



Full wwPDB EM Validation Report ⓘ

Oct 19, 2026 – 07:23 pm BST

PDB ID : 3ZTZ / pdb_000032zt
EMDB ID : EMD-59290
Title : B. subtilis RNA Polymerase with SigF
Authors : Loll, B.; Hilal, T.
Deposited on : 2026-08-03
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

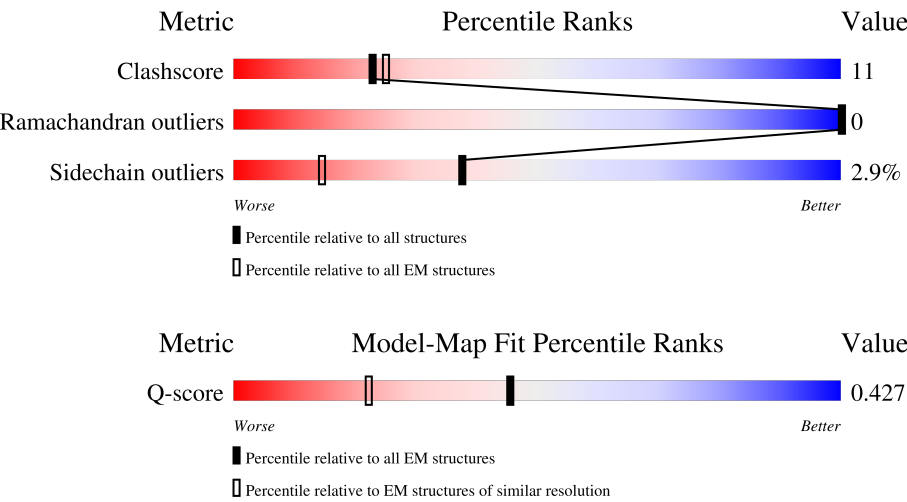
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	F	255	6% 57% 38% 5%
2	O	67	67% 22% 9%
3	E	69	72% 26%
4	U	314	56% 16% 27%

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Mol	Chain	Length	Quality of chain
4	V	314	55%18%27%
5	Y	1209	71%26%
6	D	173	30%32%21%47%
7	X	1193	69%27%
8	K	64	5%30%34%36%
9	L	64	12%39%39%22%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 27619 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 RNA polymerase sigma-F factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	242	Total	C	N	O	S	0	0
			1963	1235	343	381	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	61	Total	C	N	O	S	0	0
			485	305	83	93	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	69	Total	C	N	O	S	0	0
			580	373	92	114	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	LEU	PHE	conflict	UNP A0A9W5LJC9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	230	Total	C	N	O	S	0	0
			1770	1115	296	358	1		
4	U	228	Total	C	N	O		0	0
			1754	1104	294	356			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	1181	Total	C	N	O	S	0	0
			9291	5861	1656	1731	43		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1200	HIS	-	expression tag	UNP P37871
Y	1201	HIS	-	expression tag	UNP P37871
Y	1202	HIS	-	expression tag	UNP P37871
Y	1203	HIS	-	expression tag	UNP P37871
Y	1204	HIS	-	expression tag	UNP P37871
Y	1205	HIS	-	expression tag	UNP P37871
Y	1206	HIS	-	expression tag	UNP P37871
Y	1207	HIS	-	expression tag	UNP P37871
Y	1208	HIS	-	expression tag	UNP P37871
Y	1209	HIS	-	expression tag	UNP P37871

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	91	Total	C	N	O	S	0	0
			755	484	121	149	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	1160	Total	C	N	O	S	0	0
			9154	5738	1598	1784	34		

- Molecule 8 is a DNA chain called SigF controlled promoter PkatX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	41	Total	C	N	O	P	0	0
			840	404	148	247	41		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3	DT	-	expression tag	GB 1169001324
K	4	DT	-	expression tag	GB 1169001324
K	5	DT	-	expression tag	GB 1169001324
K	6	DT	-	expression tag	GB 1169001324
K	7	DT	-	expression tag	GB 1169001324
K	8	DT	-	expression tag	GB 1169001324
K	9	DG	-	expression tag	GB 1169001324
K	10	DA	-	expression tag	GB 1169001324
K	11	DT	-	expression tag	GB 1169001324

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Chain	Residue	Modelled	Actual	Comment	Reference
K	12	DG	-	expression tag	GB 1169001324
K	13	DC	-	expression tag	GB 1169001324
K	14	DC	-	expression tag	GB 1169001324
K	15	DA	-	expression tag	GB 1169001324
K	16	DT	-	expression tag	GB 1169001324
K	17	DT	-	expression tag	GB 1169001324
K	18	DG	-	expression tag	GB 1169001324
K	19	DT	-	expression tag	GB 1169001324
K	20	DT	-	expression tag	GB 1169001324
K	?	-	DT	deletion	GB 1169001324

- Molecule 9 is a DNA chain called SigF controlled promoter PkatX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	50	Total	C	N	O	P	0	0
			1024	492	180	302	50		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	Y	1	Total	Mg	0
			1	1	

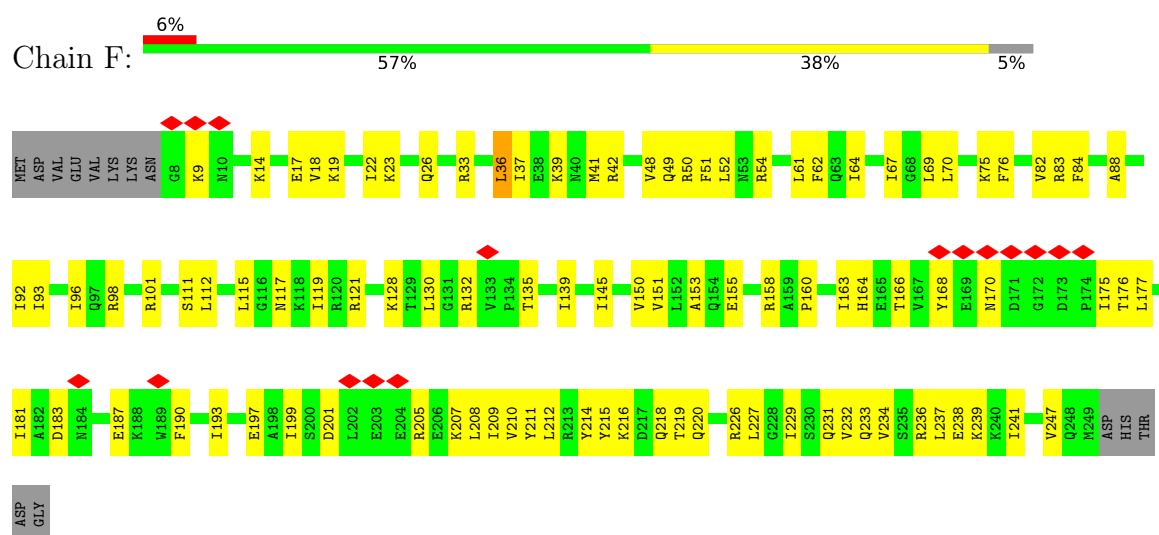
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	Y	2	Total	Zn	0
			2	2	

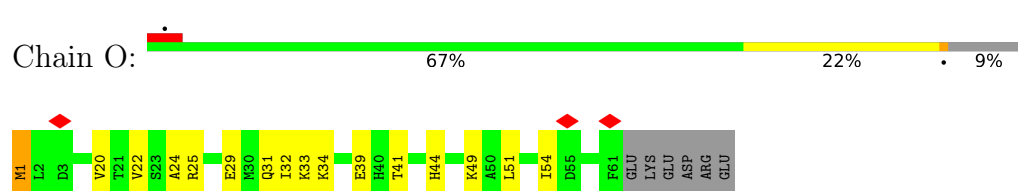
3 Residue-property plots

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.

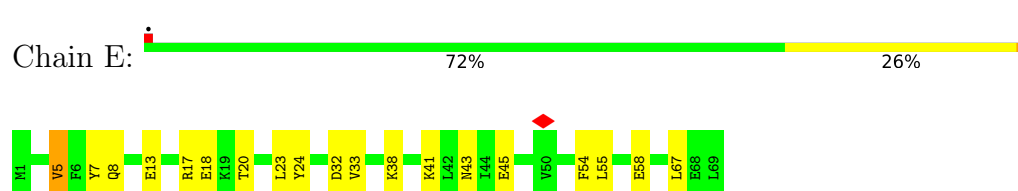
- Molecule 1: RNA polymerase sigma-F factor



- Molecule 2: DNA-directed RNA polymerase subunit omega

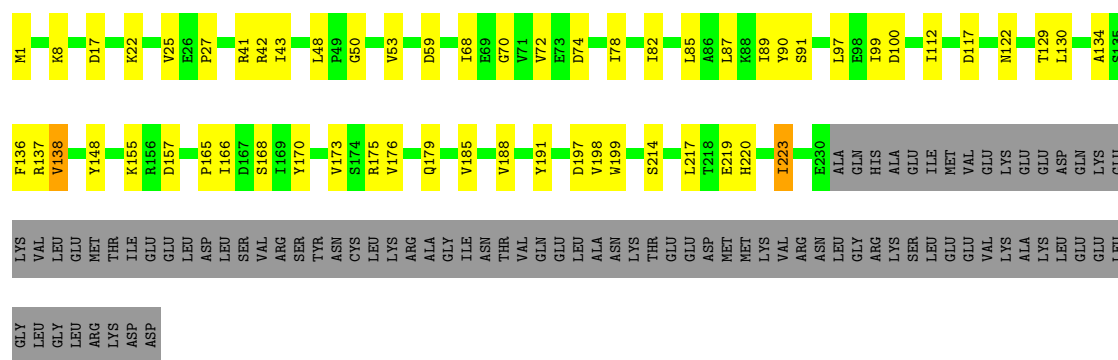


- Molecule 3: DNA-directed RNA polymerase subunit epsilon



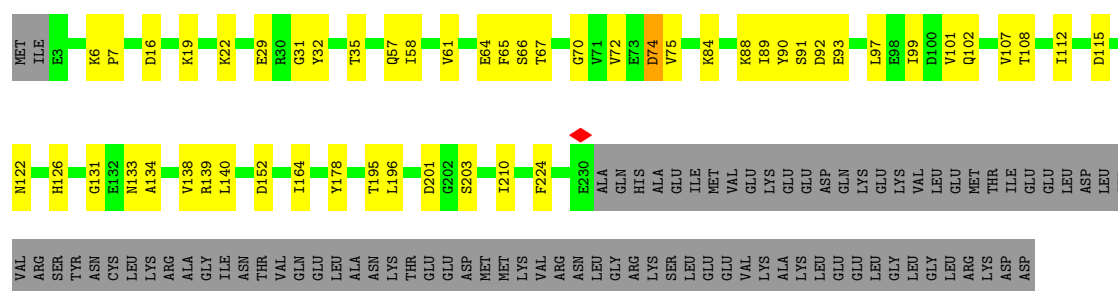
- Molecule 4: DNA-directed RNA polymerase subunit alpha





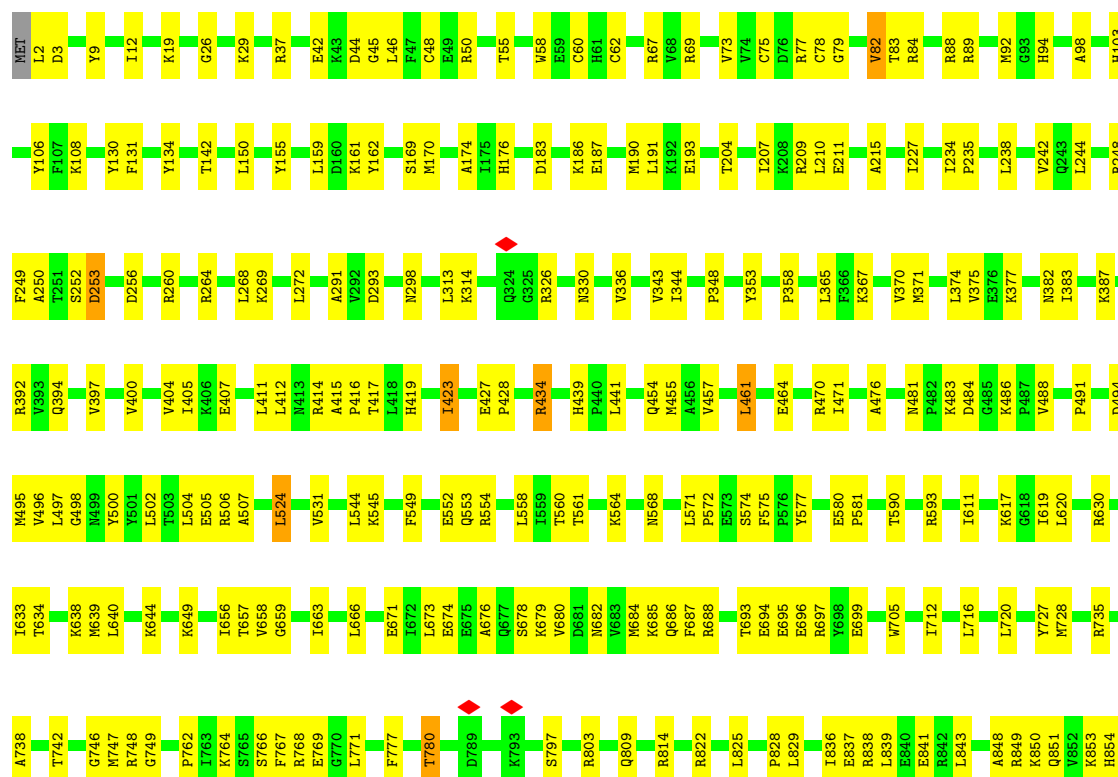
• Molecule 4: DNA-directed RNA polymerase subunit alpha

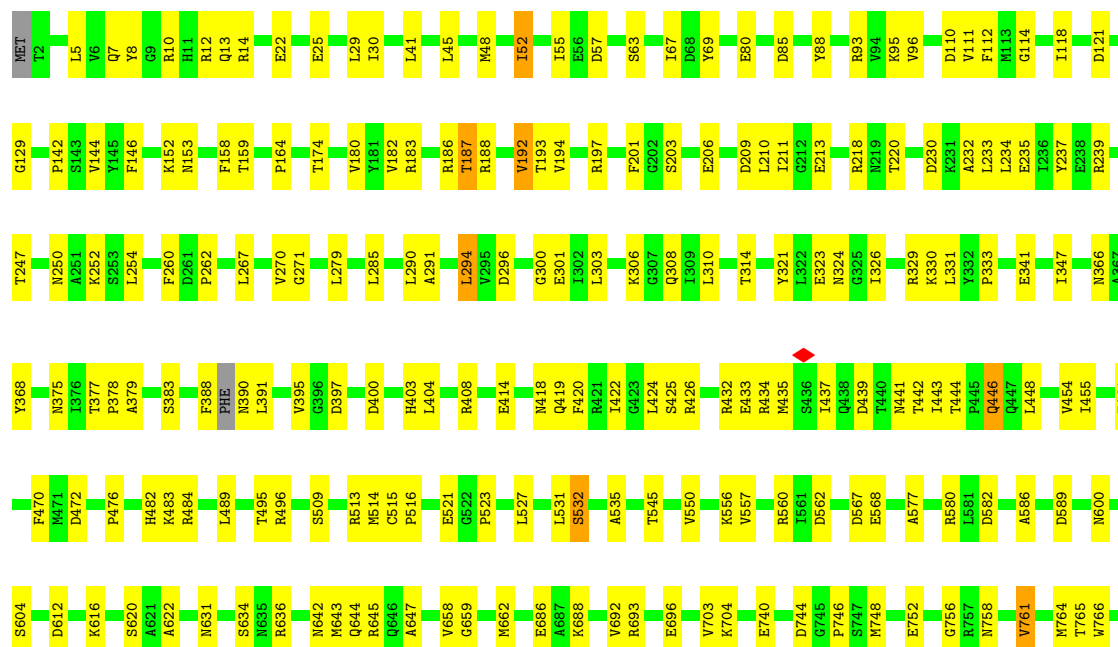
Chain U: 56% 16% 27%

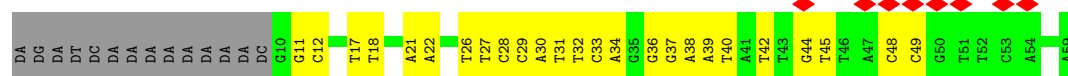


• Molecule 5: DNA-directed RNA polymerase subunit beta'

Chain Y: 71% 26% ..







