



Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 09:41 am BST

PDB ID : 7Z0H
EMDB ID : EMD-14421
Title : Structure of yeast RNA Polymerase III-Ty1 integrase complex at 2.6 Å (focus subunit AC40).
Authors : Nguyen, P.Q.; Huecas, S.; Plaza-Pegueroles, A.; Fernandez-Tornero, C.
Deposited on : 2022-02-22
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

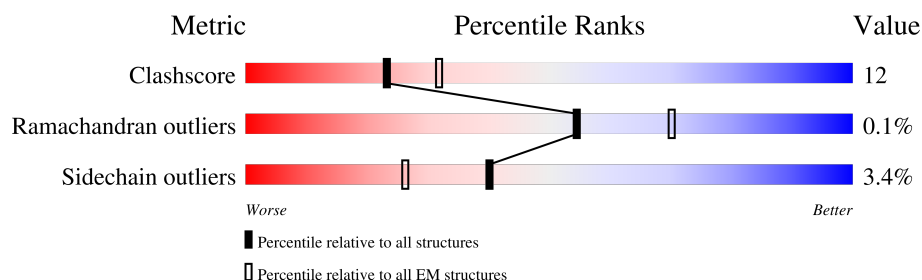
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	1460	<div> <div>18%</div> <div>67%</div> <div>29%</div> <div>• •</div> </div>
2	B	1149	<div> <div>7%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
3	C	335	<div> <div>•</div> <div>78%</div> <div>21%</div> <div>•</div> </div>
4	D	161	<div> <div>67%</div> <div>56%</div> <div>32%</div> <div>• 10%</div> </div>
5	E	215	<div> <div>19%</div> <div>65%</div> <div>34%</div> <div>•</div> </div>
6	F	155	<div> <div>•</div> <div>34%</div> <div>19%</div> <div>46%</div> </div>
7	G	212	<div> <div>42%</div> <div>65%</div> <div>25%</div> <div>10%</div> </div>
8	H	146	<div> <div>6%</div> <div>68%</div> <div>27%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	268	
18	W	635	
19	X	13	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40665 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-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0
			11123	7013	1962	2089	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1102	Total	C	N	O	S	0	0
			8701	5507	1499	1635	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1140	723	191	220	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1103	694	186	218	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			872	546	145	170	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	50	Total	C	N	O	S	0	0
			381	235	76	66	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	183	Total	C	N	O	S	0	0
			1492	953	250	288	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	151	Total	C	N	O	S	0	0
			1169	738	215	213	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	568	Total	C	N	O	S	0	0
			4558	2897	784	858	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1126	736	175	211	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			829	535	137	154	3		

- Molecule 18 is a protein called Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	17	Total	C	N	O	S	0	0
			141	86	27	27	1		

- Molecule 19 is a protein called Unknown RNA Polymerase III chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	
21	I	1	Total	Mg	0
			1	1	

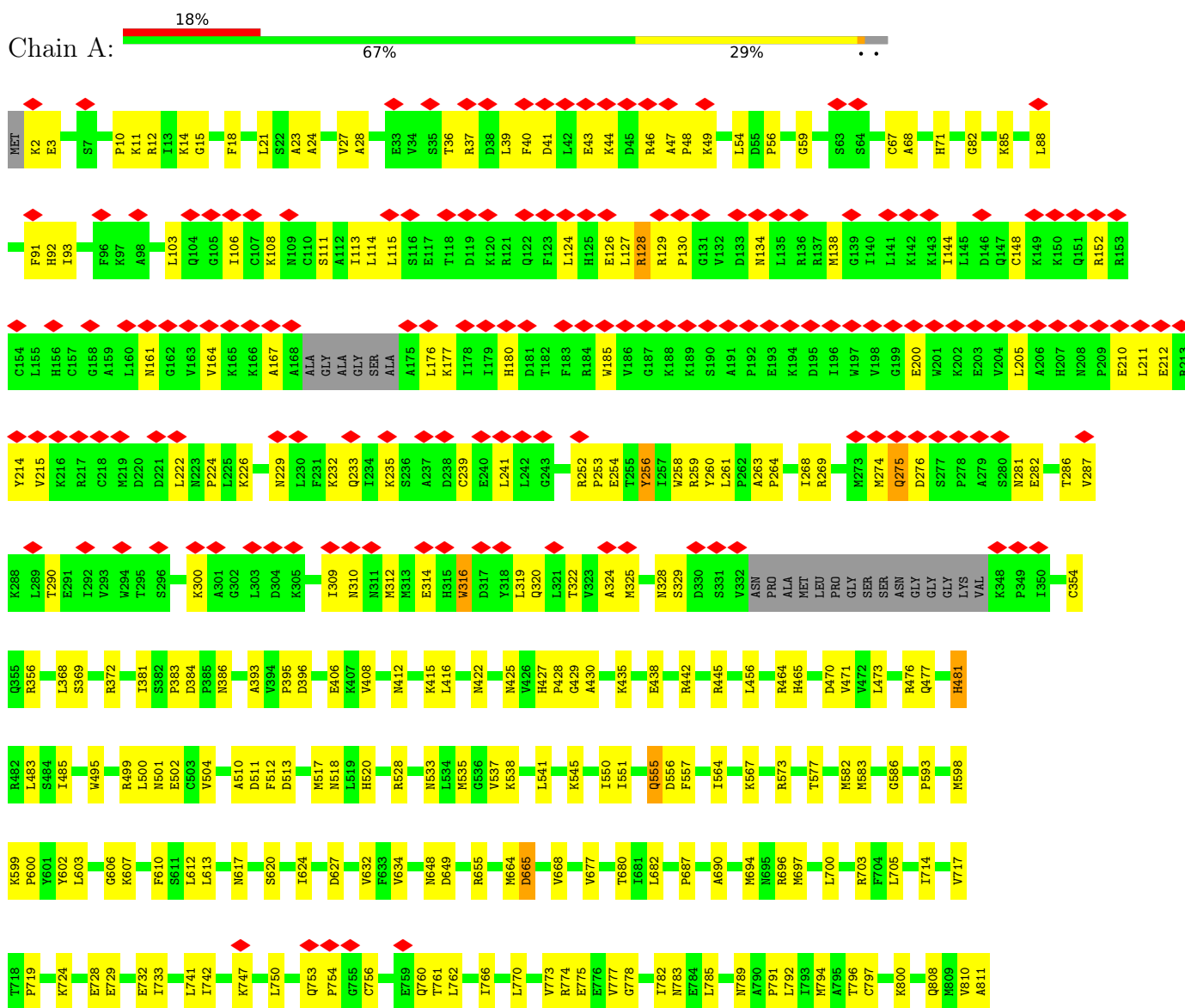
- Molecule 22 is water.

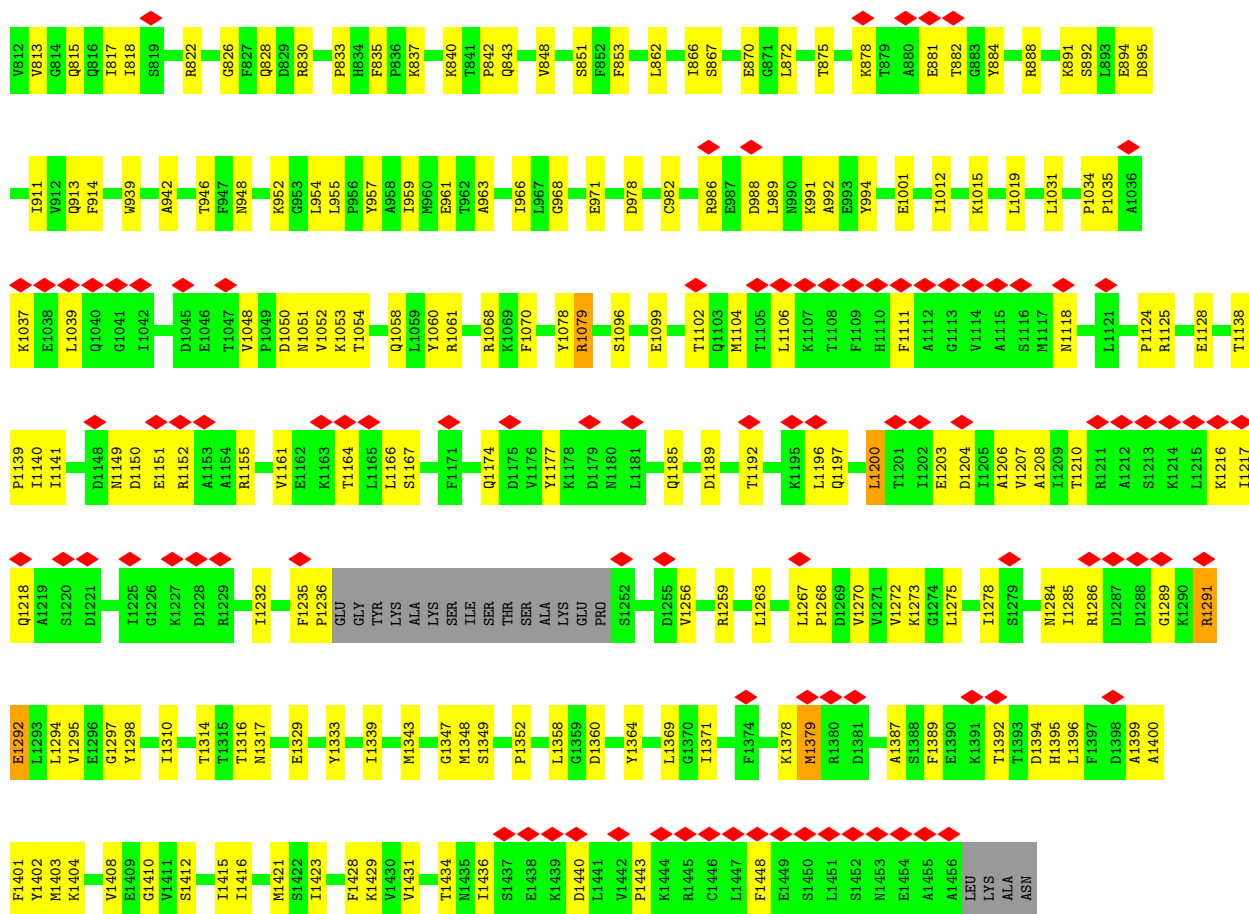
Mol	Chain	Residues	Atoms		AltConf
22	I	1	Total	O	0
			1	1	

3 Residue-property plots

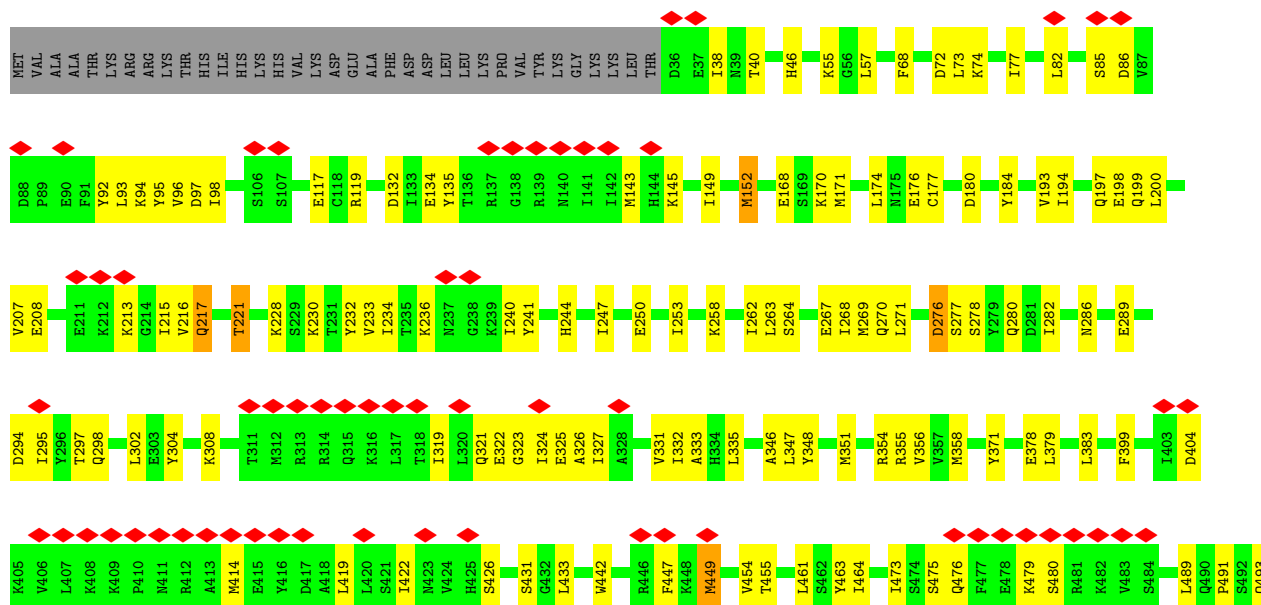
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

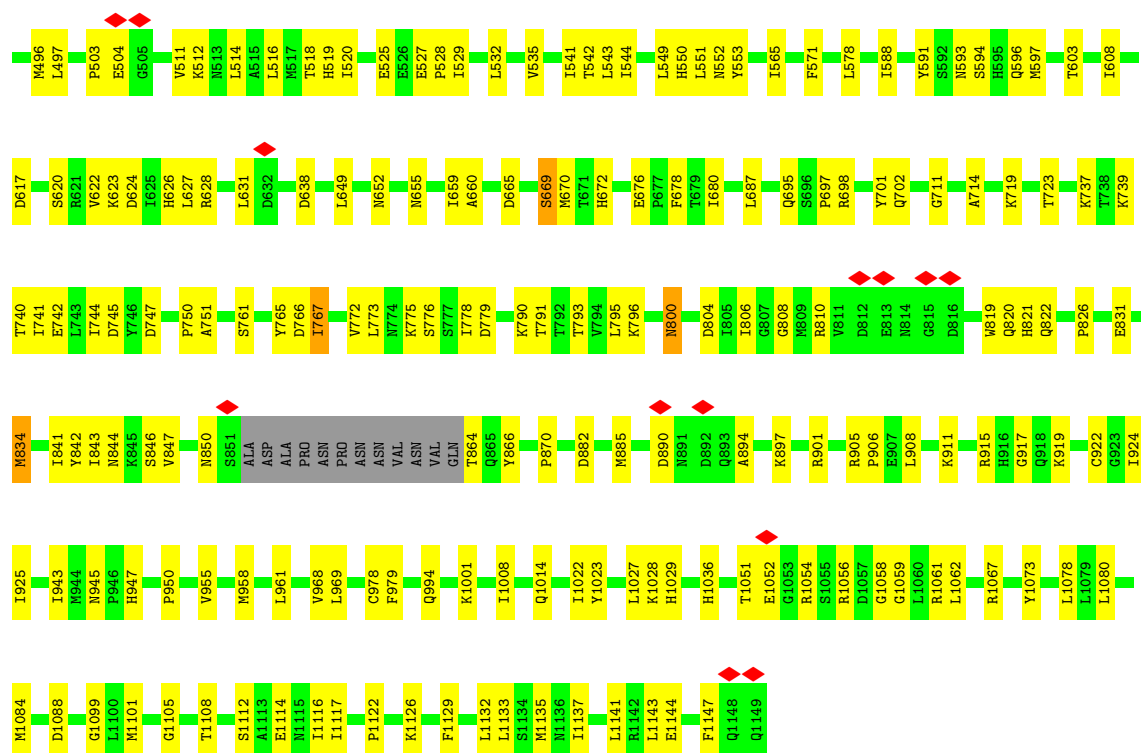
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



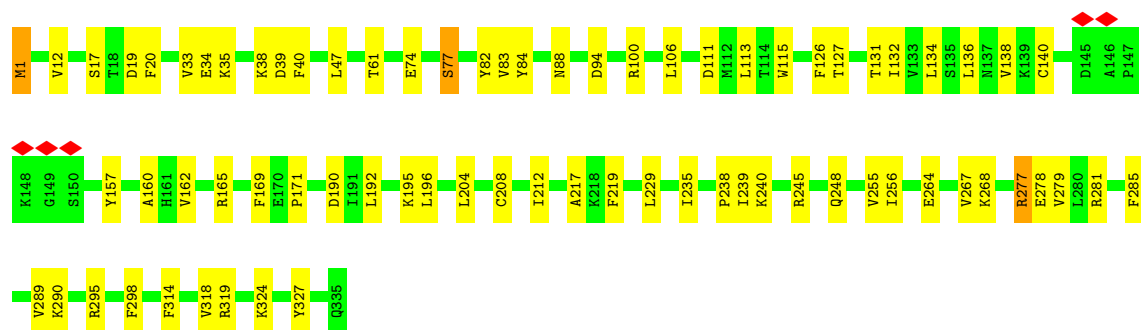
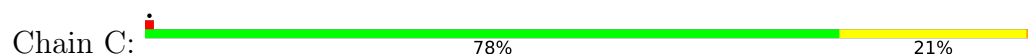


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2





• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

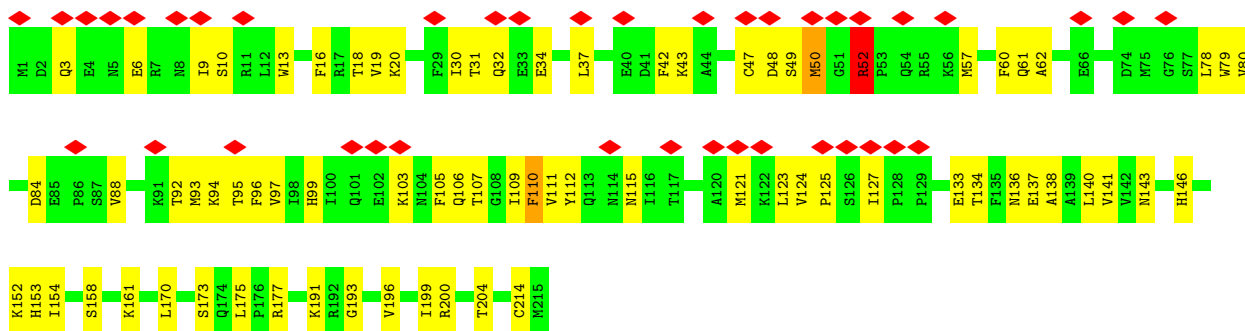


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

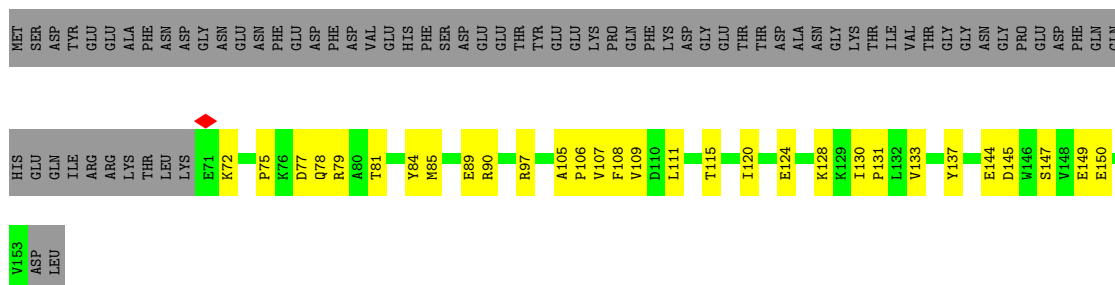
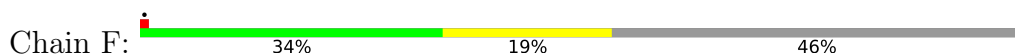




