



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:57 PM UTC

PDB ID : 8TVS / pdb_00008tvs
EMDB ID : EMD-41650
Title : Cryo-EM structure of backtracked Pol II in complex with Rad26
Authors : Sarsam, R.D.; Lahiri, I.; Leschziner, A.E.
Deposited on : 2023-08-18
Resolution : 4.40 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

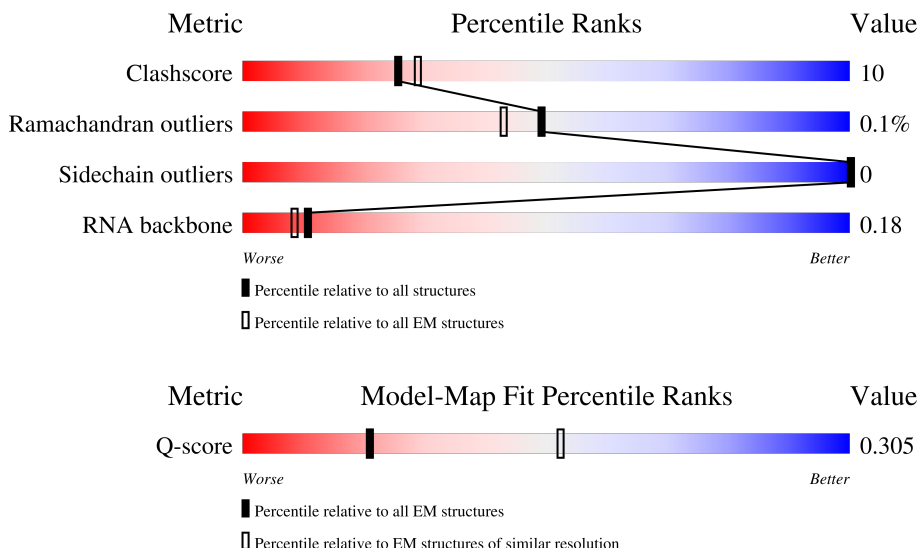
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	434	
14	N	47	
15	T	47	
16	R	17	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 56913 atoms, of which 24971 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 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1316	Total	C	H	N	O	S	0	0
			19036	6196	9180	1748	1854	58		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1041	Total	C	H	N	O	S	0	0
			14671	4865	6919	1387	1453	47		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	266	Total	C	H	N	O	S	0	0
			4149	1317	2054	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	142	Total	C	H	N	O	S	0	0
			1574	572	637	174	190	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	215	Total	C	H	N	O	S	0	0
			3548	1116	1788	310	322	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	81	Total	C	H	N	O	S	0	0
			1330	419	673	111	124	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			1730	681	642	196	207	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	133	Total	C	H	N	O	S	0	0
			2090	668	1030	174	213	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			972	426	279	129	135	3		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	65	Total	C	H	N	O	S	0	0
			1074	339	542	93	94	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	104	Total	C	H	N	O	S	0	0
			1673	534	839	142	157	1		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			752	224	388	72	64	4		

- Molecule 13 is a protein called DNA repair and recombination protein RAD26.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	434	Total	C	N	O	0	0
			2171	1302	434	435		

- Molecule 14 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	46	Total	C	N	O	P	0	0
			946	451	173	276	46		

- Molecule 15 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	46	Total	C	N	O	P	0	0
			925	443	154	282	46		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	12	Total	C	N	O	P	0	0
			263	117	53	81	12		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

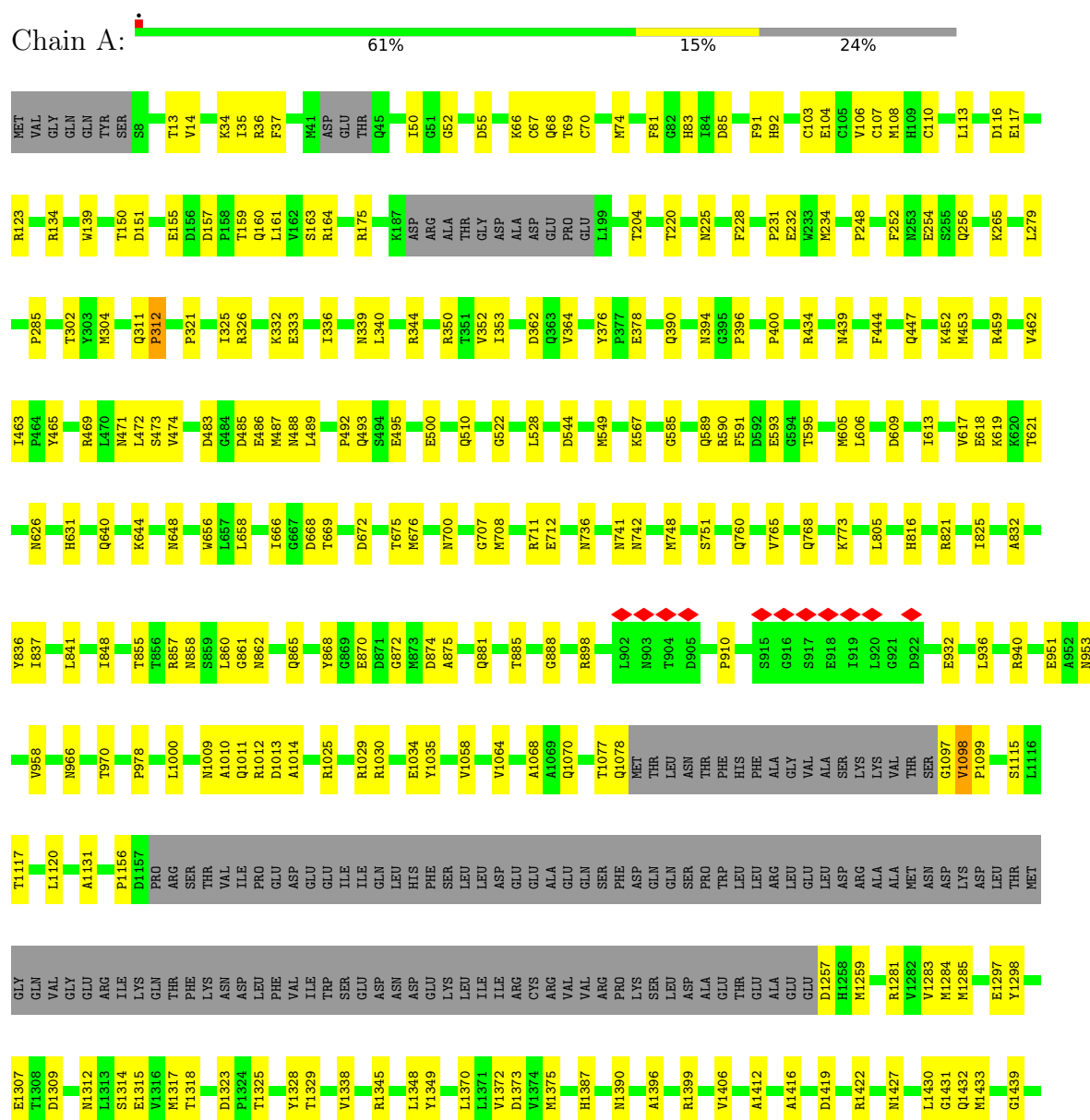
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

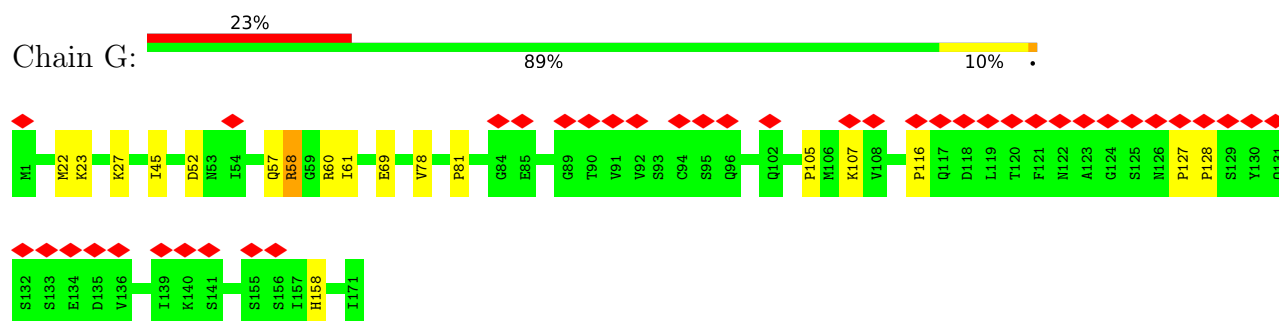
3 Residue-property plots

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

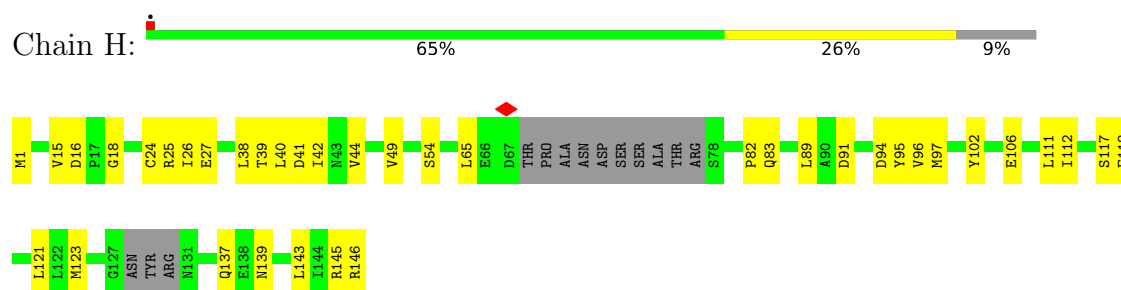
• Molecule 1: DNA-directed RNA polymerase subunit



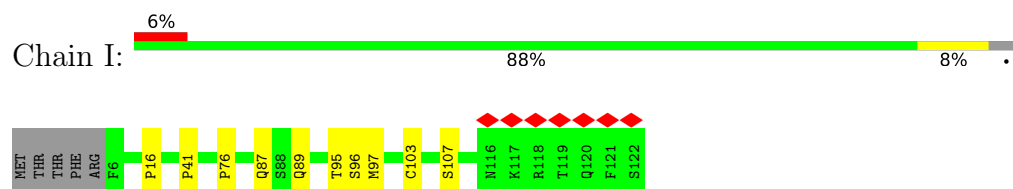
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



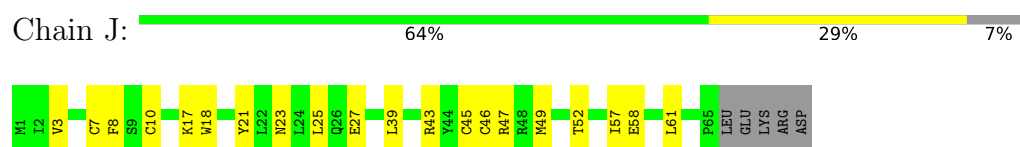
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