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.883	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	314.496, 314.496, 314.496	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.819, 0.819, 0.819	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	F	0.13	0/1987	0.39	0/2673
2	O	0.12	0/490	0.37	0/655
3	E	0.09	0/589	0.27	0/789
4	U	0.13	0/1780	0.30	0/2421
4	V	0.10	0/1796	0.27	0/2442
5	Y	0.10	0/9441	0.28	0/12734
6	D	0.10	0/771	0.33	0/1041
7	X	0.10	0/9311	0.26	0/12586
8	K	0.67	0/940	0.92	0/1446
9	L	0.65	0/1147	0.89	0/1768
All	All	0.21	0/28252	0.38	0/38555

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1963	0	2000	80	0
2	O	485	0	505	19	0
3	E	580	0	585	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	1754	0	1762	33	0
4	V	1770	0	1785	35	0
5	Y	9291	0	9531	223	0
6	D	755	0	728	25	0
7	X	9154	0	9091	219	0
8	K	840	0	468	20	0
9	L	1024	0	569	20	0
10	Y	1	0	0	0	0
11	Y	2	0	0	0	0
All	All	27619	0	27024	614	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 11.

All (614) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:657:THR:HG21	7:X:1030:VAL:HA	1.58	0.85
5:Y:244:LEU:HB2	5:Y:248:ARG:HB3	1.60	0.84
4:U:29:GLU:HB2	4:U:32:TYR:HD2	1.49	0.77
2:O:31:GLN:O	2:O:34:LYS:NZ	2.17	0.77
5:Y:685:LYS:HA	5:Y:688:ARG:HG2	1.69	0.74
5:Y:549:PHE:HB3	5:Y:554:ARG:HG3	1.68	0.74
7:X:308:GLN:HE22	7:X:314:THR:HG21	1.52	0.73
5:Y:491:PRO:HB3	5:Y:495:MET:HG2	1.70	0.72
8:K:8:DT:H2'	8:K:9:DG:C8	2.25	0.72
5:Y:62:CYS:HB3	5:Y:78:CYS:SG	2.29	0.71
3:E:17:ARG:HD3	7:X:1025:PRO:HD3	1.72	0.71
1:F:187:GLU:HA	1:F:190:PHE:HB3	1.72	0.71
1:F:166:THR:HA	1:F:176:THR:HA	1.73	0.70
7:X:158:PHE:H	7:X:174:THR:HG22	1.56	0.70
9:L:39:DA:H2''	9:L:40:DT:H5'	1.71	0.70
4:V:42:ARG:HE	4:U:35:THR:HG22	1.58	0.68
5:Y:358:PRO:HB3	5:Y:434:ARG:HA	1.77	0.67
7:X:472:ASP:HB2	7:X:482:HIS:HD2	1.61	0.66
9:L:48:DC:H2''	9:L:49:DC:H5'	1.77	0.66
1:F:128:LYS:NZ	7:X:110:ASP:O	2.28	0.66
7:X:22:GLU:N	7:X:22:GLU:OE1	2.28	0.66
9:L:17:DT:H2''	9:L:18:DT:H5'	1.76	0.66
5:Y:268:LEU:O	5:Y:272:LEU:HD22	1.94	0.65
5:Y:663:ILE:O	5:Y:768:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ILE:HG21	5:Y:242:VAL:HG21	1.78	0.65
5:Y:984:VAL:HB	5:Y:988:GLN:HB2	1.78	0.65
7:X:484:ARG:NH2	7:X:532:SER:O	2.30	0.65
5:Y:371:MET:HE1	5:Y:387:LYS:HD3	1.79	0.64
5:Y:682:ASN:HA	5:Y:685:LYS:HG3	1.78	0.64
1:F:232:VAL:HG23	1:F:236:ARG:HH21	1.60	0.64
5:Y:735:ARG:HD2	7:X:960:LEU:HB3	1.78	0.64
7:X:643:MET:HE3	7:X:926:ALA:HB1	1.80	0.64
1:F:33:ARG:HA	1:F:36:LEU:HD23	1.80	0.63
1:F:48:VAL:HG21	1:F:62:PHE:HA	1.80	0.63
5:Y:838:ARG:HB2	5:Y:841:GLU:HG3	1.80	0.63
7:X:1097:THR:HG22	7:X:1125:PRO:HG3	1.80	0.63
1:F:231:GLN:NE2	8:K:45:DA:N7	2.47	0.63
7:X:321:TYR:HB3	7:X:326:ILE:HD13	1.79	0.63
7:X:1117:ASP:OD2	7:X:1118:ASN:N	2.31	0.63
5:Y:1178:MET:SD	5:Y:1181:ARG:NH2	2.72	0.63
4:V:99:ILE:HB	4:V:138:VAL:HG13	1.79	0.63
1:F:41:MET:HE2	1:F:41:MET:HA	1.81	0.62
4:V:70:GLY:HA3	4:V:134:ALA:HB2	1.81	0.62
8:K:47:DA:H2''	8:K:48:DC:H5'	1.83	0.61
7:X:686:GLU:HG2	7:X:688:LYS:H	1.64	0.61
5:Y:684:MET:HE1	5:Y:697:ARG:HD2	1.83	0.61
5:Y:42:GLU:N	5:Y:42:GLU:OE2	2.34	0.61
7:X:765:THR:HA	7:X:770:ASN:HD21	1.66	0.61
1:F:54:ARG:NH1	8:K:22:DT:OP2	2.34	0.60
7:X:832:ILE:HA	7:X:887:ILE:HD11	1.82	0.60
4:U:93:GLU:N	4:U:93:GLU:OE2	2.34	0.60
5:Y:62:CYS:N	5:Y:78:CYS:SG	2.73	0.60
5:Y:1053:LYS:HG3	5:Y:1057:MET:HE2	1.84	0.60
1:F:220:GLN:NE2	1:F:231:GLN:O	2.34	0.60
5:Y:854:HIS:HD2	5:Y:856:GLU:H	1.48	0.60
7:X:764:MET:O	7:X:770:ASN:ND2	2.35	0.60
4:U:6:LYS:HE2	4:U:7:PRO:HD2	1.84	0.60
5:Y:1106:VAL:HG13	5:Y:1111:ASN:HB2	1.84	0.59
1:F:130:LEU:HD23	1:F:132:ARG:HH21	1.67	0.59
4:V:176:VAL:HG22	4:V:198:VAL:HG22	1.83	0.59
5:Y:1086:THR:HG23	5:Y:1088:VAL:H	1.67	0.59
7:X:1035:MET:HG2	7:X:1037:MET:HG3	1.82	0.59
7:X:1101:ASP:N	7:X:1101:ASP:OD1	2.35	0.59
8:K:6:DT:H2'	8:K:7:DT:H71	1.83	0.59
4:V:90:TYR:HB2	4:V:117:ASP:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:97:LEU:HD23	4:V:112:ILE:HG21	1.84	0.59
5:Y:1033:GLU:O	5:Y:1037:VAL:HG22	2.03	0.59
7:X:52:ILE:HD13	7:X:424:LEU:HD13	1.83	0.59
3:E:23:LEU:HD13	3:E:67:LEU:HD12	1.85	0.59
7:X:323:GLU:HA	7:X:368:TYR:HE1	1.67	0.59
5:Y:253:ASP:OD2	5:Y:253:ASP:N	2.35	0.59
1:F:160:PRO:HB3	5:Y:249:PHE:HB3	1.84	0.58
1:F:117:ASN:ND2	8:K:23:DA:N7	2.52	0.58
5:Y:434:ARG:HB2	7:X:1048:LEU:HD22	1.85	0.58
4:U:58:ILE:HB	4:U:61:VAL:HG12	1.83	0.58
7:X:980:ALA:HB2	7:X:987:ILE:HD12	1.85	0.58
7:X:811:ARG:NH2	7:X:821:LEU:O	2.36	0.58
7:X:296:ASP:HB2	7:X:301:GLU:HG3	1.85	0.58
7:X:146:PHE:HD2	7:X:391:LEU:HD22	1.68	0.58
1:F:9:LYS:HA	1:F:39:LYS:HG2	1.84	0.58
2:O:25:ARG:NH2	5:Y:1181:ARG:O	2.37	0.58
5:Y:187:GLU:OE1	5:Y:209:ARG:NH2	2.36	0.58
5:Y:298:ASN:ND2	5:Y:313:LEU:O	2.32	0.58
7:X:57:ASP:OD1	7:X:57:ASP:N	2.37	0.58
1:F:128:LYS:HE2	7:X:446:GLN:HG2	1.86	0.58
1:F:193:ILE:HD11	7:X:1107:VAL:HG13	1.85	0.58
7:X:57:ASP:HB3	7:X:432:ARG:HH21	1.68	0.58
4:U:99:ILE:HG12	4:U:112:ILE:HG12	1.87	0.57
6:D:51:LEU:HD13	6:D:54:ARG:HB3	1.86	0.57
5:Y:1160:GLY:O	5:Y:1164:ASN:ND2	2.35	0.57
8:K:40:DT:H2"	8:K:41:DT:H5"	1.86	0.57
1:F:212:LEU:HA	1:F:215:TYR:HE1	1.69	0.57
7:X:209:ASP:OD2	7:X:329:ARG:NH1	2.37	0.57
4:U:66:SER:OG	4:U:67:THR:N	2.37	0.57
4:V:155:LYS:HE2	4:V:165:PRO:HG3	1.85	0.56
7:X:388:PHE:O	7:X:390:ASN:N	2.38	0.56
7:X:279:LEU:O	7:X:366:ASN:ND2	2.38	0.56
7:X:377:THR:HG22	7:X:379:ALA:H	1.69	0.56
7:X:838:ASP:OD1	7:X:881:HIS:ND1	2.37	0.56
7:X:796:GLU:OE1	7:X:910:ARG:NH1	2.38	0.56
1:F:218:GLN:HA	5:Y:69:ARG:HH21	1.71	0.56
7:X:434:ARG:HD2	7:X:448:LEU:HA	1.87	0.56
4:U:74:ASP:OD1	4:U:74:ASP:N	2.35	0.56
1:F:163:ILE:HG23	5:Y:250:ALA:HB1	1.86	0.56
3:E:5:VAL:HG13	3:E:23:LEU:HG	1.87	0.56
5:Y:849:ARG:H	5:Y:886:ILE:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:53:ASP:OD1	6:D:53:ASP:N	2.37	0.56
7:X:642:ASN:OD1	7:X:645:ARG:NH2	2.39	0.56
2:O:51:LEU:HD21	5:Y:471:ILE:HD11	1.87	0.56
5:Y:155:TYR:O	5:Y:159:LEU:HD23	2.04	0.56
7:X:213:GLU:OE2	7:X:218:ARG:NH2	2.38	0.56
7:X:294:LEU:HB2	7:X:303:LEU:HB2	1.87	0.56
7:X:616:LYS:HD3	7:X:662:MET:HE1	1.88	0.56
7:X:489:LEU:HD21	7:X:527:LEU:HD13	1.87	0.56
5:Y:183:ASP:HB3	5:Y:186:LYS:HB3	1.86	0.55
5:Y:1096:ILE:O	5:Y:1100:THR:HG23	2.06	0.55
6:D:3:ILE:HD11	6:D:22:GLU:HB3	1.87	0.55
7:X:916:LYS:HB2	4:U:65:PHE:HZ	1.71	0.55
7:X:1055:PRO:HD3	7:X:1070:PHE:HB3	1.89	0.55
5:Y:134:TYR:N	5:Y:150:LEU:O	2.40	0.55
5:Y:666:LEU:HD22	5:Y:716:LEU:HB3	1.88	0.55
7:X:1153:GLU:OE2	7:X:1155:ARG:NH1	2.40	0.55
5:Y:344:ILE:HG21	5:Y:455:MET:HG3	1.89	0.55
5:Y:671:GLU:CD	5:Y:671:GLU:H	2.15	0.55
1:F:229:ILE:HD12	1:F:233:GLN:HB2	1.89	0.55
7:X:801:ASP:OD1	7:X:906:ASN:ND2	2.35	0.55
4:U:58:ILE:HG12	4:U:138:VAL:HG22	1.88	0.55
5:Y:405:ILE:HG23	5:Y:428:PRO:HG2	1.89	0.55
5:Y:564:LYS:O	5:Y:568:ASN:ND2	2.40	0.55
8:K:27:DC:H2''	8:K:28:DT:H5'	1.89	0.55
5:Y:965:PRO:HD3	5:Y:1030:ASP:HB2	1.88	0.54
7:X:919:ILE:HD13	7:X:1039:LYS:HD2	1.89	0.54
5:Y:930:PRO:HG2	5:Y:1062:ILE:HD11	1.89	0.54
6:D:9:GLU:HA	6:D:12:LYS:HD3	1.89	0.54
7:X:435:MET:HE3	7:X:435:MET:HA	1.87	0.54
2:O:39:GLU:OE2	2:O:39:GLU:N	2.28	0.54
4:V:22:LYS:HG2	4:V:197:ASP:HB3	1.88	0.54
4:V:179:GLN:N	4:V:179:GLN:OE1	2.40	0.54
5:Y:500:TYR:HE1	5:Y:728:MET:HG2	1.72	0.54
5:Y:483:LYS:NZ	5:Y:484:ASP:OD1	2.39	0.54
5:Y:814:ARG:NH2	5:Y:896:HIS:O	2.35	0.54
7:X:439:ASP:O	7:X:441:ASN:ND2	2.40	0.54
2:O:29:GLU:O	2:O:33:LYS:HG2	2.08	0.54
5:Y:837:GLU:OE2	5:Y:1056:ARG:NE	2.41	0.54
5:Y:439:HIS:HE1	5:Y:441:LEU:HD12	1.72	0.54
7:X:180:VAL:HG22	7:X:192:VAL:HG11	1.90	0.54
7:X:496:ARG:HD3	7:X:523:PRO:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:1130:VAL:O	7:X:1134:GLU:HG3	2.08	0.54
1:F:49:GLN:HA	1:F:52:LEU:HB2	1.90	0.53
1:F:37:ILE:HD13	1:F:69:LEU:HD23	1.91	0.53
5:Y:1039:ASP:N	5:Y:1039:ASP:OD2	2.40	0.53
7:X:556:LYS:HG2	7:X:586:ALA:HB2	1.91	0.53
4:U:108:THR:HG22	4:U:126:HIS:HA	1.90	0.53
5:Y:45:GLY:H	5:Y:48:CYS:HB2	1.73	0.53
5:Y:392:ARG:NH1	7:X:838:ASP:O	2.41	0.53
5:Y:572:PRO:HG2	5:Y:575:PHE:HB2	1.90	0.53
5:Y:375:VAL:HG21	5:Y:383:ILE:HD13	1.89	0.53
5:Y:695:GLU:OE1	5:Y:695:GLU:N	2.25	0.53
7:X:29:LEU:HB3	7:X:484:ARG:HD2	1.91	0.53
5:Y:851:GLN:N	5:Y:851:GLN:OE1	2.38	0.53
7:X:194:VAL:HG13	7:X:232:ALA:HB1	1.91	0.53
1:F:84:PHE:CE1	1:F:88:ALA:HB2	2.44	0.53
6:D:67:ARG:NH2	6:D:79:ARG:HH21	2.07	0.53
3:E:32:ASP:OD1	3:E:33:VAL:N	2.42	0.52
7:X:186:ARG:NH2	9:L:49:DC:O2	2.41	0.52
9:L:27:DT:H2''	9:L:28:DC:C5	2.44	0.52
9:L:33:DC:H2''	9:L:34:DA:C8	2.44	0.52
5:Y:370:VAL:O	5:Y:374:LEU:HG	2.09	0.52
5:Y:215:ALA:HB1	5:Y:1152:LYS:HA	1.90	0.52
5:Y:927:ILE:O	5:Y:1055:TYR:OH	2.23	0.52
6:D:22:GLU:HA	6:D:25:GLU:OE2	2.09	0.52
7:X:291:ALA:HA	7:X:306:LYS:HG3	1.90	0.52
1:F:61:LEU:HA	1:F:64:ILE:HD12	1.92	0.52
1:F:201:ASP:OD2	1:F:201:ASP:N	2.41	0.52
1:F:247:VAL:O	5:Y:382:ASN:ND2	2.37	0.52
5:Y:658:VAL:HG11	7:X:962:VAL:HG21	1.91	0.52
5:Y:809:GLN:OE1	5:Y:1162:LYS:HE2	2.10	0.52
5:Y:975:ASP:OD2	5:Y:975:ASP:N	2.38	0.52
4:U:57:GLN:OE1	4:U:139:ARG:NH1	2.42	0.52
8:K:7:DT:H2'	8:K:8:DT:C6	2.45	0.52
2:O:24:ALA:HB1	5:Y:464:GLU:HG3	1.90	0.52
5:Y:234:ILE:HG12	5:Y:235:PRO:HD2	1.91	0.52
5:Y:491:PRO:O	5:Y:617:LYS:NZ	2.42	0.52
5:Y:1161:LEU:HD22	5:Y:1171:VAL:HG13	1.91	0.52
7:X:14:ARG:NH1	7:X:752:GLU:OE2	2.42	0.52
1:F:19:LYS:O	1:F:23:LYS:HG2	2.09	0.52
5:Y:9:TYR:HB2	7:X:1145:LEU:HB2	1.91	0.52
7:X:444:THR:HB	7:X:448:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:134:TYR:O	5:Y:150:LEU:N	2.37	0.52
5:Y:374:LEU:HD23	5:Y:400:VAL:HG21	1.90	0.52
7:X:795:TYR:HB3	7:X:877:LEU:HD21	1.90	0.52
6:D:61:ASP:HA	6:D:64:ILE:HG12	1.91	0.51
7:X:1108:LYS:HG3	7:X:1120:PRO:HG2	1.92	0.51
1:F:14:LYS:HZ2	1:F:17:GLU:HB2	1.74	0.51
5:Y:336:VAL:HG11	7:X:1095:ILE:HG23	1.93	0.51
