



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:33 AM UTC

PDB ID : 8OEV / pdb_00008oev
EMDB ID : EMD-16837
Title : Structure of the mammalian Pol II-SPT6-Elongin complex, lacking ELOA latch (composite structure, structure 3)
Authors : Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.
Deposited on : 2023-03-13
Resolution : 2.86 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:

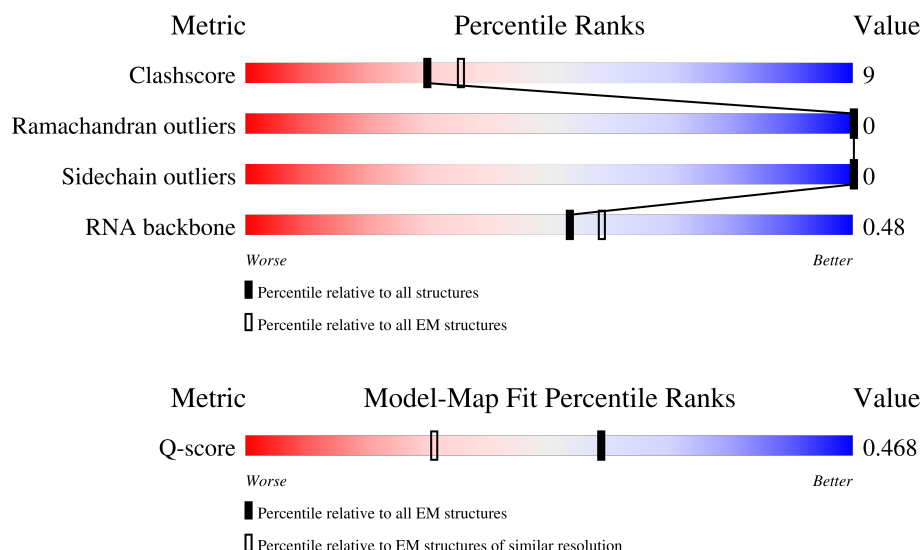
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.86 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.



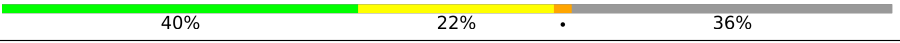
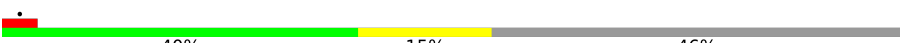
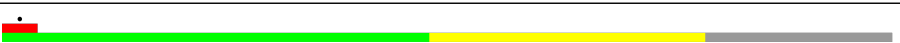
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	1970	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	48	
14	P	46	
15	T	48	
16	M	801	
17	O	112	
18	Q	118	
19	S	1729	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 41781 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11159	7024	2000	2064	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9047	5721	1592	1670	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	118	Total	C	N	O	S	0	0
			967	608	167	188	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1347	872	218	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			932	577	165	179	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	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			367	228	69	64	6		

- Molecule 13 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	26	Total	C	N	O	P	0	0
			549	255	117	151	26		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	13	Total	C	N	O	P	0	0
			280	125	54	88	13		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	38	Total	C	N	O	P	0	0
			769	365	130	236	38		

- Molecule 16 is a protein called Elongin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	128	Total	C	N	O	S	0	0
			1074	680	195	192	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q14241
M	-1	ASN	-	expression tag	UNP Q14241
M	0	ALA	-	expression tag	UNP Q14241

- Molecule 17 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	101	Total	C	N	O	S	0	0
			792	506	127	153	6		

- Molecule 18 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	88	Total	C	N	O	S	0	0
			696	437	121	135	3		

- Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	825	Total	C	N	O	S	0	0
			6744	4289	1168	1253	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP Q7KZ85
S	-1	ASN	-	expression tag	UNP Q7KZ85
S	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	C	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0

[illegible]

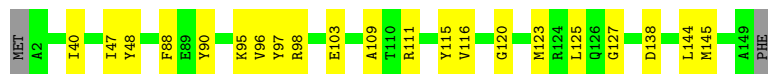
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 75% 16% 10%

[illegible]

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

Chain H:  85% 14%



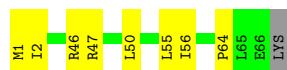
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  80% 13% 7%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  87% 12%



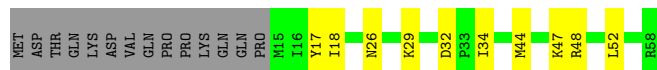
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  87% 11%

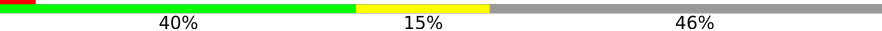


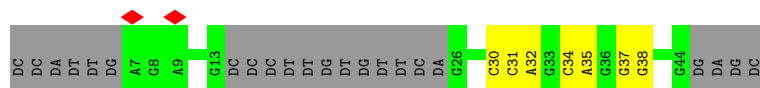
- Molecule 12: RNA polymerase II subunit K

Chain L:  59% 17% 24%



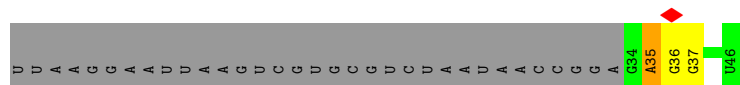
- Molecule 13: Non-Template DNA

Chain N:  40% 15% 46%

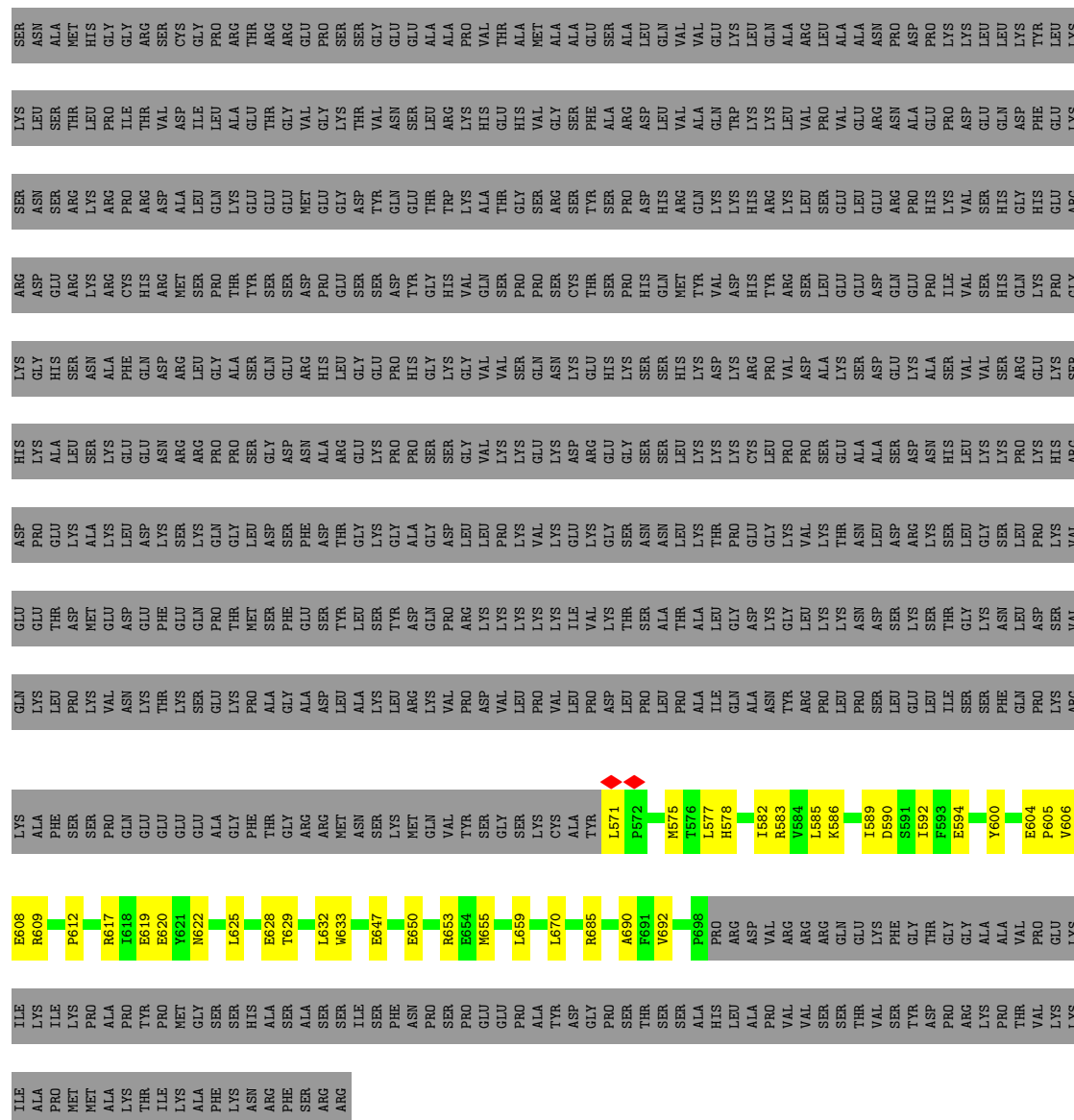
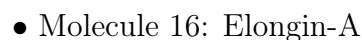


- Molecule 14: RNA

Chain P:  22% 72%



Chain T: 48% 31% 21%



Chain O: 29% 65% 25% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118642	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 ($e^-/\text{\AA}^2$)	40.09	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.253	Depositor
Minimum map value	-16.528	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.086	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/11360	0.45	2/15328 (0.0%)
2	B	0.22	0/9227	0.44	0/12454
3	C	0.21	0/2115	0.39	0/2873
4	D	0.43	0/979	0.84	2/1312 (0.2%)
5	E	0.19	0/1752	0.44	0/2366
6	F	0.19	0/636	0.45	0/859
7	G	0.24	0/1378	0.60	0/1870
8	H	0.18	0/1207	0.41	0/1628
9	I	0.17	0/954	0.43	0/1293
10	J	0.20	0/533	0.41	0/719
11	K	0.22	0/939	0.41	0/1271
12	L	0.21	0/372	0.49	0/493
13	N	0.18	0/619	0.31	0/954
14	P	0.13	0/313	0.21	0/486
15	T	0.23	0/857	0.43	0/1319
16	M	0.24	0/1098	0.58	0/1481
17	O	0.24	0/810	0.68	2/1097 (0.2%)
18	Q	0.26	0/707	0.73	2/952 (0.2%)
19	S	0.24	0/6868	0.51	1/9250 (0.0%)
All	All	0.22	0/42724	0.48	9/58005 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	1
7	G	0	1
19	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	VAL	CA-C-N	6.43	133.83	121.54
1	A	538	VAL	C-N-CA	6.43	133.83	121.54
18	Q	10	HIS	CA-C-N	5.94	136.66	126.32
18	Q	10	HIS	C-N-CA	5.94	136.66	126.32
4	D	147	PRO	N-CA-C	-5.86	102.25	111.34
19	S	414	THR	N-CA-C	-5.82	104.94	111.28
17	O	52	PHE	CA-C-N	5.23	131.53	121.54
17	O	52	PHE	C-N-CA	5.23	131.53	121.54
4	D	148	GLU	N-CA-C	-5.21	107.48	113.88

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	GLN	Mainchain
4	D	157	ILE	Mainchain
7	G	124	ASN	Peptide
19	S	415	ARG	Sidechain

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	A	11159	0	11304	148	0
2	B	9047	0	9080	127	0
3	C	2072	0	2019	28	0
4	D	967	0	973	54	0
5	E	1721	0	1737	17	0
6	F	626	0	657	8	0
7	G	1347	0	1347	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1186	0	1147	13	0
9	I	932	0	856	12	0
10	J	524	0	540	5	0
11	K	920	0	942	8	0
12	L	367	0	367	10	0
13	N	549	0	289	4	0
14	P	280	0	142	2	0
15	T	769	0	429	13	0
16	M	1074	0	1070	27	0
17	O	792	0	774	18	0
18	Q	696	0	694	16	0
19	S	6744	0	6723	272	0
20	A	1	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	41781	0	41090	743	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 9.