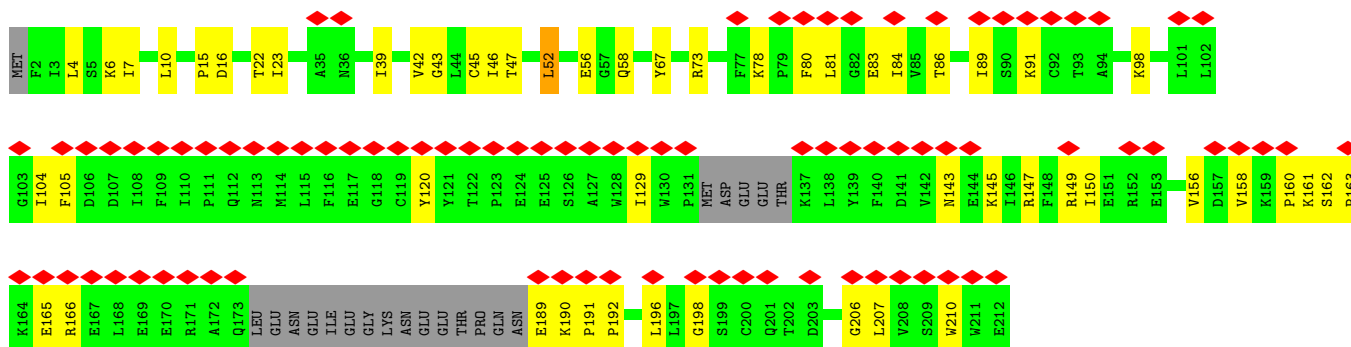
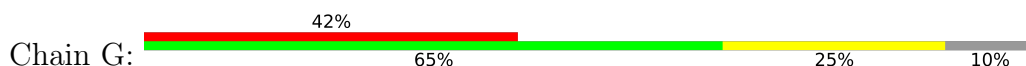
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



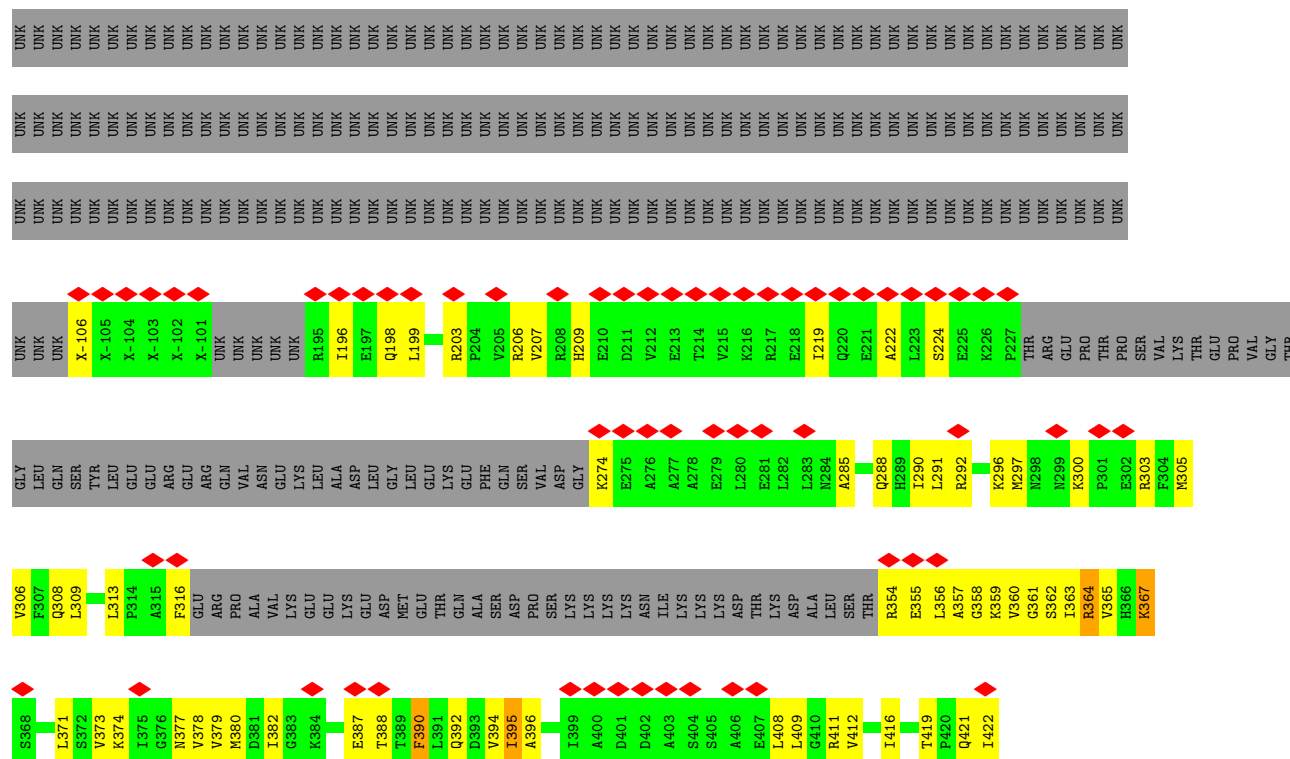
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



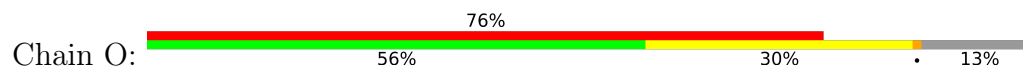
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

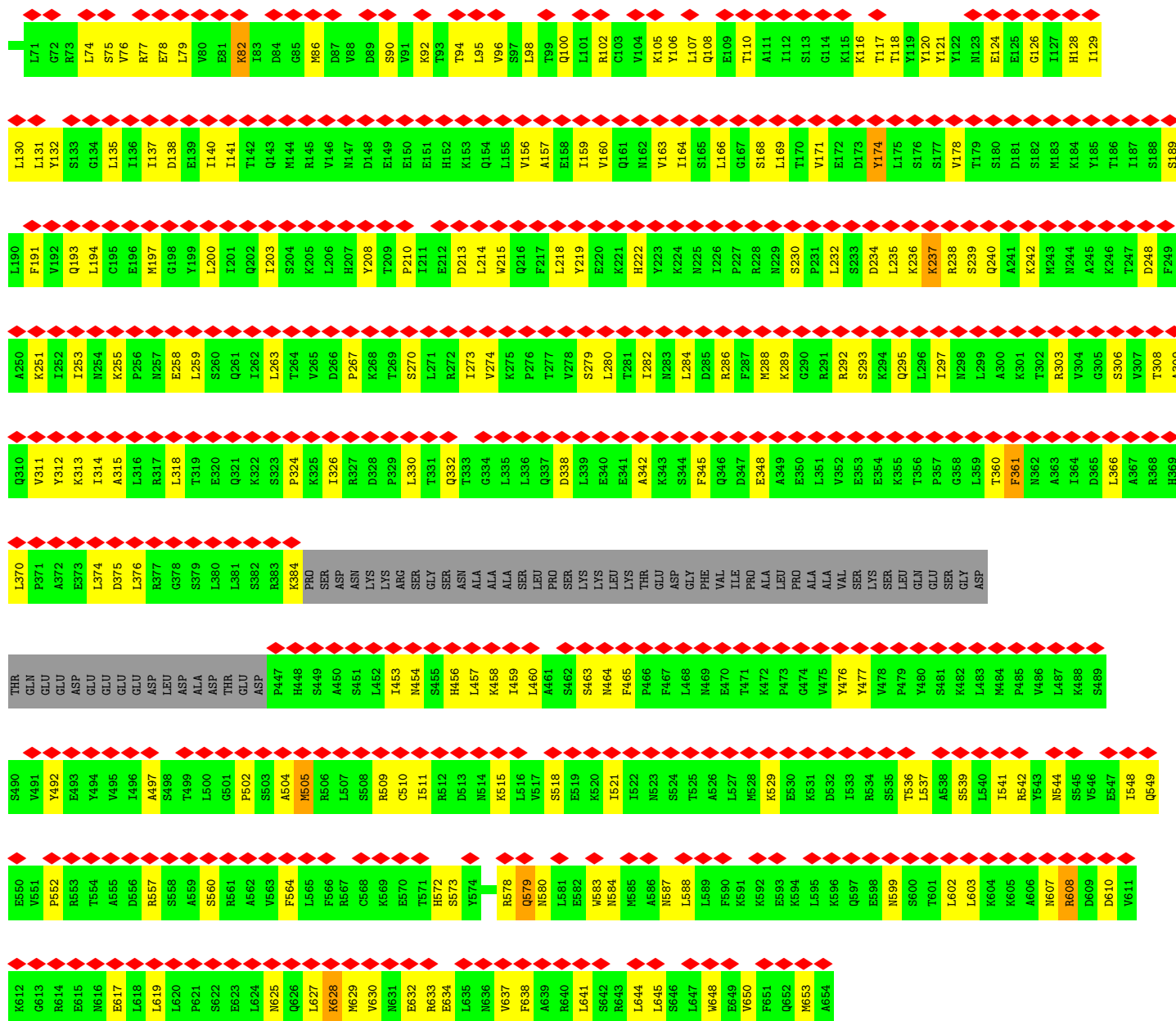


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

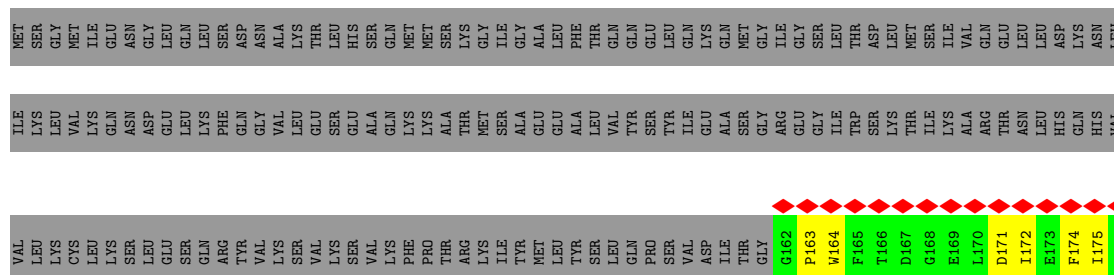
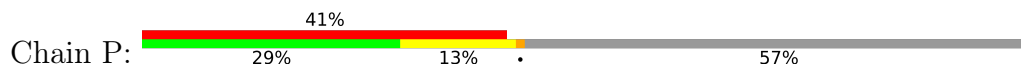


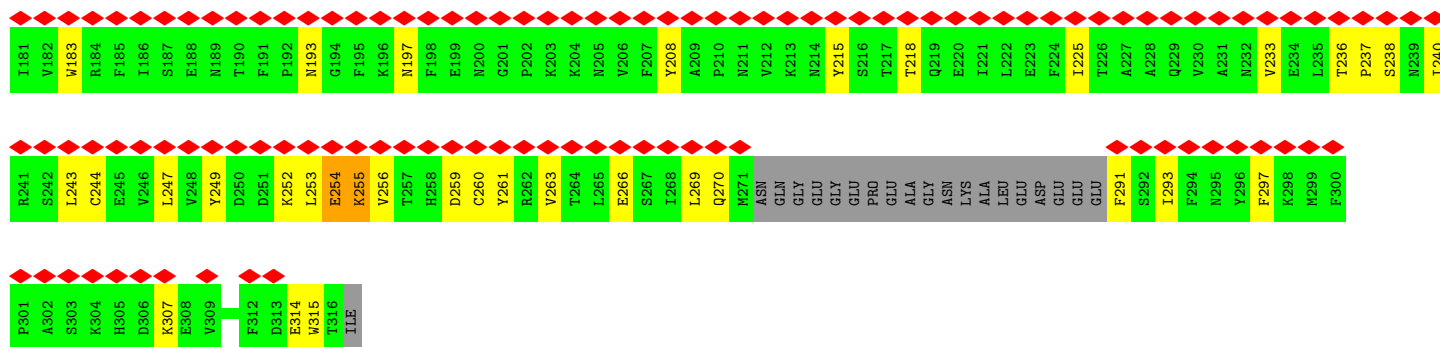
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

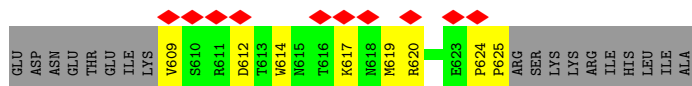




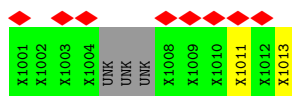
● Molecule 16: DNA-directed RNA polymerase III subunit RPC6







- Molecule 19: Unknown RNA Polymerase III chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	643858	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0213	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.27	0/11322	0.51	0/15295
2	B	0.27	0/8853	0.53	0/11940
3	C	0.26	0/2711	0.51	0/3676
4	D	0.27	0/1158	0.50	0/1550
5	E	0.31	0/1795	0.55	0/2416
6	F	0.26	0/683	0.50	0/923
7	G	0.27	0/1583	0.50	0/2146
8	H	0.27	0/1121	0.56	0/1517
9	I	0.29	0/893	0.49	0/1208
10	J	0.27	0/558	0.53	0/750
11	K	0.28	0/803	0.49	0/1083
12	L	0.25	0/353	0.59	0/468
13	M	0.28	0/1524	0.51	0/2061
14	N	0.28	0/1152	0.57	0/1546
15	O	0.26	0/4627	0.53	0/6243
16	P	0.28	0/1157	0.46	0/1571
17	Q	0.29	0/850	0.48	0/1148
18	W	0.22	0/144	0.50	0/195
All	All	0.27	0/41287	0.52	0/55736