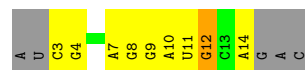


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.351	Depositor
Minimum map value	-2.554	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.209	Depositor
Recommended contour level	1.13	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	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	0.15	0/10018	0.42	7/13572 (0.1%)
2	B	0.16	0/7882	0.44	7/10660 (0.1%)
3	C	0.13	0/2133	0.33	0/2891
4	D	0.18	0/940	0.55	0/1275
5	E	0.12	0/1796	0.31	0/2416
6	F	0.13	0/669	0.33	0/903
7	G	0.22	0/1101	0.68	5/1500 (0.3%)
8	H	0.14	0/1076	0.34	0/1455
9	I	0.19	0/700	0.72	3/961 (0.3%)
10	J	0.14	0/541	0.28	0/727
11	K	0.14	0/850	0.33	0/1148
12	L	0.13	0/366	0.39	0/485
14	N	0.42	0/1061	0.56	0/1636
15	T	0.40	0/1031	0.58	0/1585
16	R	0.50	0/295	0.71	0/459
All	All	0.19	0/30459	0.45	22/41673 (0.1%)

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
4	D	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	116	PRO	N-CA-CB	8.91	111.09	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	293	PRO	N-CA-CB	8.90	111.09	103.17
1	A	321	PRO	N-CA-CB	8.76	111.11	103.31
2	B	281	PRO	N-CA-CB	8.75	111.10	103.31
1	A	978	PRO	N-CA-CB	8.37	111.12	103.33
1	A	396	PRO	N-CA-CB	7.92	111.11	103.51
7	G	127	PRO	N-CA-CB	7.73	111.10	102.60
9	I	41	PRO	N-CA-CB	7.61	111.09	103.48
2	B	100	PRO	N-CA-CB	7.49	111.11	103.25
2	B	316	PRO	N-CA-CB	7.49	111.11	103.25
9	I	16	PRO	N-CA-CB	7.49	111.11	103.25
2	B	877	PRO	N-CA-CB	7.49	111.11	103.25
2	B	274	PRO	N-CA-CB	7.48	111.11	103.25
7	G	128	PRO	N-CA-CB	7.47	111.09	103.25
1	A	400	PRO	N-CA-CB	7.46	111.09	103.25
1	A	312	PRO	N-CA-CB	7.46	111.08	103.25
7	G	105	PRO	N-CA-CB	7.44	111.11	102.33
7	G	81	PRO	N-CA-CB	7.23	111.11	102.72
1	A	910	PRO	N-CA-CB	7.14	111.10	103.39
1	A	1156	PRO	N-CA-CB	7.14	111.10	103.39
9	I	76	PRO	N-CA-CB	6.89	111.11	103.26
2	B	362	PRO	N-CA-CB	6.87	111.09	103.26

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	66	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	9856	9180	9533	198	0
2	B	7752	6919	7276	138	0
3	C	2095	2054	2054	42	0
4	D	937	637	769	13	0
5	E	1760	1788	1788	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	657	673	673	17	0
7	G	1088	642	840	10	0
8	H	1060	1030	1030	28	0
9	I	693	279	446	9	0
10	J	532	542	543	16	0
11	K	834	839	839	14	0
12	L	364	388	388	5	0
13	M	2171	0	460	64	0
14	N	946	0	520	50	0
15	T	925	0	521	72	0
16	R	263	0	132	15	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31942	24971	27812	609	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 10.

