:LEU:HD23	5:6:119:LEU:HA	1.89	0.41
5:6:279:ILE:O	5:6:280:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:40:ILE:HD11	7:A:82:ASN:HB3	2.01	0.41
9:C:169:LEU:O	9:C:174:LYS:HE3	2.21	0.41
11:E:572:ILE:HB	11:E:579:TYR:CZ	2.55	0.41
12:F:707:LEU:HD21	12:F:718:TRP:CZ2	2.56	0.41
12:G:538:PHE:HE2	12:G:540:ASN:HD21	1.68	0.41
15:M:2164:CYS:SG	15:M:2165:SER:N	2.94	0.41
16:N:24:VAL:O	16:N:28:LYS:CB	2.68	0.41
16:N:636:PRO:HG2	16:N:639:MET:CE	2.49	0.41
1:2:244:VAL:O	1:2:297:ILE:HA	2.21	0.41
1:2:339:PHE:O	1:2:348:LEU:N	2.54	0.41
2:3:284:ASP:OD1	6:7:329:ARG:NH2	2.54	0.41
3:4:340:PRO:HB2	3:4:391:PHE:CD2	2.55	0.41
4:5:149:ARG:HG3	4:5:272:ARG:HE	1.85	0.41
4:5:346:VAL:HG22	4:5:347:THR:H	1.85	0.41
4:5:575:ILE:HD13	4:5:580:ALA:HB2	2.02	0.41
5:6:440:LEU:HB2	5:6:443:LEU:HB2	2.01	0.41
6:7:638:MET:O	6:7:642:ILE:HG22	2.20	0.41
8:B:82:GLN:N	8:B:82:GLN:OE1	2.54	0.41
11:E:362:MET:HG3	11:E:399:TYR:CD1	2.56	0.41
12:F:530:ASP:OD2	12:F:533:GLY:N	2.53	0.41
12:G:538:PHE:CG	12:G:582:ALA:HA	2.56	0.41
12:H:652:LYS:HD3	12:H:652:LYS:HA	1.96	0.41
12:H:702:ASN:HB3	12:H:724:SER:HB3	2.01	0.41
15:M:1321:THR:HG23	15:M:1444:SER:HB3	2.03	0.41
16:N:63:LEU:HD12	16:N:64:GLU:N	2.36	0.41
16:N:86:GLU:O	16:N:90:GLU:OE1	2.39	0.41
1:2:335:LYS:HB3	1:2:381:VAL:HG13	2.02	0.41
1:2:533:ILE:HG21	4:5:576:HIS:NE2	2.35	0.41
2:3:150:ARG:HG3	2:3:152:PRO:HD3	2.02	0.41
2:3:476:ASP:OD1	2:3:476:ASP:N	2.54	0.41
3:4:519:TYR:OH	3:4:538:LYS:HB3	2.21	0.41
3:4:856:VAL:O	3:4:859:ARG:HG2	2.21	0.41
4:5:66:GLU:OE2	11:E:379:TYR:OH	2.29	0.41
4:5:168:SER:HB3	4:5:257:LYS:HB3	2.01	0.41
4:5:485:MET:HB3	4:5:490:ARG:HB2	2.03	0.41
5:6:578:SER:OG	5:6:717:ASP:OD2	2.32	0.41
5:6:733:ASP:O	5:6:736:MET:HB2	2.21	0.41
6:7:102:LEU:HA	6:7:105:ALA:HB3	2.02	0.41
6:7:473:ILE:HD13	6:7:476:ILE:HD11	2.02	0.41
9:C:105:PHE:HB2	9:C:172:MET:CE	2.51	0.41
10:D:195:ASN:O	10:D:200:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:62:PHE:HE1	11:E:542:PRO:HG2	1.85	0.41
11:E:347:LYS:HA	11:E:347:LYS:HD2	1.83	0.41
12:F:563:HIS:ND1	12:H:880:GLU:OE1	2.40	0.41
12:F:685:LYS:HD2	12:F:698:PHE:HE1	1.85	0.41
12:G:540:ASN:OD1	12:G:583:ALA:HB3	2.21	0.41
12:H:747:LEU:HB2	12:H:752:LEU:HD12	2.03	0.41
15:M:1489:HIS:ND1	15:M:1599:LYS:HE3	2.36	0.41
15:M:1525:ALA:HA	15:M:1632:LEU:HD21	2.03	0.41
15:M:1730:VAL:O	15:M:1870:THR:OG1	2.33	0.41
16:N:178:GLN:HE22	16:N:531:ARG:NH1	2.19	0.41
16:N:326:VAL:HG12	16:N:346:LEU:HD23	2.01	0.41
2:3:194:PRO:HA	2:3:251:ILE:O	2.21	0.41
3:4:820:GLU:HA	3:4:823:GLN:NE2	2.36	0.41
5:6:134:LYS:HB2	5:6:137:ARG:HB3	2.02	0.41
5:6:536:ALA:CA	5:6:742:ILE:HD13	2.50	0.41
6:7:417:SER:O	6:7:420:PRO:HD3	2.21	0.41
12:G:818:PRO:HG2	12:G:821:MET:HG3	2.03	0.41
12:H:680:ASN:HA	12:H:681:PRO:HD3	1.93	0.41
12:H:830:SER:HA	12:H:858:LEU:HD11	2.02	0.41
16:N:381:LYS:O	16:N:385:ILE:HG12	2.21	0.41
16:N:416:ALA:O	16:N:420:ILE:HG12	2.20	0.41
1:2:206:THR:HG23	1:2:209:ARG:HH22	1.86	0.41
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.86	0.41
1:2:300:PHE:CD1	1:2:301:PRO:HD2	2.56	0.41
1:2:370:LYS:HD2	1:2:370:LYS:HA	1.78	0.41
1:2:383:ARG:HB2	1:2:412:ALA:HB2	2.02	0.41
1:2:600:ASP:OD1	1:2:643:ARG:N	2.42	0.41
1:2:793:LEU:HB3	1:2:805:ILE:HG21	2.03	0.41
2:3:343:THR:O	2:3:347:ILE:HG13	2.20	0.41
2:3:469:VAL:HA	2:3:511:SER:O	2.21	0.41
3:4:269:ILE:HA	3:4:269:ILE:HD13	1.92	0.41
3:4:512:VAL:HG21	3:4:746:PHE:HE2	1.85	0.41
3:4:625:ASP:OD1	3:4:625:ASP:N	2.54	0.41
3:4:732:LYS:HA	6:7:649:ARG:HH21	1.85	0.41
3:4:798:LEU:HA	3:4:801:MET:HG2	2.03	0.41
3:4:907:LEU:HD23	3:4:910:LEU:HD12	2.03	0.41
4:5:650:ILE:H	4:5:650:ILE:HD12	1.86	0.41
4:5:669:SER:OG	4:5:671:ILE:O	2.37	0.41
5:6:273:VAL:HG13	5:6:289:SER:O	2.21	0.41
5:6:303:GLU:HG2	5:6:356:TRP:HB2	2.03	0.41
5:6:580:SER:HB2	20:6:1103:AGS:C5	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:717:ASP:OD1	5:6:717:ASP:N	2.49	0.41
6:7:265:CYS:SG	6:7:288:GLU:HB3	2.61	0.41
8:B:101:LYS:HA	8:B:101:LYS:HD3	1.75	0.41
9:C:112:ILE:O	9:C:116:SER:N	2.52	0.41
10:D:83:LEU:O	10:D:87:LEU:HD23	2.21	0.41
11:E:30:PHE:HB3	11:E:86:PHE:HZ	1.86	0.41
11:E:596:HIS:CD2	11:E:596:HIS:H	2.39	0.41
12:G:624:ARG:NH1	12:G:693:GLY:HA3	2.36	0.41
12:G:662:PRO:HB3	12:G:665:ASN:HB2	2.03	0.41
15:M:1810:ASP:O	15:M:1813:VAL:HG22	2.21	0.41
15:M:2143:GLN:HE21	15:M:2210:PHE:HA	1.86	0.41
16:N:66:PHE:HE1	16:N:80:ASP:HB3	1.86	0.41
16:N:272:LYS:HB2	16:N:302:SER:HB2	2.01	0.41
16:N:277:ARG:N	16:N:277:ARG:HD2	2.36	0.41
16:N:409:ASP:OD2	16:N:439:THR:OG1	2.38	0.41
16:N:443:VAL:HG11	16:N:490:LEU:HD22	2.02	0.41
16:N:604:LYS:HE2	16:N:604:LYS:HB3	1.75	0.41
1:2:300:PHE:HD2	1:2:319:ARG:HB2	1.85	0.41
1:2:368:LYS:NZ	5:6:339:GLU:OE2	2.40	0.41
1:2:803:PHE:HD2	1:2:845:PHE:HD1	1.69	0.41
2:3:372:TYR:CD2	2:3:561:ILE:HG12	2.55	0.41
3:4:587:ARG:HB2	3:4:627:GLY:HA3	2.03	0.41
3:4:618:SER:HB2	3:4:622:VAL:HG13	2.03	0.41
6:7:228:ARG:NH2	6:7:326:HIS:HB3	2.35	0.41
6:7:442:LYS:H	6:7:649:ARG:HH12	1.68	0.41
6:7:667:LEU:HA	6:7:670:ASP:OD2	2.21	0.41
12:G:624:ARG:HB2	12:G:641:SER:O	2.21	0.41
12:H:538:PHE:HE1	12:H:619:THR:HG23	1.86	0.41
15:M:2080:LEU:HD12	15:M:2087:GLU:HA	2.03	0.41
16:N:503:LEU:HD11	16:N:542:PHE:CE1	2.56	0.41
3:4:204:LYS:N	3:4:221:ASP:O	2.51	0.40
3:4:564:ILE:HA	3:4:704:LEU:O	2.21	0.40
3:4:584:ILE:O	3:4:748:THR:OG1	2.29	0.40
4:5:42:SER:O	4:5:42:SER:OG	2.31	0.40
4:5:293:THR:OG1	4:5:334:GLN:HB2	2.20	0.40
4:5:721:ARG:HB3	15:M:1778:PHE:HE2	1.86	0.40
11:E:271:TRP:CE3	11:E:318:LEU:HD11	2.56	0.40
12:F:748:ALA:O	12:F:751:THR:OG1	2.39	0.40
15:M:1411:LYS:HB3	15:M:1411:LYS:HE3	1.85	0.40
15:M:1496:TYR:CZ	15:M:1631:LEU:HD13	2.56	0.40
15:M:1945:LEU:O	15:M:1950:GLN:NE2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:2051:LEU:HD12	15:M:2054:LEU:HD23	2.02	0.40
15:M:2155:GLU:O	15:M:2159:ILE:HG12	2.21	0.40
16:N:545:ASP:HA	16:N:643:ASP:CG	2.46	0.40
2:3:649:LYS:O	2:3:650:LEU:HD23	2.21	0.40
3:4:365:ILE:HB	5:6:439:GLY:C	2.47	0.40
3:4:625:ASP:HB3	3:4:667:ALA:O	2.21	0.40
4:5:728:THR:OG1	15:M:1778:PHE:O	2.32	0.40
5:6:366:ASN:OD1	5:6:367:GLU:HG2	2.22	0.40
6:7:75:LEU:HG	6:7:77:SER:H	1.85	0.40
6:7:608:ASP:HA	6:7:611:LYS:HE3	2.03	0.40
6:7:669:GLN:HG3	6:7:673:ARG:HH21	1.87	0.40
11:E:244:GLY:H	11:E:602:LEU:HD23	1.87	0.40
12:F:688:PHE:CZ	12:F:744:PRO:HB2	2.56	0.40
12:H:740:ILE:HG22	12:H:740:ILE:O	2.21	0.40
16:N:452:ILE:O	16:N:453:SER:C	2.65	0.40
3:4:367:GLU:HG3	5:6:441:ARG:HD2	2.03	0.40
3:4:590:TYR:OH	3:4:632:ASP:OD2	2.38	0.40
3:4:610:ASP:O	3:4:611:THR:OG1	2.34	0.40
4:5:407:ARG:O	4:5:658:ARG:HD3	2.21	0.40
4:5:497:MET:HE2	4:5:549:ARG:HB3	2.02	0.40
5:6:830:LEU:O	5:6:833:GLN:HG3	2.22	0.40
6:7:82:LEU:HB3	6:7:207:LEU:HG	2.02	0.40
6:7:527:ASP:HA	6:7:586:LEU:HD21	2.03	0.40
12:F:484:THR:HG22	12:F:485:PRO:O	2.21	0.40
12:F:490:ASP:HB3	12:F:506:LYS:H	1.86	0.40
12:F:661:LEU:HA	12:F:662:PRO:HD3	1.95	0.40
12:H:488:PHE:CD2	12:H:489:THR:HG23	2.55	0.40
15:M:2062:MET:HG3	15:M:2072:ILE:HG23	2.03	0.40
16:N:86:GLU:O	16:N:89:GLN:HB2	2.20	0.40
16:N:412:LYS:O	16:N:415:THR:OG1	2.32	0.40
16:N:507:PRO:HB3	16:N:525:TRP:O	2.21	0.40
1:2:227:TYR:HA	1:2:230:ARG:HB2	2.03	0.40
2:3:132:LEU:O	2:3:136:MET:HG3	2.20	0.40
2:3:235:ASP:OD1	2:3:236:THR:N	2.53	0.40
2:3:440:VAL:HG11	13:I:53:DT:H3'	2.02	0.40
2:3:680:VAL:HG12	6:7:613:ALA:HB1	2.03	0.40
3:4:243:LEU:O	3:4:305:PRO:HA	2.22	0.40
3:4:502:THR:O	3:4:506:LEU:HG	2.21	0.40
3:4:621:LEU:O	3:4:624:SER:OG	2.31	0.40
3:4:811:MET:O	3:4:814:LYS:NZ	2.54	0.40
3:4:884:ASN:O	3:4:888:LYS:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:270:LEU:HB2	5:6:289:SER:OG	2.22	0.40
6:7:24:PHE:HA	6:7:88:TYR:CZ	2.57	0.40
6:7:419:ALA:HB1	6:7:422:ILE:HB	2.02	0.40
6:7:662:GLN:HA	6:7:665:ILE:HD12	2.03	0.40
8:B:23:GLU:HG3	8:B:118:ASN:ND2	2.37	0.40
9:C:18:CYS:HB3	9:C:74:LEU:HD23	2.04	0.40
10:D:79:TYR:CZ	10:D:84:MET:HG3	2.56	0.40
15:M:1536:PHE:CD1	15:M:1640:LEU:HB3	2.56	0.40
15:M:2056:LYS:HB3	15:M:2094:PHE:CD1	2.56	0.40
16:N:485:PRO:HG2	16:N:528:ASN:HB2	2.04	0.40
1:2:194:TYR:O	1:2:198:ILE:HG12	2.22	0.40
1:2:510:ASP:N	1:2:510:ASP:OD1	2.54	0.40
1:2:820:PHE:CE2	1:2:836:ARG:HB3	2.56	0.40
3:4:628:VAL:HA	3:4:670:SER:HB2	2.03	0.40
4:5:491:VAL:HA	4:5:494:HIS:NE2	2.37	0.40
5:6:300:VAL:HG13	5:6:386:VAL:HG11	2.04	0.40
5:6:572:CYS:HA	5:6:680:ALA:HB3	2.03	0.40
5:6:832:ARG:O	5:6:836:ILE:HG12	2.22	0.40
6:7:80:ILE:HG21	6:7:117:PHE:CE2	2.56	0.40
11:E:561:ASP:OD1	11:E:561:ASP:N	2.54	0.40
11:E:622:ILE:HG23	11:E:630:ILE:HG22	2.04	0.40
12:F:502:VAL:HG21	12:F:537:CYS:SG	2.61	0.40
12:F:667:ASP:O	12:F:669:LYS:HG2	2.22	0.40
12:F:728:ILE:HD11	12:F:742:VAL:HG23	2.03	0.40
12:F:830:SER:OG	12:F:862:TYR:HB2	2.22	0.40
12:H:878:ASN:HD22	12:H:881:LYS:HD2	1.86	0.40
15:M:1672:ILE:HD11	15:M:1815:SER:OG	2.22	0.40
15:M:2150:LEU:HD13	15:M:2201:PHE:CD2	2.56	0.40
16:N:36:ASP:HB2	16:N:78:PHE:CZ	2.57	0.40
16:N:322:PRO:HD2	16:N:553:HIS:O	2.22	0.40
16:N:676:VAL:O	16:N:680:LYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	658/868 (76%)	642 (98%)	16 (2%)	0	100	100
2	3	639/971 (66%)	617 (97%)	22 (3%)	0	100	100
3	4	685/933 (73%)	657 (96%)	28 (4%)	0	100	100
4	5	663/775 (86%)	644 (97%)	19 (3%)	0	100	100
5	6	605/1017 (60%)	586 (97%)	19 (3%)	0	100	100
6	7	633/845 (75%)	599 (95%)	34 (5%)	0	100	100
7	A	196/208 (94%)	189 (96%)	7 (4%)	0	100	100
8	B	191/213 (90%)	188 (98%)	3 (2%)	0	100	100
9	C	167/194 (86%)	165 (99%)	2 (1%)	0	100	100
10	D	237/294 (81%)	234 (99%)	3 (1%)	0	100	100
11	E	560/650 (86%)	546 (98%)	14 (2%)	0	100	100
12	F	429/927 (46%)	402 (94%)	27 (6%)	0	100	100
12	G	417/927 (45%)	390 (94%)	27 (6%)	0	100	100
12	H	415/927 (45%)	382 (92%)	33 (8%)	0	100	100
15	M	799/2222 (36%)	760 (95%)	39 (5%)	0	100	100
16	N	524/689 (76%)	493 (94%)	31 (6%)	0	100	100
All	All	7818/12660 (62%)	7494 (96%)	324 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	579/770 (75%)	579 (100%)	0	100	100
2	3	551/835 (66%)	551 (100%)	0	100	100
3	4	622/848 (73%)	622 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5	605/688 (88%)	605 (100%)	0	100	100
5	6	535/886 (60%)	535 (100%)	0	100	100
6	7	550/753 (73%)	550 (100%)	0	100	100
7	A	182/193 (94%)	181 (100%)	1 (0%)	81	81
8	B	184/198 (93%)	184 (100%)	0	100	100
9	C	156/173 (90%)	156 (100%)	0	100	100
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	509/586 (87%)	509 (100%)	0	100	100
12	F	382/825 (46%)	382 (100%)	0	100	100
12	G	370/825 (45%)	370 (100%)	0	100	100
12	H	368/825 (45%)	368 (100%)	0	100	100
15	M	720/2014 (36%)	720 (100%)	0	100	100
16	N	474/629 (75%)	474 (100%)	0	100	100
All	All	7021/11327 (62%)	7020 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	206	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	290	HIS
1	2	366	ASN
1	2	454	ASN
1	2	528	ASN
1	2	551	GLN
1	2	653	ASN
2	3	312	ASN
2	3	365	GLN
2	3	677	ASN
3	4	196	ASN
3	4	229	GLN
3	4	380	ASN
3	4	576	GLN