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	52	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11245	323	0
2	B	8701	0	8822	225	0
3	C	2655	0	2628	52	0
4	D	1140	0	1112	42	0
5	E	1759	0	1788	50	0
6	F	671	0	692	23	0
7	G	1544	0	1540	41	0
8	H	1103	0	1079	28	0
9	I	872	0	817	29	0
10	J	549	0	559	8	0
11	K	792	0	790	16	0
12	L	381	0	384	13	0
13	M	1492	0	1456	54	0
14	N	1169	0	1208	58	0
15	O	4558	0	4735	139	0
16	P	1126	0	1079	35	0
17	Q	829	0	819	28	0
18	W	141	0	137	6	0
19	X	50	0	15	1	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
21	I	1	0	0	0	0
22	I	1	0	0	0	0
All	All	40665	0	40905	1004	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1004) 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)
16:P:253:LEU:HB3	16:P:261:TYR:HB3	1.53	0.90
2:B:264:SER:HB3	2:B:267:GLU:HG2	1.55	0.87
11:K:55:SER:HB3	11:K:60:SER:HB2	1.57	0.87
1:A:85:LYS:HD3	1:A:260:TYR:HE1	1.41	0.83
1:A:300:LYS:HD2	17:Q:33:ILE:HG13	1.63	0.81
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.62	0.81
1:A:176:LEU:HB3	1:A:320:GLN:HE22	1.46	0.81
16:P:256:VAL:HB	16:P:260:CYS:HB2	1.65	0.79
17:Q:133:PRO:HD2	17:Q:136:LEU:HD12	1.64	0.78
2:B:831:GLU:HB2	2:B:834:MET:HG3	1.67	0.77
14:N:316:PHE:CE2	14:N:360:VAL:HA	2.20	0.77
1:A:1436:ILE:HD11	7:G:22:THR:HB	1.65	0.76
4:D:127:LEU:HB3	4:D:133:HIS:HB3	1.68	0.76
9:I:28:SER:HA	13:M:186:ILE:HD11	1.67	0.76
15:O:232:LEU:HD13	15:O:237:LYS:HB3	1.67	0.75
1:A:264:PRO:O	1:A:269:ARG:NH1	2.20	0.75
15:O:603:LEU:O	15:O:607:ASN:ND2	2.21	0.74
15:O:361:PHE:HE1	15:O:457:LEU:HD11	1.52	0.74
16:P:247:LEU:O	16:P:252:LYS:HB2	1.87	0.74
2:B:198:GLU:HB2	2:B:475:SER:HA	1.71	0.73
15:O:210:PRO:HG2	15:O:213:ASP:HB2	1.71	0.73
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.71	0.73
2:B:302:LEU:HB3	2:B:325:GLU:HG2	1.70	0.72
4:D:4:LEU:HB2	7:G:6:LYS:HG3	1.70	0.72
10:J:10:CYS:SG	10:J:43:ARG:NE	2.61	0.72
13:M:100:LYS:HD2	13:M:101:PRO:HD2	1.71	0.72
13:M:111:ARG:NH1	13:M:120:GLU:OE1	2.22	0.72
15:O:110:THR:HA	15:O:116:LYS:HB2	1.70	0.72
15:O:140:ILE:HG12	15:O:160:VAL:HG21	1.69	0.72
2:B:791:THR:HG21	2:B:842:TYR:HE2	1.52	0.71
15:O:194:LEU:HD23	15:O:200:LEU:HD22	1.73	0.71
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.55	0.71
13:M:89:GLN:HB3	14:N:390:PHE:HE2	1.54	0.71
2:B:119:ARG:NH2	2:B:176:GLU:OE2	2.23	0.70
1:A:368:LEU:HD12	1:A:1416:ILE:HG23	1.73	0.70
2:B:197:GLN:HB2	2:B:378:GLU:HG2	1.73	0.70
1:A:742:ILE:HD13	1:A:762:LEU:HD11	1.73	0.70
15:O:303:ARG:HH12	15:O:465:PHE:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:363:ILE:HG12	14:N:373:VAL:HG22	1.74	0.69
2:B:776:SER:HB2	3:C:217:ALA:HB2	1.75	0.69
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.74	0.69
15:O:77:ARG:HH22	15:O:117:THR:HG21	1.56	0.69
15:O:141:ILE:HD11	15:O:157:ALA:HB2	1.75	0.69
1:A:1124:PRO:O	1:A:1128:GLU:HG3	1.94	0.68
2:B:776:SER:HA	2:B:779:ASP:HB2	1.74	0.68
1:A:878:LYS:HZ1	9:I:87:ILE:HB	1.58	0.68
13:M:75:PRO:HG2	13:M:167:GLN:HG2	1.73	0.68
13:M:164:LYS:HE3	13:M:256:LYS:HD2	1.76	0.68
2:B:793:THR:HG21	2:B:843:ILE:HG21	1.75	0.68
1:A:108:LYS:O	15:O:572:HIS:NE2	2.26	0.67
16:P:253:LEU:HB3	16:P:261:TYR:CB	2.25	0.67
15:O:96:VAL:HG23	17:Q:136:LEU:HD13	1.77	0.67
15:O:52:LEU:HD11	15:O:131:LEU:HD22	1.77	0.67
13:M:168:VAL:HG11	14:N:363:ILE:HD12	1.77	0.66
1:A:665:ASP:H	1:A:668:VAL:HG12	1.60	0.66
1:A:200:GLU:HG2	15:O:515:LYS:HB3	1.76	0.66
13:M:161:ALA:HB2	13:M:170:LEU:HD13	1.77	0.66
1:A:128:ARG:HD2	1:A:128:ARG:N	2.10	0.66
15:O:253:ILE:HD11	15:O:330:LEU:HD12	1.77	0.66
1:A:93:ILE:HG12	1:A:324:ALA:HA	1.76	0.66
1:A:41:ASP:HB2	1:A:44:LYS:HG2	1.78	0.65
2:B:221:THR:HG21	2:B:333:ALA:HA	1.77	0.65
2:B:234:ILE:HD11	2:B:356:VAL:HG13	1.78	0.65
1:A:473:LEU:HB2	1:A:520:HIS:HB2	1.78	0.65
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.77	0.65
1:A:93:ILE:H	1:A:93:ILE:HD12	1.62	0.65
1:A:427:HIS:O	1:A:465:HIS:ND1	2.29	0.65
15:O:237:LYS:HD2	15:O:238:ARG:HE	1.62	0.65
1:A:599:LYS:NZ	8:H:90:ALA:O	2.29	0.65
4:D:13:ASP:OD2	4:D:125:ASN:ND2	2.30	0.65
2:B:882:ASP:HB3	2:B:901:ARG:HH11	1.62	0.65
1:A:108:LYS:HD3	1:A:222:LEU:HD21	1.79	0.65
13:M:94:PRO:HA	14:N:390:PHE:HA	1.79	0.65
3:C:111:ASP:HB3	18:W:620:ARG:H	1.61	0.65
2:B:1036:HIS:HB2	2:B:1054:ARG:HG3	1.78	0.65
15:O:628:LYS:O	15:O:632:GLU:HG2	1.97	0.64
16:P:163:PRO:HG3	16:P:233:VAL:HG11	1.78	0.64
1:A:754:PRO:HB3	9:I:53:ASP:HB3	1.79	0.64
16:P:175:ILE:HA	16:P:178:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:163:PRO:HA	7:G:166:ARG:HE	1.61	0.64
15:O:43:ASN:ND2	15:O:45:ASP:OD2	2.30	0.64
1:A:11:LYS:HD2	2:B:1117:ILE:HD13	1.80	0.64
1:A:368:LEU:HB3	1:A:1416:ILE:HG12	1.79	0.64
1:A:254:GLU:OE1	1:A:259:ARG:NH2	2.31	0.64
1:A:464:ARG:NH1	1:A:470:ASP:OD2	2.29	0.64
2:B:73:LEU:HD13	2:B:98:ILE:HG12	1.78	0.64
2:B:199:GLN:HE22	2:B:378:GLU:HB3	1.63	0.64
3:C:255:VAL:HG12	3:C:256:ILE:HG23	1.78	0.64
1:A:386:ASN:ND2	2:B:765:TYR:OH	2.30	0.64
13:M:266:LYS:HE2	14:N:357:ALA:HB1	1.80	0.64
1:A:1125:ARG:NH2	1:A:1317:ASN:O	2.30	0.64
7:G:189:GLU:HG2	7:G:191:PRO:HD3	1.80	0.64
16:P:247:LEU:C	16:P:249:TYR:N	2.49	0.63
1:A:1155:ARG:NH2	9:I:52:ASP:O	2.30	0.63
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.79	0.63
2:B:542:THR:HB	13:M:153:VAL:HG21	1.80	0.63
15:O:232:LEU:HB2	15:O:236:LYS:HG3	1.80	0.63
3:C:248:GLN:HA	3:C:256:ILE:HD11	1.80	0.63
15:O:537:LEU:O	15:O:541:ILE:HG12	1.98	0.63
15:O:541:ILE:HD12	15:O:548:ILE:HD11	1.81	0.63
1:A:892:SER:HB2	1:A:1371:ILE:HG23	1.81	0.63
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.45	0.63
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.80	0.62
2:B:1001:LYS:O	3:C:277:ARG:NH2	2.31	0.62
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.30	0.62
8:H:64:ASN:HA	8:H:88:SER:HB2	1.80	0.62
1:A:556:ASP:OD2	2:B:945:ASN:ND2	2.26	0.62
2:B:497:LEU:HD13	2:B:512:LYS:HD2	1.80	0.62
2:B:286:ASN:HA	2:B:289:GLU:HG2	1.81	0.62
4:D:107:MET:SD	4:D:107:MET:N	2.72	0.62
4:D:106:LEU:HB3	4:D:110:LEU:HD23	1.81	0.62
1:A:774:ARG:NH2	1:A:775:GLU:OE1	2.33	0.62
1:A:913:GLN:NE2	1:A:1360:ASP:OD2	2.30	0.62
2:B:1036:HIS:NE2	2:B:1058:GLY:O	2.32	0.62
4:D:152:GLU:OE1	4:D:152:GLU:N	2.23	0.62
7:G:120:TYR:HB2	7:G:129:ILE:HD11	1.82	0.62
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.81	0.62
7:G:162:SER:HB3	7:G:165:GLU:HG3	1.80	0.62
3:C:74:GLU:OE2	3:C:324:LYS:NZ	2.33	0.61
4:D:115:LEU:HD12	4:D:144:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:492:TYR:CZ	15:O:573:SER:HB2	2.34	0.61
16:P:193:ASN:HB2	16:P:197:ASN:HB2	1.82	0.61
1:A:1415:ILE:HD13	2:B:1067:ARG:HD2	1.82	0.61
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.35	0.61
2:B:267:GLU:HA	2:B:270:GLN:HB2	1.81	0.61
6:F:107:VAL:HG21	6:F:111:LEU:HD21	1.82	0.61
15:O:132:TYR:HD1	15:O:135:LEU:HD12	1.64	0.61
1:A:239:CYS:SG	1:A:252:ARG:NH2	2.72	0.61
15:O:53:VAL:HG21	15:O:65:ILE:HG21	1.83	0.61
15:O:539:SER:O	15:O:542:ARG:NH1	2.33	0.61
1:A:668:VAL:HG22	1:A:677:VAL:HG23	1.83	0.61
1:A:986:ARG:HA	1:A:989:LEU:HG	1.82	0.61
5:E:6:GLU:HA	5:E:9:ILE:HG12	1.83	0.61
13:M:270:ALA:HA	14:N:316:PHE:HA	1.82	0.61
14:N:316:PHE:CZ	14:N:360:VAL:HA	2.36	0.61
1:A:766:ILE:HD11	1:A:822:ARG:CZ	2.31	0.61
1:A:1204:ASP:HA	1:A:1207:VAL:HG22	1.81	0.61
2:B:622:VAL:O	2:B:626:HIS:ND1	2.31	0.61
2:B:819:TRP:HA	2:B:822:GLN:HG2	1.83	0.61
15:O:35:SER:O	15:O:40:ARG:NH2	2.32	0.61
17:Q:41:LEU:HD23	17:Q:43:ILE:HG12	1.81	0.61
9:I:88:ARG:HB2	9:I:92:GLU:HB2	1.83	0.61
15:O:318:LEU:HD12	15:O:366:LEU:HD22	1.83	0.60
1:A:533:ASN:OD1	6:F:90:ARG:NH1	2.35	0.60
1:A:1347:GLY:HA3	9:I:107:TRP:HA	1.82	0.60
3:C:165:ARG:NH1	3:C:190:ASP:OD1	2.35	0.60
1:A:1192:THR:O	1:A:1196:LEU:HB2	2.01	0.60
2:B:271:LEU:O	2:B:550:HIS:NE2	2.32	0.60
10:J:7:CYS:HA	10:J:49:MET:HG3	1.83	0.60
1:A:884:TYR:OH	1:A:888:ARG:NH2	2.35	0.60
1:A:1141:ILE:HB	1:A:1295:VAL:HG22	1.83	0.60
1:A:1394:ASP:OD1	1:A:1395:HIS:N	2.35	0.60
4:D:11:LEU:HD21	7:G:4:LEU:HG	1.84	0.60
13:M:134:ASP:N	13:M:134:ASP:OD1	2.35	0.60
15:O:96:VAL:HB	17:Q:136:LEU:HD22	1.84	0.60
1:A:741:LEU:HD21	1:A:750:LEU:HD13	1.83	0.60
15:O:105:LYS:O	15:O:121:TYR:N	2.33	0.59
1:A:1289:GLY:O	1:A:1291:ARG:NH1	2.35	0.59
2:B:199:GLN:NE2	2:B:378:GLU:HB3	2.17	0.59
2:B:1101:MET:HE1	2:B:1126:LYS:HA	1.83	0.59
15:O:360:THR:HG22	15:O:477:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:HD12	1:A:682:LEU:HD13	1.84	0.59
1:A:1174:GLN:HG3	1:A:1185:GLN:HB3	1.85	0.59
2:B:74:LYS:NZ	2:B:97:ASP:OD1	2.29	0.59
2:B:322:GLU:O	2:B:325:GLU:HG3	2.02	0.59
5:E:34:GLU:OE2	5:E:34:GLU:N	2.26	0.59
2:B:532:LEU:HD21	2:B:578:LEU:HD23	1.83	0.59
3:C:126:PHE:HD1	3:C:131:THR:HG1	1.49	0.59
16:P:254:GLU:O	16:P:261:TYR:HA	2.03	0.59
1:A:126:GLU:OE1	1:A:129:ARG:NH2	2.35	0.59
3:C:256:ILE:HA	3:C:268:LYS:H	1.67	0.59
15:O:289:LYS:HE2	15:O:326:ILE:HB	1.85	0.59
2:B:297:THR:HG22	13:M:183:PHE:HB2	1.84	0.58
14:N:196:ILE:HG22	14:N:198:GLN:H	1.68	0.58
14:N:196:ILE:HB	14:N:199:LEU:HB2	1.85	0.58
1:A:477:GLN:OE1	1:A:518:ASN:ND2	2.35	0.58
2:B:85:SER:OG	2:B:404:ASP:OD1	2.21	0.58
2:B:791:THR:HG21	2:B:842:TYR:CE2	2.37	0.58
2:B:152:MET:SD	2:B:433:LEU:HD21	2.43	0.58
4:D:153:MET:O	4:D:157:ILE:HG12	2.02	0.58
1:A:513:ASP:HB2	2:B:919:LYS:HE3	1.85	0.58
1:A:613:LEU:O	1:A:696:ARG:NH1	2.34	0.58
1:A:1058:GLN:NE2	8:H:134:ASN:O	2.29	0.58
4:D:72:PHE:HB3	4:D:128:PRO:HD2	1.85	0.58
15:O:106:TYR:CD2	17:Q:133:PRO:HG3	2.39	0.58
1:A:955:LEU:HD12	1:A:1031:LEU:HB2	1.86	0.58
15:O:578:ARG:HH22	15:O:648:TRP:HB2	1.69	0.58
5:E:78:LEU:HD13	5:E:107:THR:HG23	1.86	0.58
2:B:194:ILE:HG12	2:B:455:THR:HG22	1.86	0.57
13:M:114:PRO:HG2	13:M:243:ILE:HG13	1.86	0.57
16:P:253:LEU:HB3	16:P:261:TYR:CG	2.39	0.57
1:A:968:GLY:HA2	1:A:971:GLU:HB2	1.86	0.57
1:A:252:ARG:HE	1:A:253:PRO:HD2	1.69	0.57
1:A:275:GLN:HE21	1:A:281:ASN:HD22	1.50	0.57
1:A:167:ALA:HB2	1:A:177:LYS:HB2	1.87	0.57
1:A:742:ILE:HD11	1:A:840:LYS:HB2	1.86	0.57
4:D:126:GLN:NE2	7:G:84:ILE:O	2.34	0.57
13:M:89:GLN:HB3	14:N:390:PHE:CE2	2.38	0.57
13:M:253:GLU:OE2	13:M:256:LYS:HE3	2.04	0.57
17:Q:69:PRO:HB3	17:Q:120:ILE:HG23	1.87	0.57
15:O:75:SER:H	15:O:78:GLU:HG3	1.69	0.57
2:B:276:ASP:O	2:B:280:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:LYS:HB3	7:G:98:LYS:HB3	1.87	0.57
1:A:1286:ARG:HD2	1:A:1292:GLU:HG2	1.87	0.57
2:B:230:LYS:HZ3	2:B:333:ALA:HB2	1.70	0.57
3:C:1:MET:SD	3:C:1:MET:N	2.76	0.57
16:P:215:TYR:HB2	16:P:260:CYS:HB3	1.87	0.57
2:B:68:PHE:HA	2:B:72:ASP:HB2	1.87	0.56
16:P:164:TRP:HD1	16:P:175:ILE:HD12	1.70	0.56
1:A:556:ASP:HB2	2:B:767:ILE:HD13	1.87	0.56
15:O:529:LYS:HE3	16:P:172:ILE:HG12	1.86	0.56
2:B:698:ARG:NH2	2:B:917:GLY:O	2.37	0.56
4:D:66:LEU:HD12	4:D:95:ILE:HG13	1.87	0.56
2:B:217:GLN:O	2:B:232:TYR:HB3	2.05	0.56
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.85	0.56
4:D:139:GLU:OE2	17:Q:109:SER:OG	2.24	0.56
2:B:168:GLU:HA	2:B:171:MET:HB2	1.88	0.56
1:A:88:LEU:HB3	1:A:316:TRP:CE2	2.41	0.56
1:A:1192:THR:HG23	1:A:1196:LEU:HD13	1.86	0.56
2:B:665:ASP:N	2:B:665:ASP:OD1	2.37	0.56
1:A:583:MET:HG3	1:A:696:ARG:HG2	1.88	0.56
1:A:1232:ILE:HD13	1:A:1267:LEU:HD11	1.88	0.56
1:A:37:ARG:NH2	17:Q:16:MET:SD	2.71	0.56
4:D:71:ASN:HD22	7:G:86:THR:HG21	1.71	0.56
15:O:193:GLN:HG2	15:O:197:MET:SD	2.46	0.56
1:A:867:SER:O	1:A:870:GLU:HG3	2.06	0.55
12:L:32:ALA:HB3	12:L:53:HIS:CE1	2.40	0.55
15:O:168:SER:HB3	15:O:279:SER:HB2	1.88	0.55
3:C:229:LEU:HD13	3:C:295:ARG:HA	1.87	0.55
2:B:117:GLU:HG3	12:L:55:ILE:HD11	1.88	0.55
16:P:244:CYS:HA	16:P:247:LEU:HG	1.88	0.55
3:C:140:CYS:HB2	3:C:196:LEU:CD1	2.37	0.55
15:O:222:HIS:NE2	15:O:248:ASP:OD2	2.31	0.55
2:B:701:TYR:CZ	9:I:91:ASP:HB3	2.41	0.55
3:C:111:ASP:OD2	18:W:617:LYS:NZ	2.40	0.55
5:E:93:MET:O	5:E:97:VAL:HG23	2.06	0.55
1:A:770:LEU:HD11	1:A:842:PRO:HB3	1.88	0.55
15:O:263:LEU:HA	15:O:274:VAL:HA	1.88	0.55
3:C:115:TRP:HH2	3:C:212:ILE:HG12	1.72	0.55
4:D:115:LEU:HA	4:D:144:ARG:HH12	1.72	0.55
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.88	0.55
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.87	0.55
13:M:87:VAL:HG22	14:N:394:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:164:ILE:HG22	15:O:282:ILE:HG21	1.88	0.54
16:P:291:PHE:HD2	16:P:293:ILE:HG22	1.72	0.54
1:A:111:SER:OG	1:A:233:GLN:OE1	2.23	0.54
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.89	0.54
7:G:191:PRO:HG2	7:G:192:PRO:HD3	1.89	0.54
8:H:11:GLN:HE21	8:H:52:GLN:HA	1.71	0.54
11:K:87:GLU:HB3	11:K:108:TYR:CZ	2.43	0.54
15:O:288:MET:HE2	15:O:326:ILE:HG21	1.90	0.54
2:B:549:LEU:HD23	2:B:550:HIS:CE1	2.42	0.54
4:D:130:ASN:HD22	4:D:133:HIS:CD2	2.26	0.54
3:C:100:ARG:NH2	3:C:192:LEU:O	2.38	0.54
1:A:129:ARG:HD3	1:A:130:PRO:HD2	1.90	0.54
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.90	0.54
2:B:649:LEU:HD11	2:B:672:HIS:CE1	2.43	0.54
2:B:841:ILE:HG12	2:B:870:PRO:HB2	1.89	0.54
7:G:89:ILE:HG13	7:G:143:ASN:H	1.73	0.54
15:O:584:ASN:O	15:O:588:LEU:HG	2.08	0.54
15:O:239:SER:HA	15:O:242:LYS:HE3	1.90	0.54
1:A:978:ASP:N	1:A:982:CYS:O	2.40	0.53
3:C:327:TYR:OH	11:K:43:ASP:OD2	2.22	0.53
8:H:15:VAL:HG13	8:H:26:ILE:HG22	1.89	0.53
15:O:100:GLN:NE2	15:O:166:LEU:O	2.25	0.53
1:A:1360:ASP:O	1:A:1364:TYR:HB3	2.08	0.53
13:M:130:PHE:HD2	14:N:199:LEU:HD13	1.73	0.53
1:A:963:ALA:HB2	1:A:1012:ILE:HG21	1.90	0.53
13:M:82:GLU:N	13:M:82:GLU:OE1	2.41	0.53
2:B:94:LYS:HB3	2:B:134:GLU:HB2	1.91	0.53
2:B:503:PRO:HG2	2:B:511:VAL:HB	1.91	0.53
15:O:52:LEU:HD21	15:O:131:LEU:HD13	1.89	0.53
1:A:15:GLY:HA2	1:A:1408:VAL:HG23	1.89	0.53
8:H:31:THR:O	8:H:32:THR:OG1	2.22	0.53
1:A:425:ASN:OD1	1:A:445:ARG:NH1	2.39	0.53
1:A:167:ALA:N	1:A:177:LYS:O	2.42	0.53
2:B:302:LEU:HD22	2:B:325:GLU:OE2	2.09	0.53
1:A:476:ARG:HG3	1:A:517:MET:HG2	1.91	0.53
2:B:766:ASP:HB3	2:B:772:VAL:HG23	1.91	0.53
2:B:775:LYS:HB2	2:B:925:ILE:HG22	1.90	0.53
1:A:1429:LYS:HG3	6:F:137:TYR:HE2	1.73	0.52
4:D:65:TYR:OH	4:D:126:GLN:OE1	2.26	0.52
4:D:122:GLN:NE2	7:G:83:GLU:HG3	2.25	0.52
13:M:247:TRP:NE1	13:M:249:GLU:HB2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:OE2	1:A:442:ARG:NH2	2.36	0.52
2:B:698:ARG:NH1	9:I:90:ALA:O	2.42	0.52
8:H:135:LEU:HB2	8:H:137:GLN:OE1	2.08	0.52
2:B:177:CYS:HB2	2:B:714:ALA:HB1	1.90	0.52
2:B:295:ILE:HG12	9:I:28:SER:HB3	1.92	0.52
5:E:97:VAL:HG13	5:E:127:ILE:HD13	1.91	0.52
6:F:75:PRO:HD2	6:F:78:GLN:NE2	2.25	0.52
14:N:367:LYS:H	14:N:367:LYS:HD2	1.75	0.52
17:Q:20:PRO:HG2	17:Q:23:LEU:HB2	1.91	0.52
1:A:573:ARG:NH2	11:K:87:GLU:HB2	2.25	0.52
2:B:354:ARG:O	2:B:358:MET:HG3	2.09	0.52
13:M:75:PRO:HA	14:N:362:SER:HA	1.91	0.52
2:B:145:LYS:HZ2	2:B:419:LEU:HD22	1.74	0.52
2:B:215:ILE:HB	2:B:234:ILE:HD12	1.92	0.52
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.45	0.52
4:D:130:ASN:N	4:D:154:LEU:HD11	2.25	0.52
15:O:171:VAL:HG13	15:O:280:LEU:HD11	1.91	0.52
1:A:1436:ILE:HD12	7:G:23:ILE:HG12	1.91	0.52
17:Q:65:VAL:HG22	17:Q:70:PHE:HB2	1.91	0.52
1:A:268:ILE:O	1:A:356:ARG:NH2	2.41	0.52
1:A:830:ARG:HD2	1:A:835:PHE:O	2.09	0.52
1:A:911:ILE:HD12	5:E:170:LEU:HD11	1.91	0.52
1:A:1138:THR:O	1:A:1138:THR:OG1	2.25	0.52
5:E:94:LYS:HD3	5:E:123:LEU:HD21	1.92	0.52
15:O:641:LEU:O	15:O:645:LEU:HG	2.09	0.52
1:A:556:ASP:OD1	2:B:761:SER:OG	2.23	0.52
1:A:1051:ASN:O	8:H:131:ASN:ND2	2.42	0.52
2:B:298:GLN:O	2:B:302:LEU:HG	2.10	0.52
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.91	0.52
2:B:1112:SER:HB3	2:B:1114:GLU:HG2	1.91	0.52
4:D:109:LYS:HD3	4:D:156:ILE:HG13	1.92	0.52
1:A:372:ARG:NH1	2:B:1059:GLY:O	2.43	0.51
1:A:875:THR:HG21	9:I:89:SER:HA	1.91	0.51
2:B:826:PRO:HB2	12:L:27:LEU:HD11	1.92	0.51
18:W:612:ASP:OD2	18:W:614:TRP:NE1	2.43	0.51
2:B:463:TYR:OH	2:B:744:ILE:O	2.22	0.51
4:D:8:ASN:HD21	7:G:6:LYS:HB3	1.75	0.51
5:E:79:TRP:HB2	5:E:105:PHE:CD2	2.45	0.51
14:N:354:ARG:HG3	14:N:356:LEU:HB2	1.92	0.51
15:O:580:ASN:O	15:O:584:ASN:ND2	2.43	0.51
1:A:1167:SER:OG	1:A:1268:PRO:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:687:LEU:HD12	2:B:741:ILE:HG22	1.92	0.51
1:A:537:VAL:HG13	1:A:551:ILE:HD13	1.93	0.51
4:D:58:ILE:HG13	7:G:46:ILE:HG23	1.91	0.51
7:G:149:ARG:O	7:G:198:GLY:HA2	2.10	0.51
14:N:292:ARG:HG3	14:N:292:ARG:HH11	1.76	0.51
15:O:61:ALA:HB1	15:O:98:LEU:HD13	1.91	0.51
15:O:128:HIS:HB3	15:O:132:TYR:CD2	2.46	0.51
15:O:311:VAL:HG22	15:O:374:LEU:HD21	1.93	0.51
1:A:386:ASN:HB2	11:K:95:HIS:HD2	1.75	0.51
2:B:278:SER:O	2:B:282:ILE:HG13	2.09	0.51
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.92	0.51
14:N:-106:UNK:HA	14:N:207:VAL:HG12	1.93	0.51
16:P:171:ASP:HB3	16:P:174:PHE:HB3	1.92	0.51
1:A:1048:VAL:HG13	1:A:1052:VAL:HG22	1.93	0.51
1:A:1329:GLU:OE2	5:E:200:ARG:NH2	2.44	0.51
1:A:617:ASN:O	1:A:620:SER:OG	2.29	0.51
1:A:719:PRO:HG2	1:A:724:LYS:HE3	1.93	0.51
1:A:1235:PHE:CG	1:A:1236:PRO:HD2	2.46	0.51
1:A:106:ILE:HA	1:A:113:ILE:HA	1.93	0.51
1:A:599:LYS:HG3	1:A:600:PRO:HA	1.93	0.51
7:G:80:PHE:CG	7:G:81:LEU:N	2.79	0.51
1:A:1149:ASN:OD1	1:A:1150:ASP:N	2.44	0.51
2:B:747:ASP:OD1	2:B:747:ASP:N	2.42	0.51
4:D:48:ARG:HB3	4:D:50:TYR:CE2	2.46	0.51
1:A:1141:ILE:HG12	1:A:1316:THR:HB	1.94	0.50
2:B:740:THR:O	2:B:744:ILE:HG12	2.11	0.50
3:C:113:LEU:HD11	3:C:132:ILE:HG12	1.93	0.50
15:O:608:ARG:HG2	15:O:610:ASP:OD1	2.12	0.50
2:B:240:ILE:HG12	2:B:356:VAL:HG11	1.92	0.50
15:O:174:TYR:O	15:O:178:VAL:HG23	2.12	0.50
1:A:287:VAL:O	1:A:290:THR:OG1	2.27	0.50
1:A:957:TYR:HD1	1:A:1031:LEU:HB3	1.77	0.50
1:A:1054:THR:HG23	8:H:131:ASN:HB2	1.94	0.50
2:B:170:LYS:HE3	2:B:174:LEU:HD11	1.92	0.50
13:M:268:LEU:HD12	13:M:269:VAL:H	1.76	0.50
1:A:88:LEU:HB3	1:A:316:TRP:CZ2	2.47	0.50
5:E:111:VAL:HG12	5:E:137:GLU:HG3	1.94	0.50
8:H:92:ASP:OD1	8:H:92:ASP:N	2.38	0.50
14:N:316:PHE:CZ	14:N:360:VAL:HB	2.47	0.50
15:O:312:TYR:HD1	15:O:315:ALA:HB3	1.76	0.50
2:B:269:MET:HE1	2:B:280:GLN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LEU:HD21	2:B:520:ILE:HD12	1.94	0.50
2:B:527:GLU:OE2	2:B:527:GLU:N	2.30	0.50
4:D:127:LEU:HD11	7:G:84:ILE:HG21	1.93	0.50
8:H:11:GLN:NE2	8:H:52:GLN:HA	2.27	0.50
14:N:316:PHE:CZ	14:N:360:VAL:CA	2.95	0.50
15:O:171:VAL:HG12	15:O:191:PHE:CE2	2.46	0.50
1:A:412:ASN:HB3	6:F:115:THR:HB	1.92	0.50
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.94	0.50
13:M:147:THR:HG21	13:M:184:LYS:HE3	1.93	0.50
15:O:137:ILE:HG13	17:Q:57:LYS:HD3	1.92	0.50
1:A:41:ASP:HB3	1:A:43:GLU:HG3	1.94	0.50
1:A:828:GLN:NE2	2:B:593:ASN:OD1	2.40	0.50
2:B:419:LEU:O	2:B:422:ILE:HG22	2.11	0.50
2:B:719:LYS:HE2	10:J:65:PRO:HB3	1.94	0.50
1:A:384:ASP:HB2	1:A:499:ARG:HB3	1.94	0.50
1:A:573:ARG:HH21	11:K:87:GLU:HB2	1.77	0.50
1:A:603:LEU:HD12	8:H:46:LEU:HD11	1.93	0.50
1:A:785:LEU:HD23	1:A:792:LEU:HB2	1.94	0.50
2:B:678:PHE:HB2	2:B:978:CYS:HB3	1.93	0.50
5:E:112:TYR:HE2	5:E:134:THR:HG22	1.75	0.50
13:M:278:ILE:HD13	14:N:422:ILE:HG23	1.94	0.50
1:A:473:LEU:HD11	2:B:1078:LEU:HD21	1.94	0.49
1:A:613:LEU:HD11	1:A:697:MET:HA	1.94	0.49
2:B:543:LEU:HD11	13:M:176:VAL:HG21	1.94	0.49
15:O:74:LEU:HB2	15:O:78:GLU:HB2	1.94	0.49
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.76	0.49
2:B:207:VAL:HG21	2:B:355:ARG:HB3	1.95	0.49
2:B:527:GLU:HG2	2:B:528:PRO:HD3	1.92	0.49
2:B:660:ALA:HB2	2:B:670:MET:SD	2.53	0.49
2:B:911:LYS:HD2	2:B:1027:LEU:HD12	1.95	0.49
3:C:127:THR:HA	12:L:-899:UNK:HA	1.94	0.49
15:O:338:ASP:HB3	15:O:342:ALA:HA	1.94	0.49
1:A:545:LYS:NZ	1:A:1349:SER:O	2.41	0.49
1:A:567:LYS:HD3	8:H:23:VAL:HG11	1.93	0.49
1:A:891:LYS:HE2	1:A:1389:PHE:HB2	1.94	0.49
12:L:32:ALA:HB3	12:L:53:HIS:HE1	1.77	0.49
1:A:21:LEU:HD11	2:B:1133:LEU:HD22	1.92	0.49
1:A:222:LEU:HD13	1:A:226:LYS:HD3	1.95	0.49
1:A:1284:ASN:N	1:A:1292:GLU:O	2.37	0.49
4:D:115:LEU:HD12	4:D:144:ARG:NH1	2.28	0.49
15:O:29:GLU:OE1	15:O:29:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:TYR:O	4:D:68:ILE:HG22	2.12	0.49
11:K:49:LEU:HD11	11:K:61:ALA:HB1	1.95	0.49
13:M:96:LEU:HD12	14:N:224:SER:O	2.12	0.49
15:O:78:GLU:O	15:O:82:LYS:HB2	2.12	0.49
15:O:454:ASN:O	15:O:458:LYS:HG3	2.12	0.49
15:O:102:ARG:O	15:O:126:GLY:HA3	2.13	0.49
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.22	0.49
2:B:263:LEU:HD22	2:B:298:GLN:HB2	1.95	0.49
5:E:13:TRP:NE1	5:E:37:LEU:O	2.41	0.49
5:E:107:THR:OG1	5:E:133:GLU:OE1	2.31	0.49
14:N:209:HIS:O	14:N:209:HIS:ND1	2.38	0.49
1:A:583:MET:CG	1:A:696:ARG:HG2	2.43	0.49
2:B:277:SER:HB3	14:N:206:ARG:HB2	1.94	0.49
2:B:804:ASP:OD1	2:B:847:VAL:HG22	2.13	0.49
2:B:890:ASP:OD1	2:B:890:ASP:N	2.45	0.49
4:D:142:ASP:OD1	4:D:142:ASP:N	2.46	0.49
1:A:44:LYS:HE3	1:A:47:ALA:O	2.13	0.49
2:B:241:TYR:HB3	2:B:250:GLU:HB2	1.94	0.49
5:E:110:PHE:HE1	5:E:112:TYR:HB3	1.78	0.49
15:O:215:TRP:O	15:O:219:TYR:HB2	2.13	0.49
15:O:602:LEU:HB3	15:O:627:LEU:HD21	1.94	0.49
1:A:44:LYS:HD2	1:A:49:LYS:HG3	1.94	0.48
1:A:252:ARG:NE	1:A:253:PRO:HD2	2.28	0.48
5:E:9:ILE:HG13	5:E:10:SER:N	2.28	0.48
15:O:234:ASP:O	15:O:237:LYS:HG3	2.13	0.48
1:A:103:LEU:HD22	1:A:108:LYS:HE2	1.95	0.48
2:B:207:VAL:HA	2:B:217:GLN:HB2	1.95	0.48
8:H:63:LEU:HD12	8:H:89:LEU:HB3	1.95	0.48
17:Q:103:ASP:OD1	17:Q:103:ASP:N	2.45	0.48
1:A:714:ILE:HD13	2:B:958:MET:HB2	1.94	0.48
2:B:240:ILE:HG22	2:B:253:ILE:HB	1.95	0.48
13:M:173:ILE:HD11	14:N:306:VAL:HG22	1.96	0.48
15:O:166:LEU:HD11	17:Q:125:HIS:CE1	2.48	0.48
1:A:624:ILE:HD12	1:A:680:THR:HG22	1.94	0.48
7:G:158:VAL:HG22	7:G:160:PRO:HD3	1.95	0.48
15:O:625:ASN:O	15:O:629:MET:HG2	2.13	0.48
2:B:55:LYS:HD3	2:B:519:HIS:CD2	2.49	0.48
7:G:105:PHE:HE2	7:G:196:LEU:HD13	1.78	0.48
1:A:134:ASN:O	1:A:138:MET:HG2	2.12	0.48
1:A:813:VAL:O	1:A:848:VAL:HB	2.12	0.48
1:A:888:ARG:HG2	1:A:1371:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:GLU:OE1	1:A:1412:SER:OG	2.30	0.48
1:A:1443:PRO:HB3	7:G:73:ARG:CZ	2.43	0.48
1:A:1099:GLU:O	1:A:1102:THR:OG1	2.32	0.48
1:A:1400:ALA:HB2	2:B:1137:ILE:HG23	1.96	0.48
2:B:669:SER:O	2:B:669:SER:OG	2.28	0.48
7:G:81:LEU:HD22	17:Q:107:ARG:HD3	1.95	0.48
15:O:361:PHE:CE1	15:O:457:LEU:HD11	2.41	0.48
3:C:40:PHE:O	11:K:134:LYS:NZ	2.47	0.48
5:E:43:LYS:HA	5:E:47:CYS:HB2	1.96	0.48
6:F:79:ARG:NH1	6:F:145:ASP:O	2.47	0.48
1:A:40:PHE:HB3	1:A:46:ARG:HA	1.96	0.48
1:A:430:ALA:HA	1:A:464:ARG:HA	1.94	0.48
2:B:778:ILE:HG12	2:B:906:PRO:HG2	1.96	0.48
13:M:136:ALA:HB1	13:M:143:VAL:HG21	1.96	0.48
1:A:319:LEU:HA	1:A:322:THR:HG22	1.96	0.48
1:A:408:VAL:HG21	1:A:456:LEU:HD22	1.95	0.48
1:A:942:ALA:O	1:A:946:THR:OG1	2.30	0.48
2:B:473:ILE:HD11	2:B:514:LEU:HG	1.96	0.48
3:C:33:VAL:O	3:C:34:GLU:HB2	2.14	0.48
14:N:361:GLY:HA3	14:N:374:LYS:O	2.13	0.48
14:N:394:VAL:HG23	14:N:409:LEU:HB2	1.95	0.48
3:C:136:LEU:HD23	3:C:204:LEU:HD21	1.95	0.47
3:C:138:VAL:HG11	3:C:162:VAL:HG22	1.95	0.47
1:A:1079:ARG:HD3	6:F:84:TYR:CE1	2.49	0.47
2:B:216:VAL:HB	2:B:233:VAL:HG13	1.95	0.47
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.96	0.47
5:E:50:MET:SD	5:E:50:MET:N	2.88	0.47
1:A:28:ALA:N	15:O:32:MET:HE1	2.29	0.47
2:B:772:VAL:HB	2:B:943:ILE:HB	1.97	0.47
4:D:123:ILE:HG22	4:D:137:ILE:HD13	1.97	0.47
5:E:80:VAL:HG22	5:E:109:ILE:HD12	1.96	0.47
15:O:289:LYS:NZ	15:O:324:PRO:O	2.29	0.47
1:A:535:MET:HG2	2:B:1073:TYR:CG	2.49	0.47
1:A:717:VAL:HA	1:A:810:VAL:HG22	1.96	0.47
1:A:1208:ALA:HB3	1:A:1272:VAL:HG12	1.96	0.47
2:B:294:ASP:N	2:B:294:ASP:OD1	2.45	0.47
2:B:1084:MET:HG3	2:B:1122:PRO:HG3	1.96	0.47
15:O:137:ILE:O	15:O:140:ILE:HG22	2.14	0.47
1:A:325:MET:HA	1:A:329:SER:HA	1.96	0.47
1:A:1216:LYS:HB3	1:A:1217:ILE:HD12	1.95	0.47
2:B:449:MET:SD	2:B:449:MET:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.96	0.47
5:E:152:LYS:HE3	5:E:154:ILE:HD11	1.97	0.47
15:O:376:LEU:HD23	15:O:456:HIS:CE1	2.50	0.47
1:A:46:ARG:NH1	1:A:46:ARG:HB3	2.29	0.47
1:A:205:LEU:HD22	1:A:212:GLU:HG3	1.96	0.47
1:A:473:LEU:HD11	2:B:1078:LEU:HD11	1.96	0.47
3:C:17:SER:HB3	3:C:19:ASP:OD1	2.14	0.47
13:M:277:TYR:HA	13:M:280:ASN:HB3	1.96	0.47
16:P:237:PRO:O	16:P:240:ILE:HG22	2.15	0.47
1:A:54:LEU:HD11	1:A:282:GLU:HG3	1.97	0.47
1:A:406:GLU:HG2	1:A:416:LEU:HD11	1.97	0.47
1:A:471:VAL:HB	1:A:528:ARG:HG3	1.97	0.47
1:A:555:GLN:HG2	1:A:556:ASP:H	1.79	0.47
1:A:564:ILE:HD13	1:A:700:LEU:HD21	1.96	0.47