All (609) 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)
13:M:537:UNK:CB	13:M:550:UNK:CB	1.75	1.61
13:M:354:UNK:C	15:T:38:DG:OP1	1.71	1.36
13:M:447:UNK:CB	15:T:38:DG:H5''	1.60	1.31
13:M:317:UNK:CB	13:M:515:UNK:O	1.83	1.25
13:M:355:UNK:N	15:T:38:DG:P	2.21	1.13
13:M:355:UNK:CB	15:T:38:DG:OP2	2.01	1.08
1:A:832:ALA:HB1	15:T:18:DC:OP2	1.57	1.05
13:M:355:UNK:N	15:T:38:DG:OP1	1.89	1.04
14:N:8:DA:C2'	14:N:9:DT:H72	1.85	1.04
14:N:8:DA:H2'	14:N:9:DT:H72	1.35	1.03
13:M:447:UNK:CB	15:T:38:DG:C5'	2.37	1.02
13:M:537:UNK:C	13:M:550:UNK:CB	2.40	0.99
14:N:26:DA:H2''	14:N:27:DC:OP2	1.58	0.97
1:A:175:ARG:NH1	14:N:39:DA:OP1	1.97	0.97
13:M:538:UNK:N	13:M:550:UNK:CB	2.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:DG:C2'	14:N:5:DT:H72	1.95	0.96
1:A:832:ALA:CA	15:T:18:DC:OP2	2.13	0.96
1:A:832:ALA:CB	15:T:18:DC:OP2	2.15	0.95
14:N:26:DA:C4'	14:N:27:DC:H5'	1.96	0.95
13:M:537:UNK:CA	13:M:550:UNK:CB	2.46	0.94
15:T:5:DC:H2''	15:T:6:DT:H72	1.48	0.92
14:N:26:DA:C2'	14:N:27:DC:OP2	2.17	0.92
13:M:631:UNK:N	13:M:645:UNK:CB	2.32	0.92
6:F:130:ILE:HG23	6:F:148:VAL:HG21	1.52	0.91
13:M:339:UNK:O	13:M:343:UNK:CB	2.18	0.91
14:N:4:DG:H2'	14:N:5:DT:H72	1.51	0.91
1:A:252:PHE:CZ	16:R:3:C:C5	2.59	0.90
13:M:719:UNK:HA	13:M:741:UNK:CB	2.00	0.90
13:M:379:UNK:O	13:M:383:UNK:CB	2.20	0.89
14:N:8:DA:C2'	14:N:9:DT:C7	2.52	0.88
13:M:354:UNK:CA	15:T:38:DG:OP1	2.21	0.87
1:A:544:ASP:OD1	11:K:47:ARG:NH1	2.08	0.87
2:B:979:LYS:NZ	16:R:11:U:OP1	2.09	0.84
2:B:216:GLU:OE1	2:B:500:THR:OG1	1.93	0.83
15:T:3:DC:H2''	15:T:4:DT:H71	1.58	0.83
13:M:450:UNK:CB	15:T:39:DA:OP1	2.26	0.83
15:T:3:DC:C2'	15:T:4:DT:H71	2.09	0.82
14:N:26:DA:H1'	14:N:27:DC:OP2	1.79	0.82
1:A:447:GLN:NE2	1:A:488:ASN:OD1	2.13	0.82
15:T:5:DC:H2''	15:T:6:DT:C7	2.09	0.82
2:B:776:GLN:OE1	2:B:1097:HIS:NE2	2.13	0.82
15:T:5:DC:H2''	15:T:6:DT:C5	2.15	0.81
1:A:700:ASN:OD1	9:I:96:SER:OG	1.98	0.80
1:A:252:PHE:CE1	16:R:3:C:C6	2.70	0.80
14:N:8:DA:H2''	14:N:9:DT:C7	2.10	0.80
13:M:537:UNK:CB	13:M:550:UNK:CA	2.59	0.80
14:N:26:DA:H4'	14:N:27:DC:H5'	1.62	0.79
1:A:1115:SER:O	1:A:1329:THR:OG1	2.01	0.79
13:M:355:UNK:CA	15:T:38:DG:OP2	2.30	0.78
3:C:61:GLU:N	3:C:61:GLU:OE1	2.16	0.78
2:B:442:PHE:N	2:B:444:MET:SD	2.58	0.77
14:N:4:DG:C2'	14:N:5:DT:C7	2.61	0.77
1:A:832:ALA:C	15:T:18:DC:OP2	2.28	0.77
1:A:1257:ASP:N	1:A:1259:MET:SD	2.58	0.77
2:B:1133:MET:HE2	15:T:19:DA:H4'	1.67	0.77
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:DG:H2''	14:N:5:DT:C7	2.16	0.75
1:A:618:GLU:OE1	1:A:619:LYS:N	2.19	0.75
13:M:534:UNK:O	13:M:538:UNK:CB	2.35	0.75
2:B:259:TYR:O	2:B:266:ALA:N	2.18	0.75
14:N:26:DA:C1'	14:N:27:DC:OP2	2.35	0.74
3:C:73:GLN:OE1	3:C:75:MET:HE3	1.86	0.74
1:A:447:GLN:NE2	2:B:1134:GLU:OE2	2.21	0.74
1:A:452:LYS:N	1:A:1070:GLN:OE1	2.21	0.74
2:B:217:ARG:NE	2:B:407:ASP:OD2	2.19	0.74
13:M:612:UNK:CB	14:N:18:DT:O4	2.36	0.73
14:N:8:DA:H2'	14:N:9:DT:C7	2.15	0.73
14:N:26:DA:O4'	14:N:27:DC:H5'	1.88	0.73
1:A:1297:GLU:OE1	1:A:1298:TYR:N	2.22	0.73
15:T:39:DA:C2'	15:T:40:DT:H72	2.19	0.73
13:M:326:UNK:O	13:M:327:UNK:CB	2.37	0.72
2:B:546:SER:OG	2:B:632:ARG:N	2.22	0.72
13:M:767:UNK:O	13:M:768:UNK:CB	2.37	0.72
2:B:43:LEU:O	2:B:496:ARG:NH1	2.23	0.71
13:M:735:UNK:O	13:M:736:UNK:CB	2.38	0.71
2:B:1133:MET:HE2	15:T:19:DA:C4'	2.20	0.71
1:A:91:PHE:CE2	1:A:204:THR:HG22	2.25	0.71
1:A:855:THR:OG1	1:A:857:ARG:NH1	2.24	0.71
1:A:332:LYS:NZ	1:A:333:GLU:OE2	2.20	0.70
2:B:87:LYS:N	2:B:137:TYR:O	2.24	0.70
1:A:444:PHE:CE1	1:A:489:LEU:HD13	2.26	0.70
4:D:203:SER:OG	4:D:205:ASP:OD1	2.08	0.70
9:I:103:CYS:O	9:I:107:SER:N	2.24	0.70
1:A:116:ASP:OD2	1:A:164:ARG:NE	2.24	0.70
3:C:75:MET:HE2	3:C:75:MET:N	2.07	0.70
1:A:74:MET:O	2:B:1116:ARG:NH2	2.26	0.69
2:B:71:LEU:HD13	2:B:433:GLN:HE22	1.55	0.69
13:M:324:UNK:O	13:M:325:UNK:CB	2.39	0.69
1:A:252:PHE:CZ	16:R:3:C:C6	2.80	0.69
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.74	0.69
2:B:997:GLU:OE1	2:B:997:GLU:N	2.25	0.69
3:C:14:SER:OG	3:C:16:ASP:OD1	2.10	0.69
2:B:1070:GLU:OE1	2:B:1071:VAL:N	2.24	0.69
13:M:354:UNK:HA	15:T:38:DG:OP1	1.91	0.69
2:B:564:GLU:N	2:B:564:GLU:OE1	2.25	0.69
2:B:1053:GLU:N	2:B:1053:GLU:OE1	2.25	0.68
1:A:1442:ASP:OD2	6:F:137:TYR:OH	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:N	1:A:232:GLU:OE1	2.26	0.68
1:A:364:VAL:HG21	1:A:444:PHE:CZ	2.28	0.68
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.26	0.68
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.26	0.68
3:C:66:ARG:NH2	3:C:143:LEU:O	2.27	0.68
14:N:42:DA:C2	15:T:7:DG:C2	2.83	0.67
1:A:1010:ALA:O	1:A:1014:ALA:N	2.27	0.67
2:B:806:THR:OG1	2:B:809:MET:SD	2.53	0.67
1:A:760:GLN:NE2	1:A:765:VAL:O	2.27	0.67
4:D:66:ARG:NH2	4:D:133:THR:HA	2.09	0.67
1:A:439:ASN:OD1	1:A:459:ARG:NH1	2.27	0.67
2:B:122:LEU:O	2:B:207:GLY:N	2.26	0.67
1:A:1349:TYR:OH	5:E:203:GLU:OE2	2.11	0.67
2:B:526:GLU:OE2	2:B:752:ALA:N	2.29	0.66
14:N:26:DA:H1'	14:N:27:DC:P	2.34	0.66
2:B:1067:ARG:NE	3:C:194:GLU:OE2	2.29	0.66
2:B:776:GLN:NE2	16:R:9:G:O3'	2.29	0.66
13:M:719:UNK:O	13:M:741:UNK:CB	2.44	0.65
1:A:832:ALA:HA	15:T:18:DC:OP2	1.94	0.65
2:B:773:MET:HE1	2:B:987:LYS:HD3	1.78	0.65
14:N:42:DA:C2	15:T:7:DG:N1	2.65	0.65
1:A:453:MET:HE3	1:A:453:MET:HA	1.78	0.65
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.30	0.65
1:A:1348:LEU:HD21	1:A:1375:MET:HE3	1.77	0.65
1:A:966:ASN:O	1:A:970:THR:N	2.29	0.64
4:D:205:ASP:OD1	4:D:206:GLU:N	2.30	0.64
1:A:711:ARG:CZ	9:I:97:MET:HE1	2.28	0.64
10:J:23:ASN:O	10:J:27:GLU:N	2.30	0.64
14:N:19:DC:H2''	14:N:20:DA:H2'	1.80	0.64
15:T:44:DC:H2'	15:T:45:DT:H71	1.79	0.63
1:A:712:GLU:OE2	1:A:773:LYS:NZ	2.31	0.63
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.30	0.63
13:M:355:UNK:N	15:T:38:DG:OP2	2.31	0.63
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.31	0.63
8:H:27:GLU:OE1	8:H:39:THR:HG22	1.99	0.63
13:M:520:UNK:O	13:M:521:UNK:CB	2.46	0.63
8:H:137:GLN:NE2	8:H:139:ASN:O	2.30	0.63
5:E:100:ILE:O	5:E:104:ASN:N	2.31	0.63
1:A:1064:VAL:O	1:A:1068:ALA:N	2.28	0.62
2:B:815:ARG:NE	2:B:1041:GLU:OE2	2.28	0.62
2:B:996:ARG:NH2	3:C:174:ALA:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:94:ASP:OD2	8:H:146:ARG:N	2.31	0.62
14:N:42:DA:N1	15:T:7:DG:C6	2.66	0.62
1:A:658:LEU:O	2:B:1074:ASN:ND2	2.32	0.62
2:B:28:GLU:OE2	2:B:807:ARG:NH2	2.33	0.62
2:B:712:PRO:O	2:B:716:ASN:N	2.32	0.62
14:N:25:DT:H2''	14:N:26:DA:H5'	1.81	0.62
1:A:1323:ASP:OD1	1:A:1325:THR:OG1	2.09	0.62
3:C:16:ASP:OD1	3:C:17:ASN:N	2.31	0.62
5:E:76:GLY:N	5:E:106:GLN:OE1	2.30	0.62
2:B:1100:ASP:O	2:B:1122:ARG:NH2	2.32	0.62
1:A:1390:ASN:O	1:A:1399:ARG:NE	2.33	0.62
15:T:39:DA:H2'	15:T:40:DT:H72	1.80	0.62
3:C:29:MET:O	3:C:33:LEU:HD23	2.00	0.62
13:M:762:UNK:O	13:M:766:UNK:N	2.32	0.62
15:T:12:DT:H2'	15:T:13:DT:H72	1.81	0.62
2:B:1129:ARG:NH1	15:T:20:DT:OP2	2.32	0.62
6:F:103:MET:HE3	6:F:103:MET:HA	1.82	0.61
7:G:27:LYS:NZ	7:G:52:ASP:OD1	2.30	0.61
1:A:339:ASN:ND2	2:B:1117:GLN:OE1	2.33	0.61
13:M:537:UNK:CB	13:M:550:UNK:N	2.63	0.61
2:B:835:GLN:O	2:B:1013:ASN:ND2	2.33	0.61
15:T:5:DC:C2'	15:T:6:DT:H72	2.26	0.61
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.33	0.61
2:B:481:GLN:NE2	16:R:8:G:H5'	2.15	0.61
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.83	0.61
2:B:681:TRP:CH2	2:B:690:VAL:HG21	2.36	0.61
3:C:5:GLY:O	3:C:7:GLN:NE2	2.33	0.61
2:B:41:LYS:O	2:B:45:SER:OG	2.12	0.61
3:C:241:ASP:OD1	3:C:242:GLN:N	2.34	0.61
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.34	0.60
1:A:888:GLY:O	1:A:940:ARG:NH2	2.34	0.60
8:H:106:GLU:OE1	8:H:106:GLU:N	2.34	0.60
13:M:321:UNK:N	13:M:566:UNK:O	2.34	0.60
2:B:89:GLU:N	2:B:135:ARG:O	2.34	0.60
3:C:148:ARG:NE	10:J:61:LEU:O	2.33	0.60
1:A:951:GLU:OE2	1:A:953:ASN:N	2.34	0.60
11:K:24:ASP:OD1	11:K:25:THR:N	2.34	0.60
2:B:1168:LEU:HD21	2:B:1208:MET:SD	2.41	0.60
11:K:60:ALA:O	11:K:73:LEU:HD12	2.01	0.60
1:A:462:VAL:O	1:A:463:ILE:HD13	2.02	0.60
1:A:113:LEU:O	1:A:164:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ALA:O	15:T:18:DC:OP2	2.19	0.59
13:M:703:UNK:O	13:M:704:UNK:CB	2.50	0.59
2:B:71:LEU:HD13	2:B:433:GLN:NE2	2.16	0.59
2:B:841:MET:SD	2:B:846:ILE:HD11	2.42	0.59
9:I:96:SER:C	9:I:97:MET:HE2	2.28	0.59
13:M:719:UNK:CA	13:M:741:UNK:CB	2.79	0.59
1:A:644:LYS:O	1:A:648:ASN:ND2	2.35	0.59
1:A:1427:ASN:O	1:A:1431:GLY:N	2.36	0.59
4:D:187:THR:OG1	4:D:208:GLU:OE2	2.19	0.59
14:N:47:DG:C2	15:T:2:DG:C2	2.91	0.59
5:E:3:GLN:NE2	5:E:51:GLY:O	2.34	0.59
8:H:1:MET:SD	8:H:65:LEU:HD12	2.43	0.59
14:N:40:DG:H2''	14:N:41:DC:C6	2.38	0.59
1:A:364:VAL:HG11	1:A:444:PHE:CZ	2.38	0.59
2:B:233:PRO:O	2:B:260:GLY:N	2.36	0.59
10:J:17:LYS:HD2	10:J:39:LEU:HD12	1.85	0.59
13:M:533:UNK:O	13:M:550:UNK:CB	2.51	0.59
1:A:1077:THR:OG1	1:A:1078:GLN:OE1	2.16	0.58
5:E:52:ARG:NH2	5:E:84:ASP:OD1	2.35	0.58
4:D:66:ARG:NH2	4:D:132:GLN:O	2.36	0.58
1:A:66:LYS:O	1:A:69:THR:N	2.36	0.58
3:C:241:ASP:OD2	11:K:109:TRP:NE1	2.36	0.58
13:M:354:UNK:O	13:M:358:UNK:N	2.37	0.58
1:A:35:ILE:O	1:A:36:ARG:NE	2.35	0.58
15:T:39:DA:H2''	15:T:40:DT:C7	2.34	0.58
2:B:1168:LEU:HD11	2:B:1208:MET:SD	2.44	0.58
13:M:474:UNK:O	13:M:476:UNK:N	2.37	0.58
8:H:38:LEU:HD11	8:H:123:MET:HE3	1.86	0.58
1:A:885:THR:O	1:A:940:ARG:NH1	2.33	0.57
1:A:836:TYR:HB2	15:T:17:DC:O3'	2.03	0.57
1:A:870:GLU:OE1	5:E:202:SER:OG	2.13	0.57