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Mol	Chain	Res	Type
3	4	797	GLN
3	4	848	ASN
3	4	891	ASN
4	5	344	ASN
4	5	586	GLN
4	5	765	HIS
5	6	156	GLN
5	6	163	ASN
5	6	506	ASN
5	6	583	GLN
5	6	653	HIS
5	6	730	HIS
5	6	814	ASN
6	7	9	GLN
6	7	144	ASN
6	7	291	GLN
6	7	554	ASN
6	7	623	ASN
6	7	683	GLN
7	A	90	GLN
7	A	202	GLN
7	A	206	GLN
8	B	8	GLN
8	B	167	HIS
8	B	196	HIS
9	C	133	GLN
10	D	231	HIS
10	D	247	GLN
11	E	13	ASN
11	E	133	ASN
11	E	229	GLN
11	E	476	ASN
11	E	500	GLN
11	E	611	GLN
12	F	548	GLN
12	F	852	ASN
12	G	540	ASN
12	G	680	ASN
12	G	725	ASN
12	G	761	HIS
12	G	859	ASN
12	G	916	ASN

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Mol	Chain	Res	Type
12	H	527	HIS
12	H	565	ASN
12	H	601	ASN
12	H	877	GLN
12	H	878	ASN
12	H	916	ASN
15	M	1473	ASN
15	M	1587	GLN
15	M	1608	ASN
15	M	1657	ASN
15	M	1780	HIS
15	M	1814	ASN
15	M	1837	HIS
15	M	1877	ASN
15	M	1940	GLN
16	N	48	ASN
16	N	52	ASN
16	N	81	GLN
16	N	216	GLN
16	N	236	GLN
16	N	273	ASN
16	N	291	ASN
16	N	594	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	$\# Z > 2$
18	ADP	3	1001	19	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
20	AGS	7	903	19	32,33,33	0.48	1 (3%)	45,52,52	0.67	1 (2%)
20	AGS	6	1103	19	32,33,33	0.47	1 (3%)	45,52,52	0.67	1 (2%)
18	ADP	2	902	19	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
20	AGS	5	802	19	32,33,33	0.46	1 (3%)	45,52,52	0.64	1 (2%)