1:A:866:ILE:HG12	2:B:489:LEU:HB3	1.96	0.47
2:B:207:VAL:HA	2:B:217:GLN:CB	2.44	0.47
4:D:60:ARG:HA	4:D:63:VAL:HG12	1.97	0.47
5:E:153:HIS:HB3	5:E:196:VAL:HG21	1.97	0.47
8:H:132:LEU:HD23	8:H:132:LEU:H	1.80	0.47
13:M:252:PHE:CE1	13:M:256:LYS:HB2	2.50	0.47
15:O:458:LYS:HG2	15:O:476:TYR:OH	2.14	0.47
2:B:553:TYR:CE1	2:B:597:MET:HG2	2.50	0.47
5:E:43:LYS:O	5:E:47:CYS:HB2	2.14	0.47
9:I:35:ILE:HG13	9:I:38:ILE:HG13	1.97	0.47
15:O:156:VAL:O	15:O:159:ILE:HG22	2.15	0.47
1:A:14:LYS:HB2	2:B:1144:GLU:HG2	1.97	0.47
2:B:846:SER:HB3	2:B:866:TYR:HB3	1.97	0.47
15:O:263:LEU:HB3	15:O:274:VAL:HG12	1.97	0.47
15:O:633:ARG:HH12	16:P:307:LYS:HB2	1.79	0.47
1:A:800:LYS:HG2	2:B:947:HIS:O	2.15	0.47
1:A:881:GLU:HG3	1:A:1106:LEU:HD21	1.96	0.47
10:J:1:MET:HA	10:J:56:LEU:HB2	1.95	0.47
15:O:497:ALA:O	15:O:505:MET:HE1	2.15	0.47
15:O:518:SER:H	15:O:521:ILE:HB	1.80	0.47
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.96	0.47
1:A:23:ALA:O	1:A:27:VAL:HG23	2.14	0.46
1:A:229:ASN:HB3	15:O:544:ASN:OD1	2.14	0.46
2:B:911:LYS:HE3	2:B:1029:HIS:HB2	1.96	0.46
3:C:40:PHE:HD2	11:K:134:LYS:HG3	1.80	0.46
1:A:275:GLN:HB3	1:A:281:ASN:HB2	1.97	0.46
1:A:948:ASN:H	1:A:1061:ARG:HH22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:ILE:HG22	1:A:1218:GLN:HG3	1.96	0.46
2:B:518:THR:HB	2:B:608:ILE:HD11	1.96	0.46
2:B:1147:PHE:CD1	7:G:58:GLN:HG3	2.50	0.46
13:M:228:THR:OG1	13:M:229:GLY:N	2.48	0.46
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.96	0.46
14:N:388:THR:HB	14:N:390:PHE:CE1	2.50	0.46
3:C:192:LEU:HG	10:J:2:ILE:HD11	1.97	0.46
13:M:78:ILE:HG22	14:N:358:GLY:O	2.15	0.46
14:N:379:VAL:HG13	14:N:421:GLN:NE2	2.30	0.46
1:A:406:GLU:OE1	1:A:415:LYS:NZ	2.45	0.46
7:G:156:VAL:HG11	7:G:190:LYS:HB3	1.96	0.46
1:A:422:ASN:ND2	1:A:428:PRO:O	2.48	0.46
1:A:914:PHE:HZ	5:E:175:LEU:HD23	1.81	0.46
15:O:460:LEU:O	15:O:463:SER:OG	2.26	0.46
16:P:269:LEU:HG	16:P:297:PHE:HE2	1.81	0.46
13:M:274:GLN:HG3	14:N:378:VAL:HG22	1.98	0.46
15:O:230:SER:HB3	15:O:232:LEU:HG	1.98	0.46
15:O:332:GLN:HE21	15:O:345:PHE:HD2	1.64	0.46
1:A:85:LYS:HD3	1:A:260:TYR:CE1	2.33	0.46
2:B:262:ILE:HG13	2:B:346:ALA:HB1	1.97	0.46
2:B:371:TYR:OH	2:B:655:ASN:ND2	2.46	0.46
2:B:723:THR:HA	2:B:790:LYS:HG2	1.97	0.46
16:P:180:THR:HA	16:P:183:TRP:CD1	2.51	0.46
16:P:240:ILE:HD12	16:P:243:LEU:HD12	1.98	0.46
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.31	0.46
13:M:89:GLN:HB2	13:M:178:GLN:HA	1.97	0.46
15:O:361:PHE:CE1	15:O:366:LEU:HD11	2.51	0.46
1:A:593:PRO:HD3	1:A:612:LEU:HD21	1.98	0.46
1:A:627:ASP:OD1	1:A:655:ARG:NH2	2.49	0.46
2:B:77:ILE:HG13	2:B:95:TYR:HB3	1.98	0.46
14:N:364:ARG:NE	14:N:374:LYS:HG3	2.31	0.46
15:O:326:ILE:HG12	15:O:653:MET:HG2	1.97	0.46
1:A:233:GLN:HG2	15:O:579:GLN:OE1	2.16	0.45
1:A:396:ASP:OD1	1:A:396:ASP:N	2.48	0.45
1:A:473:LEU:HB3	1:A:485:ILE:HD11	1.97	0.45
2:B:228:LYS:HE2	2:B:331:VAL:HG12	1.98	0.45
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.98	0.45
2:B:737:LYS:HB2	2:B:741:ILE:HG12	1.97	0.45
4:D:7:ARG:NH2	17:Q:102:ASN:O	2.48	0.45
5:E:30:ILE:HG23	5:E:34:GLU:HG2	1.98	0.45
15:O:599:ASN:HD21	15:O:630:VAL:HG11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:138:ASP:OD2	17:Q:54:LEU:HD13	2.15	0.45
15:O:267:PRO:HD3	15:O:273:ILE:HG22	1.98	0.45
1:A:891:LYS:HG3	1:A:1389:PHE:CD1	2.50	0.45
5:E:16:PHE:O	5:E:20:LYS:HG2	2.15	0.45
6:F:97:ARG:HG2	6:F:130:ILE:HG12	1.97	0.45
1:A:12:ARG:NH2	2:B:1144:GLU:OE1	2.50	0.45
1:A:511:ASP:OD1	1:A:511:ASP:N	2.49	0.45
1:A:878:LYS:HE2	1:A:1104:MET:C	2.35	0.45
1:A:1206:ALA:O	1:A:1210:THR:HG23	2.17	0.45
2:B:831:GLU:HB3	12:L:61:THR:HB	1.98	0.45
5:E:143:ASN:HD21	5:E:146:HIS:CD2	2.34	0.45
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.84	0.45
15:O:95:LEU:HD21	15:O:120:TYR:CE1	2.52	0.45
1:A:48:PRO:HB2	1:A:56:PRO:HD3	1.99	0.45
1:A:632:VAL:HG21	1:A:796:THR:HA	1.99	0.45
2:B:262:ILE:HG22	2:B:268:ILE:HG13	1.97	0.45
3:C:38:LYS:NZ	3:C:39:ASP:OD1	2.50	0.45
15:O:650:VAL:HA	15:O:653:MET:CE	2.47	0.45
1:A:10:PRO:HG2	2:B:1147:PHE:HE2	1.82	0.45
2:B:86:ASP:OD1	2:B:86:ASP:N	2.48	0.45
5:E:52:ARG:H	5:E:52:ARG:HG2	1.44	0.45
6:F:105:ALA:HB2	7:G:15:PRO:HB3	1.97	0.45
14:N:392:GLN:HB3	14:N:412:VAL:HB	1.98	0.45
15:O:239:SER:O	15:O:242:LYS:HG2	2.16	0.45
1:A:939:TRP:CD1	1:A:1015:LYS:HE3	2.51	0.45
3:C:77:SER:HB3	3:C:219:PHE:O	2.16	0.45
3:C:235:ILE:HG23	3:C:239:ILE:HD12	1.99	0.45
4:D:6:GLU:HG3	7:G:42:VAL:HG13	1.97	0.45
17:Q:27:ASP:OD1	17:Q:28:VAL:N	2.49	0.45
17:Q:54:LEU:HA	17:Q:57:LYS:HG2	1.99	0.45
1:A:256:TYR:CE2	1:A:1401:PHE:HD1	2.35	0.45
1:A:582:MET:SD	1:A:703:ARG:HB3	2.57	0.45
1:A:774:ARG:NE	9:I:63:ASP:OD2	2.49	0.45
1:A:815:GLN:HG3	1:A:817:ILE:HG12	1.99	0.45
1:A:1421:MET:SD	1:A:1423:ILE:HB	2.56	0.45
2:B:40:THR:OG1	2:B:624:ASP:HB3	2.17	0.45
2:B:447:PHE:HB3	2:B:449:MET:CE	2.47	0.45
2:B:834:MET:SD	12:L:63:ARG:HD2	2.57	0.45
4:D:117:LYS:HA	4:D:117:LYS:HD2	1.79	0.45
5:E:19:VAL:HG13	5:E:140:LEU:HD13	1.99	0.45
15:O:292:ARG:O	15:O:295:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:O	1:A:606:GLY:HA3	2.16	0.45
1:A:813:VAL:HG23	1:A:851:SER:HA	1.99	0.45
1:A:1434:THR:HG23	7:G:56:GLU:HA	1.98	0.45
3:C:61:THR:HA	3:C:298:PHE:CZ	2.52	0.45
3:C:212:ILE:HD13	3:C:212:ILE:HA	1.83	0.45
9:I:8:CYS:SG	9:I:10:ASN:HB2	2.57	0.45
15:O:293:SER:O	15:O:297:ILE:HG12	2.17	0.45
15:O:456:HIS:O	15:O:459:ILE:HG12	2.17	0.45
16:P:269:LEU:HG	16:P:297:PHE:CE2	2.52	0.45
1:A:106:ILE:HG22	1:A:113:ILE:HA	1.99	0.45
1:A:794:MET:SD	2:B:950:PRO:HG3	2.57	0.45
2:B:476:GLN:O	2:B:479:LYS:HE3	2.16	0.45
2:B:1117:ILE:HD11	2:B:1143:LEU:HD13	1.99	0.45
6:F:72:LYS:HA	6:F:72:LYS:HD3	1.74	0.45
13:M:95:ARG:HG3	14:N:390:PHE:O	2.17	0.45
13:M:168:VAL:HG11	14:N:363:ILE:CD1	2.46	0.45
14:N:309:LEU:HD23	14:N:313:LEU:HD21	1.99	0.45
17:Q:35:GLU:H	17:Q:35:GLU:HG3	1.35	0.45
1:A:557:PHE:HB3	1:A:697:MET:HE3	1.99	0.44
1:A:742:ILE:CD1	1:A:840:LYS:HB2	2.47	0.44
2:B:208:GLU:HG2	2:B:216:VAL:O	2.17	0.44
2:B:1108:THR:O	2:B:1108:THR:OG1	2.33	0.44
9:I:107:TRP:HE1	9:I:109:GLU:HG3	1.81	0.44
12:L:28:LYS:HD2	12:L:37:LYS:HG3	1.99	0.44
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.98	0.44
1:A:1174:GLN:HB2	1:A:1185:GLN:H	1.82	0.44
1:A:1387:ALA:HB1	1:A:1392:THR:HG23	1.98	0.44
2:B:480:SER:O	2:B:480:SER:OG	2.36	0.44
8:H:30:SER:HB3	8:H:33:GLN:O	2.17	0.44
15:O:258:GLU:O	15:O:258:GLU:HG2	2.17	0.44
15:O:552:PRO:HB3	15:O:557:ARG:HG2	1.98	0.44
1:A:872:LEU:HD11	9:I:90:ALA:HB2	1.99	0.44
2:B:38:ILE:HD11	2:B:628:ARG:NH2	2.32	0.44
2:B:593:ASN:HB3	2:B:596:GLN:O	2.18	0.44
2:B:739:LYS:O	2:B:742:GLU:HG2	2.18	0.44
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.99	0.44
3:C:106:LEU:HD22	3:C:134:LEU:HD11	1.99	0.44
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.99	0.44
4:D:27:HIS:C	4:D:28:LEU:HG	2.38	0.44
6:F:97:ARG:NH2	6:F:106:PRO:O	2.51	0.44
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:137:GLN:NE2	8:H:139:ASN:O	2.43	0.44
1:A:966:ILE:HD11	1:A:1068:ARG:HG2	1.99	0.44
10:J:31:ASP:HB2	10:J:34:THR:HG22	1.99	0.44
11:K:50:LEU:HD12	11:K:62:SER:HB3	1.99	0.44
13:M:140:TRP:HB3	13:M:185:TYR:HB2	2.00	0.44
1:A:1118:ASN:O	1:A:1138:THR:HG21	2.17	0.44
1:A:1177:TYR:CE2	9:I:14:ILE:HG13	2.52	0.44
1:A:1256:VAL:HG22	1:A:1259:ARG:HH12	1.82	0.44
2:B:347:LEU:O	2:B:351:MET:HG2	2.17	0.44
2:B:885:MET:HE1	2:B:897:LYS:HD2	2.00	0.44
3:C:314:PHE:O	3:C:318:VAL:HG23	2.18	0.44
14:N:285:ALA:O	14:N:288:GLN:HG2	2.18	0.44
14:N:395:ILE:HG12	14:N:396:ALA:N	2.33	0.44
17:Q:32:HIS:O	17:Q:33:ILE:HG22	2.17	0.44
1:A:309:ILE:HA	1:A:312:MET:HB3	2.00	0.44
1:A:778:GLY:O	1:A:782:ILE:HG12	2.18	0.44
1:A:1019:LEU:HD13	1:A:1060:TYR:HB2	2.00	0.44
1:A:1140:ILE:HG21	1:A:1294:LEU:HD12	1.98	0.44
12:L:50:ASP:OD1	12:L:50:ASP:N	2.51	0.44
1:A:602:TYR:CE2	8:H:81:PRO:HB3	2.53	0.44
1:A:853:PHE:HA	2:B:955:VAL:HG11	1.99	0.44
2:B:750:PRO:HG3	10:J:54:VAL:HG21	2.00	0.44
15:O:313:LYS:HD3	15:O:314:ILE:HG13	1.98	0.44
2:B:82:LEU:HD11	2:B:92:TYR:HB2	1.99	0.44
15:O:237:LYS:O	15:O:240:GLN:HG3	2.18	0.44
15:O:288:MET:CE	15:O:326:ILE:HG21	2.48	0.44
15:O:583:TRP:HZ3	16:P:314:GLU:HB3	1.83	0.44
16:P:247:LEU:C	16:P:249:TYR:H	2.19	0.44
1:A:1155:ARG:HH21	9:I:51:VAL:HB	1.83	0.44
1:A:1369:LEU:HD13	1:A:1378:LYS:HB3	2.00	0.44
2:B:228:LYS:HD3	2:B:244:HIS:NE2	2.33	0.44
3:C:324:LYS:HE2	3:C:324:LYS:HB3	1.68	0.44
15:O:160:VAL:HA	15:O:163:VAL:HG12	2.00	0.44
1:A:82:GLY:O	1:A:263:ALA:N	2.51	0.43
1:A:91:PHE:CG	1:A:224:PRO:HG3	2.53	0.43
1:A:256:TYR:HE2	1:A:1401:PHE:HA	1.82	0.43
2:B:247:ILE:HG23	2:B:308:LYS:HB3	1.98	0.43
2:B:461:LEU:HD13	2:B:1028:LYS:HD3	2.00	0.43
2:B:591:TYR:CE1	2:B:652:ASN:HB3	2.52	0.43
2:B:1129:PHE:CE2	2:B:1141:LEU:HD21	2.52	0.43
5:E:79:TRP:HD1	5:E:96:PHE:HE1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.54	0.43
5:E:112:TYR:CE2	5:E:134:THR:HG22	2.52	0.43
6:F:128:LYS:HE3	6:F:149:GLU:HA	1.99	0.43
11:K:78:TYR:CZ	11:K:82:LYS:HD2	2.52	0.43
14:N:297:MET:O	14:N:297:MET:HG2	2.18	0.43
15:O:108:GLN:HA	15:O:118:THR:HA	1.99	0.43
1:A:114:LEU:HD11	1:A:161:ASN:ND2	2.32	0.43
1:A:664:MET:HE1	1:A:668:VAL:HG11	2.00	0.43
1:A:826:GLY:HA3	2:B:491:PRO:HB2	2.00	0.43
1:A:895:ASP:OD1	1:A:1410:GLY:HA2	2.18	0.43
1:A:1048:VAL:HG12	1:A:1053:LYS:HD3	1.99	0.43
2:B:295:ILE:CG1	9:I:28:SER:HB3	2.48	0.43
5:E:79:TRP:CD1	5:E:96:PHE:HE1	2.36	0.43
13:M:168:VAL:HG22	13:M:170:LEU:HD22	1.99	0.43
15:O:98:LEU:HD12	15:O:98:LEU:HA	1.89	0.43
15:O:289:LYS:HA	15:O:289:LYS:HD3	1.83	0.43
15:O:502:PRO:O	15:O:505:MET:HG2	2.19	0.43
16:P:177:SER:HA	16:P:180:THR:HG22	1.99	0.43
2:B:73:LEU:HD23	2:B:73:LEU:HA	1.85	0.43
3:C:35:LYS:NZ	3:C:39:ASP:OD2	2.38	0.43
3:C:82:TYR:CE2	3:C:126:PHE:HZ	2.36	0.43
4:D:5:GLU:HG3	7:G:6:LYS:HG2	2.00	0.43
14:N:308:GLN:N	14:N:416:ILE:O	2.44	0.43
1:A:124:LEU:O	1:A:127:LEU:HB2	2.18	0.43
1:A:427:HIS:O	1:A:429:GLY:N	2.51	0.43
1:A:830:ARG:HD3	1:A:837:LYS:HA	2.00	0.43
5:E:3:GLN:HA	5:E:6:GLU:HG2	2.00	0.43
15:O:159:ILE:HD11	15:O:191:PHE:CZ	2.53	0.43
1:A:872:LEU:HD21	2:B:504:GLU:OE2	2.19	0.43
1:A:1448:PHE:CD1	4:D:12:SER:HB3	2.54	0.43
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.43	0.43
5:E:31:THR:OG1	5:E:32:GLN:N	2.51	0.43
7:G:83:GLU:HB2	7:G:150:ILE:HD13	1.99	0.43
2:B:96:VAL:HB	2:B:132:ASP:HB2	2.01	0.43
9:I:7:SER:O	13:M:146:GLN:NE2	2.52	0.43
9:I:81:TYR:CE2	9:I:101:VAL:HG12	2.54	0.43
11:K:87:GLU:HG3	11:K:106:GLN:O	2.19	0.43
13:M:247:TRP:HE1	13:M:249:GLU:HB2	1.83	0.43
1:A:41:ASP:N	1:A:44:LYS:HE2	2.34	0.43
1:A:44:LYS:NZ	1:A:49:LYS:HB2	2.34	0.43
1:A:108:LYS:NZ	1:A:180:HIS:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:HG2	15:O:560:SER:OG	2.18	0.43
2:B:57:LEU:HD11	2:B:516:LEU:HD12	1.99	0.43
3:C:278:GLU:O	3:C:281:ARG:HG2	2.19	0.43
15:O:76:VAL:HA	15:O:79:LEU:HD12	2.01	0.43
17:Q:41:LEU:HD12	17:Q:41:LEU:HA	1.91	0.43
1:A:483:LEU:HD22	1:A:550:ILE:HG21	2.00	0.43
1:A:501:ASN:O	1:A:504:VAL:HG22	2.18	0.43
1:A:770:LEU:O	1:A:773:VAL:HG12	2.18	0.43
1:A:957:TYR:CD1	1:A:1031:LEU:HB3	2.53	0.43
4:D:132:VAL:HA	4:D:135:TYR:HB3	2.01	0.43
7:G:39:ILE:HD11	7:G:45:CYS:HB2	2.01	0.43
14:N:364:ARG:HG2	14:N:364:ARG:HH11	1.84	0.43
14:N:377:ASN:HD22	14:N:377:ASN:HA	1.63	0.43
1:A:2:LYS:HG3	1:A:3:GLU:OE1	2.18	0.43
1:A:481:HIS:CD2	1:A:481:HIS:H	2.37	0.43
5:E:173:SER:O	5:E:177:ARG:NH1	2.51	0.43
6:F:75:PRO:HB2	6:F:77:ASP:OD1	2.18	0.43
13:M:112:TYR:HA	13:M:118:LEU:O	2.18	0.43
15:O:60:ARG:NH2	15:O:90:SER:O	2.48	0.43
15:O:273:ILE:HG13	15:O:274:VAL:N	2.34	0.43
1:A:210:GLU:HG3	1:A:214:TYR:CE2	2.54	0.43
1:A:665:ASP:OD1	1:A:797:CYS:HA	2.19	0.43
1:A:978:ASP:HB2	1:A:982:CYS:H	1.84	0.43
1:A:1155:ARG:HB2	1:A:1197:GLN:OE1	2.18	0.43
1:A:1278:ILE:HD12	1:A:1297:GLY:HA3	2.00	0.43
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.48	0.43
2:B:565:ILE:HD13	2:B:571:PHE:HB2	2.00	0.43
2:B:702:GLN:CD	2:B:915:ARG:HA	2.39	0.43
3:C:238:PRO:HB2	3:C:240:LYS:NZ	2.34	0.43
4:D:23:LEU:HD11	7:G:47:THR:HG21	2.01	0.43
6:F:81:THR:OG1	6:F:144:GLU:OE2	2.24	0.43
7:G:147:ARG:HB3	7:G:206:GLY:H	1.84	0.43
14:N:374:LYS:HE3	14:N:374:LYS:HB3	1.68	0.43
15:O:107:LEU:HD12	15:O:107:LEU:HA	1.89	0.43
15:O:132:TYR:CD1	15:O:135:LEU:HD12	2.50	0.43
15:O:203:ILE:HD11	15:O:208:TYR:CE2	2.54	0.43
15:O:308:THR:HA	15:O:311:VAL:HG23	2.01	0.43
16:P:171:ASP:O	16:P:175:ILE:HG12	2.19	0.43
1:A:211:LEU:O	1:A:215:VAL:HG13	2.19	0.42
1:A:232:LYS:HD2	16:P:315:TRP:CZ2	2.54	0.42
1:A:1037:LYS:HD2	1:A:1039:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:ASP:OD1	1:A:1189:ASP:N	2.50	0.42
1:A:1431:VAL:O	6:F:133:VAL:HG12	2.19	0.42
2:B:535:VAL:HG11	13:M:281:LEU:HG	2.01	0.42
2:B:796:LYS:HG2	2:B:804:ASP:OD2	2.19	0.42
9:I:98:TYR:HE2	9:I:109:GLU:HB2	1.84	0.42
1:A:1200:LEU:HD13	1:A:1273:LYS:HB2	2.02	0.42
2:B:321:GLN:HG2	2:B:323:GLY:H	1.83	0.42
4:D:109:LYS:CD	4:D:156:ILE:HG13	2.48	0.42
13:M:158:GLN:HB2	13:M:173:ILE:HB	2.01	0.42
15:O:370:LEU:HD13	15:O:376:LEU:HD11	2.02	0.42
15:O:370:LEU:HD11	15:O:453:ILE:HG12	2.01	0.42
1:A:1166:LEU:HD23	1:A:1267:LEU:O	2.19	0.42
1:A:1263:LEU:O	1:A:1267:LEU:HB2	2.18	0.42
2:B:46:HIS:CG	2:B:631:LEU:HD21	2.54	0.42
2:B:778:ILE:HG23	2:B:906:PRO:HG2	2.00	0.42
7:G:105:PHE:CE2	7:G:196:LEU:HD13	2.54	0.42
16:P:225:ILE:HD12	16:P:225:ILE:HA	1.91	0.42
1:A:88:LEU:HB3	1:A:316:TRP:NE1	2.35	0.42
1:A:538:LYS:HB3	1:A:687:PRO:HB2	2.02	0.42
2:B:228:LYS:HD3	2:B:244:HIS:CE1	2.54	0.42
2:B:676:GLU:HG2	2:B:678:PHE:CE2	2.55	0.42
2:B:1014:GLN:HA	3:C:12:VAL:HB	2.00	0.42
4:D:2:LYS:HE2	4:D:2:LYS:HB2	1.85	0.42
1:A:634:VAL:HG22	1:A:648:ASN:OD1	2.20	0.42
1:A:753:GLN:HG3	1:A:761:THR:HG23	2.01	0.42
1:A:957:TYR:O	1:A:961:GLU:HG2	2.19	0.42
2:B:258:LYS:NZ	2:B:263:LEU:O	2.52	0.42
2:B:262:ILE:HD12	2:B:271:LEU:HD11	2.02	0.42
3:C:285:PHE:O	3:C:289:VAL:HG12	2.19	0.42
5:E:124:VAL:N	5:E:125:PRO:HD3	2.35	0.42
16:P:266:GLU:O	16:P:270:GLN:HG2	2.20	0.42
1:A:68:ALA:HA	1:A:71:HIS:CE1	2.54	0.42
1:A:115:LEU:HD11	1:A:144:ILE:HG23	2.02	0.42
1:A:1001:GLU:HG3	1:A:1078:TYR:HE2	1.85	0.42
5:E:92:THR:O	5:E:95:THR:HG22	2.20	0.42
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.44	0.42
15:O:92:LYS:HD3	15:O:92:LYS:HA	1.86	0.42
16:P:179:LEU:HD12	16:P:179:LEU:HA	1.79	0.42
1:A:729:GLU:O	1:A:733:ILE:HG13	2.19	0.42
2:B:198:GLU:HG2	2:B:473:ILE:HG21	2.01	0.42
2:B:232:TYR:CE1	2:B:356:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:795:LEU:HD21	2:B:806:ILE:HG23	2.02	0.42
2:B:969:LEU:O	2:B:994:GLN:NE2	2.52	0.42
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.53	0.42
11:K:126:ASP:O	11:K:130:VAL:HG23	2.20	0.42
17:Q:14:ASN:HD21	17:Q:16:MET:HB2	1.84	0.42
1:A:108:LYS:NZ	1:A:164:VAL:HG13	2.34	0.42
1:A:828:GLN:HE22	2:B:593:ASN:CG	2.23	0.42
1:A:954:LEU:HB2	1:A:959:ILE:HG13	2.02	0.42
1:A:1079:ARG:HE	1:A:1079:ARG:HB3	1.65	0.42
2:B:496:MET:HB3	2:B:608:ILE:HG12	2.02	0.42
2:B:1062:LEU:HD23	2:B:1062:LEU:HA	1.89	0.42
4:D:148:LYS:HA	4:D:148:LYS:HD3	1.80	0.42
9:I:12:LEU:HB3	9:I:24:LEU:HD22	2.00	0.42
15:O:634:GLU:O	15:O:637:VAL:HG12	2.19	0.42
1:A:92:HIS:HA	1:A:258:TRP:CD1	2.54	0.42
1:A:395:PRO:HB3	1:A:495:TRP:O	2.20	0.42
2:B:464:ILE:HA	2:B:464:ILE:HD12	1.75	0.42
2:B:1088:ASP:O	2:B:1122:PRO:HA	2.20	0.42
3:C:290:LYS:HE2	3:C:290:LYS:HB2	1.88	0.42
7:G:52:LEU:HD21	7:G:73:ARG:HG3	2.01	0.42
8:H:131:ASN:N	8:H:131:ASN:OD1	2.53	0.42
14:N:291:LEU:HD11	14:N:365:VAL:HG11	2.02	0.42
15:O:345:PHE:O	15:O:348:GLU:HG2	2.20	0.42
16:P:263:VAL:HB	16:P:266:GLU:HG3	2.01	0.42
1:A:502:GLU:HG2	2:B:767:ILE:HB	2.02	0.42
1:A:573:ARG:HB3	3:C:20:PHE:HE2	1.85	0.42
1:A:1012:ILE:HD11	1:A:1070:PHE:CD2	2.55	0.42
2:B:800:ASN:ND2	2:B:850:ASN:O	2.53	0.42
6:F:78:GLN:O	6:F:78:GLN:HG2	2.19	0.42
7:G:10:LEU:HD11	7:G:67:TYR:HB3	2.00	0.42
7:G:43:GLY:HA2	7:G:78:LYS:HZ3	1.85	0.42
14:N:303:ARG:NE	14:N:411:ARG:HH12	2.18	0.42
14:N:316:PHE:CZ	14:N:360:VAL:O	2.73	0.42
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.60	0.41
8:H:27:GLU:OE1	8:H:39:THR:OG1	2.25	0.41
1:A:24:ALA:HB2	15:O:38:GLU:HA	2.01	0.41
1:A:328:ASN:HB2	1:A:354:CYS:SG	2.60	0.41
1:A:383:PRO:HB3	1:A:512:PHE:CE2	2.56	0.41
1:A:1001:GLU:HG3	1:A:1078:TYR:CE2	2.55	0.41
2:B:324:ILE:O	2:B:327:ILE:HG22	2.20	0.41
2:B:335:LEU:HD11	2:B:348:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:LEU:HB3	2:B:442:TRP:CZ3	2.55	0.41
9:I:91:ASP:OD1	9:I:92:GLU:HG2	2.20	0.41
1:A:114:LEU:HB2	1:A:148:CYS:HB2	2.00	0.41
1:A:381:ILE:HD11	1:A:510:ALA:HB1	2.01	0.41
1:A:545:LYS:HB2	1:A:1096:SER:HB3	2.01	0.41
1:A:952:LYS:HA	1:A:952:LYS:HD2	1.86	0.41
2:B:968:VAL:CG2	10:J:44:TYR:HB2	2.51	0.41
3:C:238:PRO:HB3	3:C:264:GLU:OE2	2.20	0.41
7:G:104:ILE:HG22	7:G:105:PHE:HD1	1.84	0.41
13:M:159:TYR:HB2	13:M:170:LEU:HD12	2.02	0.41
14:N:219:ILE:HA	14:N:222:ALA:HB3	2.02	0.41
14:N:379:VAL:HG13	14:N:421:GLN:HE21	1.84	0.41
1:A:41:ASP:HB2	1:A:44:LYS:CG	2.47	0.41
1:A:598:MET:SD	8:H:141:TYR:HE2	2.43	0.41
2:B:541:ILE:HA	2:B:544:ILE:HD12	2.01	0.41
2:B:808:GLY:HA3	2:B:844:ASN:ND2	2.36	0.41
5:E:13:TRP:HB2	5:E:42:PHE:CD2	2.56	0.41
6:F:111:LEU:HD22	6:F:120:ILE:HG12	2.02	0.41
13:M:77:LYS:HG2	14:N:359:LYS:HB2	2.02	0.41
13:M:111:ARG:HB2	13:M:120:GLU:HB2	2.02	0.41
13:M:130:PHE:CD2	14:N:199:LEU:HB3	2.55	0.41
15:O:163:VAL:HG23	15:O:169:LEU:HB3	2.02	0.41
1:A:607:LYS:HD2	8:H:120:GLY:HA3	2.02	0.41
1:A:1111:PHE:HB3	9:I:62:VAL:HG11	2.01	0.41
1:A:1352:PRO:HG3	5:E:204:THR:HG21	2.01	0.41
2:B:55:LYS:HD3	2:B:519:HIS:NE2	2.35	0.41
2:B:74:LYS:HE3	2:B:74:LYS:HB3	1.88	0.41
2:B:711:GLY:HA3	2:B:751:ALA:HA	2.01	0.41
7:G:78:LYS:HD3	7:G:78:LYS:HA	1.87	0.41
13:M:81:GLU:HG3	14:N:355:GLU:HA	2.03	0.41
15:O:56:HIS:CE1	15:O:130:LEU:HB3	2.56	0.41
17:Q:123:ASP:HB2	17:Q:141:GLY:H	1.85	0.41
1:A:108:LYS:HZ3	1:A:180:HIS:HB2	1.86	0.41
1:A:728:GLU:O	1:A:732:GLU:HG2	2.20	0.41
1:A:988:ASP:HB3	1:A:994:TYR:HE2	1.85	0.41
1:A:1139:PRO:HG3	1:A:1298:TYR:CE2	2.55	0.41
3:C:169:PHE:CE2	3:C:171:PRO:HG3	2.56	0.41
12:L:62:LYS:HA	12:L:62:LYS:HD3	1.83	0.41
13:M:164:LYS:HA	13:M:164:LYS:HD3	1.44	0.41
15:O:160:VAL:O	15:O:163:VAL:HG12	2.21	0.41
1:A:577:THR:HG21	11:K:88:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ILE:HG21	1:A:866:ILE:HG22	2.03	0.41
1:A:878:LYS:HZ1	9:I:87:ILE:CB	2.32	0.41
1:A:878:LYS:O	1:A:882:THR:HG23	2.21	0.41
1:A:1118:ASN:OD1	1:A:1118:ASN:N	2.54	0.41
1:A:1164:THR:OG1	1:A:1270:VAL:O	2.39	0.41
2:B:213:LYS:NZ	2:B:216:VAL:HG12	2.35	0.41
2:B:624:ASP:HA	2:B:627:LEU:HB2	2.02	0.41
2:B:820:GLN:HB3	2:B:821:HIS:HD2	1.86	0.41
2:B:908:LEU:HD11	2:B:924:ILE:HA	2.02	0.41
5:E:94:LYS:HD2	5:E:94:LYS:HA	1.75	0.41
5:E:143:ASN:HD21	5:E:146:HIS:CG	2.38	0.41
6:F:109:VAL:HG11	6:F:124:GLU:HA	2.02	0.41
15:O:214:LEU:O	15:O:218:LEU:HG	2.21	0.41
15:O:578:ARG:HA	15:O:578:ARG:CZ	2.51	0.41
1:A:235:LYS:HA	15:O:43:ASN:HD21	1.85	0.41
1:A:435:LYS:HB3	1:A:435:LYS:HE3	1.89	0.41
2:B:779:ASP:OD1	2:B:905:ARG:NH2	2.39	0.41
5:E:99:HIS:HE1	5:E:103:LYS:HG3	1.85	0.41
5:E:143:ASN:HD21	5:E:146:HIS:CE1	2.39	0.41
15:O:549:GLN:O	15:O:564:PHE:HB2	2.21	0.41
15:O:644:LEU:HD13	17:Q:43:ILE:HD13	2.02	0.41
16:P:236:THR:HG22	16:P:238:SER:H	1.85	0.41
17:Q:128:ASN:HB2	17:Q:131:LEU:HD23	2.03	0.41
1:A:261:LEU:HA	1:A:261:LEU:HD12	1.85	0.41
1:A:286:THR:O	1:A:290:THR:HG23	2.21	0.41
1:A:690:ALA:O	1:A:694:MET:HG3	2.21	0.41
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.87	0.41
1:A:1161:VAL:HG12	1:A:1275:LEU:HD23	2.01	0.41
1:A:1236:PRO:HD3	1:A:1256:VAL:HG21	2.03	0.41
1:A:1399:ALA:HA	1:A:1404:LYS:HG3	2.02	0.41
2:B:277:SER:H	2:B:277:SER:HG	1.53	0.41
2:B:701:TYR:CE2	9:I:91:ASP:HB3	2.56	0.41
3:C:84:TYR:HD1	12:L:64:LEU:HD21	1.85	0.41
4:D:3:VAL:HG22	7:G:7:ILE:HG12	2.03	0.41
4:D:130:ASN:HD21	4:D:132:VAL:HB	1.85	0.41
5:E:161:LYS:NZ	5:E:193:GLY:O	2.44	0.41
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.88	0.41
8:H:48:PRO:HD2	8:H:146:ARG:NH2	2.36	0.41
8:H:101:ALA:O	8:H:136:LYS:HG3	2.21	0.41
9:I:99:LYS:HB2	9:I:106:ARG:HG2	2.03	0.41
14:N:296:LYS:O	14:N:300:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:259:LEU:HD12	15:O:259:LEU:HA	1.92	0.41
15:O:504:ALA:HB2	15:O:536:THR:HB	2.03	0.41
16:P:179:LEU:HD11	16:P:247:LEU:HB3	2.03	0.41
18:W:624:PRO:HA	18:W:625:PRO:HD2	1.88	0.41
1:A:115:LEU:HD12	1:A:241:LEU:HD13	2.03	0.41
1:A:152:ARG:HG2	1:A:185:TRP:CD1	2.55	0.41
1:A:372:ARG:HA	2:B:1061:ARG:HA	2.02	0.41
1:A:862:LEU:HD21	2:B:491:PRO:HA	2.02	0.41
1:A:1203:GLU:O	1:A:1207:VAL:HG13	2.20	0.41
2:B:93:LEU:HD12	2:B:135:TYR:HB3	2.03	0.41
3:C:47:LEU:HD23	18:W:609:VAL:HB	2.03	0.41
6:F:77:ASP:OD1	6:F:77:ASP:N	2.54	0.41
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.84	0.41
13:M:85:LEU:HD11	14:N:394:VAL:HB	2.03	0.41
15:O:650:VAL:HA	15:O:653:MET:HE3	2.03	0.41
17:Q:62:GLY:O	17:Q:65:VAL:HG12	2.21	0.41
1:A:756:CYS:HB2	1:A:760:GLN:NE2	2.36	0.40
1:A:789:ASN:HB3	1:A:792:LEU:HB3	2.02	0.40
1:A:1339:ILE:HD13	1:A:1358:LEU:HD23	2.02	0.40
2:B:149:ILE:C	2:B:426:SER:HB2	2.41	0.40
2:B:194:ILE:HG23	2:B:454:VAL:HG12	2.02	0.40
2:B:253:ILE:HD12	2:B:253:ILE:HA	1.85	0.40
2:B:319:ILE:HD12	2:B:321:GLN:NE2	2.36	0.40
9:I:26:CYS:HB3	9:I:31:TYR:HB3	2.02	0.40
15:O:251:LYS:O	15:O:255:LYS:HG3	2.21	0.40
16:P:255:LYS:NZ	16:P:259:ASP:HA	2.36	0.40
19:X:1011:UNK:O	19:X:1013:UNK:N	2.54	0.40
1:A:586:GLY:O	11:K:62:SER:OG	2.31	0.40
1:A:992:ALA:O	5:E:199:ILE:HG13	2.20	0.40
1:A:1150:ASP:OD1	1:A:1291:ARG:HD3	2.21	0.40
2:B:525:GLU:H	2:B:525:GLU:HG3	1.71	0.40
2:B:1080:LEU:HD23	2:B:1080:LEU:HA	1.83	0.40
3:C:83:VAL:HG13	3:C:204:LEU:HD13	2.02	0.40
14:N:380:MET:HB3	14:N:419:THR:O	2.21	0.40
15:O:306:SER:HA	15:O:309:ALA:HB3	2.03	0.40
15:O:502:PRO:HA	15:O:505:MET:SD	2.61	0.40
1:A:714:ILE:HD12	1:A:714:ILE:HA	1.98	0.40
1:A:833:PRO:HB2	2:B:659:ILE:HD12	2.02	0.40
2:B:295:ILE:HD12	2:B:295:ILE:HA	1.90	0.40
2:B:326:ALA:HB3	13:M:231:LEU:HD23	2.03	0.40
2:B:773:LEU:HB2	2:B:922:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:GLY:HA3	2:B:1141:LEU:N	2.37	0.40
5:E:191:LYS:O	5:E:214:CYS:HB3	2.20	0.40
8:H:90:ALA:CB	8:H:96:VAL:HG21	2.52	0.40
13:M:249:GLU:HG2	14:N:408:LEU:HB3	2.02	0.40
14:N:382:ILE:HD11	14:N:416:ILE:HD12	2.03	0.40
18:W:614:TRP:HA	18:W:619:MET:HE3	2.03	0.40
1:A:808:GLN:CD	9:I:84:GLN:HE22	2.23	0.40
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.22	0.40
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.39	0.40
2:B:680:ILE:HD11	2:B:979:PHE:HZ	1.87	0.40
7:G:207:LEU:HB3	7:G:210:TRP:CD1	2.56	0.40
15:O:129:ILE:HG13	15:O:284:LEU:HD11	2.03	0.40
15:O:166:LEU:HD11	17:Q:125:HIS:NE2	2.37	0.40
1:A:18:PHE:O	1:A:1403:MET:HA	2.21	0.40
1:A:369:SER:O	1:A:369:SER:OG	2.37	0.40
1:A:1034:PRO:HA	1:A:1035:PRO:HD3	1.98	0.40
1:A:1310:ILE:O	1:A:1314:THR:OG1	2.28	0.40
2:B:38:ILE:HD11	2:B:628:ARG:HH21	1.86	0.40
2:B:588:ILE:HG12	2:B:603:THR:HG22	2.02	0.40
13:M:168:VAL:HG22	13:M:170:LEU:CD2	2.52	0.40
14:N:290:ILE:HD13	14:N:382:ILE:HG12	2.03	0.40
14:N:365:VAL:HA	14:N:371:LEU:HD13	2.04	0.40
15:O:384:LYS:HA	16:P:208:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1460 (97%)	1315 (93%)	96 (7%)	0	100	100
2	B	1098/1149 (96%)	1035 (94%)	63 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	333/335 (99%)	319 (96%)	14 (4%)	0	100	100
4	D	141/161 (88%)	126 (89%)	13 (9%)	2 (1%)	11	22
5	E	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
6	F	81/155 (52%)	80 (99%)	1 (1%)	0	100	100
7	G	185/212 (87%)	167 (90%)	18 (10%)	0	100	100
8	H	134/146 (92%)	123 (92%)	11 (8%)	0	100	100
9	I	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	35
10	J	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
13	M	179/282 (64%)	168 (94%)	11 (6%)	0	100	100
14	N	139/422 (33%)	136 (98%)	3 (2%)	0	100	100
15	O	564/654 (86%)	539 (96%)	25 (4%)	0	100	100
16	P	132/317 (42%)	122 (92%)	10 (8%)	0	100	100
17	Q	100/268 (37%)	93 (93%)	6 (6%)	1 (1%)	15	32
18	W	15/635 (2%)	15 (100%)	0	0	100	100
All	All	5039/6803 (74%)	4737 (94%)	298 (6%)	4 (0%)	54	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	46	GLN
4	D	49	PRO
17	Q	33	ILE
9	I	93	PRO