11:K:57:LEU:HD21	11:K:78:THR:HG22	1.86	0.57
1:A:390:GLN:NE2	1:A:394:ASN:OD1	2.37	0.57
1:A:1284:MET:C	1:A:1285:MET:HE2	2.30	0.57
1:A:676:MET:HA	1:A:676:MET:HE3	1.87	0.57
13:M:611:UNK:O	13:M:612:UNK:CB	2.51	0.57
1:A:1285:MET:HE2	1:A:1285:MET:HA	1.87	0.57
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.37	0.57
2:B:781:PHE:CZ	2:B:782:LEU:HD12	2.40	0.57
8:H:1:MET:HE2	8:H:1:MET:HA	1.87	0.57
14:N:40:DG:H2''	14:N:41:DC:C5	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:12:DT:H2'	15:T:13:DT:C7	2.35	0.56
1:A:50:ILE:HG22	1:A:52:GLY:H	1.69	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.87	0.56
3:C:58:LEU:HD21	10:J:57:ILE:HD13	1.86	0.56
8:H:54:SER:O	8:H:146:ARG:NH1	2.38	0.56
14:N:26:DA:C1'	14:N:27:DC:P	2.91	0.56
1:A:69:THR:O	1:A:69:THR:HG22	2.04	0.56
15:T:8:DC:H2'	15:T:9:DT:H71	1.87	0.56
1:A:768:GLN:OE1	1:A:816:HIS:ND1	2.32	0.56
2:B:996:ARG:NH1	3:C:174:ALA:O	2.39	0.56
3:C:81:GLU:OE1	3:C:82:TYR:N	2.36	0.56
1:A:874:ASP:OD1	1:A:875:ALA:N	2.38	0.56
2:B:298:LEU:O	2:B:302:CYS:N	2.38	0.56
2:B:800:GLN:OE1	10:J:52:THR:OG1	2.06	0.56
2:B:1223:ASP:O	2:B:1224:PHE:HB3	2.06	0.56
1:A:364:VAL:HG21	1:A:444:PHE:CE2	2.40	0.56
9:I:97:MET:HE2	9:I:97:MET:N	2.19	0.56
15:T:37:DA:H2''	15:T:38:DG:C8	2.40	0.56
2:B:128:LEU:N	2:B:168:GLY:O	2.38	0.56
2:B:694:ASP:OD1	2:B:696:GLU:N	2.39	0.56
5:E:68:SER:O	5:E:72:PHE:N	2.35	0.56
1:A:1000:LEU:N	1:A:1011:GLN:OE1	2.39	0.55
1:A:81:PHE:CZ	2:B:1208:MET:HE3	2.41	0.55
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.89	0.55
1:A:1442:ASP:OD2	7:G:60:ARG:NH1	2.39	0.55
2:B:89:GLU:O	2:B:135:ARG:N	2.38	0.55
1:A:613:ILE:HG23	8:H:117:SER:OG	2.06	0.55
11:K:113:THR:HA	11:K:116:ALA:HB3	1.89	0.55
2:B:1174:LYS:O	2:B:1178:ASN:N	2.39	0.55
2:B:1205:GLN:HA	2:B:1208:MET:HE2	1.88	0.55
13:M:447:UNK:CB	15:T:38:DG:C4'	2.84	0.55
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.42	0.55
3:C:168:ALA:O	3:C:171:GLY:N	2.40	0.54
1:A:836:TYR:CD1	15:T:17:DC:H4'	2.41	0.54
2:B:167:ILE:HD11	2:B:424:LEU:HD11	1.87	0.54
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.34	0.54
1:A:1283:VAL:HG12	1:A:1285:MET:HE3	1.89	0.54
13:M:631:UNK:CB	13:M:645:UNK:CB	2.85	0.54
1:A:589:GLN:HA	1:A:606:LEU:HD23	1.89	0.54
2:B:101:MET:O	2:B:169:ARG:NH2	2.40	0.54
3:C:55:THR:OG1	3:C:152:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:GLN:O	9:I:89:GLN:NE2	2.40	0.54
13:M:349:UNK:O	13:M:444:UNK:N	2.41	0.54
3:C:47:ASP:OD1	3:C:169:LYS:NZ	2.37	0.54
1:A:613:ILE:HG21	8:H:102:TYR:CD1	2.43	0.54
13:M:481:UNK:O	13:M:485:UNK:N	2.40	0.54
13:M:609:UNK:O	13:M:610:UNK:CB	2.55	0.54
1:A:585:GLY:N	1:A:609:ASP:OD1	2.40	0.54
2:B:224:GLN:O	2:B:239:GLU:N	2.41	0.54
11:K:79:GLU:N	11:K:79:GLU:OE2	2.40	0.54
1:A:92:HIS:CD2	1:A:304:MET:HE1	2.43	0.54
1:A:160:GLN:NE2	1:A:161:LEU:O	2.42	0.54
2:B:189:LEU:O	2:B:193:LYS:N	2.41	0.53
5:E:169:ARG:NE	6:F:140:ASP:OD2	2.37	0.53
1:A:444:PHE:CG	1:A:487:MET:HE3	2.43	0.53
1:A:1318:THR:O	5:E:7:ARG:NH2	2.41	0.53
3:C:90:ASP:OD2	3:C:91:HIS:ND1	2.38	0.53
1:A:668:ASP:O	1:A:741:ASN:ND2	2.40	0.53
2:B:284:ILE:O	2:B:288:ALA:N	2.36	0.53
2:B:1131:GLY:HA3	15:T:20:DT:P	2.48	0.53
1:A:252:PHE:HZ	16:R:3:C:C5	2.24	0.53
2:B:120:ARG:NH2	2:B:956:THR:O	2.39	0.53
13:M:551:UNK:O	13:M:555:UNK:N	2.42	0.53
15:T:3:DC:H2'	15:T:4:DT:H71	1.89	0.53
1:A:872:GLY:O	1:A:1058:VAL:HG12	2.09	0.52
1:A:858:ASN:OD1	1:A:861:GLY:N	2.43	0.52
2:B:579:ARG:NH2	2:B:621:GLU:O	2.43	0.52
3:C:163:ILE:HG22	3:C:165:LYS:H	1.73	0.52
1:A:66:LYS:O	1:A:70:CYS:N	2.42	0.52
2:B:1187:ASN:ND2	2:B:1190:ASP:OD2	2.38	0.52
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.91	0.52
1:A:444:PHE:HE1	1:A:489:LEU:HD13	1.72	0.52
2:B:824:ILE:HD11	10:J:45:CYS:HA	1.91	0.52
1:A:1318:THR:HG22	5:E:141:VAL:HG21	1.91	0.52
4:D:72:ARG:NH2	7:G:52:ASP:OD2	2.35	0.52
1:A:1433:MET:HE2	1:A:1439:GLY:CA	2.39	0.52
5:E:13:TRP:NE1	5:E:37:LEU:O	2.42	0.52
15:T:39:DA:C2'	15:T:40:DT:C7	2.86	0.52
1:A:279:LEU:HD11	1:A:285:PRO:CG	2.39	0.52
3:C:108:GLU:OE1	3:C:108:GLU:N	2.39	0.52
2:B:87:LYS:O	2:B:137:TYR:N	2.43	0.52
11:K:24:ASP:OD2	11:K:74:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:40:DT:H2''	15:T:41:DC:C6	2.45	0.51
2:B:25:ILE:HG23	2:B:658:ILE:HD13	1.91	0.51
14:N:42:DA:H2''	14:N:43:DG:C8	2.45	0.51
1:A:150:THR:O	1:A:164:ARG:N	2.43	0.51
1:A:1443:VAL:HG12	7:G:61:ILE:HD12	1.93	0.51
13:M:570:UNK:O	13:M:574:UNK:N	2.43	0.51
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.93	0.51
1:A:92:HIS:NE2	1:A:304:MET:HE1	2.25	0.51
3:C:5:GLY:O	3:C:24:ASN:ND2	2.43	0.51
14:N:47:DG:N2	15:T:2:DG:C4	2.79	0.51
13:M:631:UNK:CA	13:M:645:UNK:CB	2.89	0.51
1:A:472:LEU:HD22	2:B:835:GLN:CG	2.40	0.51
1:A:248:PRO:HG2	2:B:1114:LEU:HD13	1.93	0.51
13:M:355:UNK:CA	15:T:38:DG:P	2.93	0.51
1:A:103:CYS:O	1:A:108:MET:HE3	2.11	0.51
1:A:500:GLU:OE1	2:B:1146:PHE:N	2.41	0.51
1:A:593:GLU:N	1:A:593:GLU:OE1	2.44	0.51
2:B:370:PHE:O	2:B:374:LYS:N	2.43	0.51
3:C:11:ARG:NH1	3:C:206:ASN:OD1	2.40	0.50
15:T:18:DC:H2'	15:T:19:DA:C8	2.47	0.50
1:A:279:LEU:HD11	1:A:285:PRO:HG2	1.93	0.50
1:A:640:GLN:OE1	1:A:640:GLN:N	2.35	0.50
14:N:8:DA:H2''	14:N:9:DT:C6	2.46	0.50
5:E:88:VAL:HG11	5:E:93:MET:HE3	1.94	0.50
13:M:666:UNK:O	13:M:667:UNK:CB	2.57	0.50
8:H:106:GLU:HG3	8:H:112:ILE:HD12	1.93	0.50
15:T:30:DG:H2'	15:T:31:DG:H4'	1.94	0.50
1:A:1097:GLY:O	1:A:1098:VAL:HB	2.12	0.50
2:B:1138:MET:HE3	2:B:1138:MET:HA	1.92	0.50
4:D:129:LEU:O	4:D:133:THR:N	2.45	0.50
2:B:834:ASN:O	2:B:1013:ASN:ND2	2.41	0.50
8:H:16:ASP:OD1	8:H:18:GLY:N	2.45	0.50
1:A:1284:MET:O	1:A:1285:MET:HE2	2.11	0.50
3:C:89:GLU:O	3:C:91:HIS:N	2.45	0.50
6:F:116:ASP:OD1	6:F:118:LEU:N	2.45	0.49
13:M:555:UNK:O	13:M:559:UNK:N	2.46	0.49
15:T:12:DT:C6	15:T:13:DT:H72	2.47	0.49
14:N:42:DA:C2	15:T:7:DG:C6	2.99	0.49
4:D:198:LEU:O	4:D:202:ILE:HG22	2.12	0.49
1:A:590:ARG:HE	1:A:621:THR:HG22	1.76	0.49
1:A:1120:LEU:HD11	1:A:1131:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1032:SER:O	2:B:1036:ALA:N	2.40	0.49
10:J:43:ARG:NH2	10:J:46:CYS:SG	2.85	0.49
1:A:472:LEU:HD22	2:B:835:GLN:HG3	1.93	0.49
3:C:75:MET:O	3:C:246:ARG:NH2	2.45	0.49
3:C:136:ASP:OD2	3:C:138:GLU:N	2.45	0.49
7:G:60:ARG:N	7:G:69:GLU:O	2.41	0.49
13:M:587:UNK:N	13:M:779:UNK:O	2.46	0.49
1:A:325:ILE:HD12	1:A:325:ILE:H	1.77	0.49
1:A:364:VAL:HG23	1:A:469:ARG:O	2.13	0.49
2:B:776:GLN:HE21	16:R:10:A:P	2.35	0.49
2:B:958:GLN:OE1	2:B:958:GLN:N	2.38	0.49
1:A:344:ARG:NH1	15:T:21:DC:OP1	2.46	0.48
1:A:471:ASN:O	1:A:474:VAL:HG22	2.13	0.48
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.46	0.48
2:B:261:ARG:O	2:B:266:ALA:HB3	2.13	0.48
5:E:74:ASP:O	5:E:106:GLN:NE2	2.37	0.48
2:B:744:HIS:CE1	2:B:746:SER:HG	2.24	0.48
14:N:42:DA:N3	15:T:7:DG:C2	2.81	0.48
1:A:344:ARG:NH2	15:T:21:DC:OP2	2.47	0.48
7:G:57:GLN:O	7:G:58:ARG:HB2	2.13	0.48
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.95	0.48
10:J:10:CYS:CB	10:J:46:CYS:SG	2.98	0.48
2:B:175:ARG:N	2:B:179:CYS:SG	2.84	0.48
12:L:47:ARG:NH1	12:L:48:CYS:O	2.47	0.48
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.95	0.48
15:T:6:DT:H73	15:T:6:DT:OP2	2.14	0.48
1:A:252:PHE:CE1	16:R:3:C:C5	2.99	0.47
1:A:672:ASP:OD1	1:A:675:THR:OG1	2.11	0.47
2:B:201:GLY:O	2:B:495:LEU:HD22	2.14	0.47
2:B:1207:LEU:HA	2:B:1210:MET:HB2	1.96	0.47
5:E:43:LYS:O	5:E:47:CYS:N	2.47	0.47
11:K:19:LEU:HD22	11:K:35:PHE:CD2	2.49	0.47
11:K:113:THR:O	11:K:117:ASP:N	2.44	0.47
13:M:671:UNK:O	13:M:746:UNK:N	2.47	0.47
1:A:668:ASP:OD1	1:A:742:ASN:N	2.47	0.47
14:N:47:DG:N1	15:T:2:DG:C6	2.82	0.47
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.44	0.47
14:N:8:DA:H2"	14:N:9:DT:H73	1.95	0.47
8:H:145:ARG:O	8:H:146:ARG:HB2	2.14	0.47
1:A:151:ASP:OD1	1:A:163:SER:OG	2.23	0.47
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:68:GLU:OE2	12:L:70:ARG:NH2	2.43	0.47
15:T:23:DT:H3	16:R:7:A:H61	1.61	0.47
16:R:14:A:O5'	16:R:14:A:H8	1.97	0.47
2:B:566:LEU:HD22	2:B:586:TRP:O	2.14	0.47
5:E:170:LEU:HD11	5:E:174:GLN:CB	2.45	0.47
2:B:841:MET:HE2	2:B:1010:LEU:HD21	1.97	0.47
3:C:233:GLU:OE1	10:J:43:ARG:NH1	2.46	0.47
5:E:143:ASN:OD1	5:E:145:THR:N	2.48	0.46
11:K:109:TRP:O	11:K:113:THR:OG1	2.31	0.46
14:N:8:DA:H2''	14:N:9:DT:C5	2.49	0.46
1:A:350:ARG:NH2	1:A:486:GLU:OE1	2.49	0.46
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.49	0.46
1:A:107:CYS:HB2	1:A:110:CYS:HB3	1.97	0.46
1:A:1444:MET:HE1	6:F:135:ARG:CZ	2.46	0.46
1:A:848:ILE:HD13	1:A:858:ASN:HA	1.96	0.46
2:B:46:GLN:OE1	2:B:46:GLN:N	2.38	0.46
8:H:95:TYR:OH	8:H:97:MET:SD	2.59	0.46
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.97	0.46
14:N:4:DG:H2''	14:N:5:DT:C6	2.51	0.46
1:A:669:THR:OG1	1:A:805:LEU:HD22	2.16	0.46
1:A:352:VAL:HG12	1:A:353:ILE:N	2.31	0.46
1:A:1312:ASN:ND2	1:A:1315:GLU:OE2	2.48	0.46
2:B:71:LEU:HD12	2:B:72:GLU:N	2.30	0.46
1:A:605:MET:HE3	1:A:621:THR:HG21	1.98	0.46
2:B:1133:MET:HE2	15:T:19:DA:O4'	2.16	0.46
1:A:117:GLU:O	1:A:123:ARG:NH1	2.39	0.45
1:A:225:ASN:OD1	1:A:228:PHE:N	2.48	0.45
1:A:325:ILE:HG21	2:B:1210:MET:HG2	1.98	0.45
2:B:198:ASP:OD1	2:B:200:GLY:N	2.49	0.45
2:B:694:ASP:OD1	2:B:694:ASP:C	2.59	0.45
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.97	0.45
3:C:177:GLU:HB3	3:C:231:ASN:HB3	1.97	0.45
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.97	0.45
1:A:14:VAL:HG21	1:A:1430:LEU:HD12	1.98	0.45