4:V:173:VAL:HG11	4:V:176:VAL:HG23	1.93	0.51
5:Y:131:PHE:CD2	5:Y:170:MET:HG2	2.46	0.51
5:Y:348:PRO:O	5:Y:644:LYS:NZ	2.43	0.51
7:X:182:VAL:HB	7:X:192:VAL:HG12	1.92	0.51
7:X:426:ARG:HG3	7:X:426:ARG:HH11	1.76	0.51
5:Y:2:LEU:HB2	7:X:1157:LEU:HD11	1.92	0.51
1:F:164:HIS:HB3	5:Y:314:LYS:HD2	1.91	0.51
7:X:580:ARG:NH2	7:X:589:ASP:OD1	2.36	0.51
1:F:183:ASP:OD1	7:X:1061:GLN:NE2	2.33	0.51
1:F:205:ARG:O	1:F:209:ILE:HG13	2.11	0.51
4:V:41:ARG:NH1	4:V:176:VAL:O	2.43	0.51
5:Y:12:ILE:HD12	7:X:1142:VAL:HG22	1.92	0.51
7:X:400:ASP:HB3	7:X:403:HIS:HB2	1.92	0.51
5:Y:581:PRO:HB2	5:Y:619:ILE:HG13	1.92	0.51
7:X:296:ASP:HB3	7:X:300:GLY:H	1.76	0.51
5:Y:211:GLU:OE2	5:Y:1152:LYS:NZ	2.44	0.50
5:Y:671:GLU:HA	5:Y:674:GLU:OE1	2.11	0.50
7:X:233:LEU:HD21	7:X:252:LYS:HG2	1.93	0.50
7:X:1135:LEU:HB3	7:X:1142:VAL:HG21	1.92	0.50
1:F:199:ILE:HG22	1:F:207:LYS:HE3	1.93	0.50
5:Y:496:VAL:HG23	5:Y:620:LEU:HD12	1.93	0.50
4:V:1:MET:SD	4:V:1:MET:N	2.82	0.50
5:Y:684:MET:O	5:Y:688:ARG:HD2	2.12	0.50
7:X:781:LEU:HD22	7:X:786:VAL:HG21	1.92	0.50
4:U:89:ILE:HG22	4:U:91:SER:H	1.77	0.50
8:K:44:DA:H2"	8:K:45:DA:H5"	1.92	0.50
5:Y:367:LYS:O	5:Y:371:MET:HG2	2.12	0.50
7:X:761:VAL:HG11	7:X:1035:MET:HB3	1.93	0.50
7:X:994:GLY:O	7:X:996:ARG:NH1	2.44	0.50
1:F:50:ARG:HD3	7:X:437:ILE:HD11	1.93	0.50
5:Y:850:LYS:HG2	5:Y:885:TRP:HB2	1.94	0.50
7:X:1102:ASP:O	7:X:1106:ARG:HG2	2.12	0.50
4:U:101:VAL:HG21	4:U:107:VAL:HG12	1.93	0.50
6:D:7:SER:OG	6:D:9:GLU:OE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:685:LYS:HD2	5:Y:686:GLN:N	2.27	0.50
6:D:37:LEU:HD22	6:D:55:ILE:HD12	1.92	0.50
4:U:70:GLY:O	4:U:131:GLY:N	2.44	0.50
5:Y:75:CYS:HB3	5:Y:78:CYS:HB2	1.93	0.49
6:D:35:GLU:HA	6:D:38:ASN:HD21	1.77	0.49
5:Y:50:ARG:HE	5:Y:79:GLY:HA3	1.77	0.49
7:X:290:LEU:HD12	7:X:308:GLN:HE21	1.77	0.49
7:X:472:ASP:HB2	7:X:482:HIS:CD2	2.46	0.49
9:L:38:DA:C8	9:L:38:DA:H5'	2.47	0.49
3:E:43:ASN:OD1	7:X:1029:ARG:NH1	2.44	0.49
5:Y:67:ARG:HG3	5:Y:69:ARG:HB3	1.93	0.49
7:X:560:ARG:NH1	7:X:562:ASP:OD1	2.45	0.49
1:F:219:THR:HG23	5:Y:69:ARG:HH22	1.75	0.49
5:Y:253:ASP:OD1	5:Y:314:LYS:N	2.45	0.49
4:U:70:GLY:HA3	4:U:134:ALA:HB2	1.95	0.49
5:Y:371:MET:HA	5:Y:374:LEU:HD12	1.95	0.49
5:Y:574:SER:OG	5:Y:630:ARG:NH2	2.46	0.49
5:Y:580:GLU:OE2	5:Y:593:ARG:NH2	2.45	0.49
4:U:64:GLU:HB2	4:U:164:ILE:HG21	1.94	0.49
7:X:974:LEU:HG	7:X:1033:GLY:HA3	1.93	0.49
9:L:29:DC:H2''	9:L:30:DA:C8	2.47	0.49
1:F:158:ARG:HH22	5:Y:248:ARG:HA	1.76	0.49
7:X:121:ASP:OD1	7:X:121:ASP:N	2.45	0.49
1:F:226:ARG:HE	1:F:227:LEU:HD22	1.77	0.49
5:Y:186:LYS:HD3	5:Y:190:MET:HE3	1.95	0.49
7:X:85:ASP:HA	7:X:129:GLY:HA3	1.93	0.49
7:X:744:ASP:HB2	7:X:748:MET:HB2	1.95	0.49
8:K:9:DG:H2'	8:K:10:DA:C8	2.48	0.49
4:V:99:ILE:HD11	4:V:112:ILE:HG13	1.93	0.48
5:Y:190:MET:HE2	5:Y:190:MET:N	2.27	0.48
5:Y:659:GLY:HA2	7:X:971:VAL:HG11	1.95	0.48
2:O:41:THR:HG21	2:O:49:LYS:HE2	1.94	0.48
5:Y:679:LYS:HA	5:Y:682:ASN:ND2	2.27	0.48
7:X:1154:MET:SD	7:X:1154:MET:N	2.78	0.48
5:Y:682:ASN:HB3	5:Y:685:LYS:HE3	1.95	0.48
5:Y:747:MET:HG3	5:Y:749:GLY:N	2.28	0.48
7:X:761:VAL:HA	7:X:955:ILE:O	2.12	0.48
7:X:848:PRO:HA	7:X:872:VAL:HG12	1.94	0.48
7:X:979:ALA:HB2	7:X:1004:LEU:HD23	1.94	0.48
3:E:8:GLN:HB2	3:E:43:ASN:HB3	1.95	0.48
5:Y:848:ALA:HB2	5:Y:868:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:678:SER:O	5:Y:682:ASN:ND2	2.47	0.48
7:X:331:LEU:HD23	7:X:333:PRO:HD3	1.96	0.48
7:X:860:LEU:O	7:X:864:ILE:HG13	2.14	0.48
7:X:868:LYS:HD2	7:X:869:ALA:O	2.13	0.48
5:Y:577:TYR:O	5:Y:590:THR:OG1	2.28	0.48
5:Y:695:GLU:O	5:Y:699:GLU:HG2	2.13	0.48
5:Y:747:MET:HG3	5:Y:749:GLY:H	1.77	0.48
6:D:13:GLU:HG3	6:D:13:GLU:O	2.13	0.48
2:O:29:GLU:HA	2:O:32:ILE:HG12	1.95	0.48
6:D:21:HIS:O	6:D:25:GLU:HG3	2.13	0.48
6:D:47:LYS:HG3	6:D:49:GLU:H	1.78	0.48
1:F:83:ARG:HA	1:F:83:ARG:HD3	1.68	0.48
1:F:220:GLN:NE2	8:K:45:DA:OP2	2.46	0.48
4:V:130:LEU:HD21	4:V:136:PHE:HB2	1.96	0.48
5:Y:161:LYS:HG3	5:Y:162:TYR:HD2	1.78	0.48
5:Y:984:VAL:HG12	5:Y:986:ASP:H	1.78	0.48
7:X:515:CYS:HB2	7:X:620:SER:HB3	1.95	0.48
7:X:769:TYR:HB2	7:X:776:ILE:HD11	1.96	0.48
1:F:18:VAL:O	1:F:22:ILE:HG12	2.14	0.48
1:F:212:LEU:HA	1:F:215:TYR:CE1	2.48	0.48
5:Y:414:ARG:HG2	5:Y:455:MET:SD	2.54	0.48
5:Y:684:MET:O	5:Y:687:PHE:N	2.45	0.48
1:F:67:ILE:HA	1:F:70:LEU:HD12	1.96	0.47
5:Y:1053:LYS:O	5:Y:1057:MET:HG2	2.14	0.47
7:X:203:SER:N	7:X:206:GLU:OE2	2.47	0.47
7:X:756:GLY:HA3	7:X:1038:ILE:HG22	1.96	0.47
7:X:1156:ASP:HB3	7:X:1159:ASP:HB2	1.94	0.47
5:Y:560:THR:OG1	5:Y:561:THR:N	2.47	0.47
1:F:82:VAL:HG21	9:L:38:DA:H1'	1.97	0.47
5:Y:937:ARG:HH21	5:Y:1057:MET:HB3	1.80	0.47
5:Y:169:SER:HB2	5:Y:174:ALA:HB2	1.95	0.47
7:X:426:ARG:HG3	7:X:426:ARG:NH1	2.29	0.47
7:X:582:ASP:OD1	7:X:586:ALA:N	2.47	0.47
4:V:17:ASP:OD1	4:V:17:ASP:N	2.37	0.47
4:V:85:LEU:HD23	4:V:87:LEU:HD22	1.97	0.47
5:Y:392:ARG:HD2	5:Y:392:ARG:N	2.30	0.47
5:Y:981:ILE:HG23	5:Y:991:ILE:HG13	1.96	0.47
5:Y:983:GLU:HG2	5:Y:989:GLN:HG3	1.97	0.47
7:X:899:ASP:N	7:X:899:ASP:OD1	2.48	0.47
7:X:1049:HIS:NE2	7:X:1071:GLY:O	2.35	0.47
7:X:1057:SER:OG	7:X:1058:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:31:DT:H2"	9:L:32:DT:H72	1.97	0.47
1:F:197:GLU:OE2	7:X:1115:LYS:NZ	2.48	0.47
5:Y:190:MET:O	5:Y:193:GLU:HG3	2.15	0.47
7:X:25:GLU:H	7:X:25:GLU:CD	2.21	0.47
2:O:31:GLN:HB3	7:X:1118:ASN:HD21	1.80	0.47
5:Y:353:TYR:HB3	5:Y:476:ALA:HB2	1.96	0.47
7:X:622:ALA:O	7:X:644:GLN:NE2	2.47	0.47
7:X:693:ARG:HD2	7:X:704:LYS:HG3	1.97	0.47
5:Y:822:ARG:HB2	5:Y:891:THR:HB	1.95	0.47
7:X:813:ILE:HD11	7:X:844:GLY:HA3	1.96	0.47
7:X:1062:GLN:NE2	7:X:1127:SER:OG	2.48	0.47
4:U:102:GLN:OE1	4:U:102:GLN:HA	2.15	0.47
5:Y:26:GLY:O	5:Y:94:HIS:ND1	2.48	0.46
5:Y:130:TYR:OH	5:Y:293:ASP:OD2	2.18	0.46
7:X:870:ARG:HG3	7:X:872:VAL:H	1.80	0.46
7:X:887:ILE:HA	7:X:913:ILE:HA	1.96	0.46
7:X:10:ARG:NE	7:X:740:GLU:OE1	2.41	0.46
7:X:279:LEU:HD13	7:X:383:SER:HB2	1.97	0.46
7:X:1133:LYS:HA	7:X:1133:LYS:HD3	1.77	0.46
7:X:192:VAL:HG22	7:X:220:THR:HG21	1.96	0.46
7:X:1056:TYR:HE1	7:X:1063:PRO:HG3	1.80	0.46
5:Y:176:HIS:HB2	5:Y:227:ILE:HG21	1.96	0.46
5:Y:1023:VAL:HB	5:Y:1029:ILE:HD11	1.97	0.46
9:L:39:DA:C8	9:L:40:DT:H72	2.50	0.46
5:Y:498:GLY:O	5:Y:502:LEU:N	2.47	0.46
7:X:8:TYR:O	7:X:12:ARG:HB3	2.15	0.46
7:X:854:LEU:HB2	7:X:858:GLU:OE2	2.16	0.46
5:Y:29:LYS:HG2	5:Y:44:ASP:HB3	1.98	0.46
5:Y:55:THR:HA	5:Y:88:ARG:HD2	1.97	0.46
5:Y:544:LEU:O	5:Y:545:LYS:HG3	2.15	0.46
5:Y:720:LEU:HG	5:Y:727:TYR:HB2	1.98	0.46
5:Y:767:PHE:O	7:X:631:ASN:ND2	2.39	0.46
5:Y:828:PRO:HG3	5:Y:839:LEU:HB2	1.97	0.46
6:D:34:GLN:O	6:D:38:ASN:ND2	2.48	0.46
7:X:187:THR:HG23	7:X:188:ARG:H	1.80	0.46
7:X:296:ASP:HB3	7:X:300:GLY:N	2.31	0.46
1:F:54:ARG:NE	8:K:23:DA:N1	2.63	0.46
7:X:419:GLN:O	7:X:422:ILE:HG12	2.16	0.46
7:X:419:GLN:HG3	7:X:461:PHE:HB2	1.97	0.46
4:U:64:GLU:O	4:U:75:VAL:HB	2.16	0.46
2:O:33:LYS:C	2:O:34:LYS:HE2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:155:TYR:CE2	5:Y:159:LEU:HD21	2.51	0.46
5:Y:1115:THR:HA	6:D:63:ASN:HD21	1.81	0.46
7:X:260:PHE:CZ	7:X:378:PRO:HG3	2.51	0.46
1:F:209:ILE:HG21	1:F:234:VAL:HG21	1.97	0.46
5:Y:639:MET:HE3	5:Y:639:MET:HB3	1.80	0.46
7:X:659:GLY:O	7:X:989:SER:N	2.39	0.46
1:F:237:LEU:O	1:F:241:ILE:HG12	2.15	0.46
3:E:13:GLU:OE1	5:Y:506:ARG:NH1	2.48	0.46
5:Y:780:THR:HG21	7:X:516:PRO:HB2	1.97	0.45
5:Y:1035:LEU:HD13	5:Y:1043:VAL:HG21	1.98	0.45
7:X:404:LEU:HB2	7:X:509:SER:HB2	1.98	0.45
7:X:616:LYS:HE2	7:X:616:LYS:HB3	1.80	0.45
7:X:839:GLY:H	7:X:879:VAL:HG23	1.81	0.45
4:U:16:ASP:OD2	4:U:16:ASP:N	2.50	0.45
7:X:142:PRO:O	7:X:271:GLY:HA2	2.17	0.45
7:X:550:VAL:HG12	7:X:557:VAL:HG22	1.98	0.45
1:F:121:ARG:NE	8:K:24:DT:OP2	2.50	0.45
3:E:54:PHE:O	3:E:58:GLU:HG2	2.17	0.45
7:X:330:LYS:HE2	7:X:330:LYS:HB3	1.70	0.45
7:X:577:ALA:HB2	7:X:612:ASP:HB2	1.97	0.45
5:Y:762:PRO:HG2	5:Y:764:LYS:HD3	1.99	0.45
7:X:514:MET:HE3	7:X:514:MET:HB2	1.78	0.45
1:F:50:ARG:O	1:F:50:ARG:NE	2.50	0.45
1:F:50:ARG:NH1	7:X:433:GLU:HG2	2.31	0.45
1:F:163:ILE:HA	1:F:177:LEU:HB3	1.98	0.45
7:X:262:PRO:HD3	7:X:375:ASN:HD22	1.81	0.45
7:X:442:THR:OG1	7:X:443:ILE:N	2.48	0.45
7:X:778:SER:HB2	7:X:944:MET:HG3	1.97	0.45
7:X:983:LEU:HD21	7:X:1006:GLU:HG2	1.99	0.45
7:X:247:THR:OG1	7:X:250:ASN:HB3	2.16	0.45
4:U:29:GLU:HB2	4:U:32:TYR:CD2	2.39	0.45
4:V:100:ASP:HA	4:V:137:ARG:HD2	1.99	0.45
5:Y:486:LYS:HA	5:Y:486:LYS:HD3	1.76	0.45
4:U:22:LYS:HB2	4:U:22:LYS:HE2	1.79	0.45
8:K:42:DT:H4'	8:K:43:DT:OP1	2.16	0.45
4:V:42:ARG:NE	4:U:35:THR:HG22	2.29	0.45
7:X:201:PHE:CE1	7:X:210:LEU:HD22	2.52	0.45
7:X:237:TYR:CE2	7:X:254:LEU:HD13	2.52	0.45
7:X:321:TYR:HA	7:X:324:ASN:ND2	2.32	0.45
7:X:780:ARG:NH1	7:X:784:ASP:OD2	2.50	0.45
7:X:1108:LYS:HA	7:X:1108:LYS:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:VAL:O	1:F:155:GLU:HG2	2.17	0.45
5:Y:83:THR:OG1	5:Y:84:ARG:N	2.50	0.45
5:Y:679:LYS:HA	5:Y:682:ASN:HD22	1.82	0.45
5:Y:797:SER:HB2	5:Y:953:LEU:HD21	1.99	0.45
4:V:148:TYR:CG	5:Y:524:LEU:HD21	2.52	0.44
7:X:5:LEU:HD12	7:X:13:GLN:HG2	1.99	0.44
5:Y:62:CYS:SG	5:Y:77:ARG:NH1	2.91	0.44
5:Y:685:LYS:HD2	5:Y:685:LYS:C	2.42	0.44
5:Y:738:ALA:O	5:Y:742:THR:HG22	2.17	0.44
5:Y:1034:LEU:HG	5:Y:1043:VAL:HG22	1.98	0.44
7:X:235:GLU:O	7:X:239:ARG:HG2	2.17	0.44
2:O:34:LYS:HE2	2:O:34:LYS:N	2.31	0.44
5:Y:108:LYS:HD2	5:Y:108:LYS:HA	1.79	0.44
7:X:770:ASN:O	7:X:958:ASN:ND2	2.50	0.44
4:U:133:ASN:OD1	4:U:133:ASN:O	2.36	0.44
5:Y:454:GLN:NE2	7:X:1047:LYS:HD3	2.32	0.44
7:X:476:PRO:HD3	7:X:746:PRO:HG2	1.99	0.44
5:Y:264:ARG:NH1	5:Y:291:ALA:HB2	2.32	0.44
5:Y:864:GLU:HG3	6:D:13:GLU:OE2	2.17	0.44
5:Y:982:ASN:OD1	5:Y:982:ASN:N	2.50	0.44
4:U:88:LYS:HD3	4:U:90:TYR:CZ	2.53	0.44
1:F:220:GLN:HB3	8:K:44:DA:O5'	2.18	0.44
5:Y:256:ASP:O	5:Y:260:ARG:HG3	2.18	0.44