All (743) 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)
7:G:171:VAL:HG22	19:S:518:ALA:CB	1.43	1.48
7:G:171:VAL:CG2	19:S:518:ALA:HB1	1.58	1.32
7:G:171:VAL:CG2	19:S:518:ALA:CB	2.07	1.32
19:S:815:THR:O	19:S:829:LYS:HD2	1.11	1.24
7:G:122:ASN:HB2	19:S:405:GLN:NE2	1.57	1.18
4:D:141:CYS:O	4:D:145:LEU:HD12	1.42	1.18
7:G:171:VAL:HG22	19:S:518:ALA:HB3	1.31	1.13
7:G:171:VAL:HG13	19:S:519:SER:O	1.51	1.08
19:S:815:THR:O	19:S:829:LYS:CD	2.00	1.07
7:G:122:ASN:CB	19:S:405:GLN:NE2	2.18	1.05
19:S:424:GLN:HE22	19:S:442:ALA:HA	1.19	1.03
7:G:171:VAL:HG22	19:S:518:ALA:HB1	1.06	0.98
4:D:152:GLU:HA	7:G:167:TYR:CE2	2.02	0.95
7:G:122:ASN:CG	19:S:405:GLN:HE21	1.74	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:VAL:CG2	19:S:518:ALA:HB3	1.87	0.94
7:G:122:ASN:CG	19:S:405:GLN:NE2	2.27	0.93
19:S:416:LEU:HA	19:S:419:LYS:HD2	1.47	0.93
7:G:122:ASN:HB2	19:S:405:GLN:HE22	1.18	0.93
7:G:122:ASN:ND2	19:S:303:ILE:CD1	2.38	0.87
4:D:75:LEU:HB3	4:D:144:ASN:OD1	1.75	0.85
19:S:925:ILE:HA	19:S:985:LEU:HD21	1.60	0.84
4:D:152:GLU:HA	7:G:167:TYR:CZ	2.12	0.83
19:S:420:MET:HG3	19:S:443:LEU:HD11	1.61	0.82
7:G:171:VAL:HG23	19:S:518:ALA:CB	2.07	0.82
19:S:424:GLN:NE2	19:S:442:ALA:HA	1.95	0.81
4:D:157:ILE:O	4:D:159:SER:N	2.14	0.81
19:S:415:ARG:HG2	19:S:419:LYS:HE3	1.60	0.80
7:G:167:TYR:HE1	19:S:516:LYS:HD3	1.46	0.80
19:S:1167:ILE:HD12	19:S:1232:LEU:HD11	1.62	0.80
4:D:149:THR:OG1	4:D:152:GLU:HB2	1.83	0.78
7:G:122:ASN:ND2	19:S:303:ILE:HD11	1.96	0.78
19:S:755:VAL:HG23	19:S:923:PRO:HG2	1.64	0.78
19:S:420:MET:HG2	19:S:467:PHE:HE1	1.47	0.77
19:S:414:THR:O	19:S:418:GLU:HG2	1.84	0.77
19:S:420:MET:CG	19:S:443:LEU:HD11	2.15	0.77
19:S:417:PHE:CD2	19:S:451:LEU:HD22	2.20	0.76
7:G:122:ASN:ND2	19:S:303:ILE:HD13	2.01	0.76
7:G:122:ASN:OD1	19:S:405:GLN:NE2	2.20	0.75
7:G:171:VAL:CG1	19:S:519:SER:O	2.33	0.75
19:S:414:THR:HA	19:S:451:LEU:CD2	2.16	0.75
7:G:122:ASN:O	19:S:405:GLN:NE2	2.22	0.73
19:S:586:GLU:HA	19:S:589:ARG:HE	1.54	0.73
19:S:441:ARG:NH1	19:S:471:TYR:OH	2.21	0.72
19:S:562:PHE:O	19:S:701:GLN:NE2	2.22	0.72
7:G:171:VAL:HG21	19:S:518:ALA:HB1	1.71	0.71
19:S:1228:VAL:HB	19:S:1240:ILE:HB	1.72	0.71
18:Q:7:ILE:HB	18:Q:14:ILE:HB	1.73	0.70
16:M:585:LEU:HG	16:M:606:VAL:HG21	1.74	0.70
4:D:152:GLU:O	4:D:156:LEU:HG	1.91	0.69
19:S:837:LYS:HG2	19:S:867:ILE:HG23	1.74	0.69
2:B:825:ALA:HB3	2:B:888:TYR:HB2	1.75	0.69
7:G:122:ASN:CB	19:S:405:GLN:HE21	1.97	0.69
17:O:104:LEU:O	17:O:107:ALA:HB3	1.92	0.69
7:G:122:ASN:O	19:S:405:GLN:CD	2.36	0.69
19:S:1136:ASP:OD2	19:S:1138:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:421:GLN:HA	19:S:443:LEU:HD12	1.75	0.69
19:S:316:GLU:OE2	19:S:367:ARG:NH1	2.24	0.69
19:S:333:GLN:HE22	19:S:740:TYR:HB2	1.57	0.69
7:G:166:ASP:HB3	7:G:167:TYR:CE2	2.28	0.68
19:S:589:ARG:NH1	19:S:711:MET:SD	2.65	0.68
19:S:552:ASP:OD2	19:S:556:ARG:NE	2.26	0.68
19:S:598:ARG:HG3	19:S:598:ARG:HH11	1.59	0.68
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.75	0.68
19:S:1036:LYS:HG2	19:S:1134:TYR:CE2	2.28	0.68
19:S:593:ALA:HA	19:S:716:ALA:HB2	1.76	0.67
18:Q:9:ARG:HD3	18:Q:12:THR:OG1	1.93	0.67
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.77	0.66
8:H:95:LYS:HD3	8:H:138:ASP:HA	1.77	0.66
4:D:155:ALA:HB3	7:G:167:TYR:HE2	1.60	0.66
19:S:697:GLU:HB3	19:S:702:VAL:HG11	1.78	0.66
19:S:650:ASP:HB3	19:S:740:TYR:CZ	2.31	0.66
19:S:414:THR:HA	19:S:451:LEU:HD23	1.76	0.66
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.78	0.65
19:S:1240:ILE:HG12	19:S:1279:LEU:HB2	1.77	0.65
19:S:565:GLU:HB3	19:S:568:GLU:HG2	1.78	0.65
19:S:1148:GLU:O	19:S:1152:MET:HG3	1.97	0.65
17:O:23:SER:HB2	17:O:65:ILE:HB	1.78	0.65
19:S:563:PRO:HA	19:S:701:GLN:HE22	1.61	0.65
4:D:78:GLU:HG3	4:D:122:ILE:HG21	1.78	0.64
19:S:810:ARG:HG2	19:S:812:PRO:HD3	1.79	0.64
7:G:122:ASN:CG	19:S:303:ILE:HD11	2.22	0.64
19:S:906:TYR:O	19:S:911:ARG:NH1	2.31	0.64
19:S:938:LEU:HD11	19:S:955:LEU:HD21	1.79	0.64
2:B:854:ASN:O	10:J:47:ARG:NH1	2.31	0.64
19:S:424:GLN:O	19:S:427:GLN:HB2	1.98	0.64
6:F:100:ARG:NH2	6:F:121:ASP:O	2.31	0.63
19:S:1054:ASP:OD1	19:S:1063:TYR:OH	2.15	0.63
7:G:122:ASN:CB	19:S:405:GLN:HE22	1.97	0.63
19:S:913:ALA:HA	19:S:916:LEU:HD12	1.79	0.63
1:A:902:GLU:OE1	1:A:985:ARG:NH2	2.31	0.63
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.81	0.63
1:A:514:GLU:O	1:A:518:LEU:HB2	1.99	0.63
19:S:695:ARG:HB3	19:S:706:ASN:HD21	1.63	0.63
19:S:580:THR:HG22	19:S:582:GLU:H	1.63	0.62
19:S:787:SER:HB2	19:S:909:VAL:HG11	1.80	0.62
19:S:318:ASP:OD1	19:S:319:TRP:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:322:ARG:O	19:S:327:THR:OG1	2.16	0.62
6:F:80:MET:HE3	6:F:103:PRO:HG3	1.81	0.62
19:S:1265:CYS:SG	19:S:1279:LEU:HD23	2.39	0.62
16:M:586:LYS:HD3	16:M:609:ARG:HD2	1.82	0.61
19:S:618:ILE:HD12	19:S:640:LEU:HD12	1.82	0.61
19:S:890:ALA:HB1	19:S:912:GLN:HG3	1.81	0.61
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.83	0.61
4:D:166:ASP:HA	4:D:169:LEU:HD12	1.83	0.61
19:S:420:MET:SD	19:S:477:LYS:HD3	2.40	0.61
1:A:728:THR:H	1:A:736:THR:HG21	1.66	0.61
7:G:122:ASN:HD21	19:S:303:ILE:HD13	1.65	0.61
16:M:619:GLU:OE1	16:M:653:ARG:NH1	2.32	0.60
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.82	0.60
1:A:1285:LEU:HA	1:A:1288:ILE:HG12	1.83	0.60
19:S:618:ILE:HG12	19:S:667:THR:HG22	1.83	0.60
19:S:1090:GLU:HA	19:S:1093:LEU:HB3	1.82	0.60
7:G:166:ASP:HB3	7:G:167:TYR:CD2	2.36	0.60
18:Q:46:LYS:HD3	18:Q:51:LEU:H	1.66	0.60
19:S:1017:LEU:O	19:S:1021:CYS:HB2	2.02	0.60
18:Q:4:PHE:HB3	18:Q:72:PRO:HB3	1.84	0.60
4:D:87:LYS:O	4:D:90:ASN:N	2.35	0.59
19:S:414:THR:HA	19:S:451:LEU:HD21	1.83	0.59
19:S:853:GLU:HB2	19:S:887:ASN:HD21	1.67	0.59
1:A:59:ASP:HB3	1:A:62:GLN:HG3	1.84	0.59
19:S:420:MET:HG2	19:S:467:PHE:CE1	2.34	0.59
19:S:914:VAL:O	19:S:918:ARG:HG3	2.02	0.59
4:D:76:ASN:N	4:D:144:ASN:OD1	2.33	0.59
19:S:800:ASN:HB2	19:S:804:GLU:O	2.02	0.59
2:B:208:THR:HA	2:B:217:LEU:O	2.02	0.59
1:A:192:ARG:HH12	1:A:213:LYS:HZ2	1.50	0.59
16:M:575:MET:SD	16:M:583:ARG:NH1	2.76	0.59
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.85	0.59
1:A:34:MET:HA	2:B:1215:ARG:HB2	1.85	0.59
7:G:122:ASN:OD1	19:S:405:GLN:HG2	2.03	0.59
12:L:29:LYS:HG3	12:L:32:ASP:HB2	1.85	0.59
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.85	0.58
5:E:82:VAL:HB	5:E:110:MET:HG2	1.83	0.58
19:S:352:GLY:O	19:S:355:THR:OG1	2.15	0.58
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.85	0.58
2:B:914:CYS:HB2	2:B:917:MET:HE3	1.86	0.58
5:E:26:TYR:HA	5:E:64:HIS:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:590:ASP:HA	16:M:617:ARG:HH22	1.67	0.58
4:D:76:ASN:O	4:D:110:THR:OG1	2.21	0.58
4:D:112:ARG:NH1	7:G:140:ASP:OD1	2.36	0.58
19:S:297:ARG:NH2	19:S:992:LEU:O	2.37	0.58
2:B:919:HIS:HB2	14:P:35:A:H61	1.68	0.58
1:A:1173:THR:H	9:I:56:ASN:HB2	1.69	0.57
4:D:149:THR:O	4:D:150:ALA:C	2.45	0.57
18:Q:28:LYS:O	18:Q:42:GLN:NE2	2.37	0.57
7:G:167:TYR:O	7:G:169:GLY:N	2.38	0.57
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	1.86	0.57
4:D:152:GLU:HG3	7:G:167:TYR:CE1	2.40	0.57
7:G:122:ASN:HD21	19:S:303:ILE:CD1	2.16	0.57
1:A:544:ALA:O	1:A:548:PHE:HB2	2.05	0.57
1:A:129:ILE:HD13	1:A:143:HIS:HB3	1.87	0.57
1:A:192:ARG:NH1	1:A:201:GLU:OE2	2.37	0.57
19:S:408:ILE:O	19:S:412:ASN:ND2	2.38	0.57
19:S:424:GLN:HE22	19:S:442:ALA:CA	2.04	0.57
19:S:644:PRO:HG2	19:S:647:GLU:HB2	1.85	0.57
2:B:209:VAL:HB	2:B:217:LEU:HB3	1.87	0.57
19:S:1007:ASN:ND2	19:S:1020:MET:SD	2.78	0.57
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.87	0.56
19:S:420:MET:HG3	19:S:443:LEU:CD1	2.34	0.56
4:D:149:THR:O	4:D:152:GLU:N	2.38	0.56
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.87	0.56
4:D:152:GLU:HG3	7:G:167:TYR:CD1	2.39	0.56
19:S:423:TYR:CD2	19:S:477:LYS:HG2	2.40	0.56
19:S:465:ASN:HD22	19:S:603:ARG:HH12	1.54	0.56
19:S:1110:GLU:HA	19:S:1113:ARG:HG2	1.87	0.56
16:M:582:ILE:O	16:M:586:LYS:HB2	2.05	0.56
19:S:829:LYS:HE3	19:S:863:ASP:OD2	2.06	0.56
19:S:548:GLU:OE1	19:S:557:HIS:NE2	2.39	0.56
19:S:786:PHE:CE1	19:S:857:ALA:HB2	2.40	0.56
1:A:1139:LEU:HD21	1:A:1343:LEU:HA	1.88	0.56
2:B:1112:ARG:NH1	2:B:1113:LYS:O	2.38	0.56
2:B:1186:GLU:HA	2:B:1190:PRO:HG3	1.86	0.56
7:G:122:ASN:HB2	19:S:405:GLN:HE21	1.56	0.56
4:D:147:PRO:O	4:D:177:GLN:NE2	2.39	0.56
19:S:1057:ARG:HG3	19:S:1134:TYR:CE1	2.40	0.56
19:S:893:TYR:CD2	19:S:915:SER:HB3	2.41	0.56
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.39	0.55
2:B:763:GLU:HG2	2:B:764:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.86	0.55
7:G:6:SER:HB3	7:G:73:LYS:HD3	1.88	0.55
7:G:122:ASN:O	19:S:405:GLN:OE1	2.25	0.55
19:S:983:GLN:O	19:S:986:ILE:HG12	2.06	0.55
19:S:1098:ARG:NH2	19:S:1101:ASP:OD2	2.40	0.55
2:B:300:SER:OG	2:B:427:HIS:ND1	2.33	0.55
2:B:702:LEU:HD13	2:B:752:LEU:HD21	1.87	0.55
19:S:301:ARG:HD2	19:S:401:GLU:OE2	2.07	0.55
19:S:829:LYS:CE	19:S:863:ASP:OD2	2.54	0.55
2:B:387:VAL:HG13	2:B:388:ILE:HD12	1.87	0.55
2:B:421:GLN:NE2	2:B:432:ASP:OD1	2.39	0.55
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.39	0.55