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	A	1230/1257 (98%)	1202 (98%)	28 (2%)	50	75
2	B	965/1006 (96%)	930 (96%)	35 (4%)	35	61
3	C	296/296 (100%)	290 (98%)	6 (2%)	55	78
4	D	123/145 (85%)	117 (95%)	6 (5%)	25	48
5	E	197/197 (100%)	183 (93%)	14 (7%)	14	29
6	F	73/137 (53%)	71 (97%)	2 (3%)	44	71
7	G	170/190 (90%)	166 (98%)	4 (2%)	49	74
8	H	121/128 (94%)	119 (98%)	2 (2%)	60	81
9	I	98/98 (100%)	95 (97%)	3 (3%)	40	66
10	J	62/65 (95%)	60 (97%)	2 (3%)	39	65
11	K	91/130 (70%)	90 (99%)	1 (1%)	73	88
12	L	39/39 (100%)	37 (95%)	2 (5%)	24	46
13	M	159/249 (64%)	152 (96%)	7 (4%)	28	53
14	N	125/200 (62%)	117 (94%)	8 (6%)	17	35
15	O	521/593 (88%)	497 (95%)	24 (5%)	27	51
16	P	126/285 (44%)	123 (98%)	3 (2%)	49	74
17	Q	92/212 (43%)	88 (96%)	4 (4%)	29	54
18	W	17/586 (3%)	17 (100%)	0	100	100
All	All	4505/5813 (78%)	4354 (97%)	151 (3%)	40	63