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
18	ADP	3	1001	19	-	3/16/32/32	0/3/3/3
20	AGS	7	903	19	-	2/21/38/38	0/3/3/3
20	AGS	6	1103	19	-	4/21/38/38	0/3/3/3
18	ADP	2	902	19	-	2/16/32/32	0/3/3/3
20	AGS	5	802	19	-	1/21/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	902	ADP	C5-C4	4.73	1.47	1.39
18	3	1001	ADP	C5-C4	4.70	1.47	1.39
18	3	1001	ADP	C5-C6	2.79	1.48	1.41
18	2	902	ADP	C5-C6	2.77	1.48	1.41
18	2	902	ADP	C8-N7	2.38	1.36	1.31
18	3	1001	ADP	C8-N7	2.35	1.36	1.31
18	2	902	ADP	C5-N7	-2.23	1.35	1.39
18	3	1001	ADP	C5-N7	-2.21	1.35	1.39
20	5	802	AGS	PG-S1G	2.18	1.95	1.90
20	6	1103	AGS	PG-S1G	2.12	1.95	1.90
20	7	903	AGS	PG-S1G	2.10	1.95	1.90

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	1001	ADP	C5-C4-N3	-5.88	118.63	126.72
18	2	902	ADP	C5-C4-N3	-5.83	118.69	126.72
18	3	1001	ADP	N3-C4-N9	4.60	134.98	127.17
18	2	902	ADP	N3-C4-N9	4.50	134.83	127.17
18	3	1001	ADP	C2-N3-C4	3.73	120.93	111.83
18	2	902	ADP	C2-N3-C4	3.70	120.86	111.83
20	7	903	AGS	PB-O3B-PG	-3.58	120.06	133.17
18	2	902	ADP	C4-C5-N7	-3.57	106.50	110.58
20	5	802	AGS	PB-O3B-PG	-3.54	120.23	133.17
18	3	1001	ADP	C4-C5-N7	-3.50	106.58	110.58
20	6	1103	AGS	PB-O3B-PG	-3.42	120.66	133.17
18	3	1001	ADP	N3-C2-N1	-3.19	123.75	128.58
18	2	902	ADP	N3-C2-N1	-3.19	123.76	128.58
18	2	902	ADP	C5-N7-C8	2.58	107.50	103.45
18	3	1001	ADP	C5-N7-C8	2.52	107.42	103.45
18	3	1001	ADP	C4-N9-C8	2.51	108.38	105.74
18	2	902	ADP	C4-N9-C8	2.51	108.38	105.74
18	2	902	ADP	C6-C5-N7	2.15	136.23	132.09
18	3	1001	ADP	C3'-C2'-C1'	2.09	105.42	101.46
18	3	1001	ADP	C6-C5-N7	2.09	136.12	132.09
18	2	902	ADP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

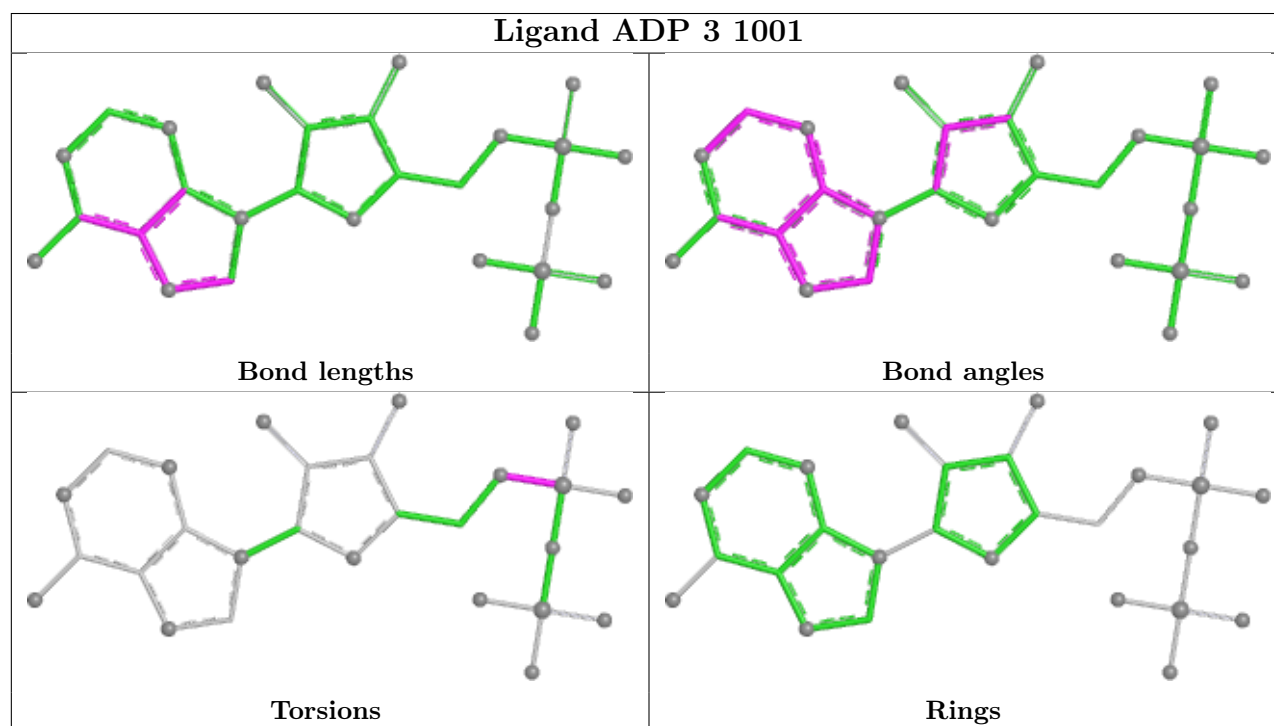
Mol	Chain	Res	Type	Atoms
18	2	902	ADP	C5'-O5'-PA-O3A
18	3	1001	ADP	C5'-O5'-PA-O1A
18	3	1001	ADP	C5'-O5'-PA-O2A
18	3	1001	ADP	C5'-O5'-PA-O3A
20	6	1103	AGS	C5'-O5'-PA-O1A
20	6	1103	AGS	C5'-O5'-PA-O3A
18	2	902	ADP	C5'-O5'-PA-O1A
20	6	1103	AGS	C5'-O5'-PA-O2A
20	7	903	AGS	PA-O3A-PB-O2B
20	5	802	AGS	PB-O3A-PA-O1A
20	6	1103	AGS	C4'-C5'-O5'-PA
20	7	903	AGS	PA-O3A-PB-O1B

There are no ring outliers.

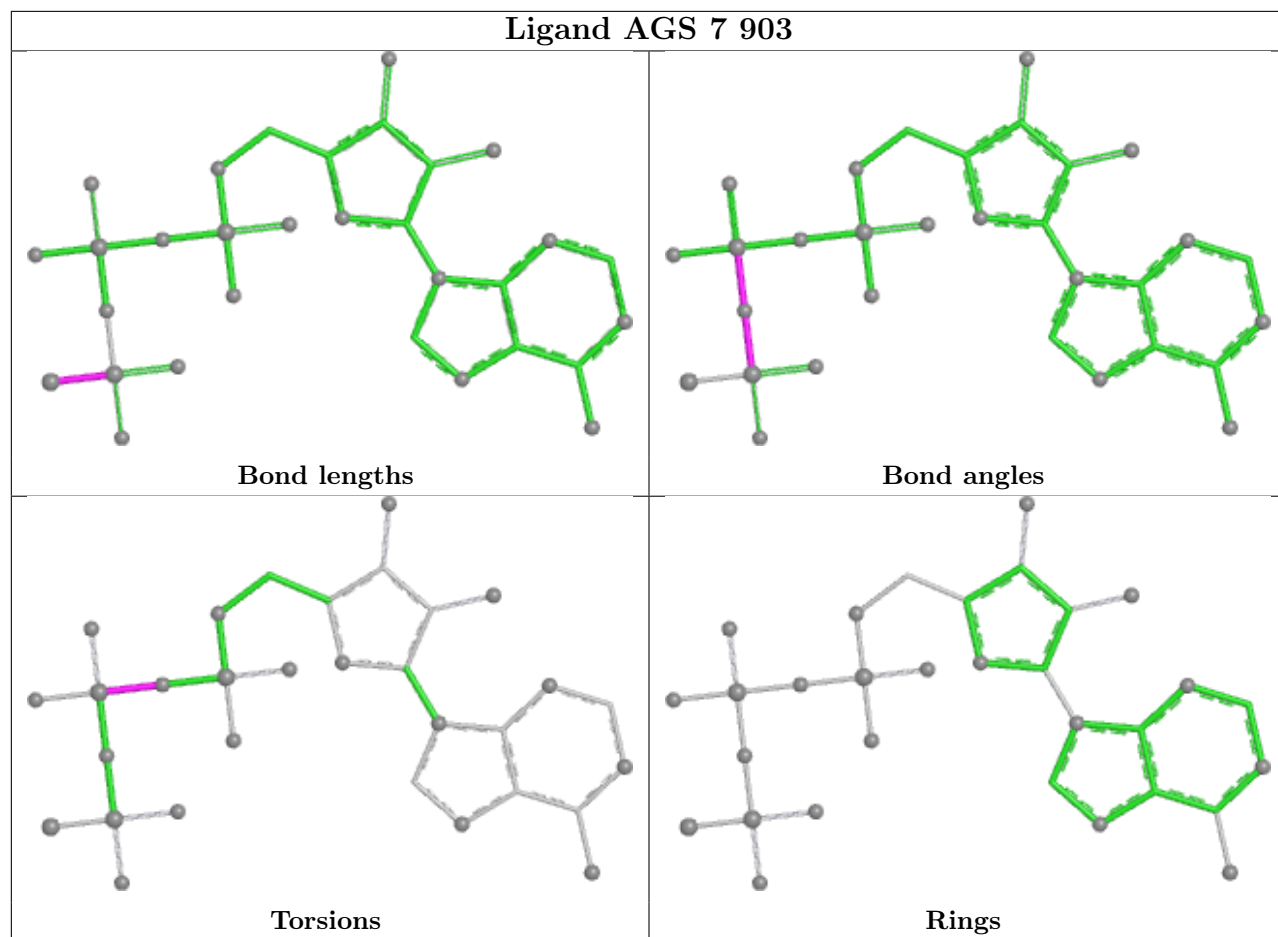
5 monomers are involved in 18 short contacts:

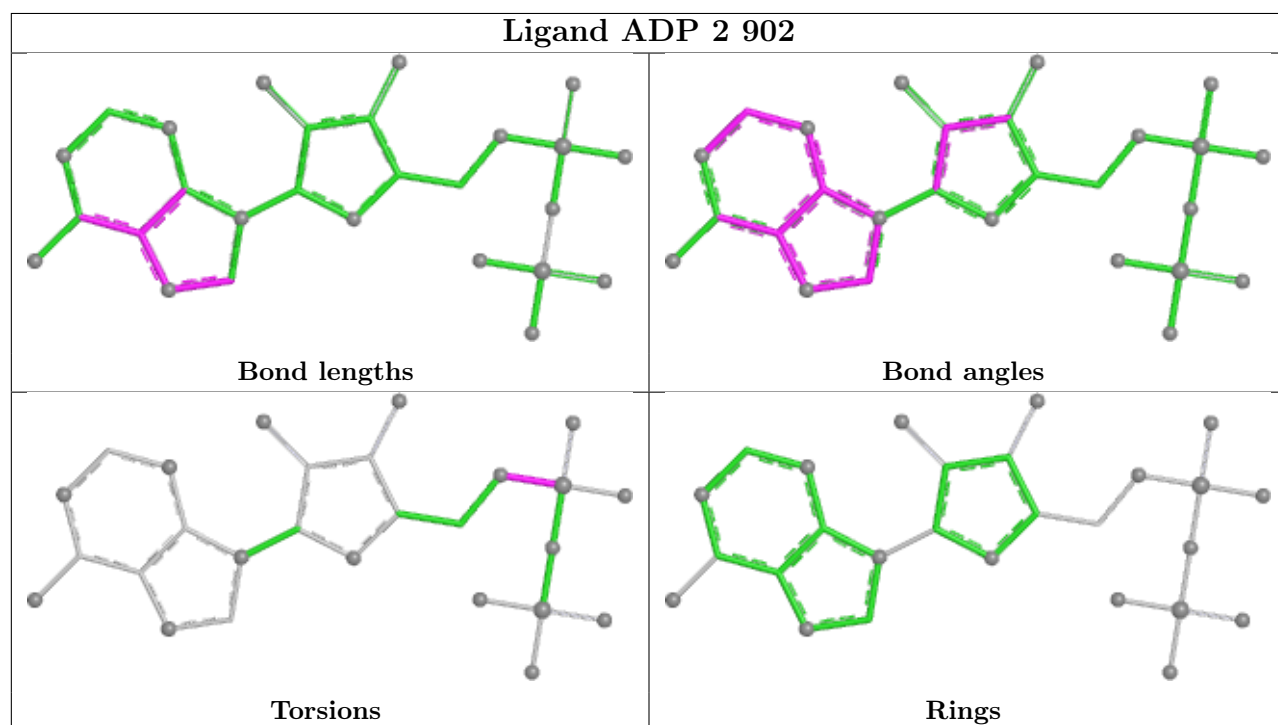
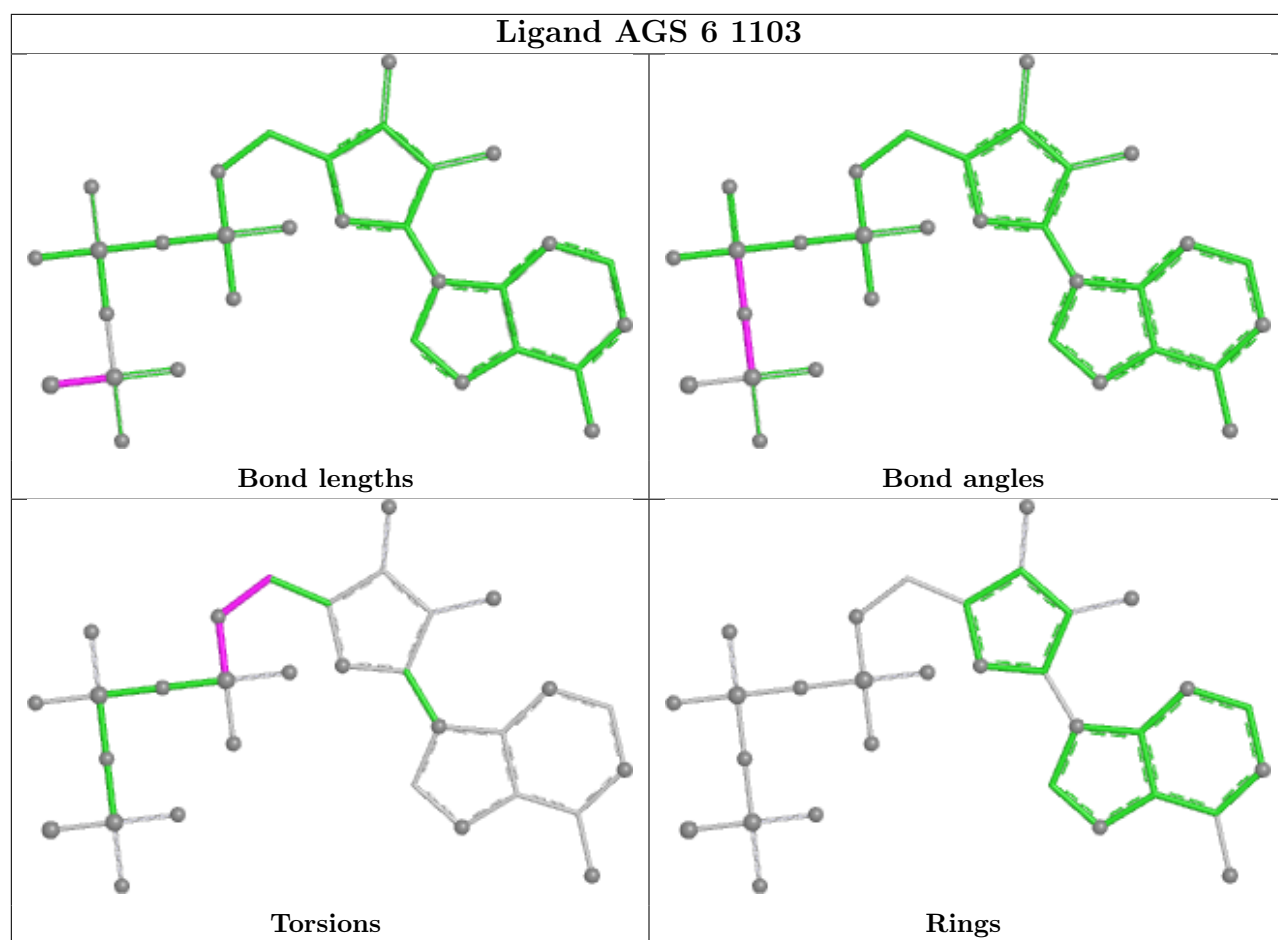
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	1001	ADP	3	0
20	7	903	AGS	1	0
20	6	1103	AGS	6	0
18	2	902	ADP	3	0
20	5	802	AGS	5	0

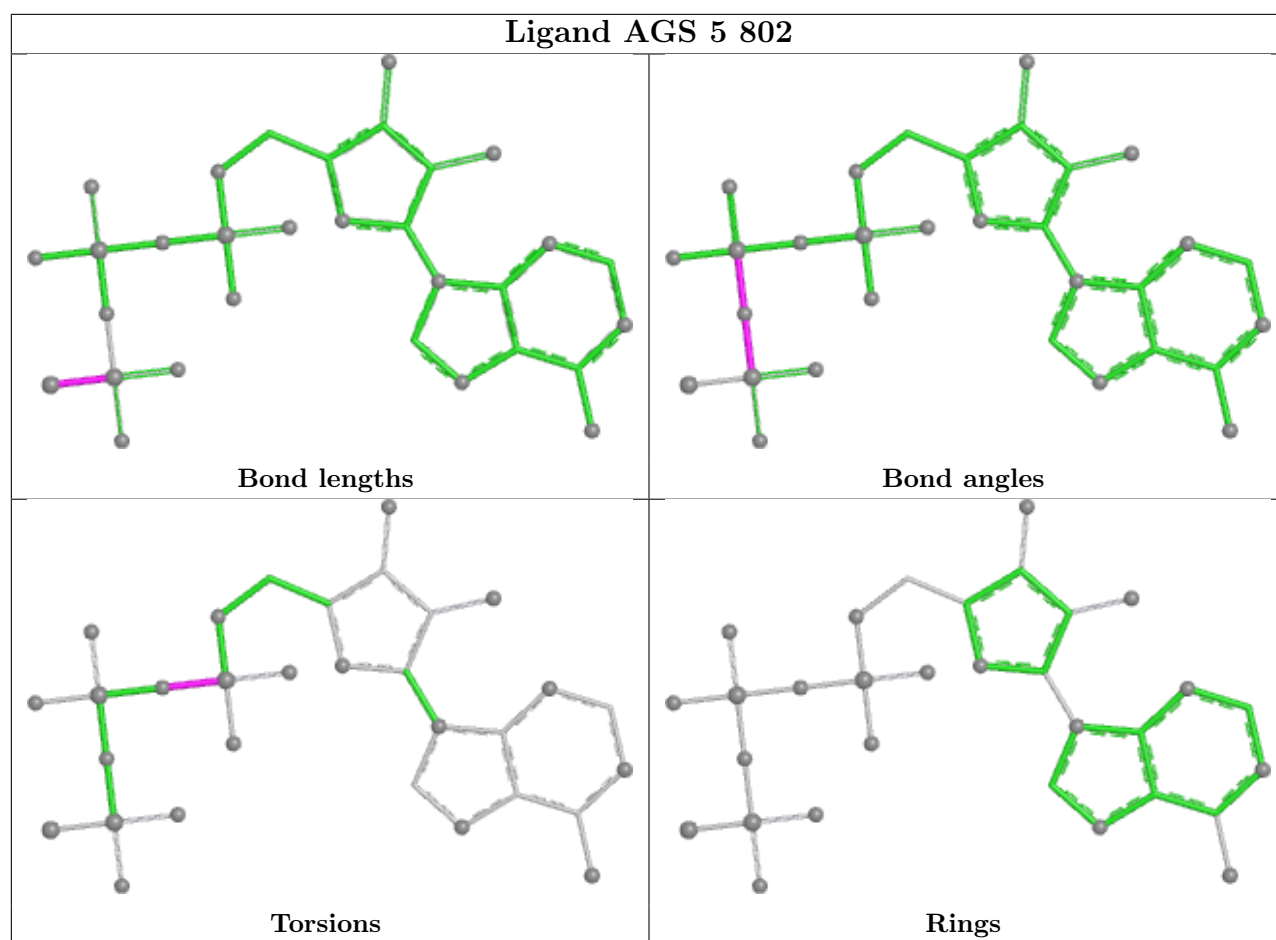
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand AGS 7 903







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.

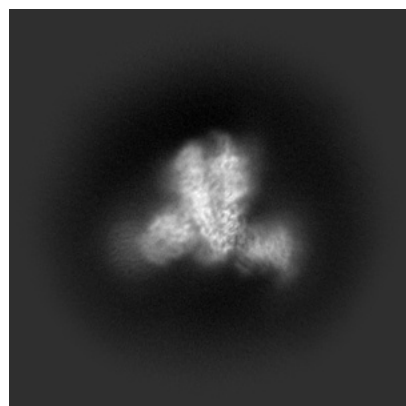
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37213. These allow visual inspection of the internal detail of the map and identification of artifacts.