1:A:123:ARG:NH2	1:A:155:GLU:OE1	2.48	0.45
1:A:350:ARG:NE	15:T:21:DC:H4'	2.31	0.45
3:C:235:VAL:HG23	3:C:237:SER:H	1.81	0.45
6:F:127:GLU:OE1	6:F:127:GLU:N	2.49	0.45
8:H:96:VAL:HG13	8:H:143:LEU:HD23	1.97	0.45
4:D:69:ALA:HA	4:D:72:ARG:HE	1.81	0.45
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:373:UNK:O	13:M:442:UNK:N	2.49	0.45
2:B:778:MET:O	2:B:819:ALA:HB1	2.15	0.45
10:J:7:CYS:HA	10:J:49:MET:HE3	1.98	0.45
13:M:447:UNK:CB	15:T:38:DG:H4'	2.47	0.45
1:A:81:PHE:CE1	2:B:1208:MET:HE3	2.51	0.45
1:A:626:ASN:O	1:A:631:HIS:ND1	2.42	0.45
2:B:239:GLU:C	2:B:240:ILE:HD13	2.41	0.45
2:B:354:ASP:O	2:B:358:LYS:N	2.49	0.45
2:B:638:PHE:CE2	2:B:743:ILE:HG23	2.52	0.45
5:E:82:PHE:CE1	5:E:111:VAL:HG21	2.52	0.45
3:C:172:PRO:O	3:C:235:VAL:HG22	2.16	0.45
13:M:672:UNK:O	13:M:728:UNK:N	2.50	0.45
14:N:4:DG:H2'	14:N:5:DT:C7	2.29	0.45
1:A:1314:SER:HA	1:A:1317:MET:HE3	1.99	0.45
2:B:638:PHE:CZ	2:B:743:ILE:HG23	2.52	0.45
2:B:776:GLN:NE2	16:R:10:A:OP1	2.50	0.45
15:T:12:DT:C2'	15:T:13:DT:H72	2.47	0.45
1:A:549:MET:HE3	1:A:656:TRP:HB2	1.99	0.45
2:B:167:ILE:HD11	2:B:424:LEU:CD1	2.47	0.45
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.99	0.45
2:B:1194:ILE:HG22	2:B:1196:ILE:HG23	1.98	0.45
3:C:75:MET:HE1	3:C:237:SER:O	2.17	0.45
5:E:138:ALA:O	5:E:141:VAL:HG22	2.18	0.44
12:L:32:ALA:O	12:L:33:GLU:HB2	2.17	0.44
15:T:14:DC:H2''	15:T:15:DT:H5'	2.00	0.44
2:B:790:ASP:O	2:B:858:SER:OG	2.27	0.44
5:E:112:TYR:N	5:E:135:PHE:O	2.45	0.44
14:N:7:DG:C2	15:T:42:DA:C2	3.05	0.44
1:A:748:MET:HA	1:A:748:MET:HE2	1.99	0.44
2:B:762:ASN:CG	2:B:1024:ALA:HB3	2.42	0.44
2:B:806:THR:H	2:B:809:MET:HE2	1.82	0.44
6:F:130:ILE:O	6:F:148:VAL:HG21	2.17	0.44
7:G:22:MET:O	7:G:23:LYS:C	2.60	0.44
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.99	0.44
2:B:1131:GLY:HA3	15:T:20:DT:OP1	2.17	0.44
13:M:317:UNK:CB	13:M:515:UNK:C	2.84	0.44
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.57	0.44
16:R:7:A:H2'	16:R:8:G:C8	2.52	0.44
1:A:881:GLN:OE1	1:A:1025:ARG:NH1	2.51	0.44
5:E:116:ILE:HD13	5:E:121:MET:SD	2.58	0.44
1:A:447:GLN:OE1	15:T:20:DT:H4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG22	8:H:26:ILE:HG12	2.00	0.44
1:A:591:PHE:CD2	1:A:595:THR:HG21	2.53	0.44
1:A:932:GLU:OE2	1:A:936:LEU:HD11	2.18	0.44
14:N:13:DA:N6	15:T:34:DA:C2	2.86	0.44
1:A:134:ARG:NH1	1:A:220:THR:O	2.51	0.44
1:A:898:ARG:O	1:A:1029:ARG:NH2	2.47	0.44
1:A:1097:GLY:O	1:A:1099:PRO:HD2	2.17	0.44
9:I:103:CYS:O	9:I:107:SER:CA	2.65	0.44
13:M:354:UNK:CB	15:T:37:DA:H4'	2.48	0.44
1:A:1387:HIS:CD2	14:N:36:DA:H5'	2.53	0.43
2:B:239:GLU:O	2:B:240:ILE:HD13	2.18	0.43
6:F:96:THR:O	6:F:100:GLN:OE1	2.35	0.43
6:F:83:PRO:O	6:F:151:LEU:HD23	2.18	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.61	0.43
13:M:585:UNK:O	13:M:779:UNK:N	2.51	0.43
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.54	0.43
6:F:109:VAL:HG13	6:F:124:GLU:OE2	2.18	0.43
1:A:858:ASN:OD1	1:A:862:ASN:N	2.48	0.43
1:A:1281:ARG:NH2	1:A:1309:ASP:OD1	2.52	0.43
5:E:157:SER:N	5:E:160:GLU:OE2	2.45	0.43
6:F:97:ARG:CZ	6:F:101:ILE:HD11	2.48	0.43
1:A:1013:ASP:OD1	5:E:207:ARG:NE	2.39	0.43
5:E:32:GLN:O	5:E:36:GLU:N	2.36	0.43
14:N:4:DG:H2''	14:N:5:DT:H73	2.00	0.43
14:N:44:DA:H2''	14:N:45:DG:C8	2.54	0.43
15:T:41:DC:H2''	15:T:42:DA:C8	2.54	0.43
1:A:453:MET:HE1	1:A:510:GLN:CB	2.48	0.43
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.54	0.43
8:H:82:PRO:O	8:H:83:GLN:HB3	2.18	0.43
8:H:111:LEU:O	8:H:112:ILE:HD13	2.18	0.43
1:A:1285:MET:HE2	1:A:1285:MET:CA	2.48	0.43
2:B:262:GLU:OE1	2:B:262:GLU:N	2.43	0.43
2:B:408:LEU:HD11	2:B:545:ILE:CD1	2.47	0.43
1:A:123:ARG:NH1	1:A:155:GLU:OE1	2.50	0.43
13:M:719:UNK:C	13:M:741:UNK:CB	2.97	0.43
1:A:492:PRO:O	1:A:493:GLN:NE2	2.52	0.43
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.39	0.43
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.00	0.43
7:G:107:LYS:O	7:G:158:HIS:HA	2.19	0.43
14:N:11:DT:H3	15:T:37:DA:H61	1.67	0.43
1:A:1396:ALA:N	1:A:1419:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.01	0.43
14:N:13:DA:H2'	14:N:14:DT:O4'	2.18	0.43
1:A:528:LEU:HD23	1:A:751:SER:HB2	2.00	0.42
1:A:605:MET:HE2	1:A:617:VAL:HG22	2.01	0.42
1:A:711:ARG:NH2	9:I:95:THR:OG1	2.45	0.42
2:B:444:MET:SD	2:B:444:MET:N	2.90	0.42
8:H:89:LEU:HD21	8:H:91:ASP:OD2	2.19	0.42
1:A:485:ASP:OD1	16:R:12:G:H5'	2.19	0.42
2:B:805:THR:O	2:B:1044:ALA:N	2.50	0.42
2:B:956:THR:HG22	12:L:46:VAL:HG21	2.00	0.42
2:B:973:ILE:O	2:B:974:PRO:C	2.62	0.42
1:A:483:ASP:HB2	2:B:987:LYS:HE3	2.01	0.42
2:B:832:GLY:O	2:B:835:GLN:HG2	2.19	0.42
5:E:52:ARG:NH1	5:E:54:GLN:O	2.52	0.42
1:A:473:SER:OG	1:A:522:GLY:O	2.37	0.42
1:A:1283:VAL:N	1:A:1307:GLU:O	2.47	0.42
2:B:59:LEU:O	2:B:59:LEU:HD23	2.18	0.42
13:M:685:UNK:O	13:M:689:UNK:N	2.53	0.42
3:C:34:ARG:HG3	3:C:176:ILE:HG21	2.02	0.42
13:M:451:UNK:O	13:M:455:UNK:N	2.53	0.42
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.46	0.42
6:F:130:ILE:HG23	6:F:130:ILE:O	2.18	0.42
1:A:68:GLN:HA	1:A:68:GLN:OE1	2.19	0.42
1:A:106:VAL:HG12	1:A:107:CYS:N	2.35	0.42
1:A:1412:ALA:O	1:A:1416:ALA:N	2.53	0.42
2:B:978:ASP:O	2:B:989:THR:HA	2.20	0.42
8:H:118:PHE:O	8:H:121:LEU:N	2.50	0.42
1:A:362:ASP:OD1	1:A:362:ASP:N	2.49	0.42
15:T:42:DA:C2	15:T:43:DA:C6	3.07	0.42
2:B:71:LEU:HB2	2:B:432:MET:HE3	2.02	0.42
3:C:38:ILE:HG13	3:C:176:ILE:HD12	2.02	0.42
3:C:167:HIS:CD2	12:L:70:ARG:HG3	2.55	0.42
14:N:21:DT:H6	14:N:21:DT:H2'	1.61	0.42
1:A:344:ARG:NE	2:B:1120:GLU:OE2	2.47	0.42
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.53	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:HG12	2.02	0.42
2:B:183:GLU:OE1	2:B:183:GLU:N	2.43	0.42
1:A:231:PRO:O	1:A:234:MET:HB3	2.19	0.41
1:A:1433:MET:HE2	1:A:1439:GLY:HA2	2.01	0.41
2:B:220:GLY:HA2	2:B:241:ARG:HB2	2.02	0.41
2:B:957:ASN:OD1	2:B:961:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:ILE:HG21	4:D:207:LEU:HD11	2.02	0.41
9:I:97:MET:HE2	9:I:97:MET:CA	2.50	0.41
1:A:157:ASP:OD1	1:A:159:THR:OG1	2.28	0.41
1:A:336:ILE:HD13	1:A:340:LEU:HD12	2.02	0.41
1:A:376:TYR:OH	1:A:495:GLU:OE2	2.35	0.41
1:A:821:ARG:HG2	1:A:825:ILE:HD12	2.01	0.41
6:F:116:ASP:OD1	6:F:116:ASP:C	2.63	0.41
13:M:480:UNK:O	13:M:484:UNK:N	2.53	0.41
14:N:4:DG:H2''	14:N:5:DT:C5	2.55	0.41
1:A:35:ILE:N	1:A:83:HIS:O	2.47	0.41
1:A:837:ILE:O	1:A:841:LEU:N	2.48	0.41
2:B:47:GLN:NE2	2:B:495:LEU:O	2.53	0.41
3:C:265:MET:HG2	11:K:21:ILE:HD12	2.01	0.41
4:D:39:ASN:ND2	4:D:45:GLU:OE2	2.54	0.41
5:E:117:THR:HG22	14:N:45:DG:H5''	2.01	0.41
6:F:79:ARG:NH1	6:F:145:ASP:O	2.53	0.41
14:N:17:DT:H6	14:N:17:DT:H2'	1.71	0.41
2:B:285:ILE:O	2:B:288:ALA:HB3	2.21	0.41
2:B:651:LEU:O	2:B:654:ARG:NH2	2.50	0.41
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.55	0.41
2:B:227:LYS:N	2:B:395:GLN:OE1	2.47	0.41
4:D:66:ARG:HH21	4:D:133:THR:HA	1.81	0.41
1:A:37:PHE:HB2	1:A:50:ILE:HG21	2.01	0.41
1:A:311:GLN:O	1:A:312:PRO:C	2.63	0.41
10:J:8:PHE:CD2	10:J:49:MET:HE1	2.55	0.41
13:M:317:UNK:CB	13:M:493:UNK:O	2.69	0.41
15:T:6:DT:C7	15:T:6:DT:OP2	2.69	0.41
1:A:606:LEU:HD12	8:H:102:TYR:OH	2.21	0.41
1:A:666:ILE:HG13	2:B:1026:LEU:HB3	2.02	0.41
5:E:16:PHE:O	5:E:17:ARG:C	2.64	0.41
6:F:97:ARG:NH2	6:F:101:ILE:HD11	2.36	0.41
13:M:370:UNK:O	13:M:371:UNK:C	2.68	0.41
14:N:35:DA:H2''	14:N:36:DA:C8	2.56	0.41
1:A:66:LYS:O	1:A:67:CYS:C	2.64	0.41
1:A:613:ILE:HG23	8:H:117:SER:CB	2.51	0.41
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.50	0.41
5:E:1:MET:HE1	5:E:7:ARG:HD3	2.02	0.41
13:M:533:UNK:O	13:M:537:UNK:N	2.54	0.41
1:A:55:ASP:OD1	1:A:55:ASP:C	2.64	0.41
1:A:254:GLU:O	1:A:256:GLN:NE2	2.41	0.41
1:A:860:LEU:O	1:A:1422:ARG:NH2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:ARG:NE	1:A:1034:GLU:OE1	2.44	0.41
4:D:211:LEU:O	4:D:215:SER:N	2.42	0.41
2:B:562:GLY:O	2:B:590:HIS:ND1	2.54	0.40
6:F:84:TYR:C	6:F:151:LEU:HD22	2.46	0.40
1:A:567:LYS:NZ	8:H:91:ASP:O	2.50	0.40
2:B:780:VAL:O	2:B:780:VAL:HG13	2.20	0.40
11:K:44:ASN:OD1	11:K:47:ARG:NH2	2.53	0.40
1:A:13:THR:HG1	1:A:1432:GLN:CD	2.23	0.40
1:A:265:LYS:NZ	1:A:302:THR:OG1	2.48	0.40
3:C:75:MET:HE1	3:C:238:ILE:HA	2.04	0.40
15:T:39:DA:C8	15:T:40:DT:H72	2.56	0.40
2:B:466:TRP:CD2	2:B:479:VAL:HG11	2.57	0.40
2:B:597:MET:HE3	2:B:617:ARG:HB2	2.04	0.40
2:B:694:ASP:OD1	2:B:697:GLU:N	2.42	0.40
16:R:3:C:H2'	16:R:4:G:C8	2.55	0.40
1:A:707:GLY:O	1:A:708:MET:HE2	2.20	0.40
1:A:1117:THR:N	1:A:1328:TYR:O	2.53	0.40
1:A:1317:MET:HE1	1:A:1338:VAL:CG1	2.52	0.40
2:B:105:SER:N	2:B:958:GLN:O	2.46	0.40
2:B:1085:ILE:HG22	2:B:1086:PHE:O	2.22	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	1306/1733 (75%)	1240 (95%)	64 (5%)	2 (0%)	43	77
2	B	1019/1224 (83%)	973 (96%)	46 (4%)	0	100	100
3	C	264/318 (83%)	255 (97%)	9 (3%)	0	100	100
4	D	138/221 (62%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
6	F	79/155 (51%)	78 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	158 (94%)	10 (6%)	1 (1%)	21	58
8	H	127/146 (87%)	116 (91%)	11 (9%)	0	100	100
9	I	115/122 (94%)	110 (96%)	5 (4%)	0	100	100
10	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
11	K	102/120 (85%)	101 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	42 (96%)	2 (4%)	0	100	100
All	All	3639/4565 (80%)	3474 (96%)	162 (4%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1098	VAL
1	A	958	VAL
7	G	58	ARG