19:S:971:VAL:HG11	19:S:986:ILE:HG22	1.88	0.55
2:B:578:LEU:HD12	2:B:582:LEU:HD12	1.89	0.55
18:Q:24:VAL:HG12	18:Q:55:LYS:HA	1.87	0.55
17:O:40:GLY:HA3	17:O:111:ASP:HB2	1.88	0.55
1:A:1207:ILE:N	1:A:1262:MET:SD	2.80	0.55
2:B:994:LYS:HE2	12:L:34:ILE:HD11	1.88	0.55
4:D:157:ILE:O	4:D:158:PRO:C	2.50	0.55
7:G:167:TYR:CD1	19:S:516:LYS:HB2	2.42	0.55
19:S:410:LYS:O	19:S:414:THR:HG23	2.06	0.54
19:S:1148:GLU:N	19:S:1148:GLU:OE1	2.35	0.54
2:B:351:ARG:NH2	2:B:358:ASP:OD1	2.41	0.54
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.88	0.54
17:O:79:TYR:OH	17:O:92:GLU:O	2.26	0.54
2:B:211:LYS:HB2	2:B:214:GLU:HB3	1.90	0.54
2:B:375:MET:HB3	9:I:14:ILE:HG12	1.89	0.54
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.41	0.54
2:B:664:LEU:HD22	2:B:674:ILE:HD11	1.90	0.54
3:C:81:LYS:HZ1	3:C:126:ARG:HH22	1.55	0.54
1:A:96:HIS:HB3	1:A:99:PHE:HB2	1.89	0.54
4:D:149:THR:OG1	4:D:152:GLU:N	2.34	0.54
18:Q:6:MET:HE3	18:Q:13:THR:HG21	1.89	0.54
2:B:171:SER:HB3	2:B:200:PRO:HG2	1.90	0.54
2:B:484:MET:HE1	2:B:521:LEU:HG	1.89	0.54
2:B:563:ASN:OD1	2:B:568:ARG:NH2	2.40	0.54
19:S:316:GLU:HG2	19:S:403:TRP:CD1	2.43	0.54
19:S:896:SER:HB3	19:S:899:SER:HB3	1.89	0.54
19:S:418:GLU:HA	19:S:448:MET:HE1	1.89	0.54
1:A:329:MET:HA	1:A:335:PRO:HA	1.90	0.54
2:B:1192:GLN:HB3	2:B:1225:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:34:DC:H2'	13:N:35:DA:C8	2.43	0.54
19:S:546:PHE:HZ	19:S:689:ILE:HG23	1.73	0.54
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.90	0.53
1:A:798:ILE:O	1:A:820:ARG:NH1	2.41	0.53
19:S:833:ILE:HA	19:S:836:LEU:HD12	1.89	0.53
4:D:153:SER:HB3	4:D:173:LEU:HD21	1.90	0.53
7:G:167:TYR:CE1	19:S:516:LYS:HD3	2.35	0.53
19:S:757:PRO:HB2	19:S:758:TYR:HD1	1.73	0.53
19:S:995:ARG:HG3	19:S:995:ARG:HH11	1.73	0.53
19:S:1149:ILE:HA	19:S:1152:MET:HE3	1.90	0.53
1:A:42:LYS:O	1:A:288:ASN:ND2	2.33	0.53
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.41	0.53
2:B:461:ASP:HB3	2:B:464:HIS:HB2	1.90	0.53
1:A:1030:SER:OG	5:E:162:ARG:NE	2.40	0.53
17:O:18:TYR:HB2	18:Q:34:ILE:HG21	1.91	0.53
19:S:926:GLU:O	19:S:930:VAL:HG12	2.09	0.53
1:A:1147:SER:HB3	1:A:1157:ILE:HD11	1.91	0.53
4:D:86:ARG:NH1	7:G:35:GLU:OE2	2.37	0.53
19:S:866:ARG:HG3	19:S:867:ILE:HD12	1.91	0.53
19:S:971:VAL:O	19:S:1036:LYS:N	2.42	0.53
2:B:1117:GLN:NE2	3:C:195:THR:OG1	2.34	0.53
18:Q:1:MET:N	18:Q:20:GLU:OE2	2.42	0.53
3:C:190:ASN:O	3:C:193:ARG:NH1	2.43	0.52
7:G:167:TYR:HD1	19:S:516:LYS:HB2	1.73	0.52
16:M:647:GLU:HG2	16:M:650:GLU:HG3	1.92	0.52
17:O:100:ALA:O	17:O:104:LEU:N	2.41	0.52
19:S:621:THR:O	19:S:625:ARG:N	2.42	0.52
19:S:642:ASN:HD21	19:S:674:LYS:H	1.56	0.52
1:A:120:ASP:O	1:A:123:ASN:ND2	2.43	0.52
4:D:149:THR:C	4:D:151:GLU:N	2.66	0.52
7:G:165:ASP:OD1	7:G:166:ASP:N	2.41	0.52
11:K:42:LEU:HD23	11:K:45:ILE:HD11	1.91	0.52
17:O:96:ALA:HB3	17:O:99:ILE:HG12	1.92	0.52
1:A:245:PRO:HA	1:A:248:MET:HE2	1.92	0.52
19:S:294:LEU:O	19:S:299:GLN:NE2	2.42	0.52
19:S:426:GLU:O	19:S:427:GLN:C	2.52	0.52
19:S:795:PHE:HB2	19:S:909:VAL:HG23	1.91	0.52
1:A:358:ARG:NH1	15:T:27:DT:OP1	2.43	0.52
2:B:944:ILE:HB	2:B:971:THR:HB	1.92	0.52
7:G:50:THR:HG22	7:G:73:LYS:HB2	1.92	0.52
1:A:374:SER:OG	1:A:376:ASP:OD1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:ILE:O	4:D:160:LEU:N	2.38	0.52
19:S:559:THR:O	19:S:695:ARG:NH2	2.36	0.52
19:S:850:VAL:HG21	19:S:861:ILE:HG22	1.92	0.52
19:S:903:PHE:CE2	19:S:914:VAL:HG11	2.44	0.52
1:A:272:ASN:HB3	15:T:35:DG:H22	1.75	0.52
19:S:365:PHE:HB3	19:S:371:PHE:HB2	1.92	0.52
1:A:1129:ASN:OD1	1:A:1415:THR:OG1	2.27	0.52
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.92	0.52
17:O:105:MET:O	17:O:108:ASN:HB2	2.09	0.52
19:S:425:TYR:O	19:S:426:GLU:C	2.53	0.52
7:G:96:GLY:HA3	7:G:108:ILE:O	2.10	0.51
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.92	0.51
16:M:594:GLU:HA	16:M:622:ASN:HD21	1.75	0.51
10:J:1:MET:HA	10:J:55:LEU:HB2	1.92	0.51
16:M:577:LEU:HD11	17:O:103:LEU:HD21	1.93	0.51
1:A:1143:LEU:HD22	1:A:1157:ILE:HD13	1.91	0.51
2:B:171:SER:OG	2:B:172:LYS:N	2.43	0.51
3:C:51:GLN:NE2	12:L:52:LEU:HD22	2.25	0.51
19:S:814:PHE:HE1	19:S:825:GLU:HB3	1.74	0.51
7:G:122:ASN:OD1	19:S:405:GLN:CD	2.54	0.51
17:O:18:TYR:HB3	17:O:30:ILE:HD11	1.92	0.51
19:S:541:LEU:HB2	19:S:693:TYR:CE1	2.45	0.51
3:C:56:SER:HB2	3:C:158:GLU:H	1.76	0.51
7:G:152:VAL:HG22	7:G:157:ILE:HD12	1.92	0.51
3:C:19:VAL:HG12	3:C:241:PRO:HB2	1.93	0.51
19:S:378:PHE:O	19:S:381:LYS:NZ	2.35	0.51
19:S:1236:VAL:HG12	19:S:1275:PHE:HD2	1.76	0.51
5:E:172:ARG:NH1	5:E:210:GLN:OE1	2.43	0.51
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.76	0.51
2:B:871:VAL:HG12	2:B:1044:ILE:HG22	1.92	0.51
2:B:123:SER:HB3	2:B:474:GLY:H	1.76	0.50
2:B:470:LEU:HD22	2:B:562:LEU:HD22	1.93	0.50
18:Q:23:THR:HA	18:Q:56:THR:HA	1.92	0.50
2:B:722:GLU:HB3	2:B:725:TYR:HB2	1.93	0.50
13:N:31:DC:H2'	13:N:32:DA:C8	2.45	0.50
16:M:690:ALA:HB1	16:M:692:VAL:HG23	1.93	0.50
17:O:35:HIS:HA	17:O:81:VAL:HG11	1.92	0.50
19:S:589:ARG:HG2	19:S:712:ALA:HB2	1.93	0.50
12:L:18:ILE:HD11	12:L:47:LYS:HD2	1.91	0.50
1:A:461:GLN:NE2	2:B:1167:GLU:OE2	2.42	0.50
2:B:1016:HIS:NE2	2:B:1060:GLU:OE1	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:GLU:OE2	4:D:155:ALA:HB2	2.11	0.50
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.93	0.50
19:S:414:THR:CA	19:S:451:LEU:HD21	2.42	0.50
1:A:911:PRO:O	1:A:963:ARG:NH2	2.40	0.50
4:D:141:CYS:C	4:D:145:LEU:HD12	2.26	0.50
4:D:152:GLU:HG3	7:G:167:TYR:CZ	2.47	0.50
15:T:13:DC:H2"	15:T:14:DT:H5"	1.94	0.50
19:S:411:GLU:C	19:S:411:GLU:CD	2.79	0.50
1:A:132:LYS:HE3	1:A:139:LYS:HZ1	1.77	0.50
1:A:466:LYS:O	2:B:1174:HIS:NE2	2.45	0.50
1:A:753:GLY:O	1:A:757:GLN:OE1	2.29	0.50
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.94	0.50
11:K:40:HIS:O	11:K:44:ASN:HB2	2.11	0.50
1:A:893:GLU:OE1	5:E:197:SER:OG	2.27	0.49
2:B:924:LYS:NZ	2:B:941:ASP:OD2	2.40	0.49
19:S:421:GLN:HA	19:S:443:LEU:CD1	2.41	0.49
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.93	0.49
2:B:606:MET:HE2	2:B:701:PRO:HG2	1.94	0.49
3:C:250:SER:OG	11:K:102:GLU:OE2	2.29	0.49
4:D:152:GLU:HG3	7:G:167:TYR:CG	2.46	0.49
16:M:585:LEU:HD11	16:M:592:ILE:HD11	1.93	0.49
19:S:421:GLN:OE1	19:S:448:MET:HE2	2.11	0.49
1:A:133:SER:OG	1:A:139:LYS:NZ	2.43	0.49
9:I:57:LYS:HB3	9:I:60:HIS:HB3	1.93	0.49
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.94	0.49
2:B:1018:GLN:NE2	2:B:1054:THR:OG1	2.46	0.49
7:G:171:VAL:HG23	19:S:518:ALA:HB3	1.77	0.49
19:S:638:LYS:HE2	19:S:639:TYR:HE1	1.78	0.49
19:S:710:THR:HA	19:S:713:ILE:HG22	1.94	0.49
19:S:814:PHE:CE1	19:S:825:GLU:HB3	2.48	0.49
8:H:40:ILE:O	8:H:123:MET:HA	2.12	0.49
1:A:60:PRO:HB2	1:A:72:GLN:HG3	1.95	0.49
1:A:78:MET:O	2:B:1149:ARG:NH2	2.46	0.49
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.49
3:C:61:ASP:OD2	12:L:48:ARG:NH2	2.40	0.49
2:B:145:GLN:OE1	2:B:160:ARG:NH1	2.45	0.49
1:A:1458:ILE:HD13	2:B:1168:ARG:HD3	1.95	0.49
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.78	0.49
4:D:110:THR:O	4:D:114:SER:OG	2.26	0.49
19:S:556:ARG:HG2	19:S:557:HIS:CD2	2.48	0.49
19:S:598:ARG:HA	19:S:603:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:992:LEU:HD23	19:S:993:GLY:N	2.28	0.49
2:B:690:ARG:NH1	2:B:692:TYR:OH	2.46	0.49
4:D:150:ALA:C	4:D:154:LYS:HZ3	2.20	0.49
1:A:65:ILE:O	1:A:271:ARG:NH2	2.46	0.49
1:A:129:ILE:O	1:A:133:SER:N	2.42	0.49
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.78	0.49
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.81	0.48
19:S:974:ASN:O	19:S:977:ILE:HG22	2.13	0.48
19:S:980:PRO:HA	19:S:983:GLN:HG3	1.95	0.48
2:B:1196:CYS:HB3	2:B:1199:CYS:SG	2.53	0.48
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.95	0.48
19:S:297:ARG:NH2	19:S:989:VAL:O	2.46	0.48
19:S:840:LEU:HD12	19:S:867:ILE:HG22	1.95	0.48
19:S:849:THR:HG21	19:S:920:ILE:HG21	1.96	0.48
19:S:1112:GLU:HA	19:S:1117:GLY:HA2	1.94	0.48
1:A:34:MET:HE1	2:B:1240:MET:HE1	1.96	0.48
16:M:578:HIS:HD2	17:O:107:ALA:HB1	1.78	0.48
19:S:786:PHE:HE1	19:S:857:ALA:HB2	1.78	0.48
1:A:373:LEU:O	1:A:485:ASN:ND2	2.45	0.48
1:A:733:LEU:HD23	9:I:107:ALA:HA	1.96	0.48
2:B:706:GLU:HB2	2:B:711:LEU:HD21	1.95	0.48
19:S:1241:PRO:HG2	19:S:1244:PHE:HB2	1.94	0.48
1:A:1020:LEU:HD21	1:A:1073:GLU:HA	1.94	0.48
2:B:137:GLU:OE2	16:M:685:ARG:NH1	2.43	0.48
15:T:34:DT:H3'	15:T:35:DG:H3'	1.95	0.48
19:S:800:ASN:O	19:S:921:GLN:NE2	2.44	0.48
1:A:416:ALA:HA	1:A:448:ARG:HA	1.95	0.48
16:M:578:HIS:CD2	17:O:107:ALA:HB1	2.48	0.48
1:A:481:THR:H	1:A:483:ARG:HH12	1.61	0.48
2:B:557:SER:OG	2:B:590:GLU:OE2	2.29	0.48
7:G:3:TYR:N	7:G:76:VAL:O	2.43	0.48
8:H:48:TYR:HE2	8:H:145:MET:HE2	1.79	0.48
19:S:546:PHE:CZ	19:S:713:ILE:HD11	2.49	0.48
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.96	0.48
9:I:73:SER:HB2	9:I:115:THR:HA	1.94	0.48
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.96	0.48
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.94	0.48
2:B:160:ARG:HB3	2:B:210:ILE:HB	1.96	0.48
2:B:644:ILE:HD11	2:B:654:HIS:HB2	1.95	0.48