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	39	LEU
1	A	128	ARG
1	A	256	TYR
1	A	274	MET
1	A	275	GLN
1	A	276	ASP
1	A	310	ASN
1	A	316	TRP
1	A	481	HIS
1	A	500	LEU
1	A	555	GLN
1	A	610	PHE
1	A	649	ASP

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Mol	Chain	Res	Type
1	A	665	ASP
1	A	747	LYS
1	A	783	ASN
1	A	843	GLN
1	A	991	LYS
1	A	1050	ASP
1	A	1079	ARG
1	A	1200	LEU
1	A	1291	ARG
1	A	1292	GLU
1	A	1333	TYR
1	A	1348	MET
1	A	1379	MET
1	A	1402	TYR
2	B	143	MET
2	B	152	MET
2	B	193	VAL
2	B	200	LEU
2	B	217	GLN
2	B	221	THR
2	B	236	LYS
2	B	276	ASP
2	B	304	TYR
2	B	332	ILE
2	B	399	PHE
2	B	414	MET
2	B	431	SER
2	B	449	MET
2	B	493	GLN
2	B	529	ILE
2	B	551	LEU
2	B	552	ASN
2	B	594	SER
2	B	617	ASP
2	B	620	SER
2	B	623	LYS
2	B	638	ASP
2	B	669	SER
2	B	745	ASP
2	B	767	ILE
2	B	800	ASN
2	B	810	ARG