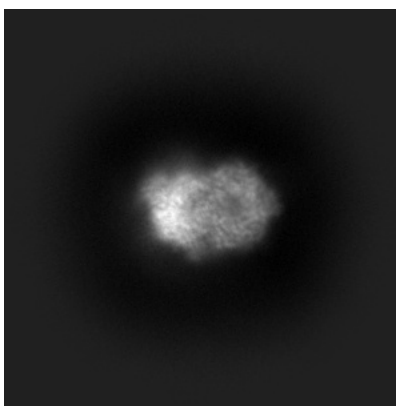
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

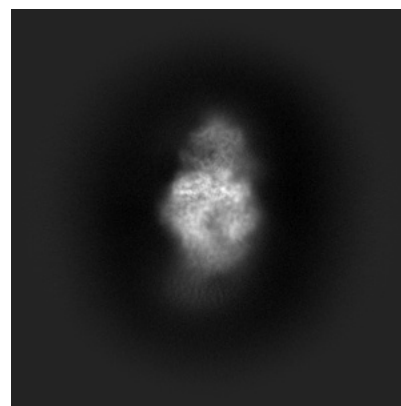
6.1.1 Primary map



X

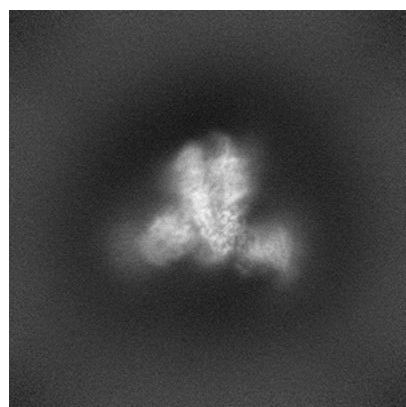


Y

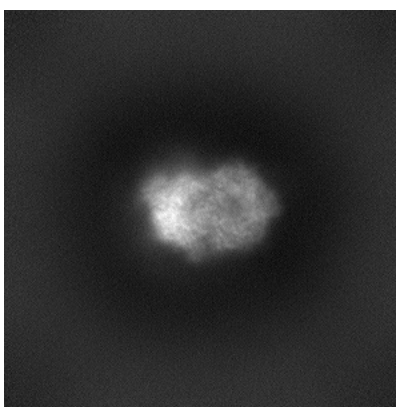


Z

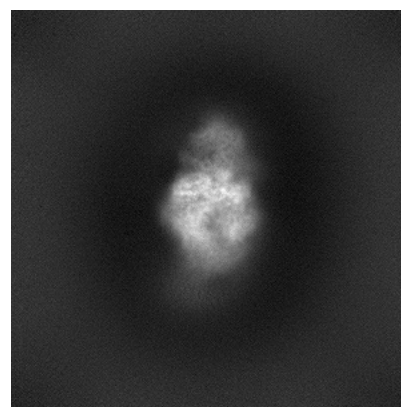
6.1.2 Raw map



X



Y

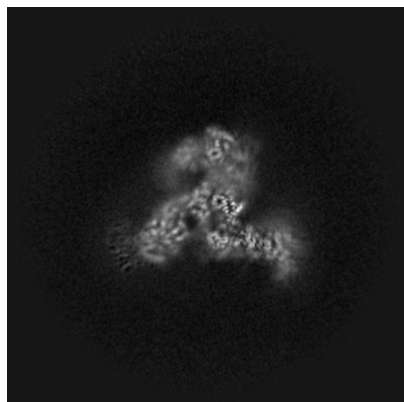


Z

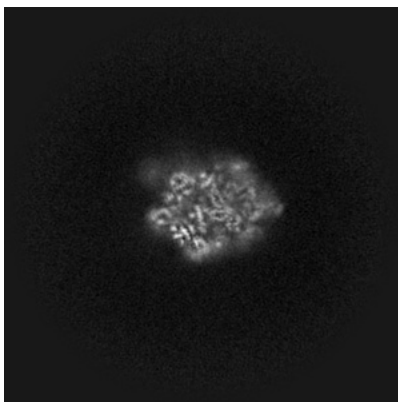
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

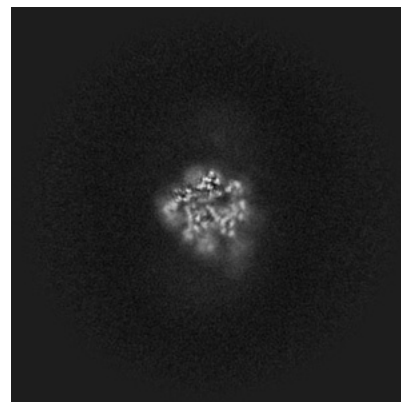
6.2.1 Primary map



X Index: 270

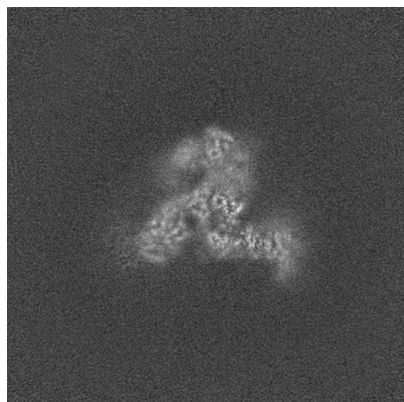


Y Index: 270

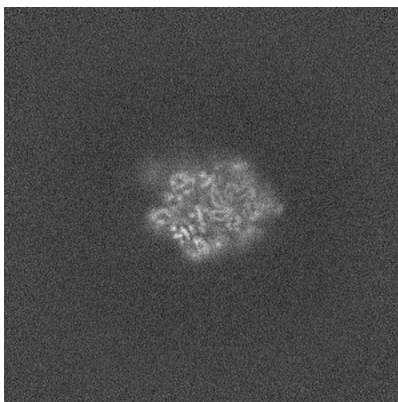


Z Index: 270

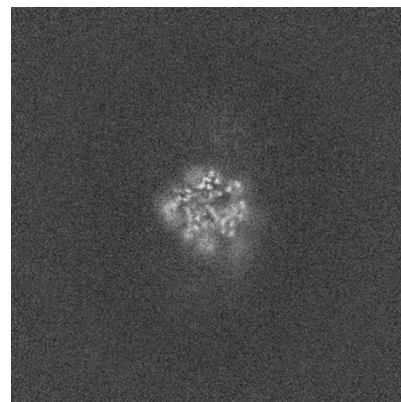
6.2.2 Raw map



X Index: 270



Y Index: 270

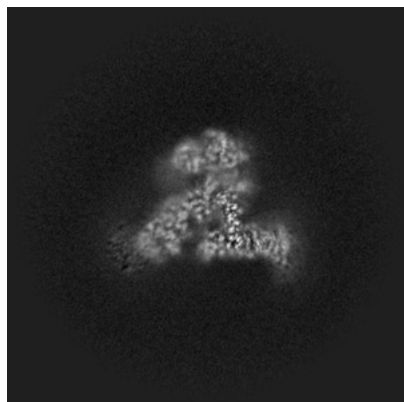


Z Index: 270

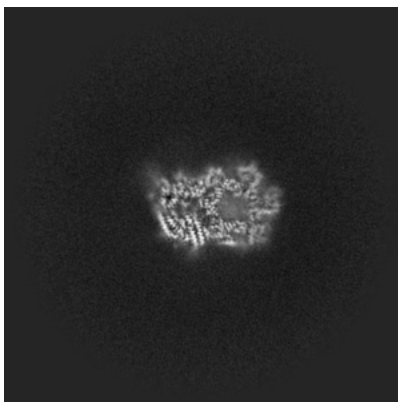
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

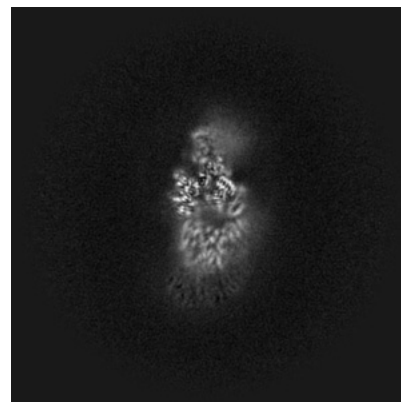
6.3.1 Primary map



X Index: 263

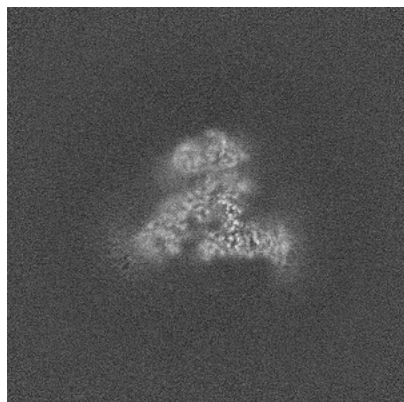


Y Index: 292

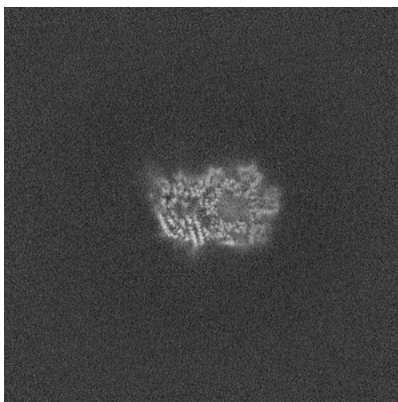


Z Index: 236

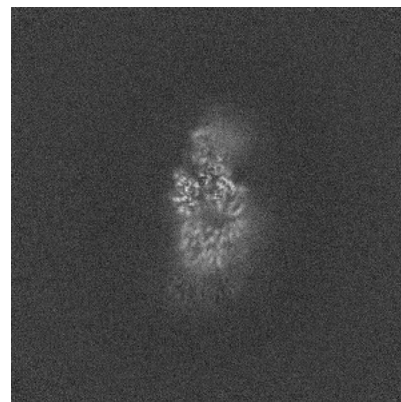
6.3.2 Raw map



X Index: 262



Y Index: 292

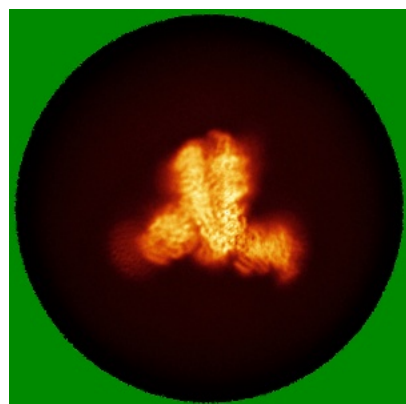


Z Index: 236

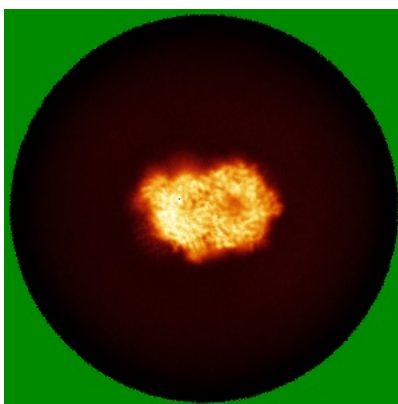
The images above show the largest variance slices of the map in three orthogonal directions.