4:D:74:LEU:HD13	7:G:4:HIS:HB2	1.95	0.48
19:S:421:GLN:NE2	19:S:443:LEU:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:454:VAL:HG11	19:S:460:LEU:HB2	1.96	0.48
1:A:360:ASP:OD1	2:B:1139:ARG:NE	2.40	0.47
9:I:29:ASP:O	9:I:33:ARG:N	2.47	0.47
19:S:556:ARG:HG2	19:S:557:HIS:HD2	1.77	0.47
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.96	0.47
4:D:151:GLU:HG3	7:G:167:TYR:OH	2.13	0.47
19:S:1057:ARG:H	19:S:1129:GLU:CD	2.22	0.47
1:A:955:GLU:OE2	1:A:1051:SER:OG	2.27	0.47
1:A:26:LEU:HG	2:B:1245:ALA:HB2	1.96	0.47
1:A:1173:THR:HG22	1:A:1214:VAL:HG13	1.96	0.47
1:A:1184:THR:N	1:A:1190:GLN:OE1	2.45	0.47
2:B:627:MET:HG3	2:B:644:ILE:HD12	1.96	0.47
4:D:172:ILE:O	4:D:176:ILE:HD12	2.15	0.47
7:G:93:ASN:OD1	7:G:94:LYS:N	2.47	0.47
2:B:312:ILE:HG23	2:B:445:MET:HE1	1.95	0.47
1:A:808:PRO:HG2	2:B:752:LEU:HD12	1.96	0.47
2:B:360:ASP:O	2:B:364:HIS:ND1	2.37	0.47
4:D:153:SER:O	4:D:156:LEU:HB2	2.14	0.47
12:L:17:TYR:HB2	12:L:44:MET:HE2	1.96	0.47
19:S:474:ASP:O	19:S:477:LYS:HE2	2.15	0.47
1:A:90:LEU:HD22	1:A:310:LEU:HD11	1.96	0.47
7:G:13:LEU:HD21	7:G:17:TYR:HB2	1.96	0.47
16:M:600:TYR:CD2	16:M:628:GLU:HB3	2.50	0.47
19:S:833:ILE:HG22	19:S:837:LYS:NZ	2.29	0.47
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.97	0.47
1:A:614:ASP:HA	1:A:619:LYS:HG3	1.96	0.47
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.48	0.47
4:D:138:GLU:OE1	4:D:157:ILE:HG21	2.15	0.47
4:D:157:ILE:HB	4:D:160:LEU:HB3	1.97	0.47
6:F:79:VAL:HG11	6:F:83:LEU:HD23	1.96	0.47
7:G:124:ASN:OD1	7:G:125:PRO:HD3	2.14	0.47
4:D:150:ALA:CB	4:D:169:LEU:HB3	2.45	0.47
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.79	0.47
9:I:29:ASP:O	9:I:33:ARG:HA	2.14	0.47
16:M:605:PRO:O	16:M:608:GLU:HG3	2.14	0.47
19:S:757:PRO:HB3	19:S:921:GLN:O	2.15	0.47
4:D:154:LYS:HD3	4:D:169:LEU:CD1	2.45	0.46
4:D:156:LEU:O	4:D:158:PRO:HD3	2.15	0.46
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.97	0.46
19:S:374:PRO:HG2	19:S:990:CYS:HB3	1.96	0.46
19:S:1059:HIS:ND1	19:S:1061:GLU:HG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.15	0.46
19:S:398:GLN:HA	19:S:401:GLU:OE1	2.14	0.46
2:B:812:VAL:HG23	2:B:831:PRO:HG3	1.97	0.46
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.98	0.46
2:B:994:LYS:HG3	12:L:34:ILE:HD11	1.98	0.46
17:O:74:CYS:HA	17:O:77:PHE:HD2	1.81	0.46
19:S:316:GLU:HG2	19:S:403:TRP:NE1	2.31	0.46
19:S:473:ARG:HH22	19:S:524:TYR:HE1	1.62	0.46
19:S:1069:MET:HE3	19:S:1102:LEU:HD11	1.96	0.46
1:A:89:GLU:O	1:A:291:ARG:NH2	2.47	0.46
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.97	0.46
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.98	0.46
19:S:297:ARG:NE	19:S:372:GLU:OE2	2.38	0.46
19:S:412:ASN:HA	19:S:415:ARG:CZ	2.46	0.46
1:A:497:ASP:HB2	2:B:1019:LYS:HG3	1.97	0.46
2:B:127:PHE:HB2	2:B:474:GLY:HA2	1.96	0.46
4:D:152:GLU:HG3	7:G:167:TYR:CD2	2.51	0.46
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.98	0.46
19:S:410:LYS:HD2	19:S:454:VAL:HB	1.98	0.46
19:S:568:GLU:HA	19:S:571:LYS:HE2	1.97	0.46
19:S:688:GLU:OE1	19:S:688:GLU:N	2.44	0.46
19:S:1002:LYS:HA	19:S:1002:LYS:HD3	1.76	0.46
19:S:1157:THR:H	19:S:1160:THR:HG1	1.64	0.46
2:B:177:GLU:HG2	2:B:179:ASP:H	1.81	0.46
2:B:568:ARG:HG3	2:B:599:LEU:HD12	1.98	0.46
2:B:712:LEU:HD21	2:B:717:ILE:HD11	1.98	0.46
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.98	0.46
16:M:655:MET:HG3	16:M:659:LEU:HD13	1.97	0.46
19:S:285:GLN:O	19:S:289:ILE:HG12	2.16	0.46
3:C:11:ILE:HD13	3:C:21:PHE:HB3	1.98	0.46
19:S:1119:LYS:HD3	19:S:1119:LYS:HA	1.73	0.46
1:A:70:ARG:HH12	2:B:1208:ARG:HH21	1.64	0.45
1:A:481:THR:HG22	2:B:1132:VAL:HG21	1.98	0.45
4:D:75:LEU:HD12	4:D:122:ILE:HG23	1.98	0.45
19:S:1228:VAL:HG23	19:S:1245:LEU:HD11	1.98	0.45
7:G:167:TYR:H	19:S:515:LEU:HA	1.81	0.45
19:S:1088:ALA:HA	19:S:1091:GLU:HG2	1.98	0.45
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.98	0.45
4:D:75:LEU:CB	4:D:144:ASN:OD1	2.56	0.45
8:H:123:MET:HE3	8:H:125:LEU:HB2	1.96	0.45
16:M:608:GLU:HA	16:M:632:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:622:ASN:HB3	16:M:625:LEU:HD13	1.99	0.45
19:S:418:GLU:N	19:S:448:MET:HE1	2.31	0.45
4:D:146:CYS:O	4:D:148:GLU:OE2	2.34	0.45
1:A:481:THR:OG1	1:A:483:ARG:NH1	2.48	0.45
1:A:1443:ALA:HB2	2:B:1244:ILE:HG23	1.99	0.45
19:S:320:ILE:HG12	19:S:399:TRP:HB3	1.98	0.45
1:A:413:TYR:O	1:A:449:HIS:ND1	2.49	0.45
17:O:46:LEU:HD12	17:O:55:ASN:HA	1.97	0.45
18:Q:10:HIS:O	18:Q:11:LYS:HG2	2.16	0.45
19:S:633:TYR:OH	19:S:662:GLU:OE2	2.35	0.45
1:A:1439:LEU:HD13	2:B:1239:LEU:HD21	1.99	0.45
2:B:664:LEU:HB3	2:B:680:MET:SD	2.57	0.45
2:B:1065:LYS:O	2:B:1069:ASN:ND2	2.49	0.45
19:S:308:ALA:HB3	19:S:313:LEU:HD12	1.98	0.45
19:S:415:ARG:HB3	19:S:419:LYS:HZ1	1.82	0.45
19:S:606:LEU:HD23	19:S:721:LEU:HD22	1.99	0.45
19:S:867:ILE:HD12	19:S:867:ILE:H	1.82	0.45
1:A:931:ARG:NE	1:A:936:GLU:OE2	2.44	0.45
2:B:569:ASP:OD1	2:B:569:ASP:N	2.44	0.45
9:I:29:ASP:O	9:I:33:ARG:CA	2.64	0.45
15:T:22:DC:H2'	15:T:23:DC:C6	2.52	0.45
16:M:629:THR:O	16:M:632:LEU:HB3	2.16	0.45
19:S:786:PHE:CE2	19:S:856:ASP:HB2	2.52	0.45
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.28	0.45
1:A:1138:SER:N	1:A:1360:ASN:OD1	2.49	0.45
1:A:1283:VAL:O	1:A:1286:ARG:HB3	2.17	0.45
3:C:103:LEU:HB3	3:C:161:LEU:HG	1.98	0.45
7:G:122:ASN:OD1	19:S:405:GLN:CG	2.65	0.45
19:S:403:TRP:NE1	19:S:407:ARG:HD2	2.32	0.45
19:S:658:LEU:O	19:S:662:GLU:HG3	2.16	0.45
1:A:1085:GLU:OE2	6:F:59:LYS:NZ	2.49	0.44
4:D:152:GLU:HG3	7:G:167:TYR:CE2	2.53	0.44
19:S:411:GLU:O	19:S:414:THR:OG1	2.35	0.44
19:S:1102:LEU:HG	19:S:1107:PHE:CE2	2.52	0.44
2:B:894:GLN:HB3	2:B:995:PHE:HD1	1.81	0.44
13:N:37:DG:H2'	13:N:38:DG:C8	2.53	0.44
1:A:589:LYS:HD2	8:H:120:GLY:HA3	1.98	0.44
1:A:823:VAL:HG11	1:A:831:LEU:HD22	2.00	0.44
2:B:252:ASN:HB3	2:B:819:VAL:HG21	1.98	0.44
2:B:526:ALA:HB1	15:T:32:DT:H5''	1.99	0.44
19:S:754:ARG:O	19:S:1139:THR:OG1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:1108:ALA:O	19:S:1112:GLU:HG3	2.18	0.44
4:D:134:LEU:HB3	4:D:164:PHE:HE2	1.82	0.44
6:F:51:ARG:NH1	6:F:117:ASP:O	2.51	0.44
15:T:30:DG:H2'	15:T:31:DT:C6	2.52	0.44
16:M:600:TYR:HD2	16:M:628:GLU:HB3	1.83	0.44
16:M:620:GLU:OE2	16:M:653:ARG:NH2	2.51	0.44
19:S:690:LYS:O	19:S:694:TYR:HB2	2.17	0.44
19:S:706:ASN:CG	19:S:709:ARG:HH21	2.26	0.44
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.98	0.44
2:B:341:LYS:NZ	2:B:403:ALA:O	2.51	0.44
1:A:406:VAL:HG11	1:A:419:ILE:HD11	2.00	0.44
1:A:1228:MET:HE2	1:A:1247:PHE:HB2	2.00	0.44
4:D:78:GLU:OE1	4:D:126:ARG:NH2	2.43	0.44
5:E:15:LYS:NZ	5:E:33:LEU:O	2.47	0.44
5:E:104:ILE:HD11	5:E:127:LEU:HD23	1.99	0.44
8:H:88:PHE:CG	8:H:144:LEU:HB3	2.53	0.44
18:Q:38:PRO:HD2	18:Q:41:GLU:HG3	2.00	0.44
2:B:234:ARG:NH2	2:B:254:CYS:O	2.51	0.44
19:S:813:HIS:HE1	19:S:836:LEU:HD11	1.81	0.44
19:S:885:VAL:HG13	19:S:916:LEU:HD22	1.99	0.44
1:A:388:MET:HA	2:B:1140:ALA:HB2	1.99	0.44
2:B:146:ALA:HB3	2:B:158:PRO:HB3	1.98	0.44
2:B:834:PRO:HG2	2:B:841:MET:HE1	2.00	0.44
16:M:589:ILE:HD12	16:M:589:ILE:H	1.81	0.44
1:A:317:MET:HE2	1:A:317:MET:HB3	1.87	0.44
1:A:1221:MET:HE3	1:A:1221:MET:HB3	1.75	0.44
7:G:166:ASP:C	7:G:167:TYR:CG	2.96	0.44
19:S:986:ILE:O	19:S:992:LEU:HD22	2.18	0.44
19:S:999:HIS:O	19:S:1003:ILE:HG12	2.18	0.44
19:S:1066:ALA:O	19:S:1069:MET:HB2	2.18	0.44
1:A:462:PRO:HG3	15:T:24:DG:H21	1.83	0.43
2:B:234:ARG:HH21	2:B:248:LEU:HD13	1.82	0.43
2:B:313:TRP:HB2	2:B:336:THR:HB	1.99	0.43
2:B:763:GLU:HG3	16:M:571:LEU:HG	1.99	0.43
2:B:821:MET:HE2	2:B:983:GLN:HB3	2.00	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.18	0.43
19:S:533:ASP:N	19:S:533:ASP:OD1	2.51	0.43
19:S:752:TRP:HZ3	19:S:940:LEU:HD23	1.83	0.43
19:S:794:VAL:HB	19:S:811:LEU:O	2.18	0.43
19:S:1145:ASN:HB3	19:S:1148:GLU:OE1	2.18	0.43
1:A:349:ARG:O	1:A:353:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	2.00	0.43
2:B:670:GLN:NE2	2:B:672:ASP:OD2	2.33	0.43
19:S:848:VAL:HG13	19:S:882:VAL:HG23	2.00	0.43
16:M:600:TYR:O	16:M:604:GLU:N	2.51	0.43
1:A:376:ASP:HB3	1:A:522:PRO:HD3	2.00	0.43
1:A:397:PHE:HB3	6:F:87:THR:HG23	2.00	0.43
1:A:413:TYR:O	1:A:415:GLY:N	2.52	0.43
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.00	0.43
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
2:B:185:MET:HE3	2:B:197:TYR:HA	2.00	0.43
4:D:115:ARG:HD2	4:D:146:CYS:SG	2.58	0.43
15:T:24:DG:H2'	15:T:25:DA:H8	1.84	0.43
19:S:558:GLU:HB3	19:S:695:ARG:HH22	1.83	0.43
2:B:805:MET:SD	2:B:1019:LYS:HB3	2.59	0.43
2:B:1171:GLN:HB2	2:B:1180:LEU:HD13	2.00	0.43
3:C:130:VAL:HG11	3:C:237:GLY:HA3	2.01	0.43
4:D:148:GLU:HA	4:D:177:GLN:NE2	2.34	0.43
18:Q:10:HIS:HB2	18:Q:88:LEU:H	1.83	0.43
19:S:294:LEU:C	19:S:299:GLN:HE21	2.26	0.43
19:S:833:ILE:O	19:S:836:LEU:HB2	2.18	0.43
2:B:1189:ASP:N	2:B:1189:ASP:OD1	2.51	0.43
11:K:61:TYR:HA	11:K:72:ILE:O	2.19	0.43
19:S:330:ILE:O	19:S:646:LYS:HA	2.18	0.43
1:A:457:ILE:HD11	1:A:515:ILE:HD12	2.00	0.43
1:A:1307:VAL:HA	1:A:1337:GLU:O	2.19	0.43
2:B:176:TRP:HE1	2:B:182:PRO:HG3	1.84	0.43
2:B:169:TYR:HB2	2:B:202:TYR:HB2	2.01	0.43