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	1007/1520 (66%)	1007 (100%)	0	100	100
2	B	753/1061 (71%)	753 (100%)	0	100	100
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	69/200 (34%)	69 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	70/152 (46%)	70 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	35/116 (30%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	89/102 (87%)	89 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	2743/4009 (68%)	2743 (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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	287	HIS
1	A	451	HIS
1	A	802	ASN
1	A	935	GLN
1	A	1387	HIS
2	B	215	GLN
2	B	449	ASN
2	B	842	ASN
2	B	1025	HIS
2	B	1104	HIS
4	D	179	GLN
5	E	101	GLN
5	E	153	HIS
8	H	11	GLN
8	H	33	GLN
9	I	87	GLN
11	K	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	R	11/17 (64%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	R	12	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	631:UNK	C	645:UNK	N	3.62
1	M	388:UNK	C	442:UNK	N	3.32

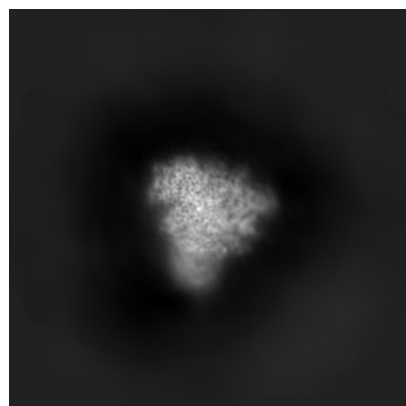
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41650. These allow visual inspection of the internal detail of the map and identification of artifacts.