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

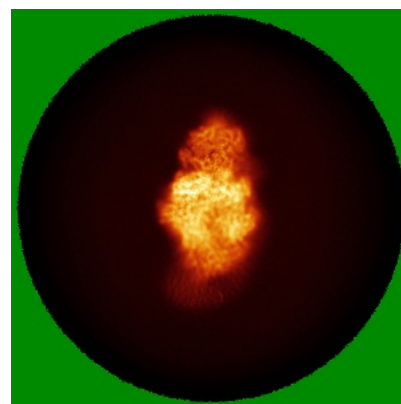
6.4.1 Primary map



X

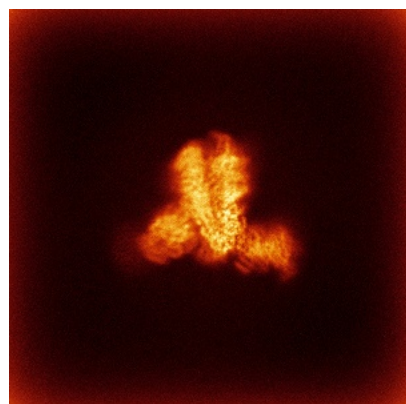


Y

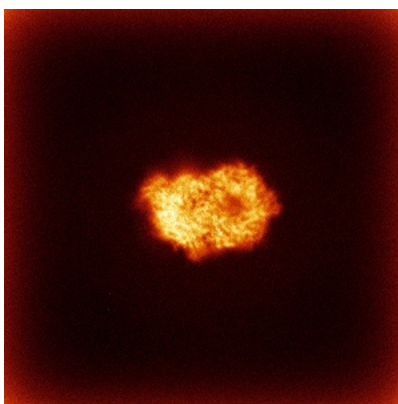


Z

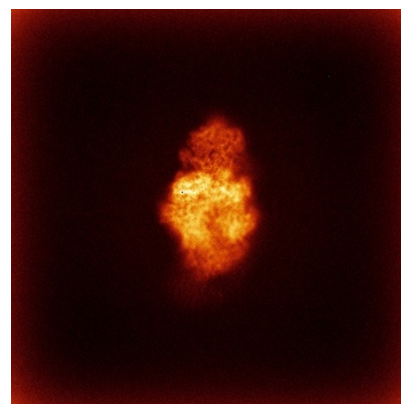
6.4.2 Raw map



X



Y

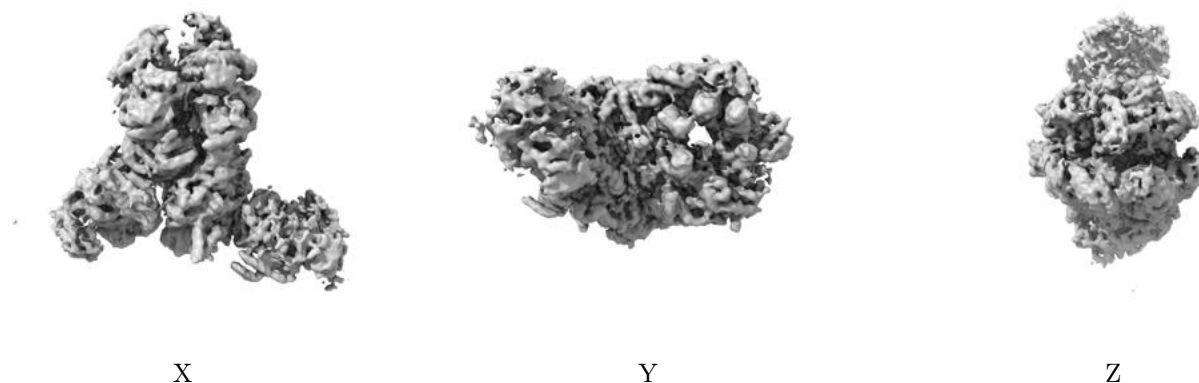


Z

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.

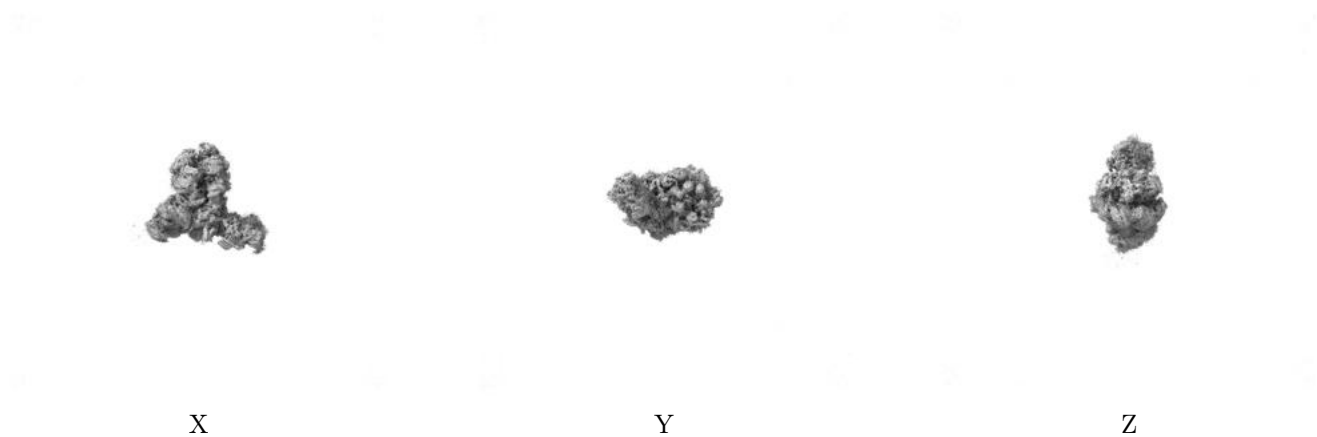
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

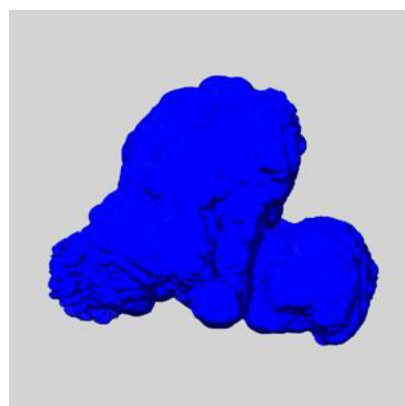
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

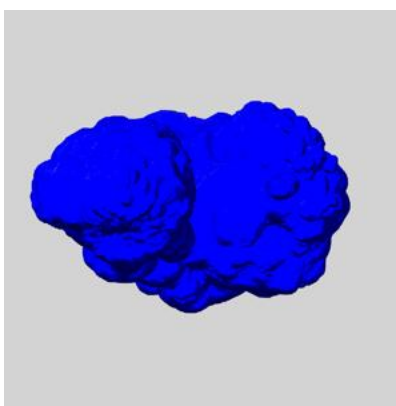
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

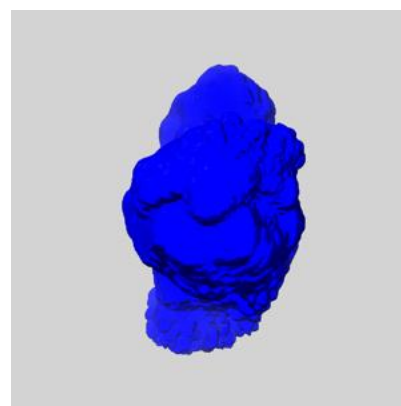
6.6.1 emd_37213_msk_1.map [i](#)