2:B:791:PRO:HG2	2:B:1078:PRO:HG3	2.00	0.43
2:B:896:SER:OG	2:B:904:GLU:OE1	2.28	0.43
19:S:548:GLU:HA	19:S:551:ARG:HG2	2.00	0.43
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	2.00	0.42
2:B:232:MET:O	2:B:235:SER:OG	2.35	0.42
17:O:86:SER:OG	17:O:87:SER:N	2.51	0.42
19:S:523:MET:HB2	19:S:526:ILE:HD12	2.00	0.42
19:S:910:LEU:O	19:S:914:VAL:HG23	2.19	0.42
2:B:175:HIS:HB2	2:B:185:MET:HB2	2.01	0.42
2:B:347:ILE:HB	2:B:385:ALA:HB3	2.01	0.42
2:B:928:ASP:OD2	12:L:17:TYR:OH	2.33	0.42
16:M:670:LEU:HD23	16:M:670:LEU:HA	1.73	0.42
19:S:333:GLN:NE2	19:S:740:TYR:HB2	2.30	0.42
19:S:550:LEU:HD23	19:S:692:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:1004:LEU:HD11	19:S:1011:LEU:HG	2.01	0.42
2:B:1115:THR:HA	3:C:195:THR:HA	2.01	0.42
5:E:77:PRO:HG3	5:E:90:TYR:HE2	1.83	0.42
19:S:290:ARG:NE	19:S:999:HIS:HB2	2.34	0.42
1:A:879:VAL:HB	1:A:888:GLN:HB2	2.02	0.42
4:D:155:ALA:CB	7:G:167:TYR:HE2	2.31	0.42
9:I:118:HIS:O	9:I:118:HIS:ND1	2.45	0.42
13:N:30:DC:H2'	13:N:31:DC:C6	2.54	0.42
18:Q:80:ARG:HG2	18:Q:83:ASP:HB2	2.01	0.42
19:S:541:LEU:HB2	19:S:693:TYR:HE1	1.83	0.42
19:S:1107:PHE:O	19:S:1111:LEU:HG	2.19	0.42
1:A:467:MET:HE1	1:A:527:THR:HA	2.01	0.42
2:B:1032:PRO:HB2	2:B:1105:LEU:HD23	2.01	0.42
2:B:1139:ARG:NH1	2:B:1158:ASP:O	2.52	0.42
19:S:721:LEU:O	19:S:725:MET:HG2	2.20	0.42
1:A:464:LEU:HD13	1:A:1100:THR:HG21	2.00	0.42
1:A:1011:GLU:O	1:A:1015:GLU:HG2	2.19	0.42
2:B:194:ASN:HA	2:B:266:GLY:HA3	2.01	0.42
9:I:65:LEU:HD23	9:I:68:ILE:HD12	2.02	0.42
19:S:550:LEU:HB3	19:S:605:VAL:HG11	2.01	0.42
19:S:756:ALA:HB3	19:S:1140:ALA:HA	2.02	0.42
2:B:629:ASN:HB2	2:B:632:GLU:HG2	2.02	0.42
9:I:91:HIS:CG	9:I:116:ALA:HB2	2.55	0.42
19:S:375:PHE:CE1	19:S:379:TYR:HD2	2.38	0.42
19:S:550:LEU:HD12	19:S:602:VAL:HG13	2.01	0.42
2:B:897:LYS:HB3	2:B:897:LYS:HE2	1.94	0.42
5:E:9:ARG:O	5:E:13:ILE:HG12	2.20	0.42
19:S:414:THR:N	19:S:451:LEU:HD21	2.34	0.42
19:S:570:ALA:O	19:S:574:VAL:HG13	2.19	0.42
1:A:883:ILE:HD13	1:A:1423:ASP:HB2	2.00	0.42
2:B:267:SER:HB3	2:B:269:LYS:HE2	2.01	0.42
2:B:1197:ASN:HB2	2:B:1222:GLN:HB3	2.00	0.42
4:D:129:LEU:HD12	4:D:134:LEU:HD21	2.01	0.42
4:D:138:GLU:HA	4:D:141:CYS:SG	2.60	0.42
5:E:192:LYS:HE3	5:E:194:ILE:HD11	2.00	0.42
17:O:32:LYS:HE2	17:O:32:LYS:HB2	1.96	0.42
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.48	0.42
1:A:542:LEU:HD23	1:A:774:ALA:HA	2.01	0.42
1:A:918:LYS:O	1:A:1052:ARG:NH1	2.53	0.42
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.20	0.42
9:I:17:CYS:SG	9:I:18:GLN:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:39:SER:HB3	17:O:42:ILE:HB	2.02	0.42
19:S:1070:ALA:HB1	19:S:1088:ALA:HB1	2.02	0.42
1:A:541:THR:HG23	1:A:676:ILE:HB	2.02	0.41
1:A:981:CYS:HB3	1:A:986:MET:HE1	2.01	0.41
2:B:893:GLU:OE1	2:B:971:THR:OG1	2.37	0.41
3:C:59:LEU:HD13	3:C:63:PHE:CE1	2.55	0.41
18:Q:80:ARG:HB3	18:Q:84:THR:O	2.20	0.41
19:S:612:GLU:HG3	19:S:613:ARG:N	2.35	0.41
1:A:132:LYS:HB3	1:A:132:LYS:HE2	1.80	0.41
1:A:456:VAL:HG11	1:A:503:LEU:HD21	2.01	0.41
1:A:831:LEU:H	2:B:792:ASP:HB2	1.85	0.41
1:A:865:ILE:HG21	2:B:1169:ASP:CG	2.45	0.41
2:B:438:LYS:HB2	2:B:438:LYS:HE2	1.76	0.41
2:B:458:GLU:OE1	2:B:458:GLU:N	2.50	0.41
19:S:418:GLU:CA	19:S:448:MET:HE1	2.48	0.41
19:S:851:ALA:HB2	19:S:916:LEU:CD1	2.50	0.41
19:S:951:LYS:O	19:S:955:LEU:HD23	2.20	0.41
1:A:340:LYS:HD2	1:A:1436:VAL:HG11	2.02	0.41
2:B:371:ASP:OD2	2:B:456:ARG:NH1	2.42	0.41
2:B:703:LEU:HG	2:B:775:ILE:HG12	2.01	0.41
19:S:308:ALA:HB1	19:S:313:LEU:HB2	2.02	0.41
19:S:781:VAL:HG13	19:S:847:VAL:O	2.20	0.41
19:S:1258:LYS:HB2	19:S:1261:MET:HE1	2.02	0.41
1:A:91:ALA:HB3	1:A:290:LEU:HD22	2.02	0.41
1:A:91:ALA:HB2	1:A:291:ARG:HE	1.85	0.41
1:A:365:THR:OG1	1:A:366:VAL:N	2.53	0.41
1:A:1075:LYS:HD3	1:A:1075:LYS:HA	1.87	0.41
2:B:918:ARG:O	14:P:35:A:N6	2.53	0.41
3:C:7:PRO:HB3	3:C:26:THR:HB	2.02	0.41
10:J:46:ARG:O	10:J:50:LEU:HB2	2.20	0.41
15:T:36:DC:H6	15:T:36:DC:H2'	1.71	0.41
19:S:618:ILE:HG21	19:S:665:LEU:HD13	2.02	0.41
19:S:1263:VAL:HG13	19:S:1265:CYS:SG	2.61	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.92	0.41
1:A:463:THR:HG23	1:A:468:SER:HB2	2.02	0.41
1:A:1357:THR:O	5:E:142:HIS:NE2	2.41	0.41
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.55	0.41
19:S:379:TYR:OH	19:S:1033:GLY:O	2.38	0.41
19:S:650:ASP:HB3	19:S:740:TYR:CE2	2.55	0.41
19:S:954:LEU:O	19:S:958:LEU:HG	2.20	0.41
2:B:226:ILE:HG22	2:B:512:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:THR:OG1	2:B:809:ALA:O	2.30	0.41
2:B:810:MET:SD	2:B:826:HIS:ND1	2.94	0.41
2:B:823:THR:HG21	15:T:30:DG:H5''	2.03	0.41
19:S:313:LEU:HD11	19:S:364:GLY:HA2	2.01	0.41
19:S:586:GLU:HB2	19:S:589:ARG:HH21	1.85	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.20	0.41
1:A:865:ILE:HD12	2:B:1169:ASP:HB3	2.03	0.41
2:B:346:ILE:HD11	2:B:442:LEU:HD11	2.02	0.41
3:C:37:VAL:HG13	3:C:41:GLU:HB2	2.03	0.41
7:G:59:ILE:HG12	7:G:66:VAL:HG22	2.02	0.41
18:Q:3:VAL:HG12	18:Q:18:ALA:H	1.85	0.41
1:A:386:ALA:HB2	1:A:413:TYR:HD1	1.84	0.41
2:B:623:GLU:OE2	2:B:629:ASN:ND2	2.47	0.41
7:G:138:GLN:N	7:G:141:ASP:OD2	2.54	0.41
15:T:24:DG:H2'	15:T:25:DA:C8	2.56	0.41
19:S:629:ASP:OD1	19:S:632:HIS:N	2.44	0.41
19:S:651:ASP:HB3	19:S:740:TYR:CD2	2.56	0.41
1:A:381:PRO:HB3	1:A:480:SER:HA	2.03	0.41
1:A:631:GLU:HG2	1:A:992:LYS:HD2	2.02	0.41
1:A:1304:ILE:HG23	1:A:1338:THR:HB	2.03	0.41
2:B:699:CYS:HA	2:B:743:ASP:HA	2.03	0.41
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.41	0.41
4:D:71:ALA:HB2	7:G:5:ILE:HD13	2.02	0.41
11:K:9:SER:HA	11:K:69:HIS:CG	2.55	0.41
11:K:41:THR:O	11:K:45:ILE:HG12	2.21	0.41
12:L:26:ASN:HB2	12:L:44:MET:HE1	2.02	0.41
15:T:41:DC:H2''	15:T:42:DT:H5''	2.03	0.41
19:S:357:GLN:O	19:S:360:LYS:HB3	2.21	0.41
19:S:829:LYS:NZ	19:S:863:ASP:OD2	2.54	0.41
19:S:864:VAL:HA	19:S:867:ILE:HD13	2.03	0.41
19:S:1098:ARG:HB2	19:S:1101:ASP:HB2	2.03	0.41
1:A:530:SER:HB2	1:A:532:ARG:HG2	2.03	0.41
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.91	0.41
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	2.02	0.41
1:A:1480:CYS:HA	6:F:80:MET:HE1	2.03	0.41
2:B:190:ALA:HA	2:B:195:LEU:HB2	2.02	0.41
4:D:63:ILE:HG13	4:D:65:PRO:HD2	2.03	0.41
19:S:351:LYS:HA	19:S:351:LYS:HD2	1.87	0.41
19:S:384:VAL:HB	19:S:388:LEU:HB2	2.03	0.41
19:S:413:LEU:C	19:S:451:LEU:HD21	2.46	0.41
19:S:1232:LEU:HB2	19:S:1236:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.56	0.40
1:A:790:GLN:HA	1:A:822:PHE:HA	2.01	0.40
2:B:301:CYS:HB2	2:B:309:THR:HG22	2.03	0.40
2:B:480:LEU:HB3	2:B:484:MET:HE2	2.02	0.40
7:G:30:LEU:HD22	7:G:70:VAL:HG11	2.03	0.40
19:S:319:TRP:CZ3	19:S:403:TRP:HB2	2.56	0.40
19:S:538:LYS:HD3	19:S:538:LYS:HA	1.76	0.40
1:A:642:LYS:HE2	1:A:642:LYS:HB3	1.84	0.40
2:B:162:LEU:HB3	2:B:208:THR:OG1	2.21	0.40
3:C:51:GLN:HE21	12:L:52:LEU:HD22	1.86	0.40
19:S:382:GLU:HG2	19:S:383:TYR:CD1	2.56	0.40
19:S:454:VAL:HG22	19:S:459:GLU:HG2	2.02	0.40
19:S:865:LYS:O	19:S:868:VAL:HB	2.21	0.40
19:S:1097:GLU:HG2	19:S:1098:ARG:N	2.36	0.40
1:A:706:ILE:HD11	1:A:787:VAL:HG21	2.02	0.40
1:A:1343:LEU:N	1:A:1364:GLU:OE2	2.54	0.40
2:B:916:GLY:O	2:B:918:ARG:NH2	2.53	0.40
16:M:612:PRO:HB3	16:M:633:TRP:HZ3	1.86	0.40
19:S:851:ALA:HB2	19:S:916:LEU:HD11	2.03	0.40
2:B:950:LEU:HD23	2:B:950:LEU:HA	1.97	0.40
19:S:301:ARG:HH21	19:S:303:ILE:HB	1.86	0.40
19:S:1057:ARG:HG3	19:S:1134:TYR:HE1	1.83	0.40
1:A:1454:VAL:HG13	1:A:1464:ALA:HB1	2.04	0.40
1:A:1481:LYS:HA	7:G:20:PRO:HA	2.03	0.40
2:B:127:PHE:HA	2:B:131:SER:HB2	2.03	0.40
2:B:860:ALA:O	2:B:866:ASN:ND2	2.54	0.40
7:G:38:CYS:HB3	7:G:157:ILE:HG12	2.04	0.40
8:H:111:ARG:HD2	8:H:127:GLY:O	2.21	0.40
19:S:545:GLN:HG2	19:S:557:HIS:ND1	2.37	0.40
19:S:621:THR:OG1	19:S:663:GLY:O	2.36	0.40
19:S:995:ARG:HG3	19:S:995:ARG:NH1	2.36	0.40
19:S:1062:THR:HA	19:S:1065:TRP:CE3	2.57	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	A	1395/1970 (71%)	1365 (98%)	30 (2%)	0	100	100
2	B	1123/1251 (90%)	1088 (97%)	35 (3%)	0	100	100
3	C	254/275 (92%)	247 (97%)	7 (3%)	0	100	100
4	D	114/184 (62%)	106 (93%)	8 (7%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
16	M	126/801 (16%)	119 (94%)	7 (6%)	0	100	100
17	O	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
18	Q	86/118 (73%)	73 (85%)	13 (15%)	0	100	100
19	S	799/1729 (46%)	770 (96%)	29 (4%)	0	100	100
All	All	4927/7466 (66%)	4757 (96%)	170 (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	A	1239/1749 (71%)	1239 (100%)	0	100	100
2	B	953/1084 (88%)	953 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55 (73%)	40 (100%)	0	100	100
16	M	118/706 (17%)	118 (100%)	0	100	100
17	O	88/96 (92%)	88 (100%)	0	100	100
18	Q	75/103 (73%)	75 (100%)	0	100	100
19	S	731/1524 (48%)	731 (100%)	0	100	100
All	All	4388/6590 (67%)	4388 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	296	ASN
1	A	377	GLN
1	A	529	GLN
1	A	599	HIS
1	A	671	ASN
1	A	731	ASN
1	A	757	GLN
1	A	783	GLN
1	A	792	ASN
1	A	1220	HIS
1	A	1236	ASN
1	A	1310	HIS
2	B	175	HIS
2	B	188	ASN
2	B	265	ASN