7:X:88:TYR:CZ	7:X:118:ILE:HD11	2.53	0.44
1:F:238:GLU:HB3	7:X:864:ILE:HD11	1.99	0.44
2:O:51:LEU:HD12	5:Y:470:ARG:HD3	2.00	0.44
5:Y:838:ARG:HG3	5:Y:838:ARG:HH11	1.83	0.44
1:F:247:VAL:HG12	5:Y:382:ASN:HB3	1.99	0.44
2:O:20:VAL:HG23	5:Y:471:ILE:HD12	1.99	0.44
5:Y:1170:LEU:HD12	5:Y:1170:LEU:HA	1.91	0.44
7:X:152:LYS:NZ	7:X:153:ASN:OD1	2.41	0.44
1:F:158:ARG:NH2	5:Y:248:ARG:HA	2.32	0.44
5:Y:103:HIS:HB3	5:Y:106:TYR:HD1	1.82	0.44
7:X:567:ASP:OD2	7:X:568:GLU:N	2.50	0.44
4:U:196:LEU:HD13	4:U:210:ILE:HD11	1.99	0.44
1:F:42:ARG:H	1:F:42:ARG:HG2	1.52	0.43
1:F:92:ILE:O	1:F:96:ILE:HG12	2.18	0.43
5:Y:748:ARG:HD3	5:Y:771:LEU:HD21	1.99	0.43
5:Y:853:LYS:HE2	5:Y:853:LYS:HB2	1.88	0.43
5:Y:950:THR:O	5:Y:955:ARG:HB2	2.17	0.43
6:D:83:PRO:HG2	6:D:86:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:330:LYS:HE3	7:X:341:GLU:HG3	2.00	0.43
7:X:636:ARG:HA	7:X:636:ARG:HD2	1.74	0.43
5:Y:419:HIS:HB3	5:Y:929:GLU:HB2	2.00	0.43
1:F:26:GLN:NE2	1:F:76:PHE:O	2.51	0.43
1:F:170:ASN:HB3	7:X:496:ARG:HH12	1.82	0.43
4:V:27:PRO:HB2	4:V:191:TYR:HD2	1.82	0.43
4:V:82:ILE:HD13	4:V:82:ILE:HA	1.87	0.43
5:Y:394:GLN:HB2	5:Y:397:VAL:HG23	1.99	0.43
5:Y:411:LEU:HD13	5:Y:423:ILE:HD11	2.00	0.43
5:Y:673:LEU:HD23	5:Y:673:LEU:HA	1.85	0.43
7:X:531:LEU:HG	7:X:535:ALA:HB3	2.01	0.43
6:D:61:ASP:O	6:D:65:ASP:N	2.51	0.43
7:X:925:MET:HE3	7:X:925:MET:HB2	1.91	0.43
7:X:925:MET:HE3	7:X:935:ILE:HD11	2.00	0.43
4:U:84:LYS:HB2	4:U:84:LYS:HE2	1.74	0.43
1:F:208:LEU:O	1:F:212:LEU:HG	2.19	0.43
2:O:44:HIS:H	5:Y:407:GLU:CD	2.27	0.43
4:U:122:ASN:OD1	4:U:122:ASN:N	2.51	0.43
8:K:45:DA:H2"	8:K:46:DA:C8	2.53	0.43
1:F:75:LYS:NZ	9:L:36:DG:OP2	2.42	0.43
3:E:38:LYS:HD3	3:E:38:LYS:HA	1.71	0.43
3:E:41:LYS:HB2	3:E:41:LYS:HE2	1.77	0.43
4:V:53:VAL:HB	4:V:166:ILE:HD11	2.01	0.43
4:V:157:ASP:OD1	4:V:157:ASP:N	2.43	0.43
5:Y:58:TRP:HA	5:Y:82:VAL:HG23	1.99	0.43
5:Y:439:HIS:HD1	5:Y:441:LEU:HB2	1.84	0.43
5:Y:1170:LEU:HD23	5:Y:1181:ARG:HH11	1.83	0.43
6:D:67:ARG:HH22	6:D:79:ARG:HH21	1.66	0.43
7:X:112:PHE:CZ	7:X:114:GLY:HA2	2.54	0.43
7:X:183:ARG:HH21	7:X:186:ARG:HB2	1.83	0.43
7:X:193:THR:O	7:X:197:ARG:HG2	2.19	0.43
7:X:306:LYS:HE3	7:X:306:LYS:HB2	1.79	0.43
7:X:855:THR:HG23	7:X:858:GLU:H	1.83	0.43
1:F:163:ILE:HG22	1:F:177:LEU:HG	1.99	0.43
5:Y:494:ASP:HA	5:Y:497:LEU:HB2	2.00	0.43
7:X:164:PRO:HA	7:X:267:LEU:HD23	2.01	0.43
1:F:98:ARG:HG2	1:F:101:ARG:HH22	1.84	0.43
2:O:1:MET:SD	5:Y:427:GLU:HB2	2.58	0.43
4:V:175:ARG:HG2	4:V:199:TRP:HB2	2.01	0.43
7:X:766:TRP:HB3	7:X:776:ILE:HD12	2.00	0.43
4:U:178:TYR:HA	4:U:195:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:VAL:HB	1:F:214:TYR:CE1	2.54	0.43
5:Y:412:LEU:HD22	5:Y:457:VAL:HG22	2.01	0.43
7:X:696:GLU:HB2	7:X:703:VAL:HB	2.00	0.43
7:X:1017:LEU:HD12	7:X:1017:LEU:HA	1.88	0.43
5:Y:777:PHE:O	5:Y:780:THR:HG22	2.18	0.42
5:Y:836:ILE:HD11	5:Y:1056:ARG:HB3	2.01	0.42
6:D:57:GLN:O	6:D:60:THR:HB	2.19	0.42
7:X:114:GLY:HA3	7:X:455:ILE:HD11	2.01	0.42
7:X:397:ASP:OD1	7:X:397:ASP:N	2.52	0.42
7:X:946:TYR:HA	7:X:952:PRO:HA	2.01	0.42
3:E:24:TYR:OH	3:E:58:GLU:OE2	2.20	0.42
5:Y:377:LYS:HE2	5:Y:377:LYS:HB2	1.92	0.42
5:Y:392:ARG:HH12	7:X:839:GLY:HA3	1.84	0.42
7:X:41:LEU:O	7:X:69:TYR:OH	2.32	0.42
4:V:25:VAL:HG21	4:U:224:PHE:CZ	2.55	0.42
4:V:59:ASP:HB2	4:V:137:ARG:HB2	2.01	0.42
5:Y:191:LEU:HB3	5:Y:210:LEU:HD23	2.01	0.42
6:D:71:LEU:HD21	6:D:82:TYR:HE1	1.84	0.42
8:K:34:DG:H2'	8:K:35:DA:C5	2.54	0.42
3:E:7:TYR:CE2	3:E:23:LEU:HD23	2.55	0.42
5:Y:98:ALA:HB2	5:Y:269:LYS:HG3	2.00	0.42
5:Y:461:LEU:HD21	7:X:1099:LYS:HD3	2.02	0.42
7:X:455:ILE:HD13	7:X:455:ILE:HA	1.85	0.42
4:V:219:GLU:O	4:V:223:ILE:HG23	2.19	0.42
5:Y:837:GLU:OE1	5:Y:1056:ARG:NH2	2.52	0.42
6:D:58:PHE:CE1	6:D:62:LEU:HD21	2.55	0.42
7:X:30:ILE:HD12	7:X:483:LYS:HD2	2.00	0.42
7:X:48:MET:HE1	7:X:420:PHE:CE2	2.54	0.42
1:F:193:ILE:O	1:F:197:GLU:HG2	2.19	0.42
5:Y:264:ARG:HH11	5:Y:291:ALA:HB2	1.84	0.42
5:Y:507:ALA:HB2	5:Y:611:ILE:HD11	2.01	0.42
5:Y:634:THR:O	5:Y:638:LYS:NZ	2.41	0.42
7:X:835:GLU:OE2	7:X:836:VAL:N	2.53	0.42
9:L:11:DG:H2''	9:L:12:DC:C6	2.55	0.42
1:F:84:PHE:CD1	1:F:84:PHE:C	2.96	0.42
4:V:43:ILE:HG13	4:V:217:LEU:HD22	2.02	0.42
4:V:122:ASN:OD1	4:V:122:ASN:N	2.52	0.42
4:V:220:HIS:O	4:V:223:ILE:HG13	2.20	0.42
7:X:67:ILE:HG12	7:X:95:LYS:HB2	2.02	0.42
7:X:285:LEU:HD21	7:X:347:ILE:HG21	2.01	0.42
7:X:940:PRO:HB2	7:X:942:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:LYS:HA	7:X:864:ILE:HG23	2.02	0.42
2:O:1:MET:HB3	5:Y:470:ARG:NH2	2.35	0.42
2:O:22:VAL:HG12	2:O:54:ILE:HD11	2.01	0.42
7:X:408:ARG:NH1	7:X:414:GLU:OE2	2.35	0.42
3:E:45:GLU:HG2	7:X:1016:VAL:HG21	2.01	0.42
1:F:119:ILE:HD11	1:F:150:VAL:HG22	2.02	0.42
1:F:163:ILE:HD11	5:Y:252:SER:HB2	2.01	0.42
2:O:33:LYS:HE3	2:O:33:LYS:HB3	1.66	0.42
3:E:67:LEU:HA	3:E:67:LEU:HD23	1.85	0.42
5:Y:204:THR:O	5:Y:207:ILE:HG22	2.20	0.42
5:Y:1134:LEU:HD23	5:Y:1134:LEU:HA	1.89	0.42
7:X:513:ARG:HG3	7:X:545:THR:OG1	2.20	0.42
1:F:42:ARG:HG3	9:L:42:DT:H1'	2.01	0.41
3:E:8:GLN:HE21	3:E:20:THR:HG22	1.86	0.41
7:X:111:VAL:HG12	7:X:446:GLN:NE2	2.36	0.41
7:X:422:ILE:O	7:X:426:ARG:HG2	2.19	0.41
9:L:21:DA:H2''	9:L:22:DA:O5'	2.20	0.41
9:L:26:DT:H2''	9:L:27:DT:H5'	2.02	0.41
5:Y:434:ARG:NH1	7:X:1045:ASP:OD1	2.53	0.41
5:Y:633:ILE:HG22	5:Y:634:THR:H	1.85	0.41
5:Y:1047:LEU:O	5:Y:1051:VAL:HG23	2.20	0.41
7:X:758:ASN:HA	7:X:1036:TYR:HA	2.01	0.41
3:E:18:GLU:OE2	3:E:18:GLU:N	2.50	0.41
5:Y:19:LYS:HB2	5:Y:19:LYS:HE2	1.90	0.41
5:Y:92:MET:HE2	5:Y:92:MET:HB3	1.80	0.41
5:Y:1158:LEU:HD13	5:Y:1167:ILE:HD13	2.01	0.41
7:X:764:MET:HE1	7:X:1026:PHE:CE2	2.56	0.41
7:X:888:HIS:N	7:X:912:TYR:O	2.48	0.41
1:F:211:TYR:O	1:F:215:TYR:HD1	2.03	0.41
5:Y:326:ARG:HA	5:Y:326:ARG:HD3	1.90	0.41
5:Y:558:LEU:HD21	5:Y:577:TYR:CE1	2.55	0.41
5:Y:705:TRP:CE3	5:Y:762:PRO:HG3	2.55	0.41
6:D:29:LYS:HB2	6:D:29:LYS:HE2	1.86	0.41
7:X:230:ASP:O	7:X:234:LEU:HD23	2.19	0.41
7:X:800:ARG:HB2	7:X:904:GLY:O	2.21	0.41
8:K:24:DT:H2''	8:K:25:DC:H4'	2.02	0.41
5:Y:495:MET:HE2	5:Y:495:MET:HB2	1.81	0.41
7:X:434:ARG:NH1	7:X:448:LEU:O	2.53	0.41
1:F:49:GLN:HG2	9:L:44:DG:H4'	2.03	0.41
1:F:112:LEU:HD12	1:F:153:ALA:HA	2.02	0.41
4:V:89:ILE:HG22	4:V:91:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:25:GLU:OE1	7:X:25:GLU:N	2.41	0.41
7:X:829:ILE:HD13	7:X:829:ILE:HA	1.88	0.41
4:U:31:GLY:O	4:U:35:THR:HG23	2.20	0.41
5:Y:676:ALA:O	5:Y:680:VAL:HG23	2.20	0.41
5:Y:766:SER:H	5:Y:769:GLU:HB3	1.85	0.41
7:X:390:ASN:HB3	7:X:395:VAL:HB	2.03	0.41
7:X:999:ASP:O	7:X:1003:THR:HG22	2.20	0.41
4:V:8:LYS:HE3	4:V:8:LYS:HB2	1.84	0.41
5:Y:415:ALA:HB3	5:Y:416:PRO:HD3	2.02	0.41
5:Y:553:GLN:C	5:Y:554:ARG:HE	2.29	0.41
5:Y:693:THR:OG1	5:Y:696:GLU:HG2	2.21	0.41
7:X:7:GLN:OE1	7:X:13:GLN:NE2	2.43	0.41
7:X:647:ALA:HB2	7:X:1038:ILE:HD12	2.03	0.41
1:F:51:PHE:HE2	1:F:93:ILE:HG12	1.85	0.41
1:F:111:SER:O	1:F:115:LEU:HB2	2.21	0.41
4:V:48:LEU:HD12	4:V:48:LEU:HA	1.81	0.41
5:Y:37:ARG:NH1	9:L:31:DT:O5'	2.51	0.41
5:Y:504:LEU:HD12	5:Y:505:GLU:H	1.86	0.41
5:Y:687:PHE:HE2	5:Y:694:GLU:HA	1.86	0.41
5:Y:803:ARG:NH1	5:Y:961:GLU:OE2	2.54	0.41
7:X:418:ASN:O	7:X:422:ILE:HG23	2.21	0.41
7:X:761:VAL:CG1	7:X:1035:MET:HB3	2.51	0.41
7:X:770:ASN:HA	7:X:774:ALA:HB3	2.03	0.41
7:X:1004:LEU:HD13	7:X:1013:ALA:HB2	2.03	0.41
4:U:92:ASP:N	4:U:93:GLU:OE2	2.54	0.41
9:L:44:DG:H2''	9:L:45:DT:C6	2.55	0.41
1:F:190:PHE:HD2	7:X:1107:VAL:HG22	1.85	0.41
4:V:74:ASP:O	4:V:78:ILE:HG12	2.21	0.41
5:Y:330:ASN:HB3	7:X:1062:GLN:HE22	1.86	0.41
8:K:34:DG:H2'	8:K:35:DA:N7	2.36	0.41
5:Y:1103:ASN:OD1	6:D:59:TYR:OH	2.25	0.40
7:X:1154:MET:HA	7:X:1157:LEU:HD13	2.02	0.40
5:Y:3:ASP:OD2	5:Y:3:ASP:N	2.55	0.40
5:Y:545:LYS:NZ	5:Y:571:LEU:O	2.55	0.40
5:Y:1037:VAL:C	6:D:79:ARG:HH22	2.29	0.40
4:U:19:LYS:NZ	4:U:201:ASP:O	2.54	0.40
9:L:37:DG:H2''	9:L:38:DA:OP1	2.21	0.40
1:F:166:THR:OG1	1:F:168:TYR:O	2.35	0.40
5:Y:238:LEU:HD22	7:X:1059:VAL:HG23	2.02	0.40
5:Y:656:ILE:O	7:X:959:PRO:HG3	2.22	0.40
5:Y:746:GLY:O	5:Y:766:SER:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:45:LEU:HD23	7:X:45:LEU:HA	1.92	0.40
7:X:80:GLU:OE1	7:X:80:GLU:N	2.51	0.40
5:Y:46:LEU:HD23	5:Y:46:LEU:HA	1.89	0.40
5:Y:89:ARG:HG2	5:Y:89:ARG:HH11	1.86	0.40
7:X:55:ILE:O	7:X:63:SER:HA	2.22	0.40
7:X:801:ASP:HA	7:X:806:PRO:HA	2.03	0.40
1:F:139:ILE:HD12	1:F:139:ILE:HA	1.94	0.40
1:F:216:LYS:HD2	1:F:216:LYS:HA	1.90	0.40
2:O:51:LEU:HD23	2:O:51:LEU:HA	1.90	0.40
4:V:50:GLY:HA3	4:V:170:TYR:O	2.21	0.40
5:Y:481:ASN:HB2	5:Y:488:VAL:HB	2.03	0.40
5:Y:825:LEU:HD13	5:Y:885:TRP:CE2	2.57	0.40
5:Y:829:LEU:HD21	5:Y:1049:HIS:HA	2.04	0.40
5:Y:900:LYS:HG3	5:Y:913:VAL:HG12	2.03	0.40
5:Y:1170:LEU:HD23	5:Y:1181:ARG:HD3	2.04	0.40
7:X:321:TYR:HA	7:X:324:ASN:HD21	1.86	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	F	240/255 (94%)	224 (93%)	16 (7%)	0	100	100
2	O	59/67 (88%)	56 (95%)	3 (5%)	0	100	100
3	E	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
4	U	226/314 (72%)	223 (99%)	3 (1%)	0	100	100
4	V	228/314 (73%)	224 (98%)	4 (2%)	0	100	100
5	Y	1179/1209 (98%)	1152 (98%)	27 (2%)	0	100	100
6	D	89/173 (51%)	88 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	X	1156/1193 (97%)	1126 (97%)	30 (3%)	0	100	100
All	All	3244/3594 (90%)	3157 (97%)	87 (3%)	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	F	218/230 (95%)	214 (98%)	4 (2%)	51	77
2	O	55/61 (90%)	54 (98%)	1 (2%)	51	77
3	E	65/65 (100%)	63 (97%)	2 (3%)	35	68
4	U	196/273 (72%)	189 (96%)	7 (4%)	31	65
4	V	198/273 (72%)	189 (96%)	9 (4%)	24	59
5	Y	1009/1037 (97%)	981 (97%)	28 (3%)	38	70
6	D	81/159 (51%)	79 (98%)	2 (2%)	42	72
7	X	1000/1026 (98%)	970 (97%)	30 (3%)	36	69
All	All	2822/3124 (90%)	2739 (97%)	83 (3%)	38	70