X



Y

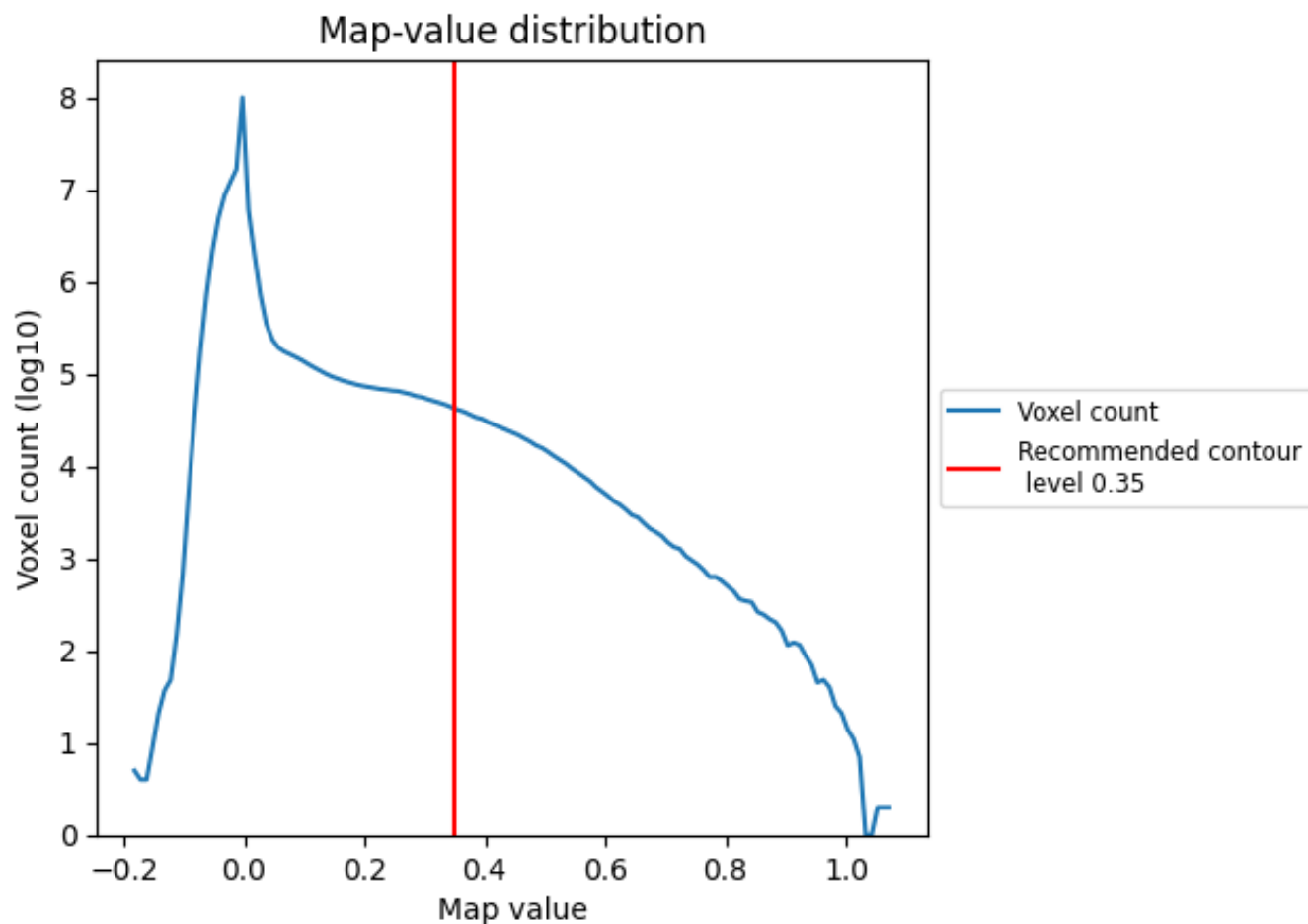


Z

7 Map analysis [i](#)

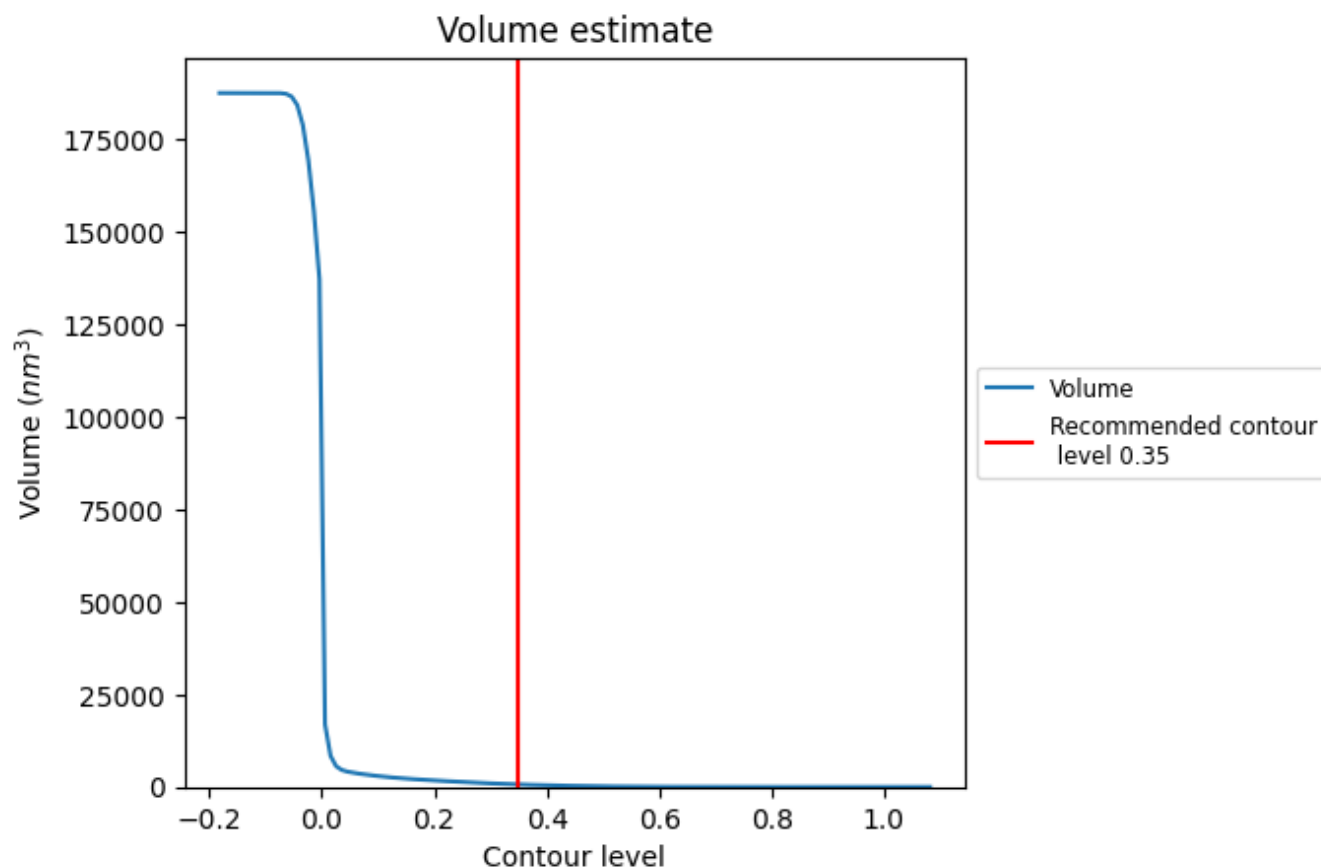
This section contains the results of statistical analysis of the map.

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.

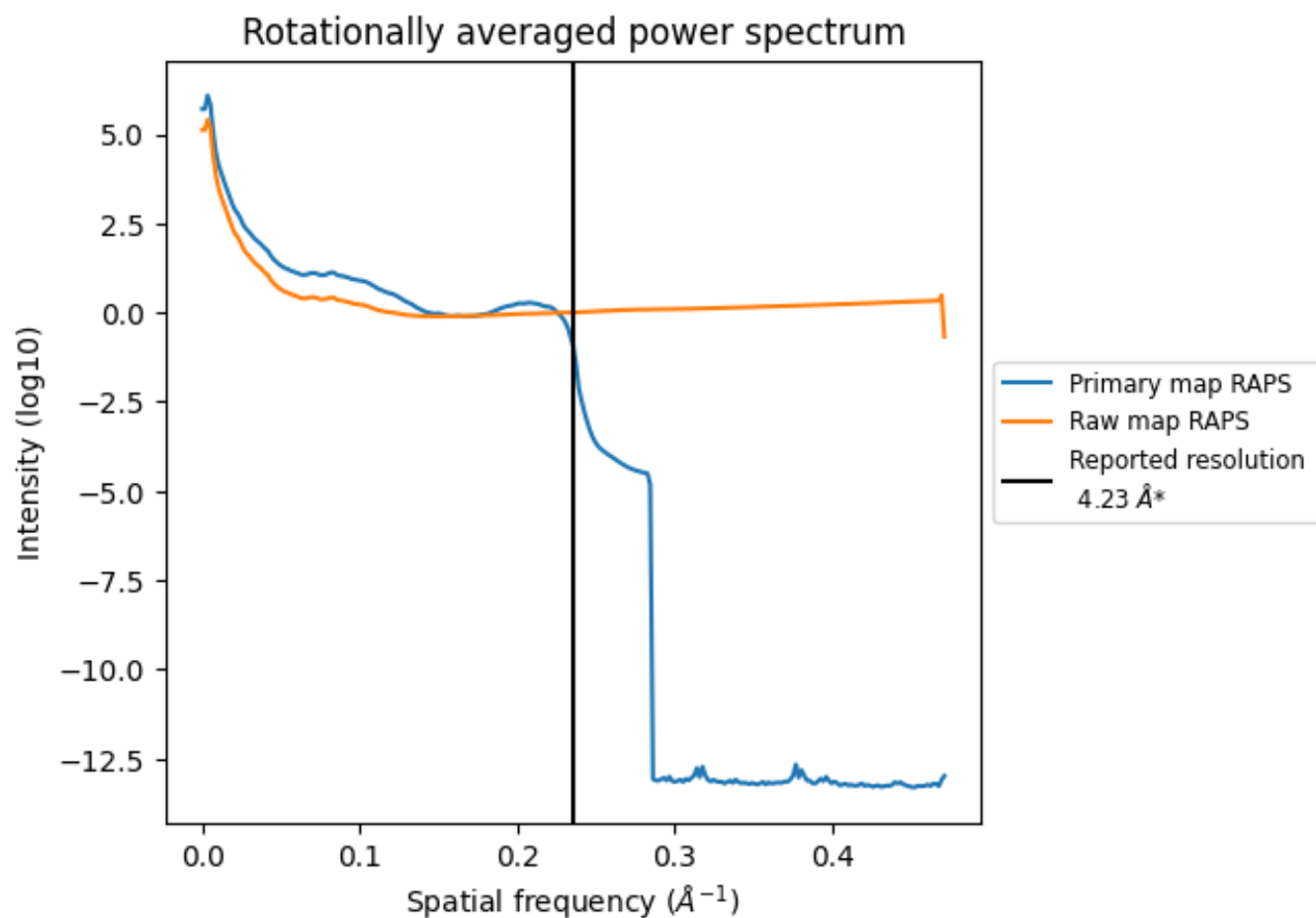
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 676 nm³; this corresponds to an approximate mass of 611 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 ⓘ

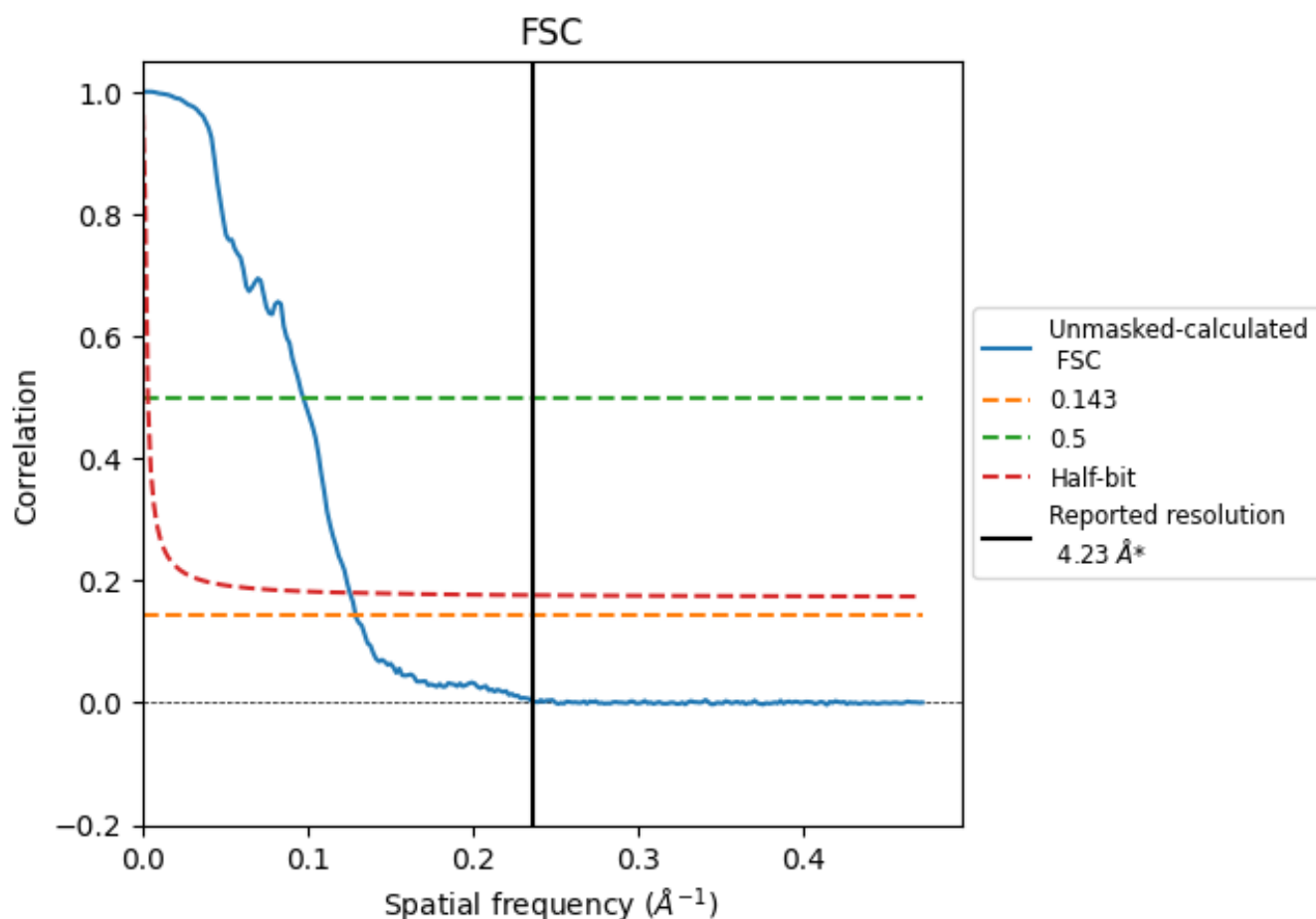


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.236 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