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Mol	Chain	Res	Type
2	B	538	GLN
2	B	708	GLN
2	B	731	GLN
2	B	802	GLN
2	B	874	ASN
2	B	983	GLN
2	B	1063	GLN
2	B	1126	GLN
3	C	268	GLN
4	D	90	ASN
5	E	30	GLN
5	E	107	GLN
5	E	116	GLN
8	H	131	ASN
9	I	22	ASN
11	K	69	HIS
11	K	89	ASN
12	L	26	ASN
16	M	638	HIS
17	O	68	HIS
19	S	405	GLN
19	S	465	ASN
19	S	701	GLN
19	S	813	HIS
19	S	887	ASN
19	S	1006	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/46 (26%)	3 (25%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	A
14	P	36	G
14	P	37	G

There are no RNA pucker outliers to report.

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 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 [i](#)

There are no chain breaks in this entry.

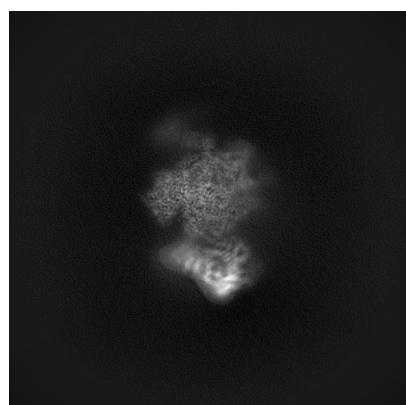
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16837. These allow visual inspection of the internal detail of the map and identification of artifacts.

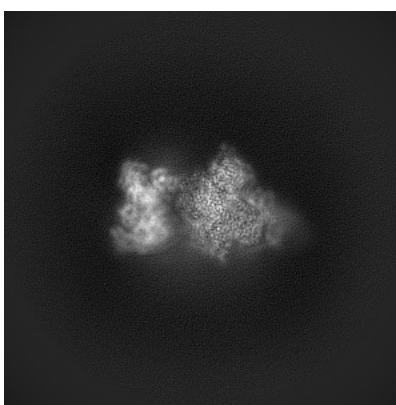
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

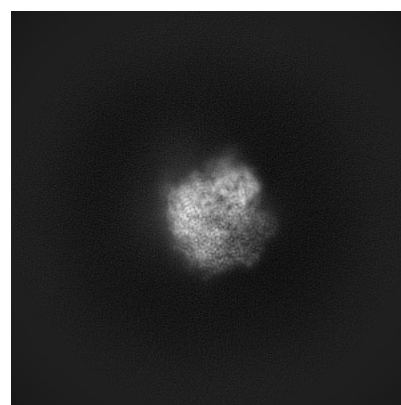
6.1.1 Primary map



X



Y

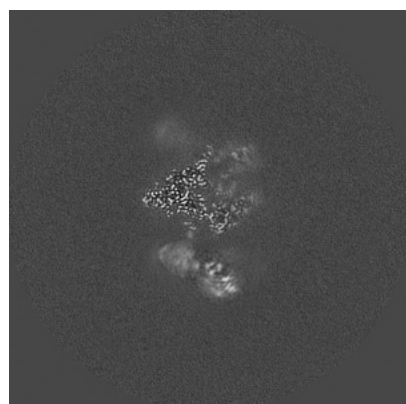


Z

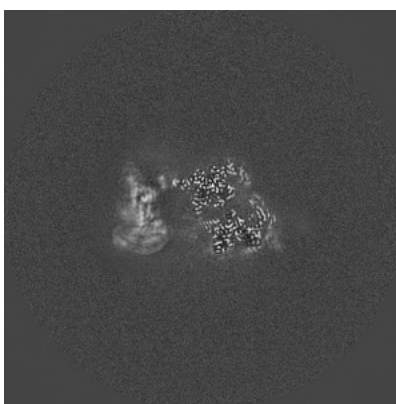
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