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Mol	Chain	Res	Type
2	B	834	MET
2	B	864	THR
2	B	1008	ILE
2	B	1051	THR
2	B	1052	GLU
2	B	1056	ARG
2	B	1135	MET
3	C	1	MET
3	C	77	SER
3	C	245	ARG
3	C	277	ARG
3	C	279	VAL
3	C	319	ARG
4	D	5	GLU
4	D	8	ASN
4	D	18	LYS
4	D	22	ASP
4	D	28	LEU
4	D	131	MET
5	E	48	ASP
5	E	49	SER
5	E	50	MET
5	E	52	ARG
5	E	57	MET
5	E	60	PHE
5	E	61	GLN
5	E	84	ASP
5	E	88	VAL
5	E	106	GLN
5	E	110	PHE
5	E	115	ASN
5	E	121	MET
5	E	158	SER
6	F	85	MET
6	F	147	SER
7	G	16	ASP
7	G	52	LEU
7	G	145	LYS
7	G	161	LYS
8	H	13	SER
8	H	77	ARG
9	I	44	LYS

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Mol	Chain	Res	Type
9	I	88	ARG
9	I	89	SER
10	J	7	CYS
10	J	48	ARG
11	K	55	SER
12	L	37	LYS
12	L	50	ASP
13	M	81	GLU
13	M	90	TYR
13	M	133	LYS
13	M	164	LYS
13	M	165	ASP
13	M	168	VAL
13	M	252	PHE
14	N	203	ARG
14	N	274	LYS
14	N	305	MET
14	N	364	ARG
14	N	367	LYS
14	N	387	GLU
14	N	390	PHE
14	N	395	ILE
15	O	82	LYS
15	O	86	MET
15	O	94	THR
15	O	124	GLU
15	O	174	TYR
15	O	189	SER
15	O	235	LEU
15	O	237	LYS
15	O	270	SER
15	O	286	ARG
15	O	361	PHE
15	O	375	ASP
15	O	464	ASN
15	O	505	MET
15	O	509	ARG
15	O	510	CYS
15	O	511	ILE
15	O	579	GLN
15	O	587	ASN
15	O	608	ARG

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Mol	Chain	Res	Type
15	O	617	GLU
15	O	619	LEU
15	O	628	LYS
15	O	638	PHE
16	P	218	THR
16	P	254	GLU
16	P	255	LYS
17	Q	15	TYR
17	Q	33	ILE
17	Q	34	THR
17	Q	35	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	310	ASN
1	A	760	GLN
1	A	783	ASN
1	A	1180	ASN
1	A	1185	GLN
2	B	159	ASN
2	B	199	GLN
2	B	275	ASN
2	B	321	GLN
2	B	423	ASN
2	B	1025	GLN
3	C	14	ASN
3	C	130	ASN
4	D	8	ASN
4	D	52	HIS
4	D	130	ASN
5	E	106	GLN
5	E	115	ASN
5	E	143	ASN
8	H	11	GLN
10	J	23	ASN
12	L	53	HIS
13	M	89	GLN
13	M	92	ASN
13	M	132	ASN
13	M	155	ASN

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Mol	Chain	Res	Type
13	M	178	GLN
14	N	287	HIS
14	N	366	HIS
14	N	377	ASN
15	O	43	ASN
15	O	254	ASN
15	O	587	ASN
15	O	607	ASN
16	P	176	ASN
17	Q	14	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

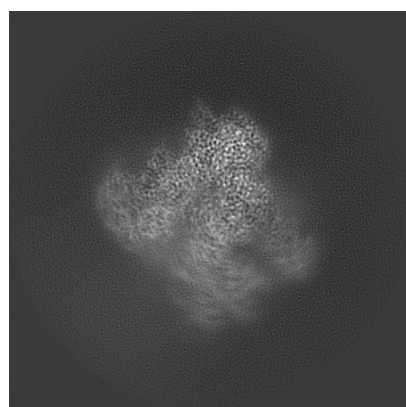
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14421. These allow visual inspection of the internal detail of the map and identification of artifacts.

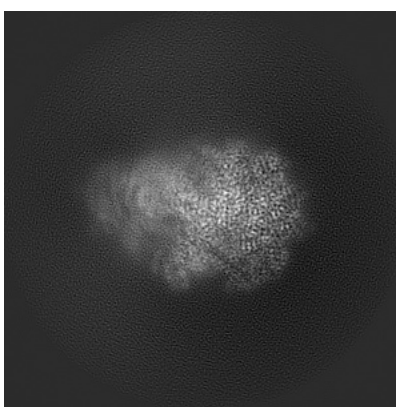
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

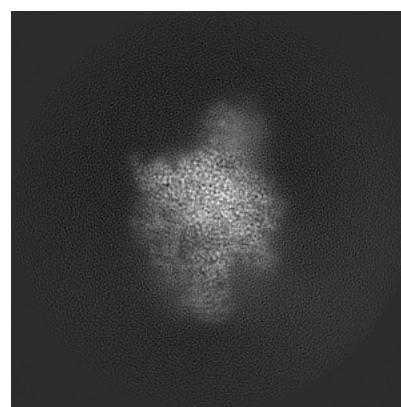
6.1.1 Primary map



X



Y

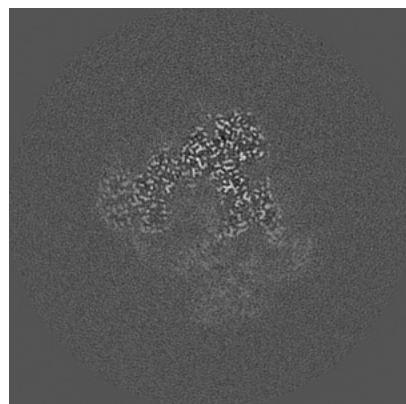


Z

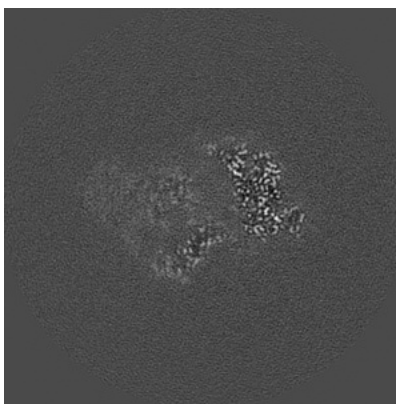
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

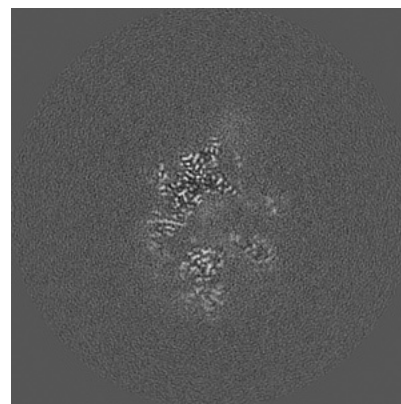
6.2.1 Primary map



X Index: 150



Y Index: 150

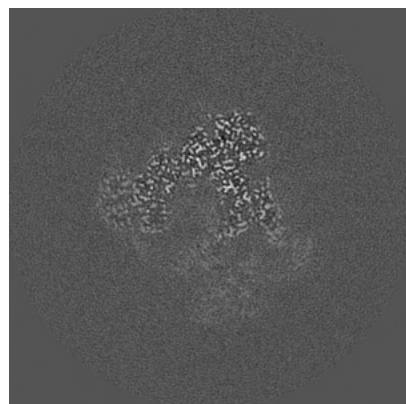


Z Index: 150

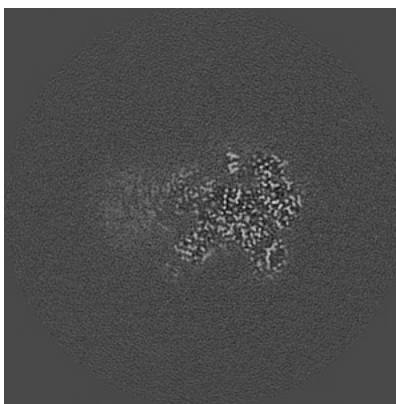
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

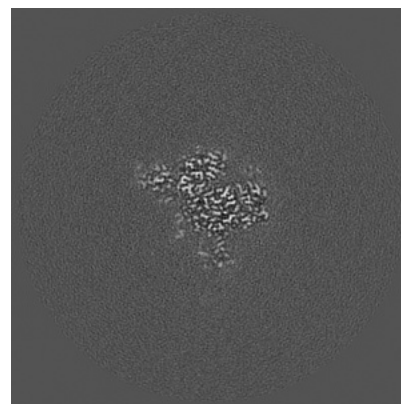
6.3.1 Primary map



X Index: 150



Y Index: 164

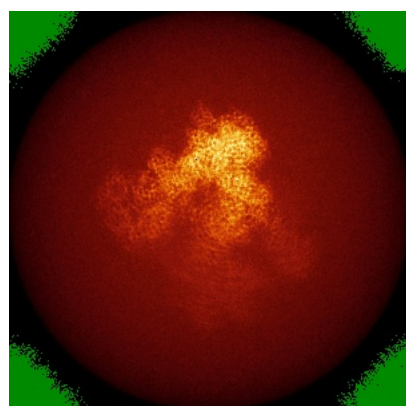


Z Index: 191

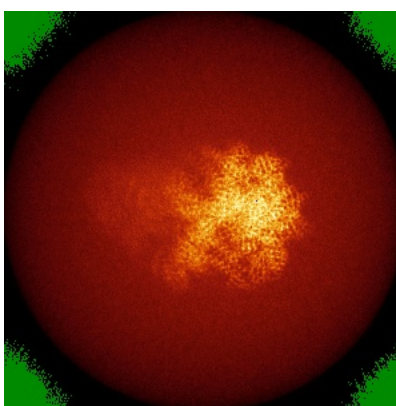
The images above show the largest variance slices of the map in three orthogonal directions.

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

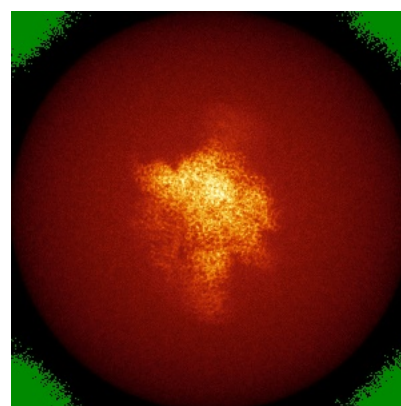
6.4.1 Primary map



X



Y

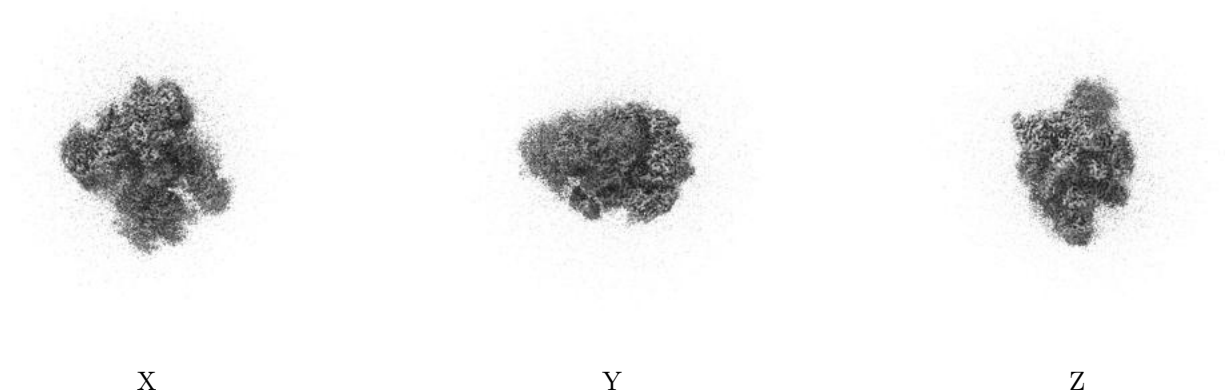


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0213. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

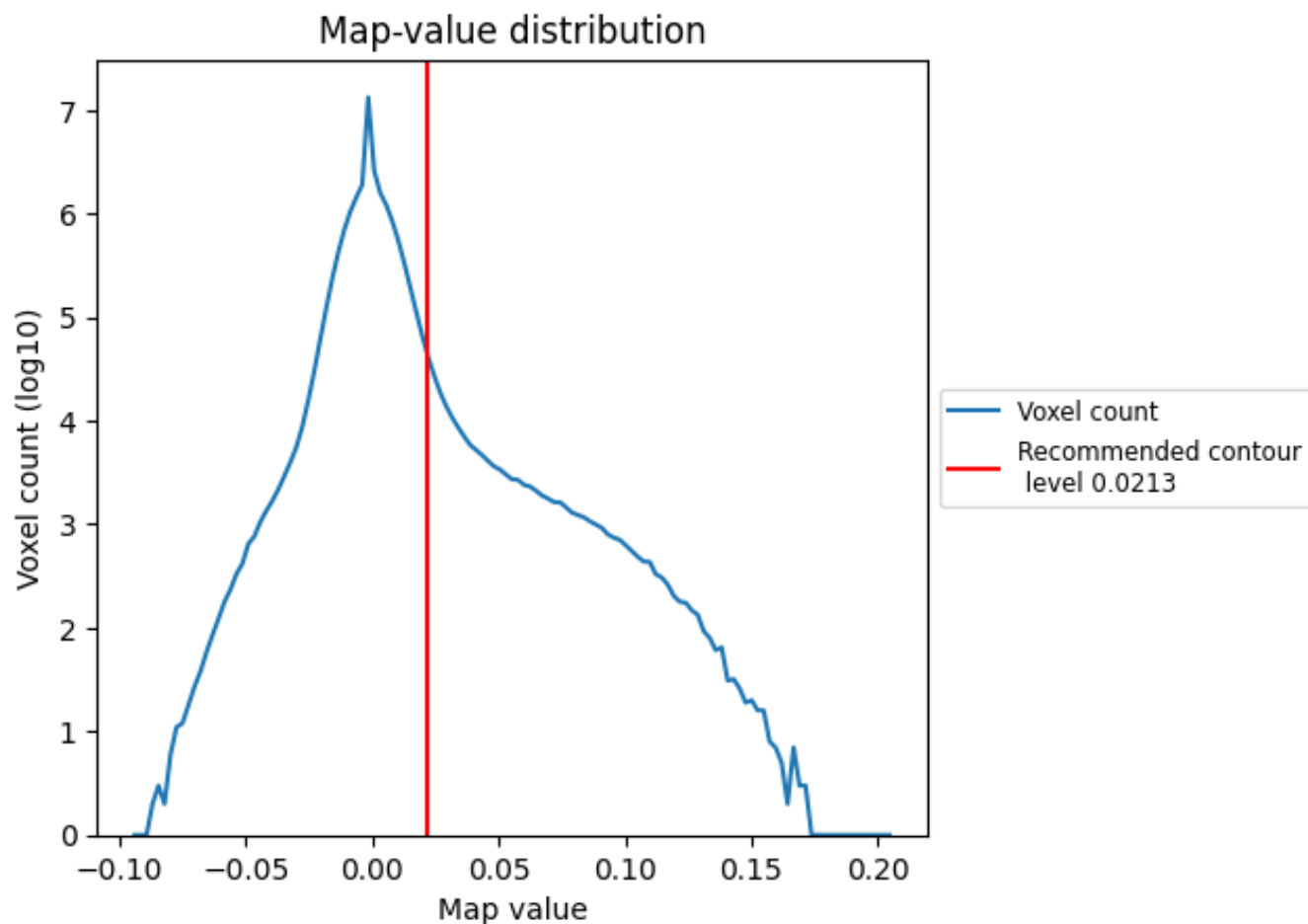
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