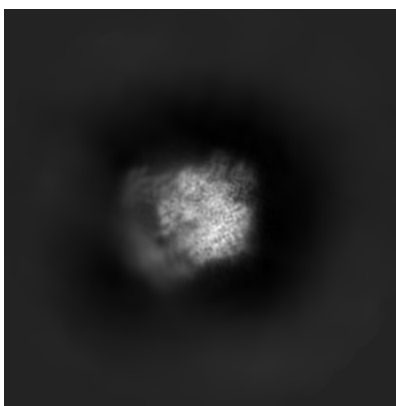
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

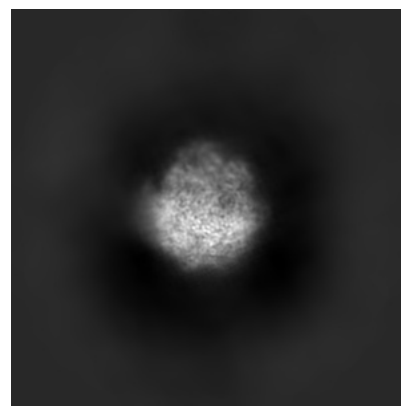
6.1.1 Primary map



X

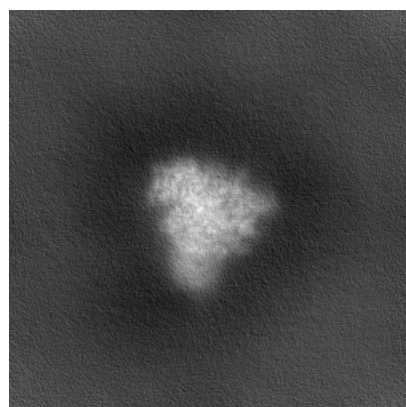


Y

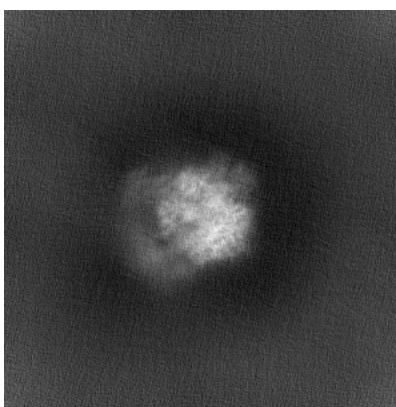


Z

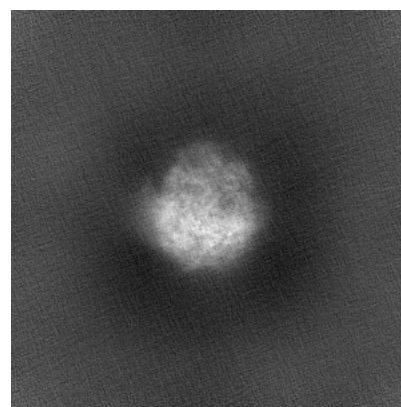
6.1.2 Raw map



X



Y

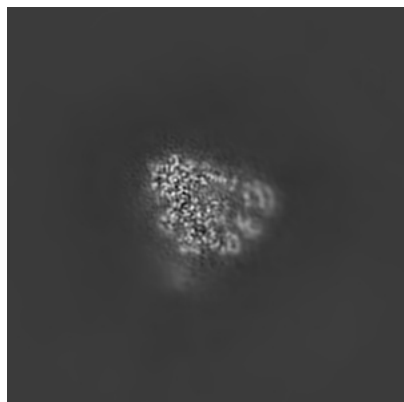


Z

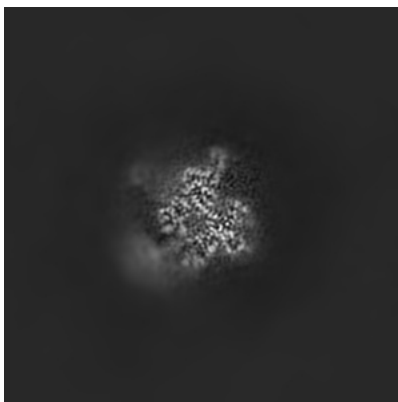
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

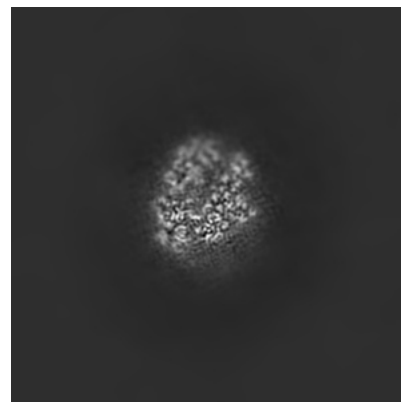
6.2.1 Primary map



X Index: 192

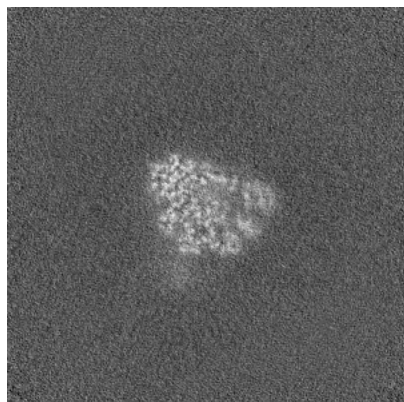


Y Index: 192

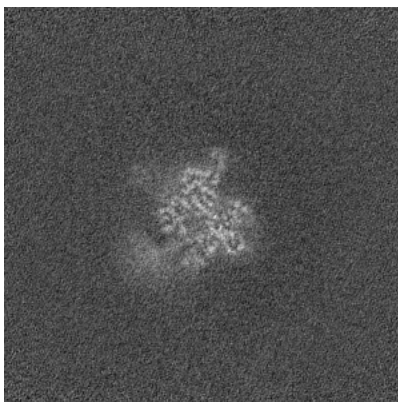


Z Index: 192

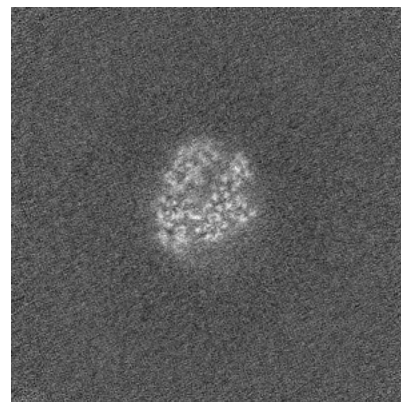
6.2.2 Raw map



X Index: 192



Y Index: 192

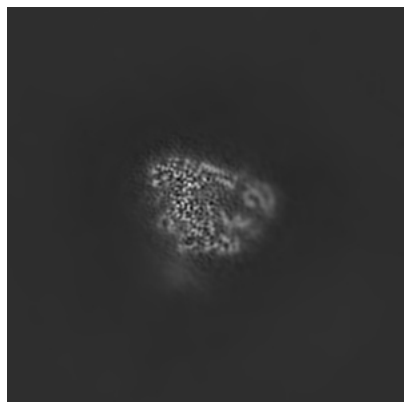


Z Index: 192

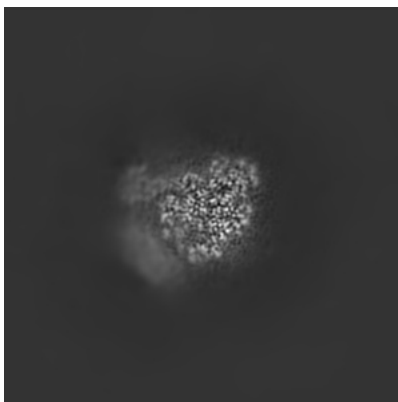
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

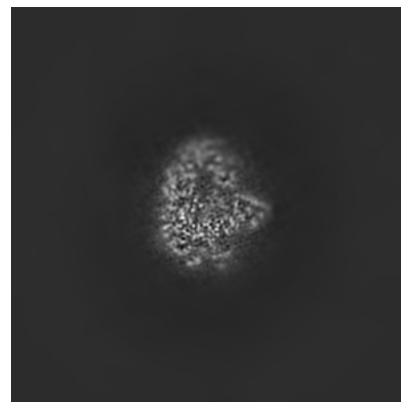
6.3.1 Primary map



X Index: 189

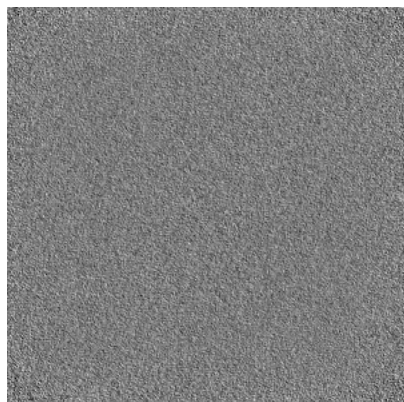


Y Index: 174

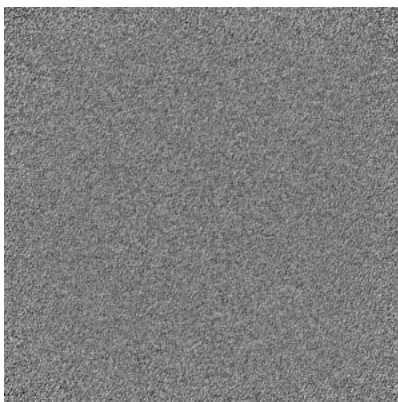


Z Index: 201

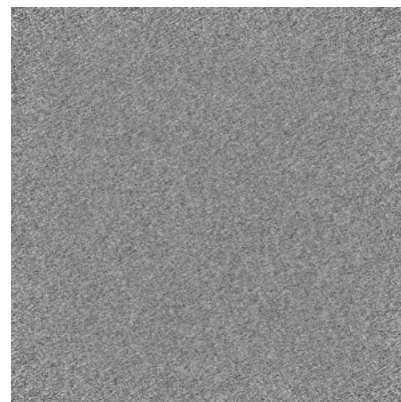
6.3.2 Raw map



X Index: 0



Y Index: 0

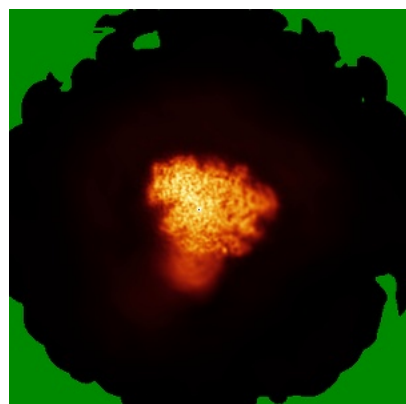


Z Index: 0

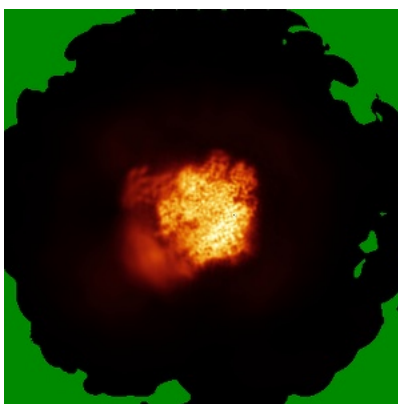
The images above show the largest variance slices of the map in three orthogonal directions.

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

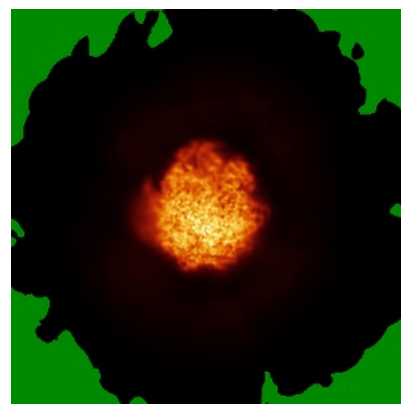
6.4.1 Primary map



X

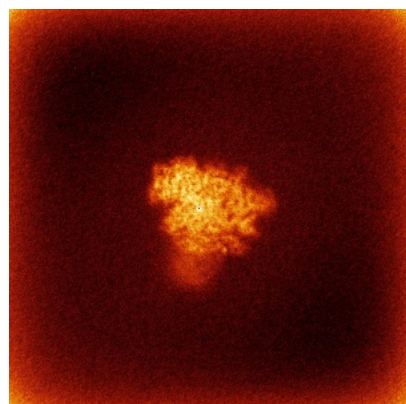


Y

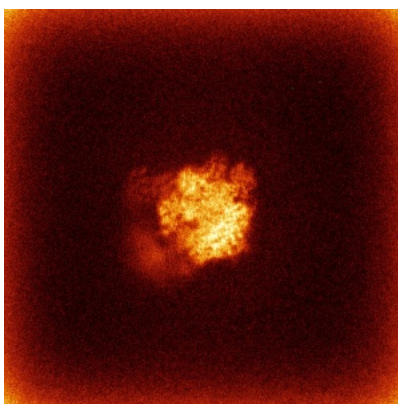


Z

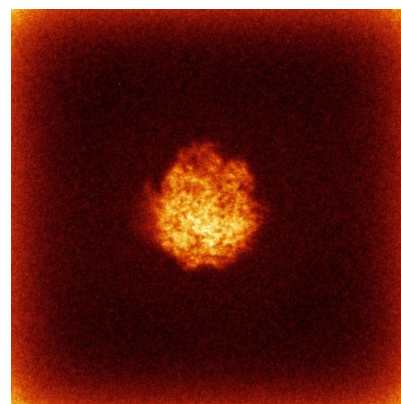
6.4.2 Raw map



X



Y

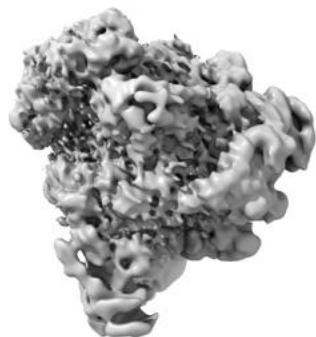


Z

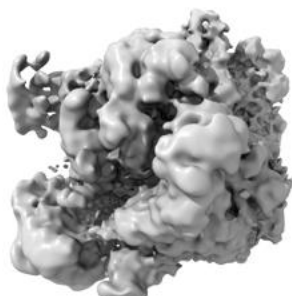
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