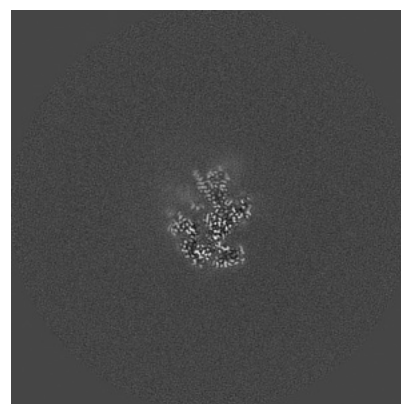
6.2.1 Primary map



X Index: 220



Y Index: 220

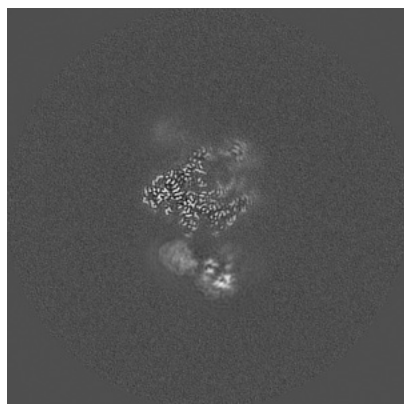


Z Index: 220

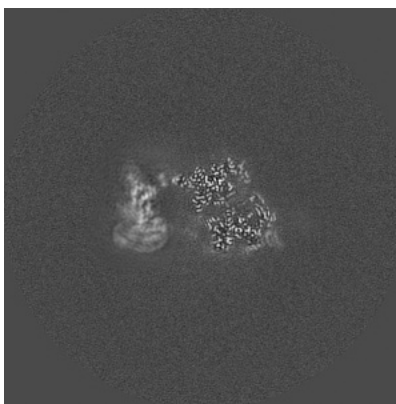
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

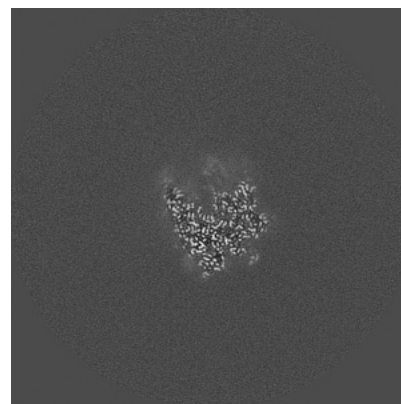
6.3.1 Primary map



X Index: 223



Y Index: 219

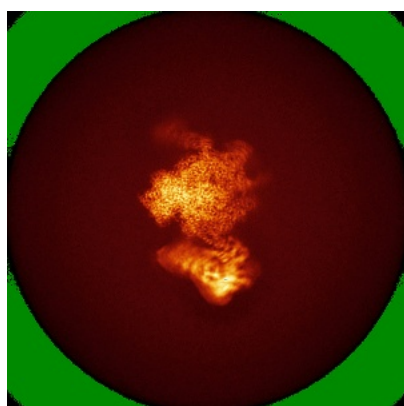


Z Index: 235

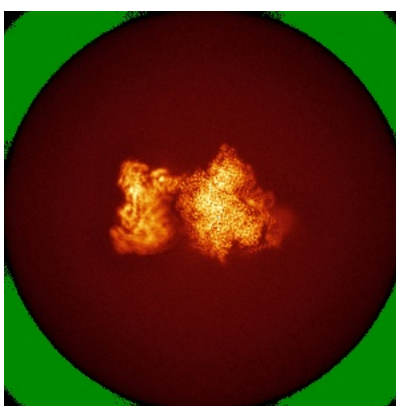
The images above show the largest variance slices of the map in three orthogonal directions.

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

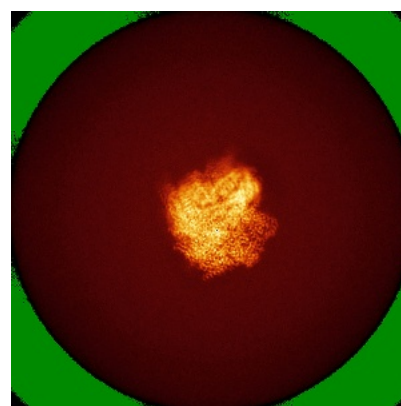
6.4.1 Primary map



X



Y

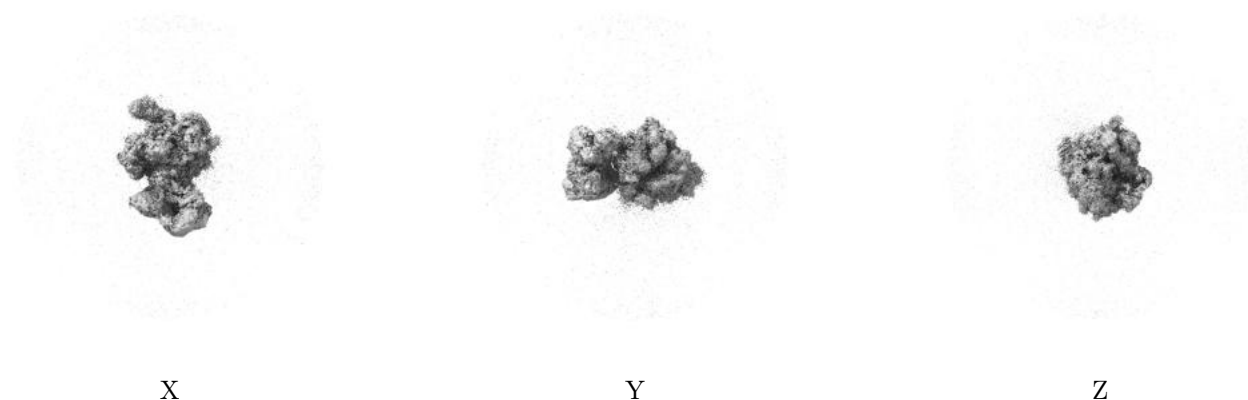


Z

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

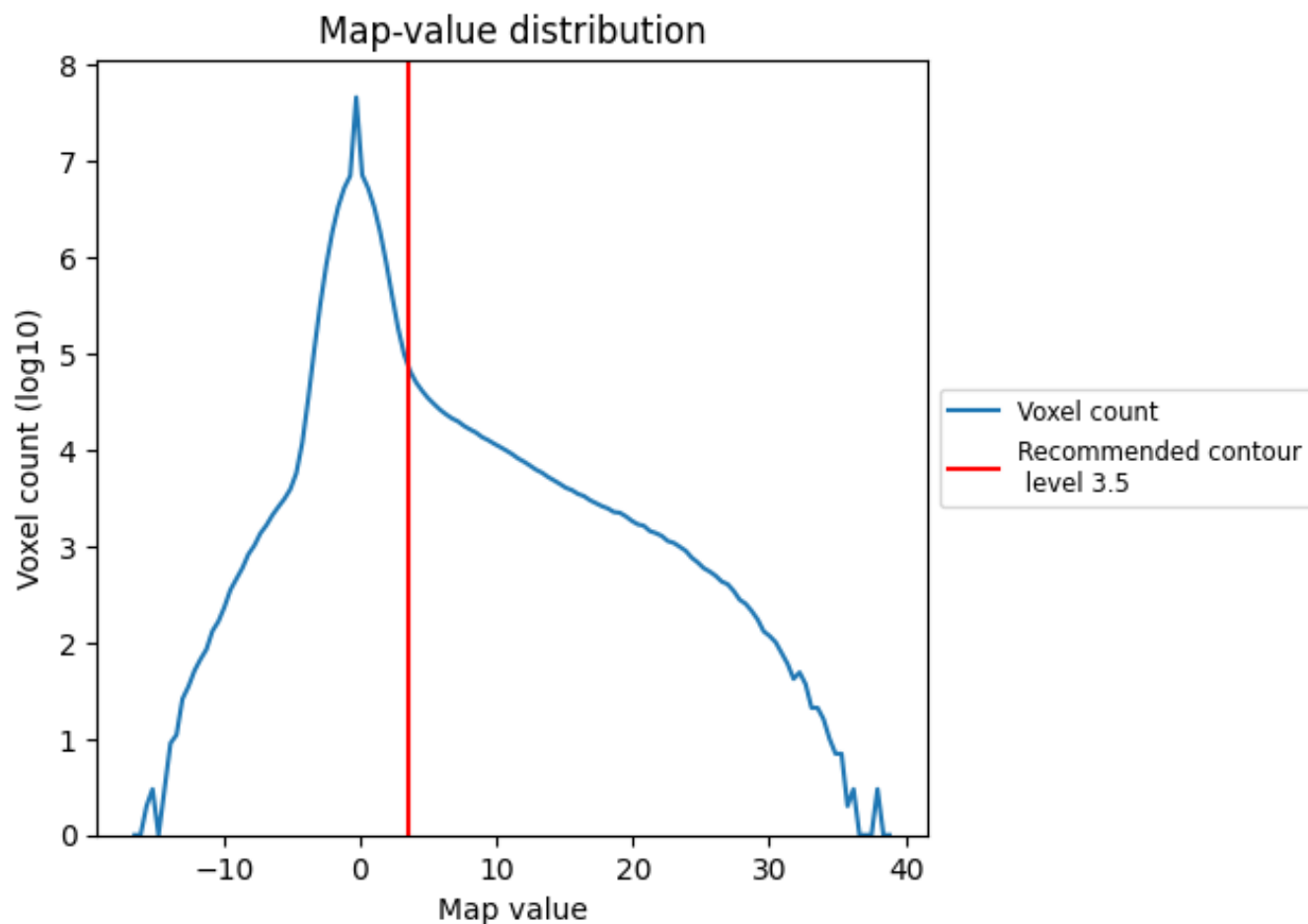
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

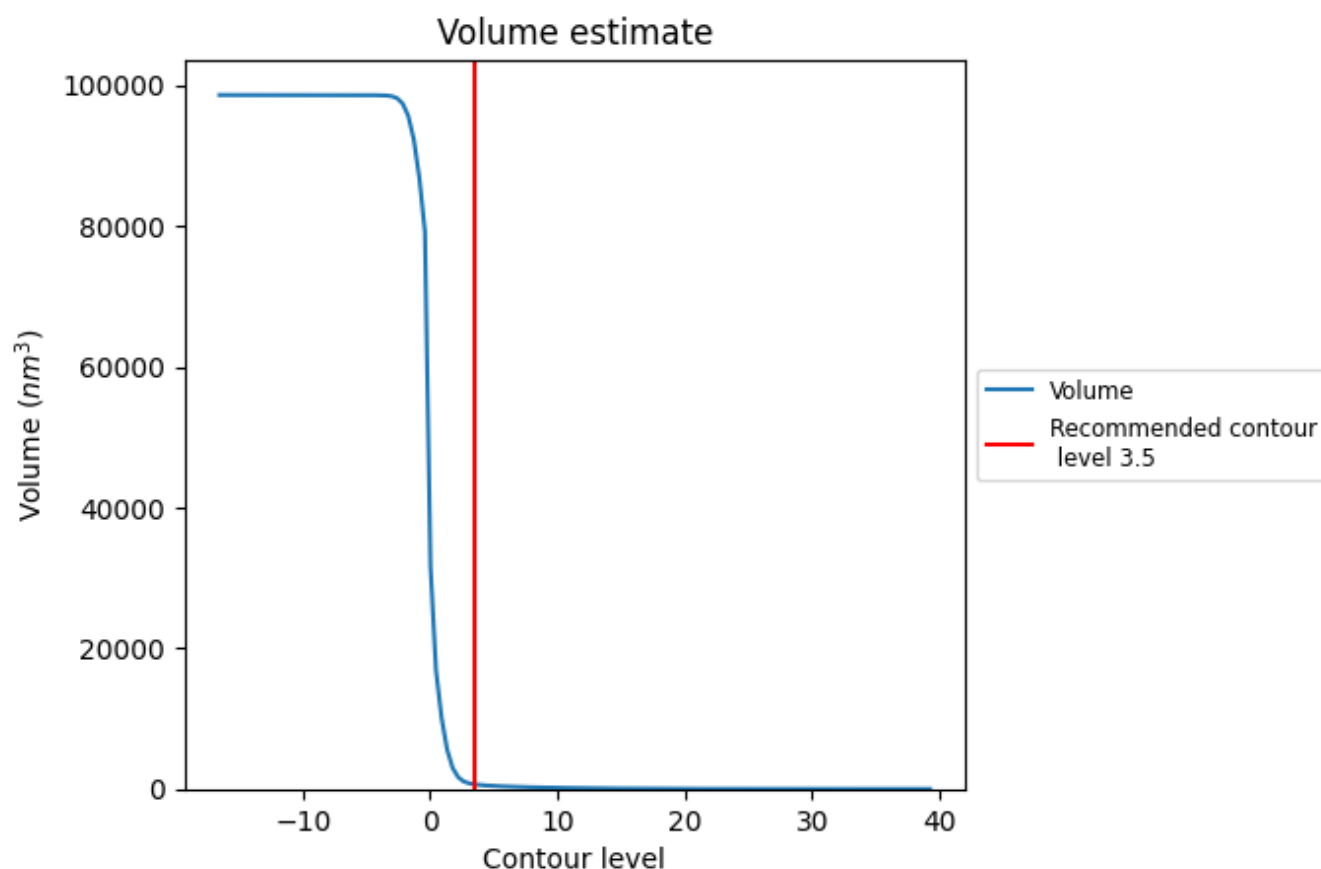
This section contains the results of statistical analysis of the map.