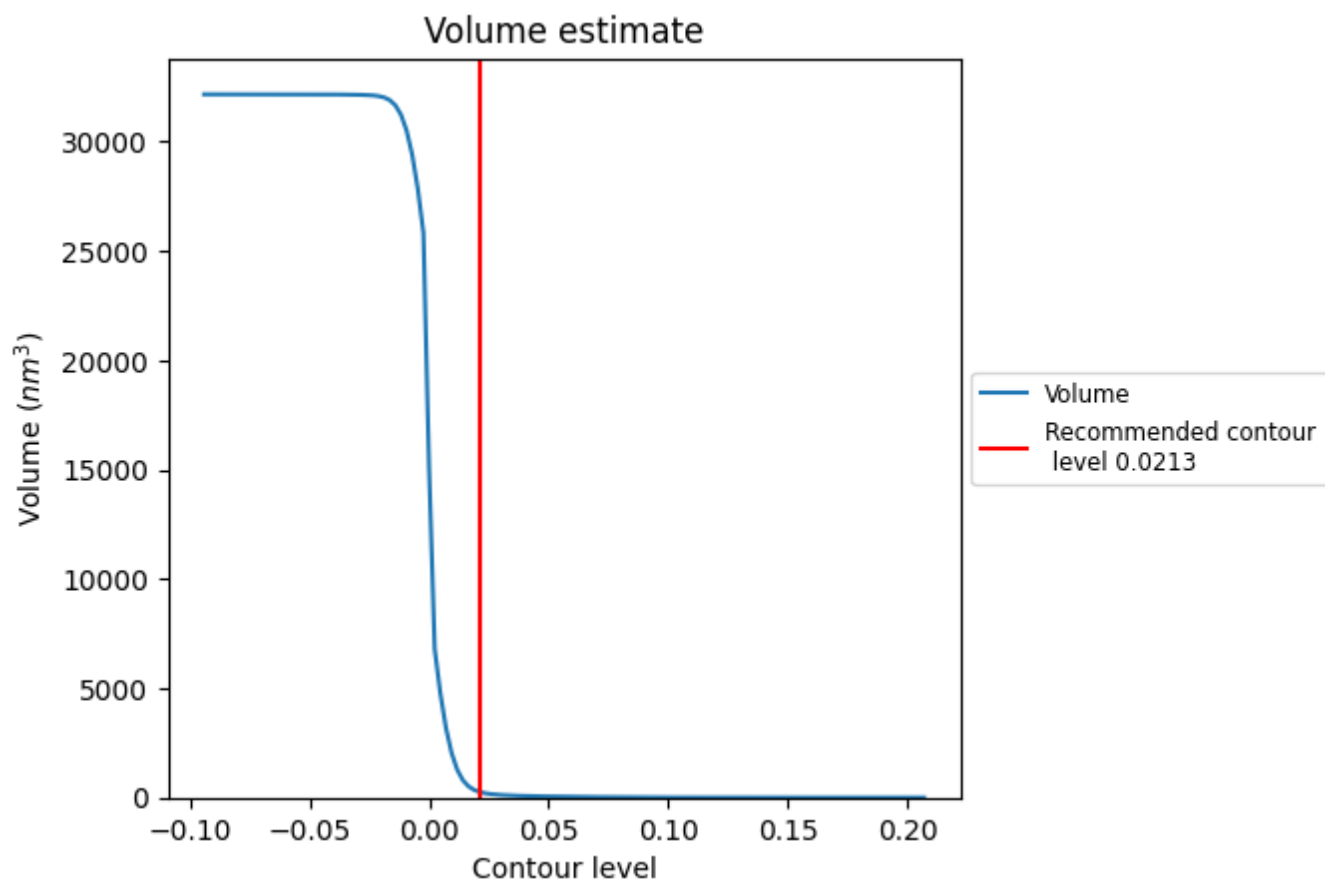
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

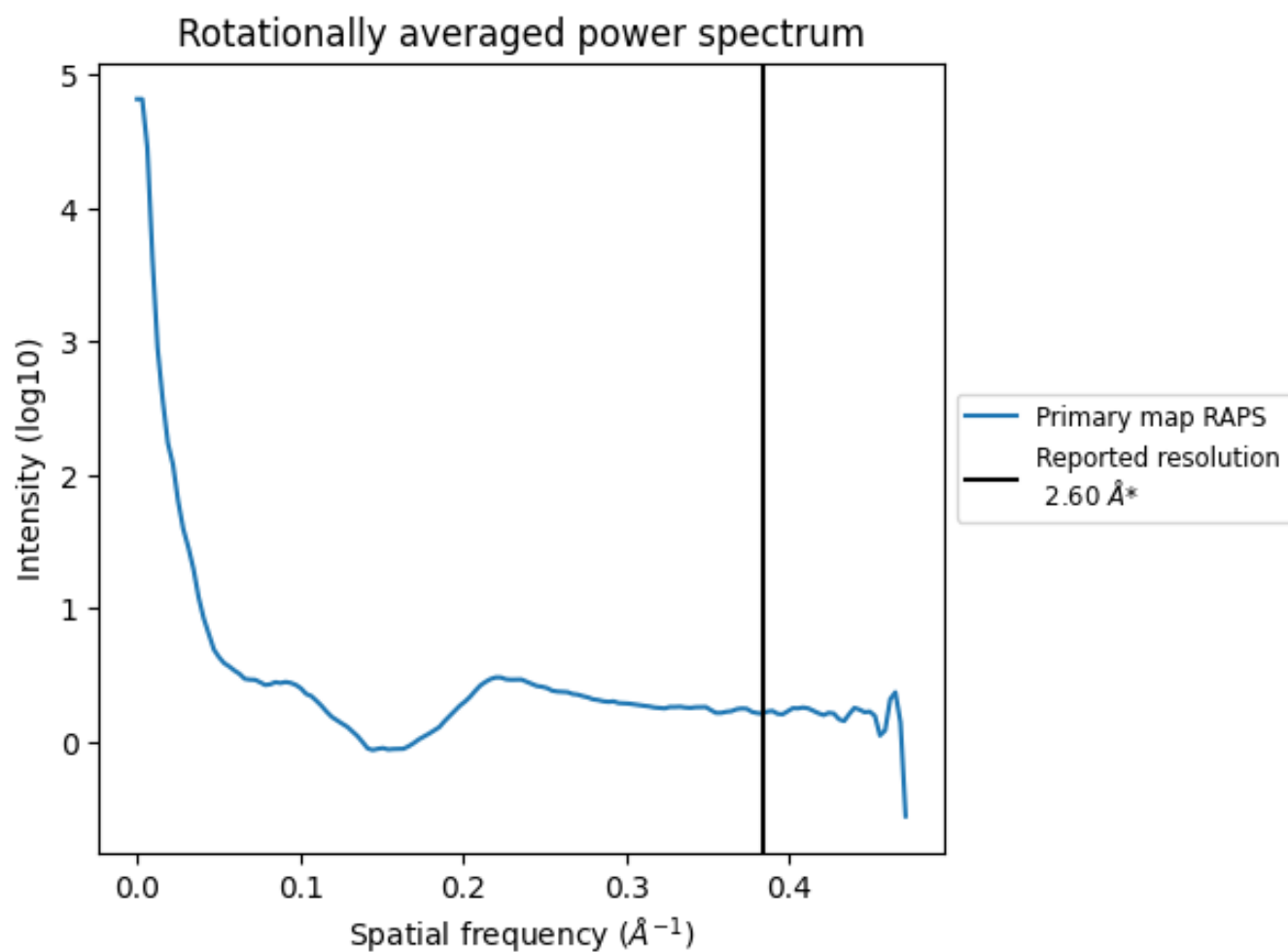
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm³; this corresponds to an approximate mass of 227 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 ⓘ

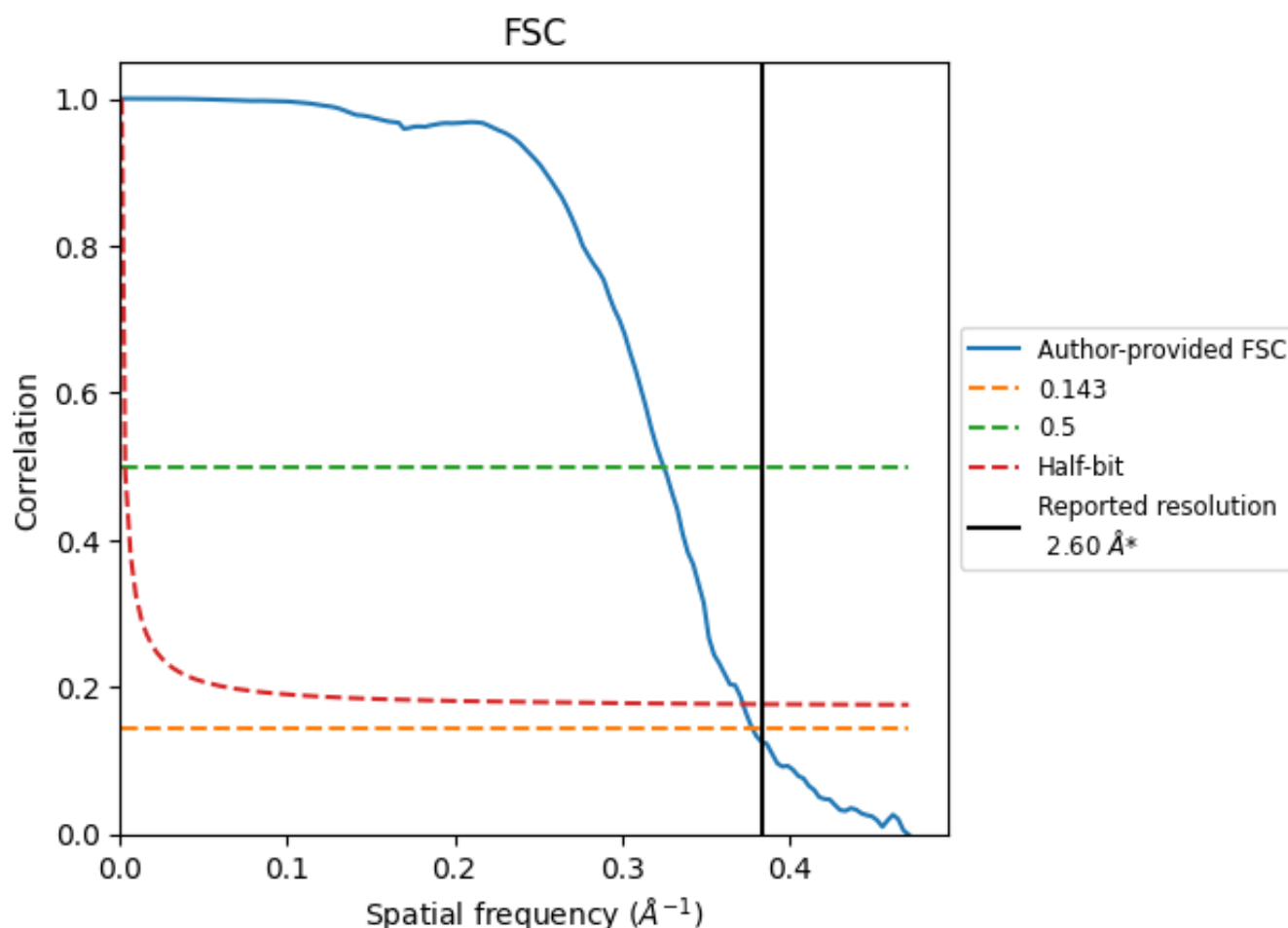


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

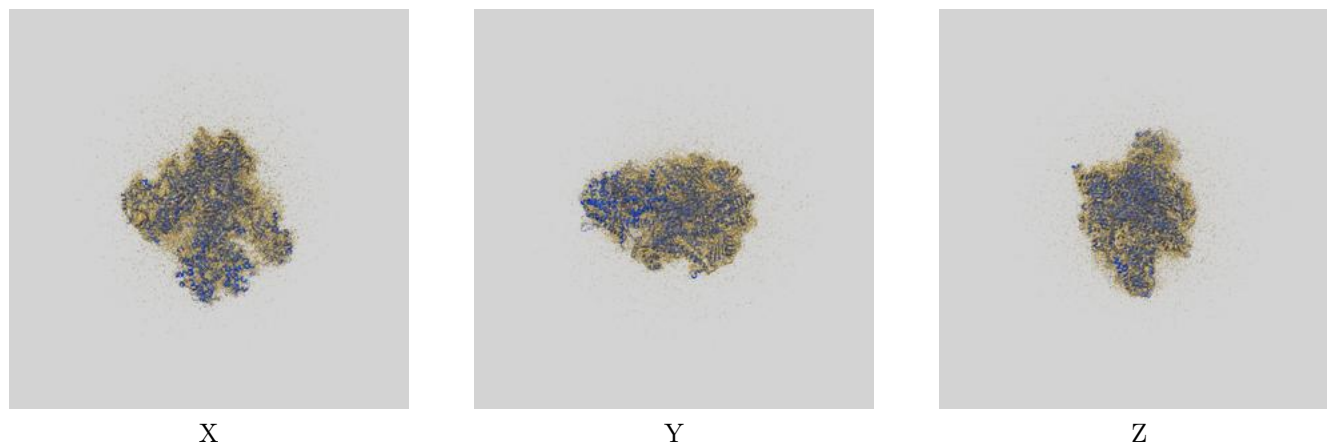
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.60	-
Author-provided FSC curve	2.64	3.08	2.68
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.08 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

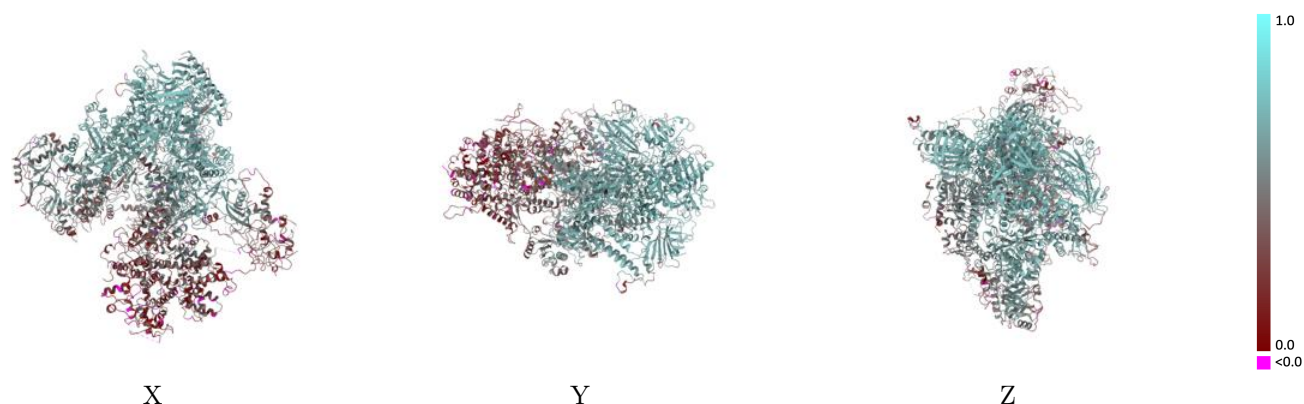
This section contains information regarding the fit between EMDB map EMD-14421 and PDB model 7Z0H. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



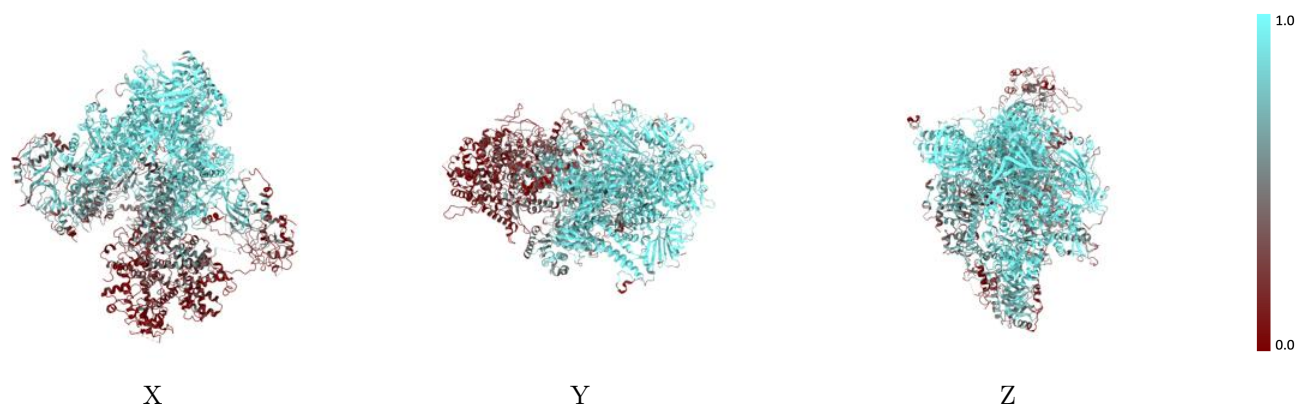
The images above show the 3D surface view of the map at the recommended contour level 0.0213 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



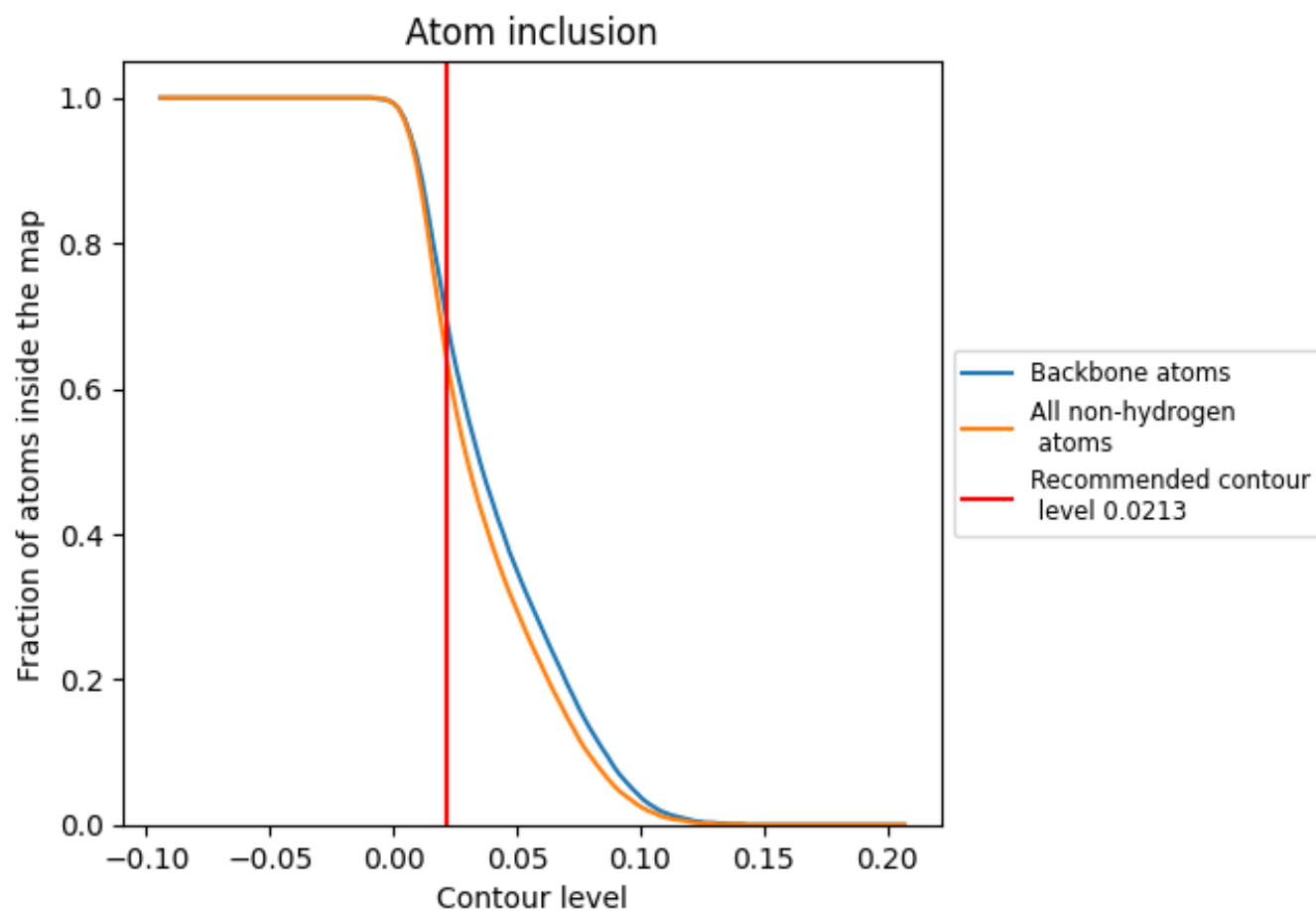
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0213).









































9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.0213) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.5100
A	 0.7380	 0.5510
B	 0.8500	 0.6130
C	 0.9230	 0.6540
D	 0.2660	 0.2980
E	 0.6920	 0.5080
F	 0.9230	 0.6540
G	 0.4930	 0.4220
H	 0.8790	 0.6170
I	 0.4190	 0.4550
J	 0.9490	 0.6710
K	 0.9360	 0.6680
L	 0.8270	 0.6000
M	 0.5270	 0.4540
N	 0.4530	 0.4380
O	 0.1920	 0.2890
P	 0.0970	 0.1930
Q	 0.1460	 0.2310
W	 0.4120	 0.4670
X	 0.3400	 0.3920