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	36	LEU
1	F	135	THR
1	F	145	ILE
1	F	175	ILE
2	O	1	MET
3	E	5	VAL
3	E	55	LEU
4	V	68	ILE
4	V	72	VAL
4	V	129	THR

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Mol	Chain	Res	Type
4	V	138	VAL
4	V	168	SER
4	V	185	VAL
4	V	188	VAL
4	V	214	SER
4	V	223	ILE
5	Y	60	CYS
5	Y	73	VAL
5	Y	82	VAL
5	Y	142	THR
5	Y	253	ASP
5	Y	343	VAL
5	Y	365	LEU
5	Y	404	VAL
5	Y	417	THR
5	Y	423	ILE
5	Y	434	ARG
5	Y	461	LEU
5	Y	524	LEU
5	Y	531	VAL
5	Y	552	GLU
5	Y	640	LEU
5	Y	649	LYS
5	Y	712	ILE
5	Y	780	THR
5	Y	843	LEU
5	Y	898	VAL
5	Y	911	SER
5	Y	949	ILE
5	Y	971	ILE
5	Y	992	VAL
5	Y	1023	VAL
5	Y	1093	LEU
5	Y	1120	LEU
6	D	11	LEU
6	D	73	ASP
7	X	52	ILE
7	X	93	ARG
7	X	96	VAL
7	X	144	VAL
7	X	159	THR
7	X	187	THR