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.

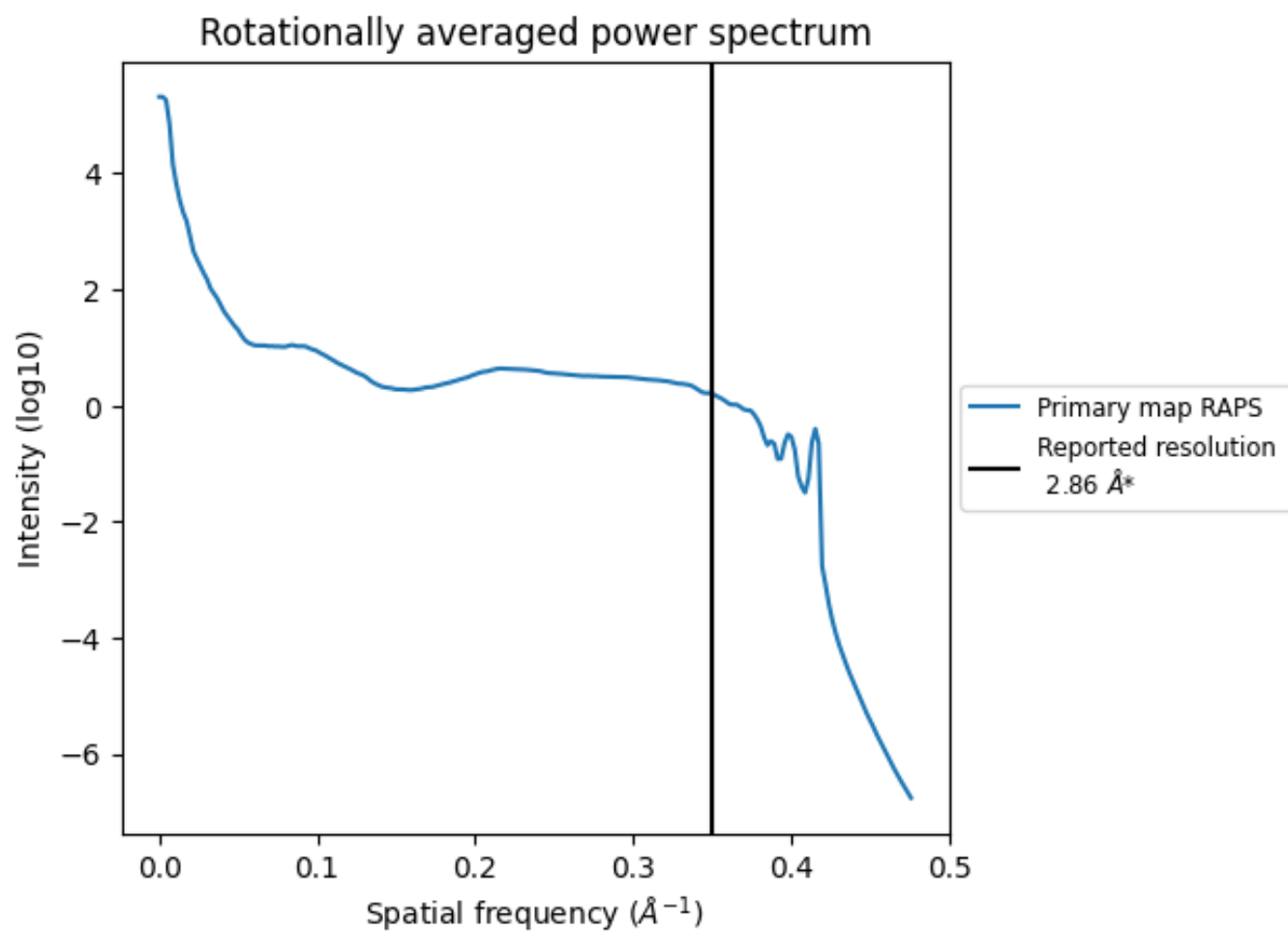
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656 nm^3 ; this corresponds to an approximate mass of 593 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 0.350 Å⁻¹

8 Fourier-Shell correlation

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

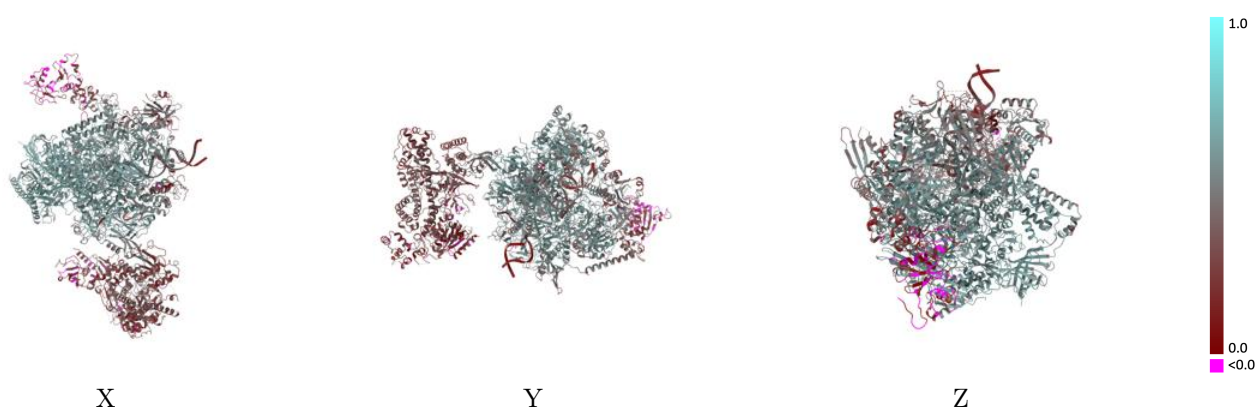
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16837 and PDB model 80EV. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

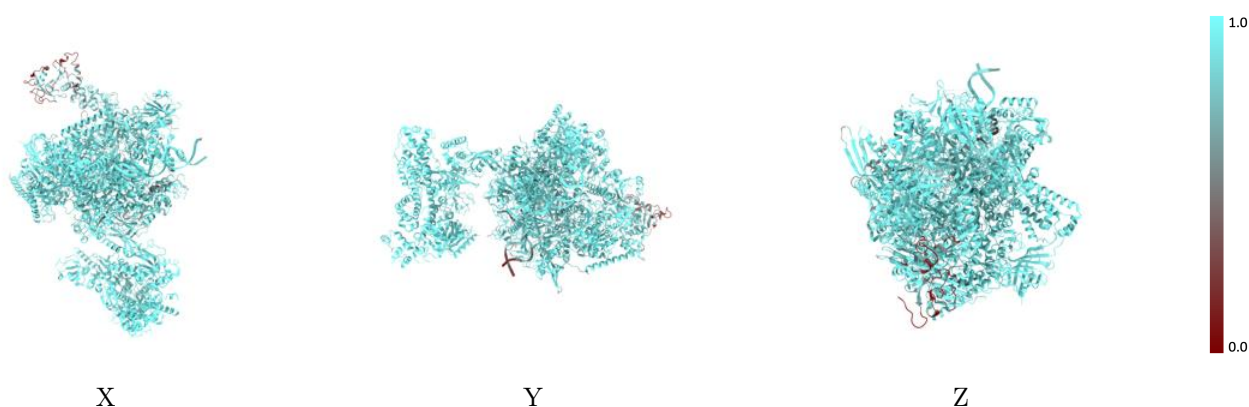
This section was not generated.

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



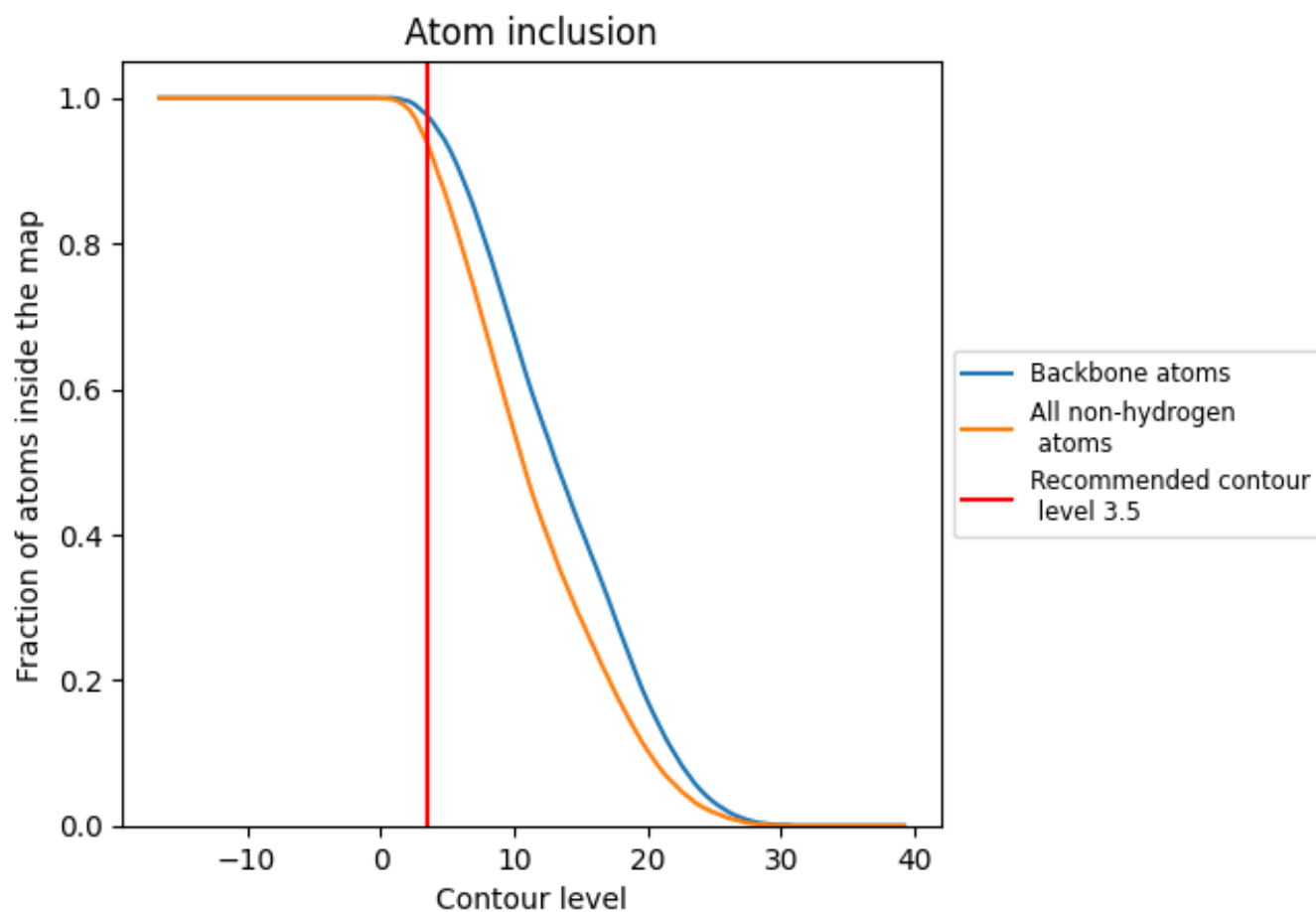
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.4680
A	 0.9550	 0.5510
B	 0.9600	 0.5650
C	 0.9690	 0.5950
D	 0.9610	 0.3040
E	 0.9520	 0.5160
F	 0.9620	 0.5790
G	 0.9500	 0.4070
H	 0.9650	 0.5760
I	 0.9310	 0.4670
J	 0.9750	 0.6040
K	 0.9670	 0.5950
L	 0.9410	 0.5120
M	 0.8590	 0.3090
N	 0.8140	 0.2840
O	 0.5700	 0.1210
P	 0.8820	 0.4980
Q	 0.4420	 0.0670
S	 0.9830	 0.2530
T	 0.8450	 0.3850