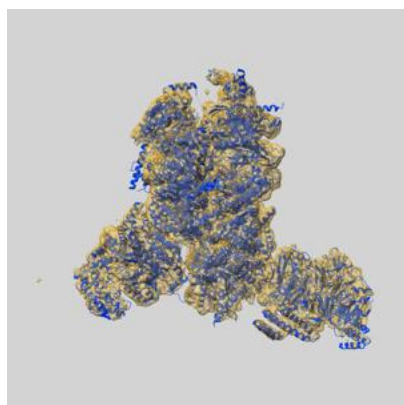
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.75	10.28	7.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.75 differs from the reported value 4.23 by more than 10 %

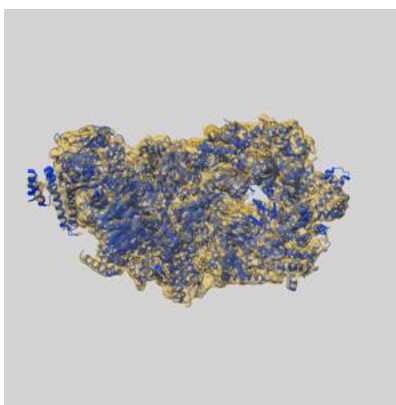
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37213 and PDB model 8KG8. Per-residue inclusion information can be found in section 3 on page 9.

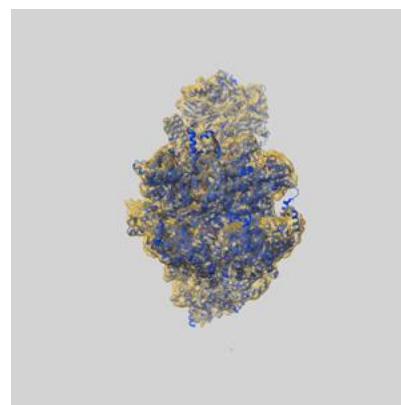
9.1 Map-model overlay [i](#)



X



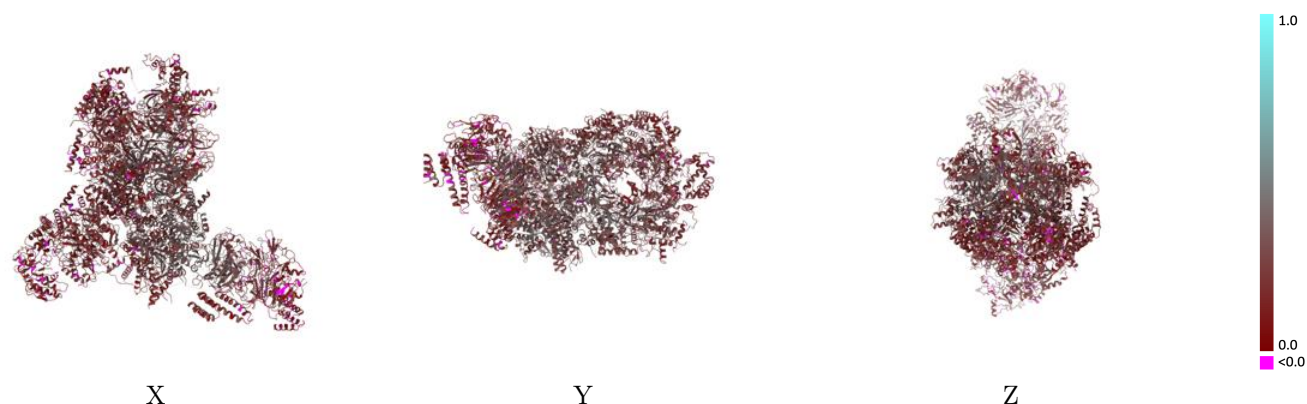
Y



Z

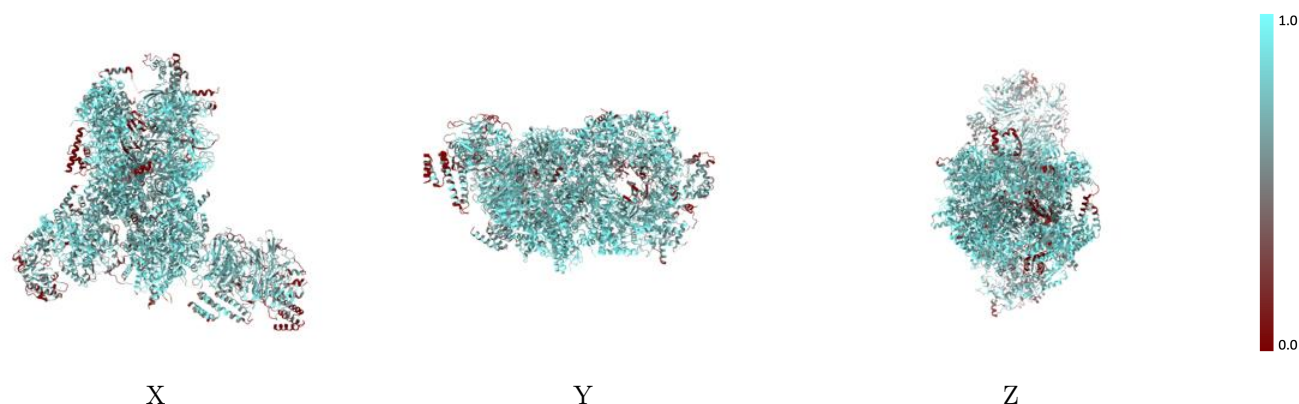
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



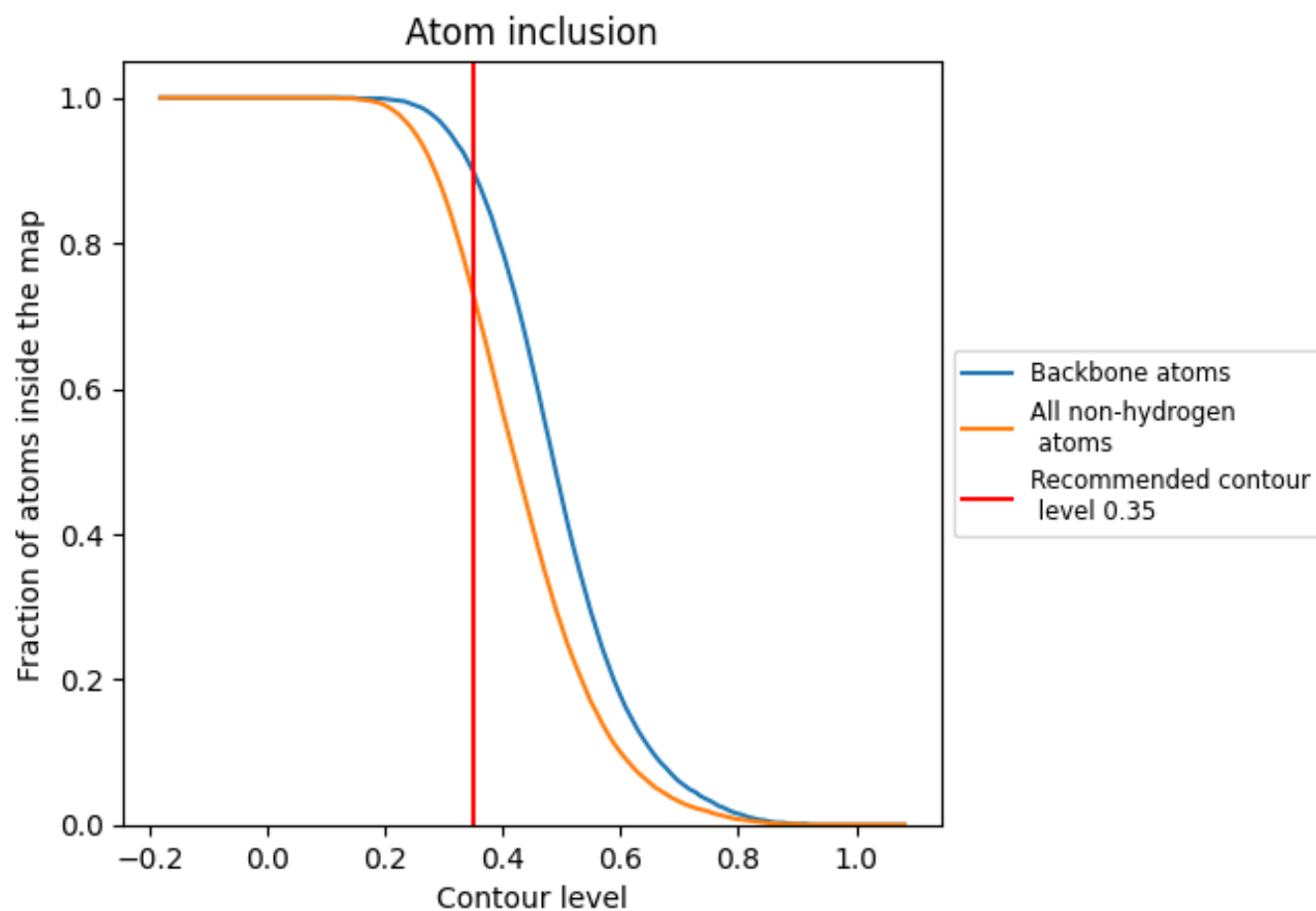
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.2460
2	 0.7570	 0.2480
3	 0.8300	 0.2940
4	 0.6210	 0.1970
5	 0.7680	 0.2840
6	 0.7480	 0.2230
7	 0.7220	 0.2290
A	 0.8010	 0.2770
B	 0.8490	 0.3650
C	 0.8530	 0.3160
D	 0.8280	 0.3410
E	 0.7900	 0.2920
F	 0.7130	 0.2950
G	 0.5620	 0.1870
H	 0.5890	 0.1930
I	 0.5300	 0.2420
J	 0.1920	 0.1970
M	 0.6830	 0.1930
N	 0.7750	 0.2090