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Mol	Chain	Res	Type
7	X	192	VAL
7	X	211	ILE
7	X	270	VAL
7	X	294	LEU
7	X	310	LEU
7	X	425	SER
7	X	446	GLN
7	X	454	VAL
7	X	470	PHE
7	X	495	THR
7	X	521	GLU
7	X	532	SER
7	X	600	ASN
7	X	604	SER
7	X	634	SER
7	X	658	VAL
7	X	692	VAL
7	X	761	VAL
7	X	854	LEU
7	X	886	ILE
7	X	1056	TYR
7	X	1059	VAL
7	X	1101	ASP
7	X	1152	ILE
4	U	72	VAL
4	U	74	ASP
4	U	97	LEU
4	U	115	ASP
4	U	140	LEU
4	U	152	ASP
4	U	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	16	HIS
1	F	24	GLN
1	F	49	GLN
1	F	117	ASN
1	F	220	GLN
1	F	231	GLN
4	V	220	HIS

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Mol	Chain	Res	Type
5	Y	11	ASN
5	Y	318	HIS
5	Y	413	ASN
5	Y	424	GLN
5	Y	454	GLN
5	Y	528	ASN
5	Y	546	ASN
5	Y	632	HIS
5	Y	682	ASN
5	Y	863	ASN
5	Y	865	ASN
5	Y	951	GLN
5	Y	988	GLN
5	Y	1058	GLN
5	Y	1073	GLN
6	D	38	ASN
7	X	50	GLN
7	X	61	ASN
7	X	100	ASN
7	X	219	ASN
7	X	308	GLN
7	X	355	GLN
7	X	417	GLN
7	X	419	GLN
7	X	446	GLN
7	X	466	GLN
7	X	473	GLN
7	X	482	HIS
7	X	529	ASN
7	X	576	GLN
4	U	38	ASN
4	U	179	GLN
4	U	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

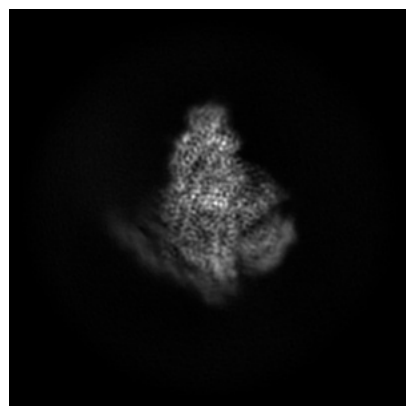
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-59290. These allow visual inspection of the internal detail of the map and identification of artifacts.

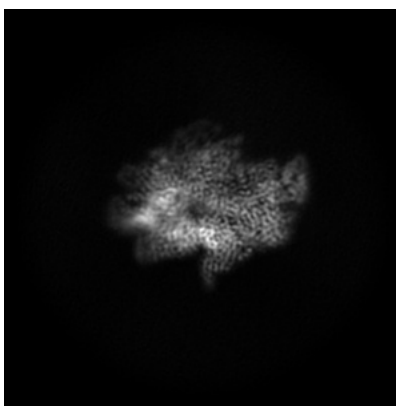
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

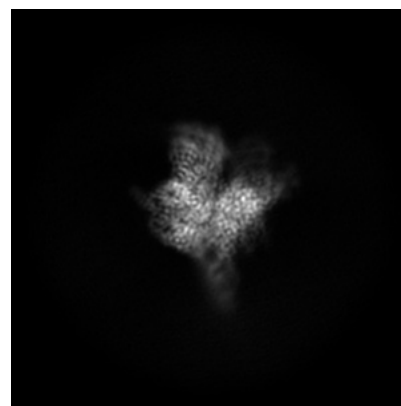
6.1.1 Primary map



X

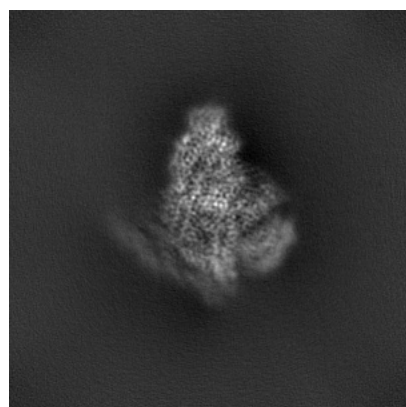


Y

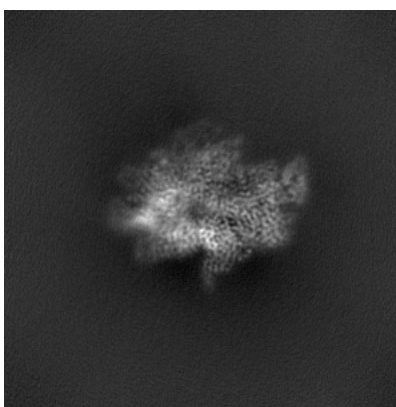


Z

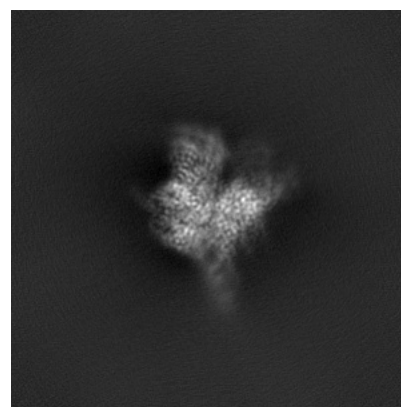
6.1.2 Raw map



X



Y

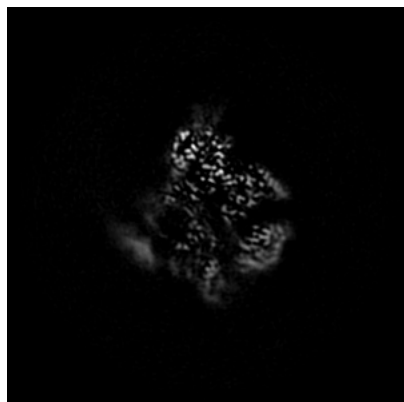


Z

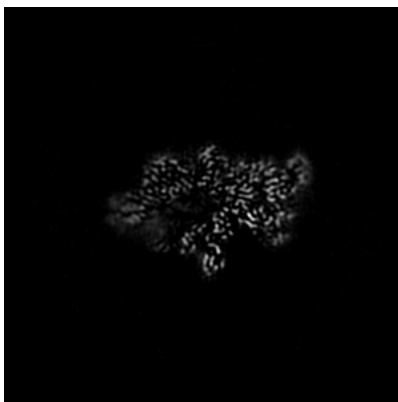
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192

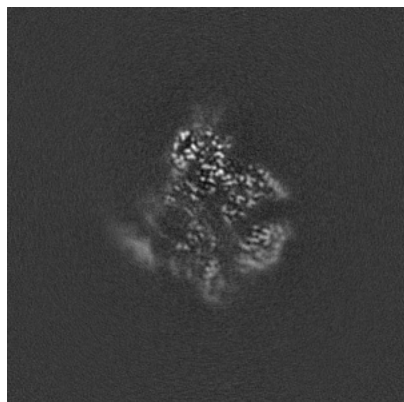


Y Index: 192

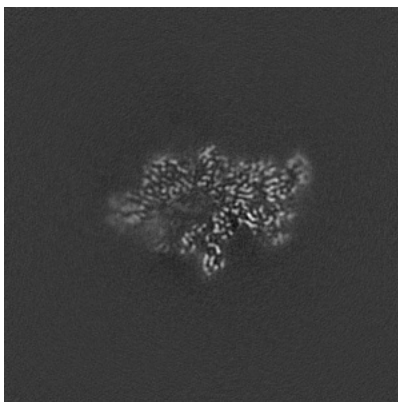


Z Index: 192

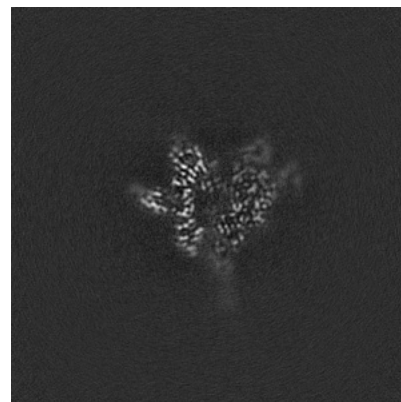
6.2.2 Raw map



X Index: 192



Y Index: 192

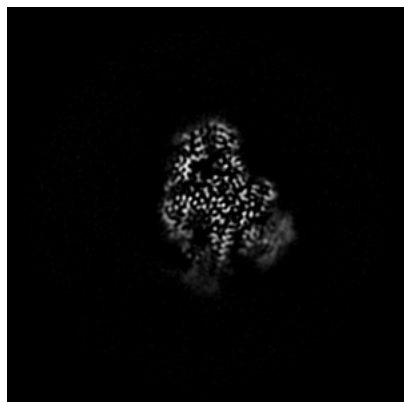


Z Index: 192

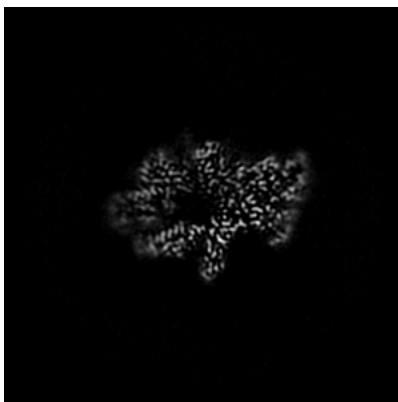
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

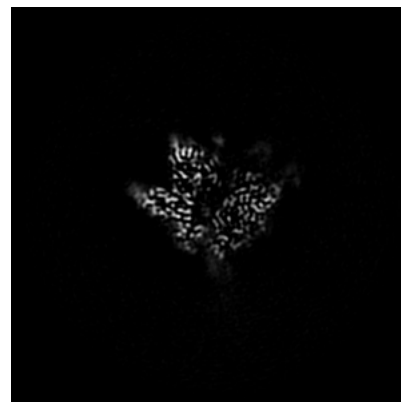
6.3.1 Primary map



X Index: 168

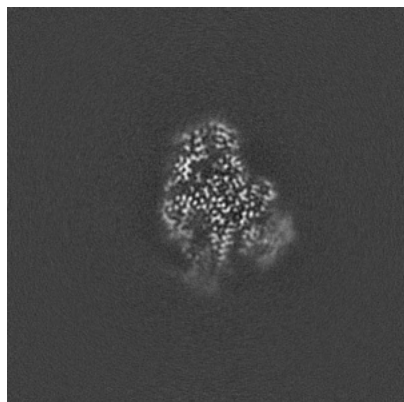


Y Index: 198

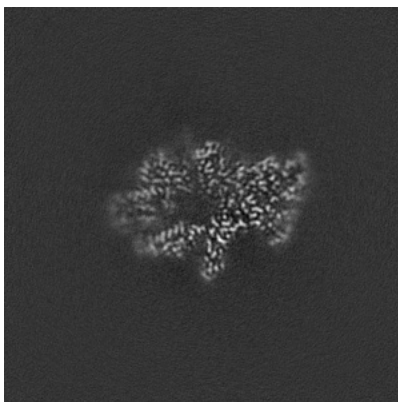


Z Index: 197

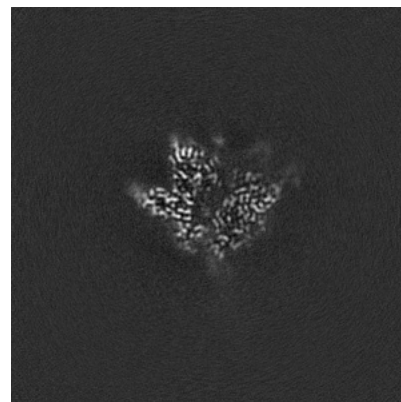
6.3.2 Raw map



X Index: 168



Y Index: 198

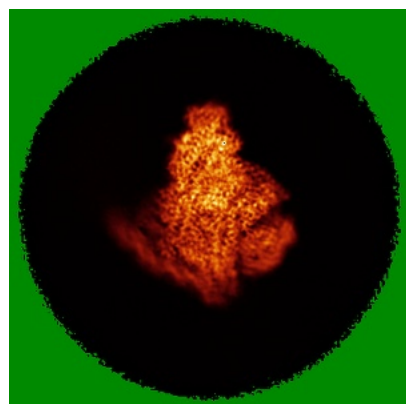


Z Index: 197

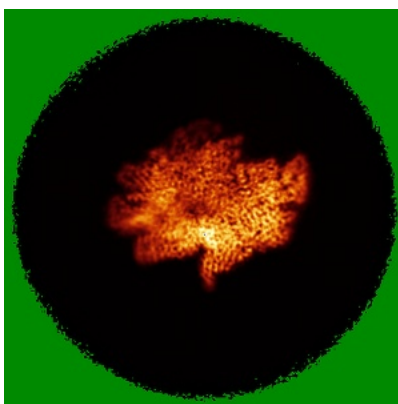
The images above show the largest variance slices of the map in three orthogonal directions.

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

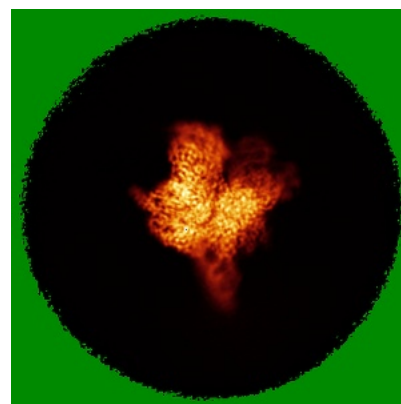
6.4.1 Primary map



X

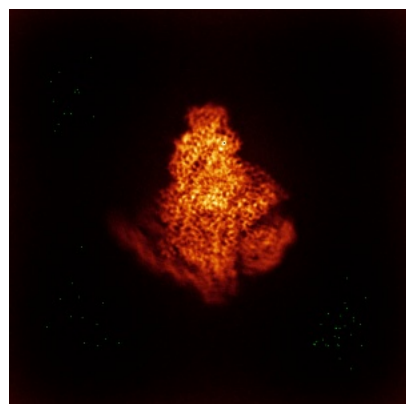


Y

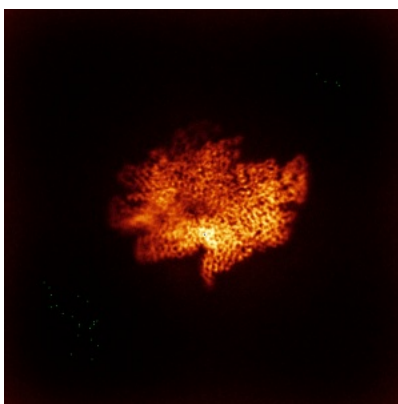


Z

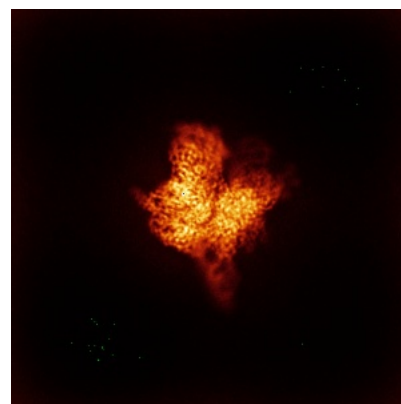
6.4.2 Raw map



X



Y



Z

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

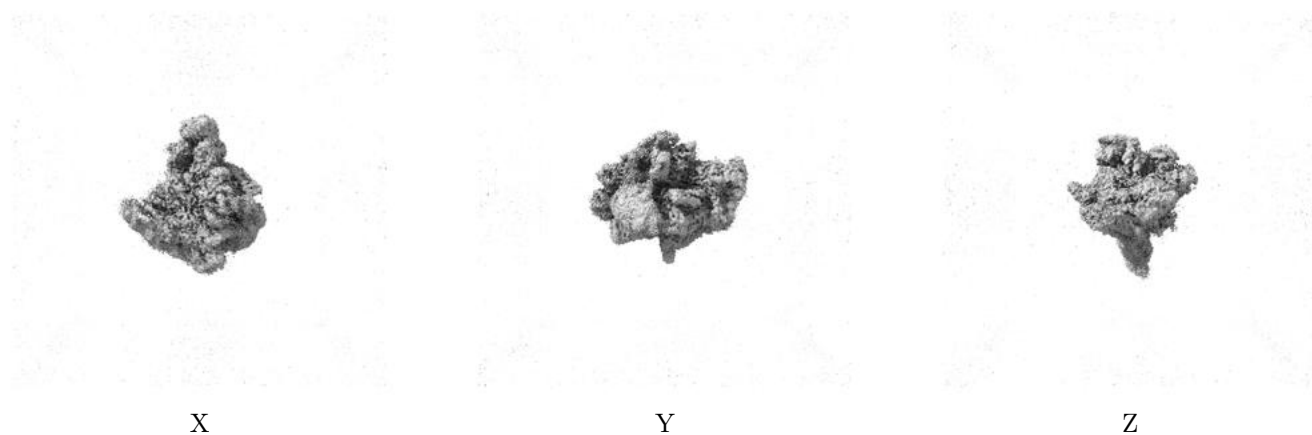
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

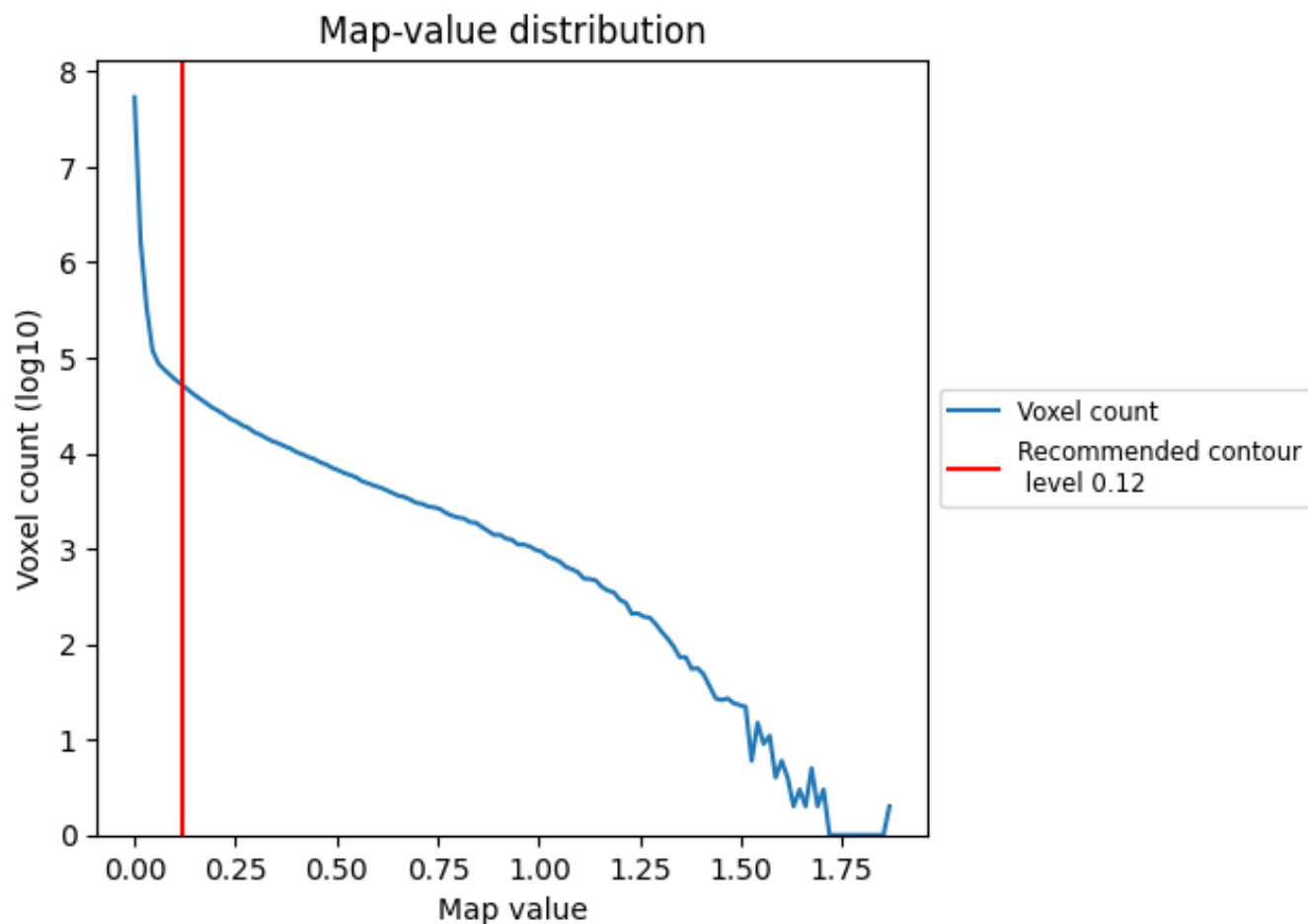
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

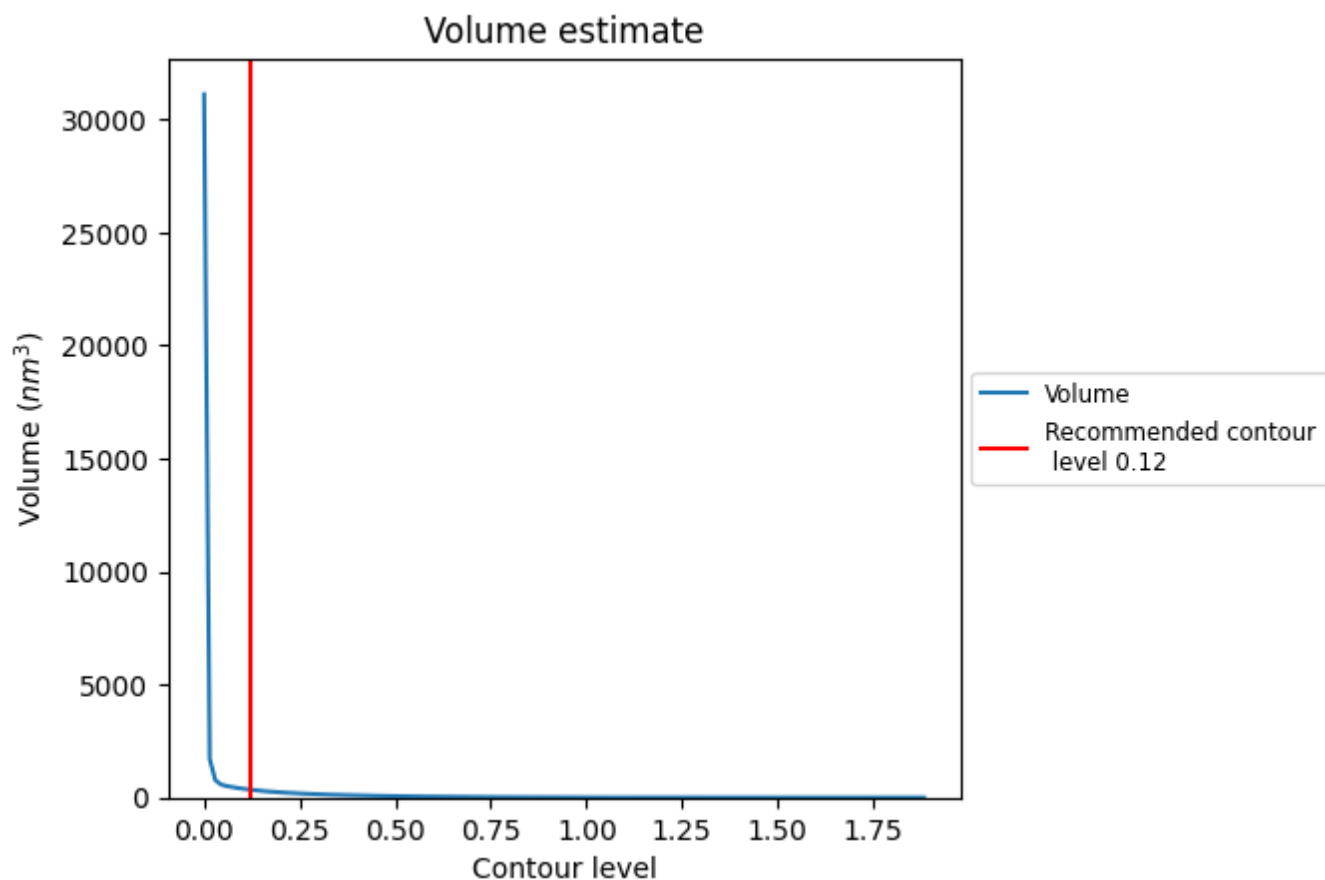
This section contains the results of statistical analysis of the map.

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.

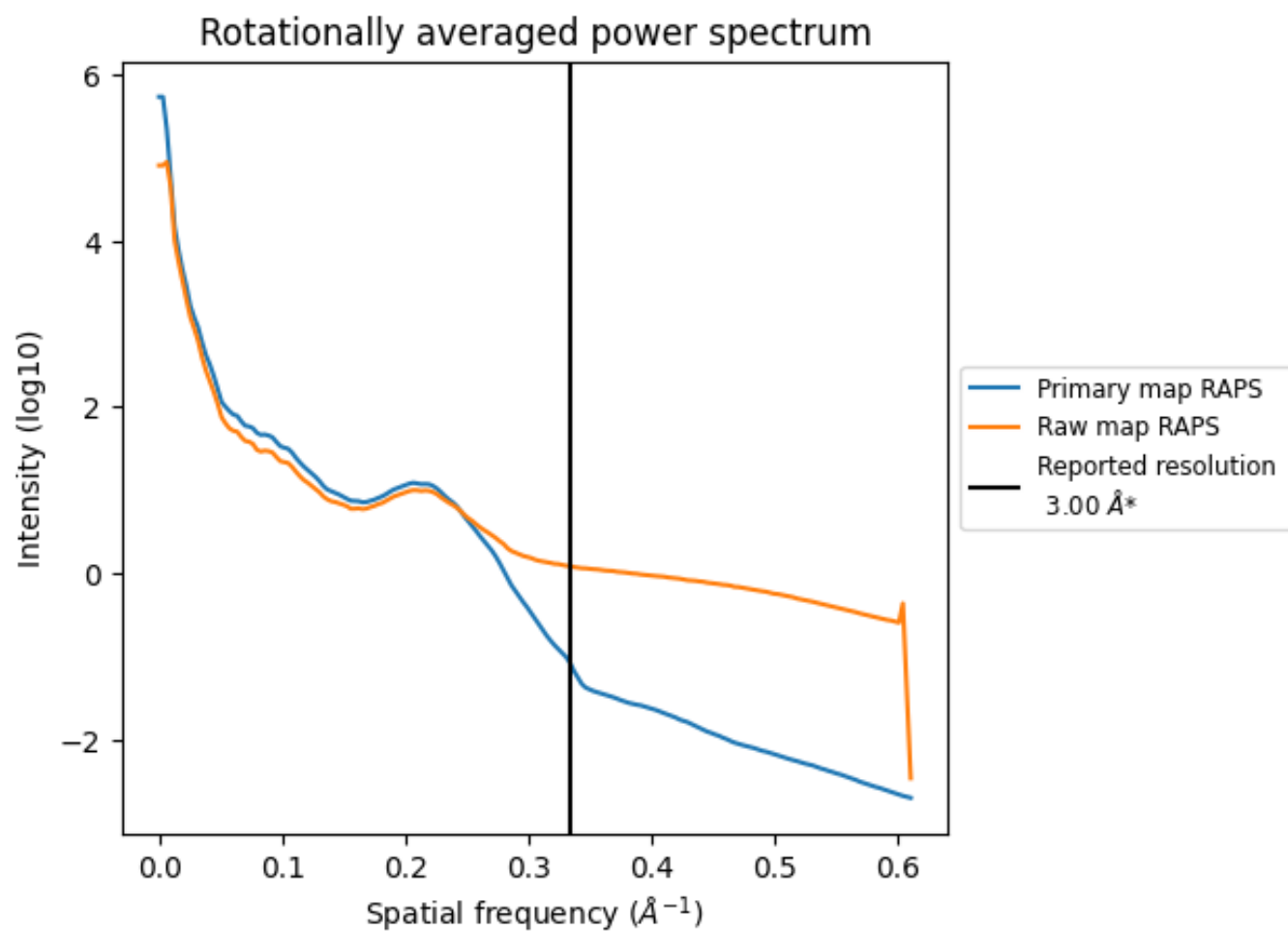
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm³; this corresponds to an approximate mass of 316 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 ⓘ

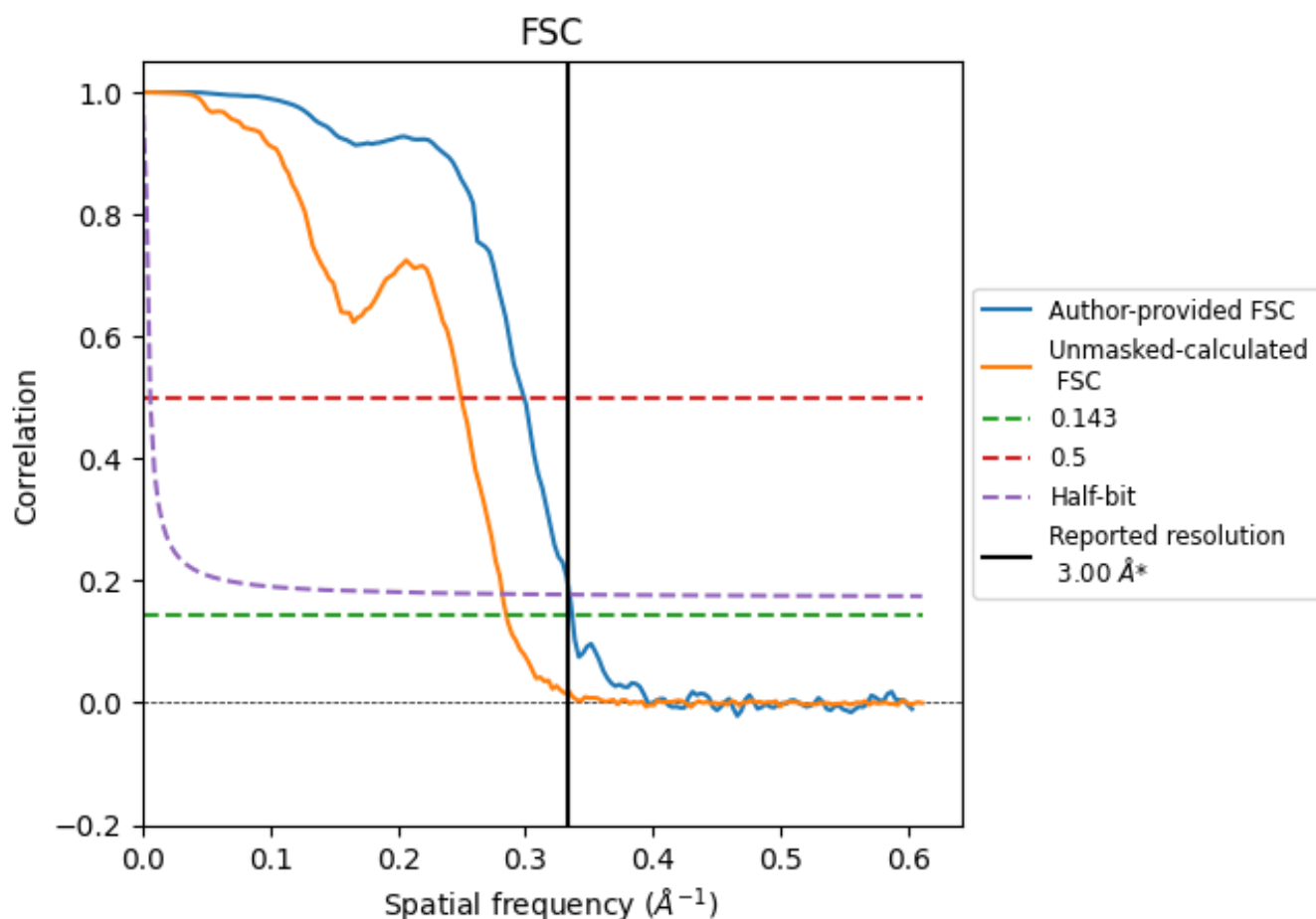


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

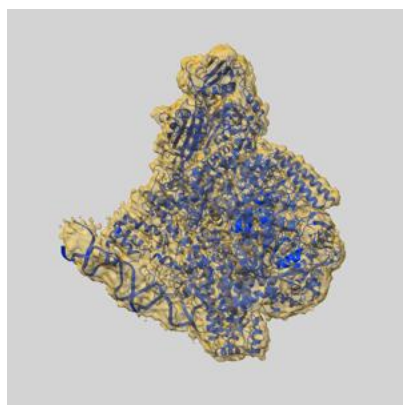
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.35	2.99
Unmasked-calculated*	3.51	4.00	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.0 by more than 10 %

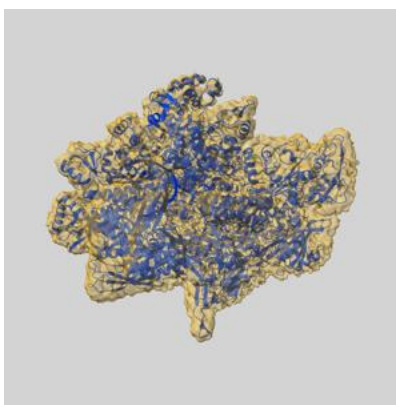
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-59290 and PDB model 3Z2T. Per-residue inclusion information can be found in section [3](#) on page [7](#).

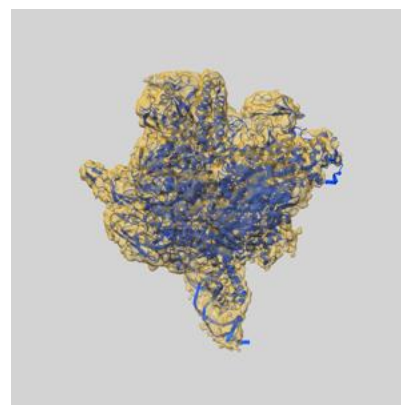
9.1 Map-model overlay [i](#)



X



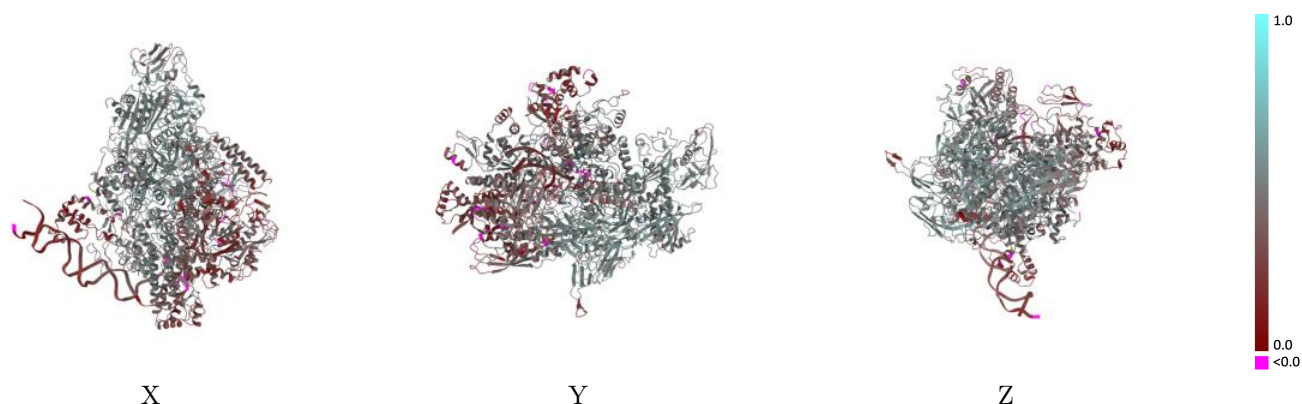
Y



Z

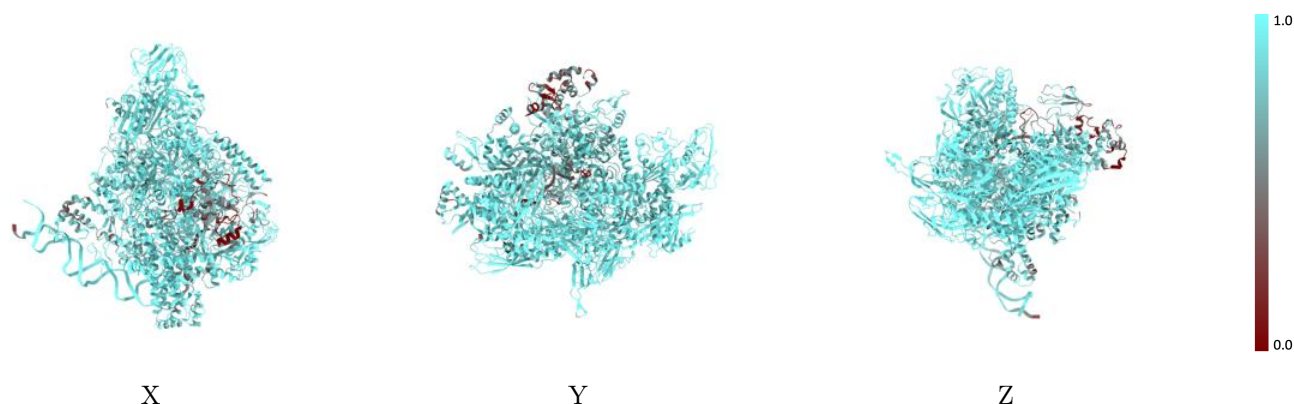
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



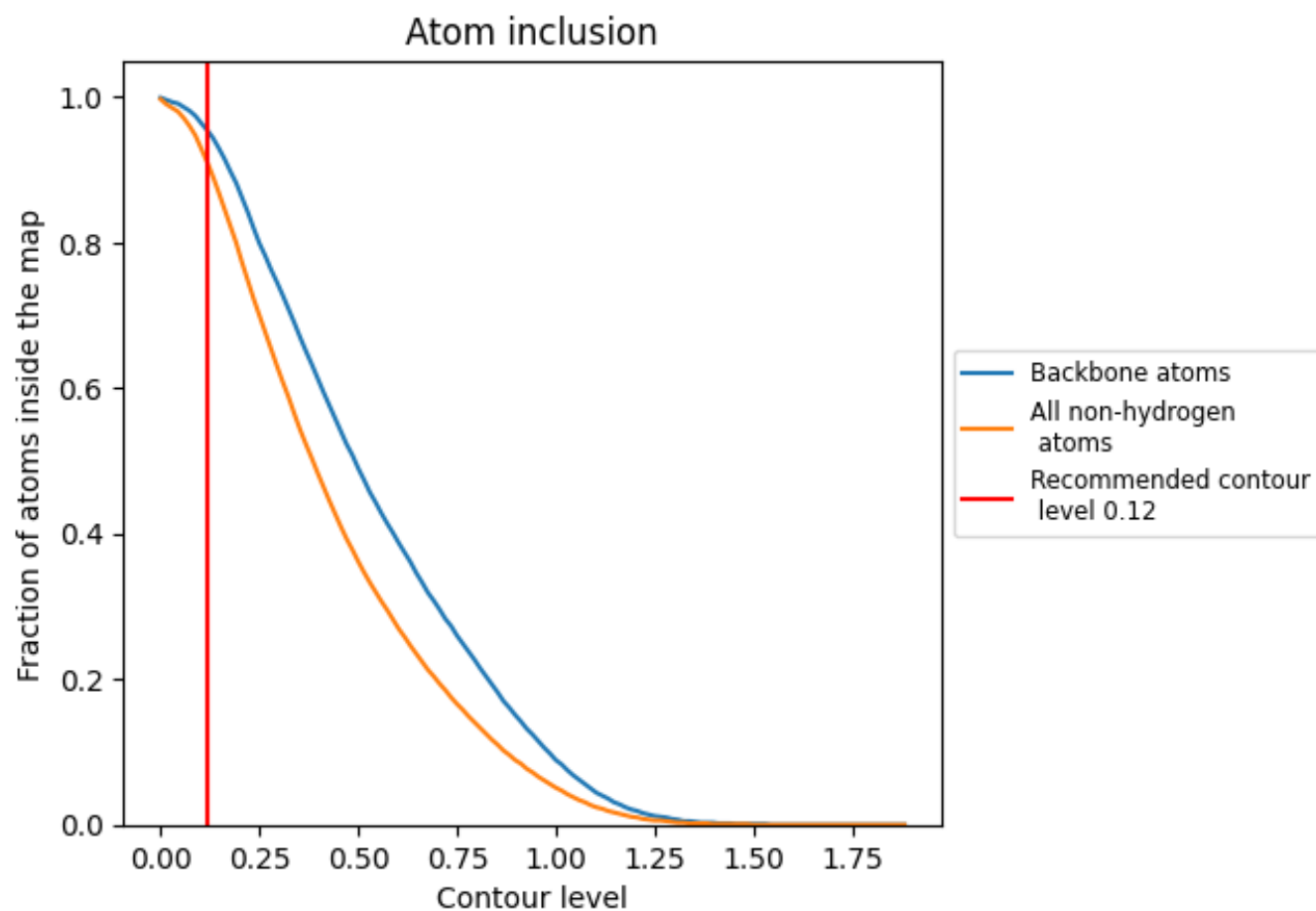
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.4270
D	0.3390	0.2360
E	0.9720	0.5000
F	0.8100	0.3030
K	0.8500	0.1920
L	0.7560	0.1900
O	0.8320	0.4380
U	0.9850	0.5230
V	0.9820	0.4710
X	0.9630	0.4600
Y	0.9140	0.4520

1.0
0.0
<0.0