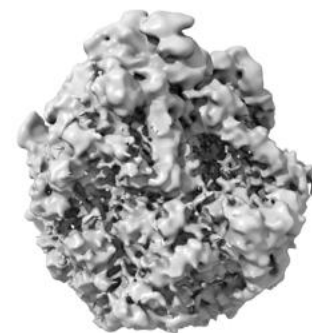
6.5.1 Primary map



X



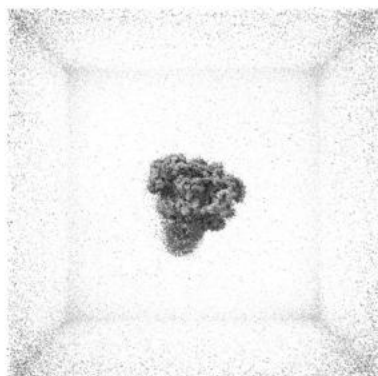
Y



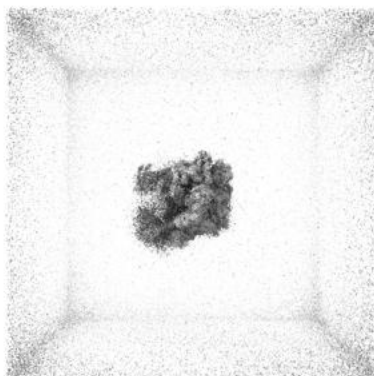
Z

The images above show the 3D surface view of the map at the recommended contour level 1.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

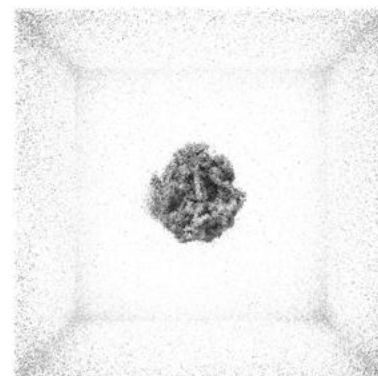
6.5.2 Raw map



X



Y



Z

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.

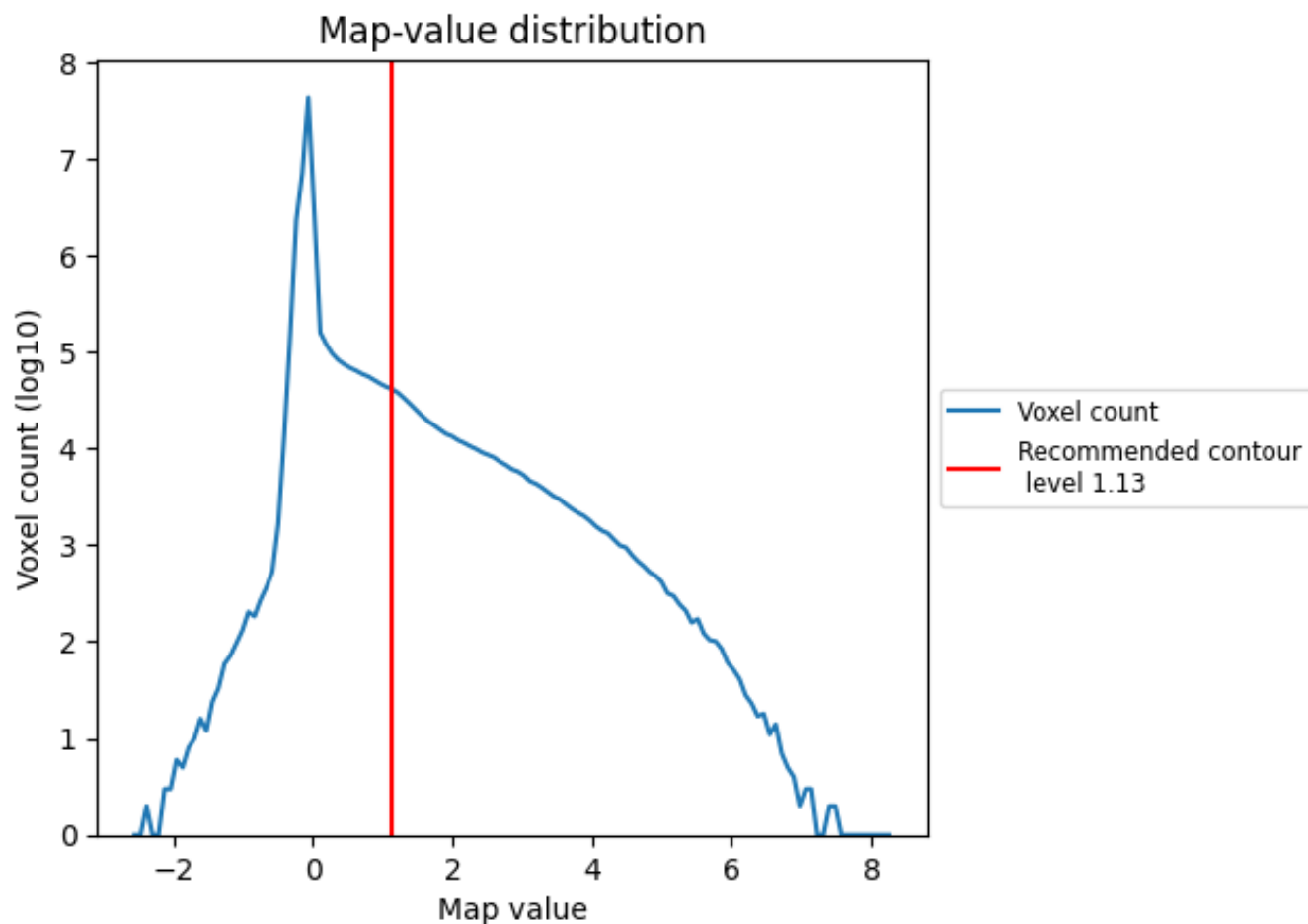
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

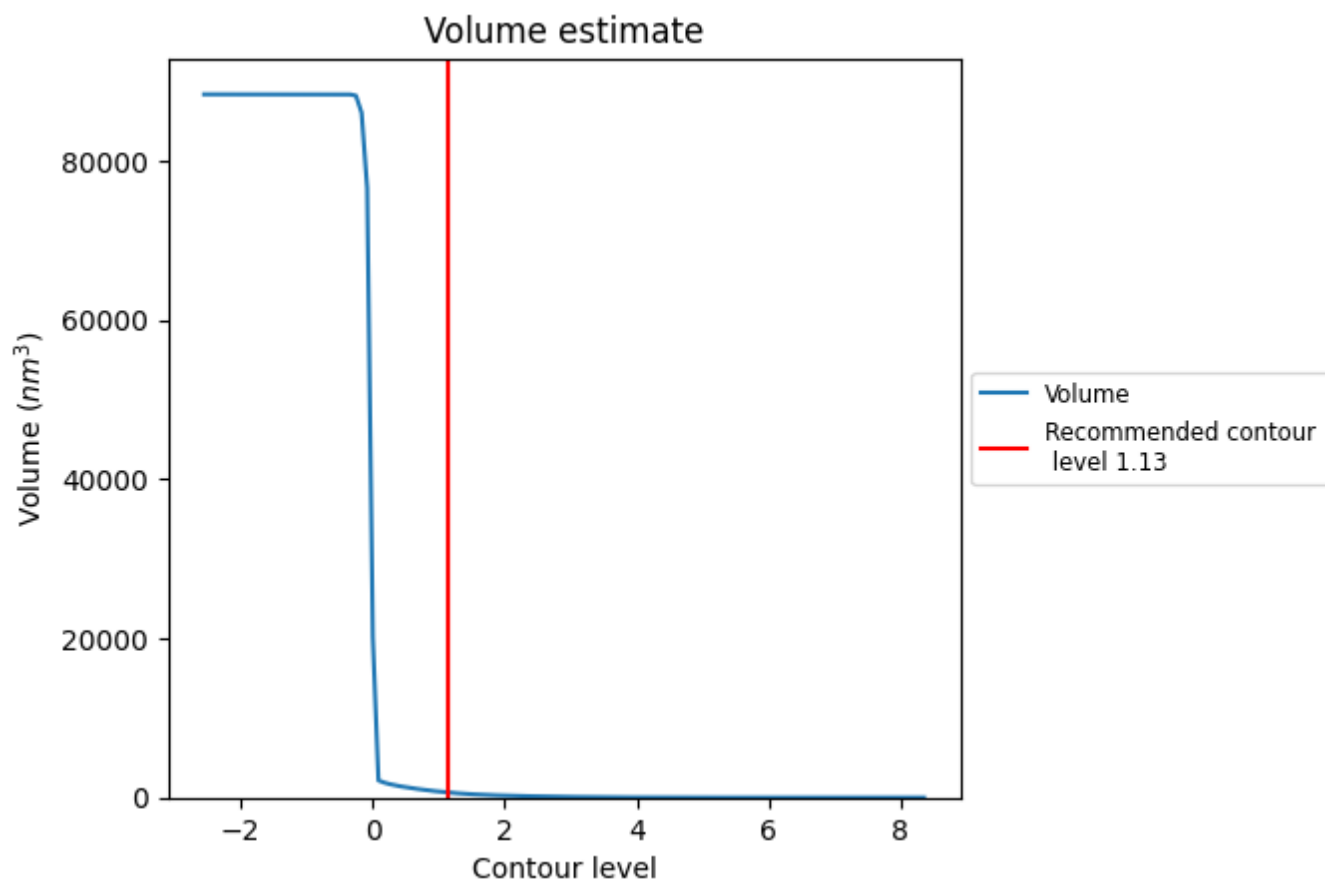
This section contains the results of statistical analysis of the map.

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.

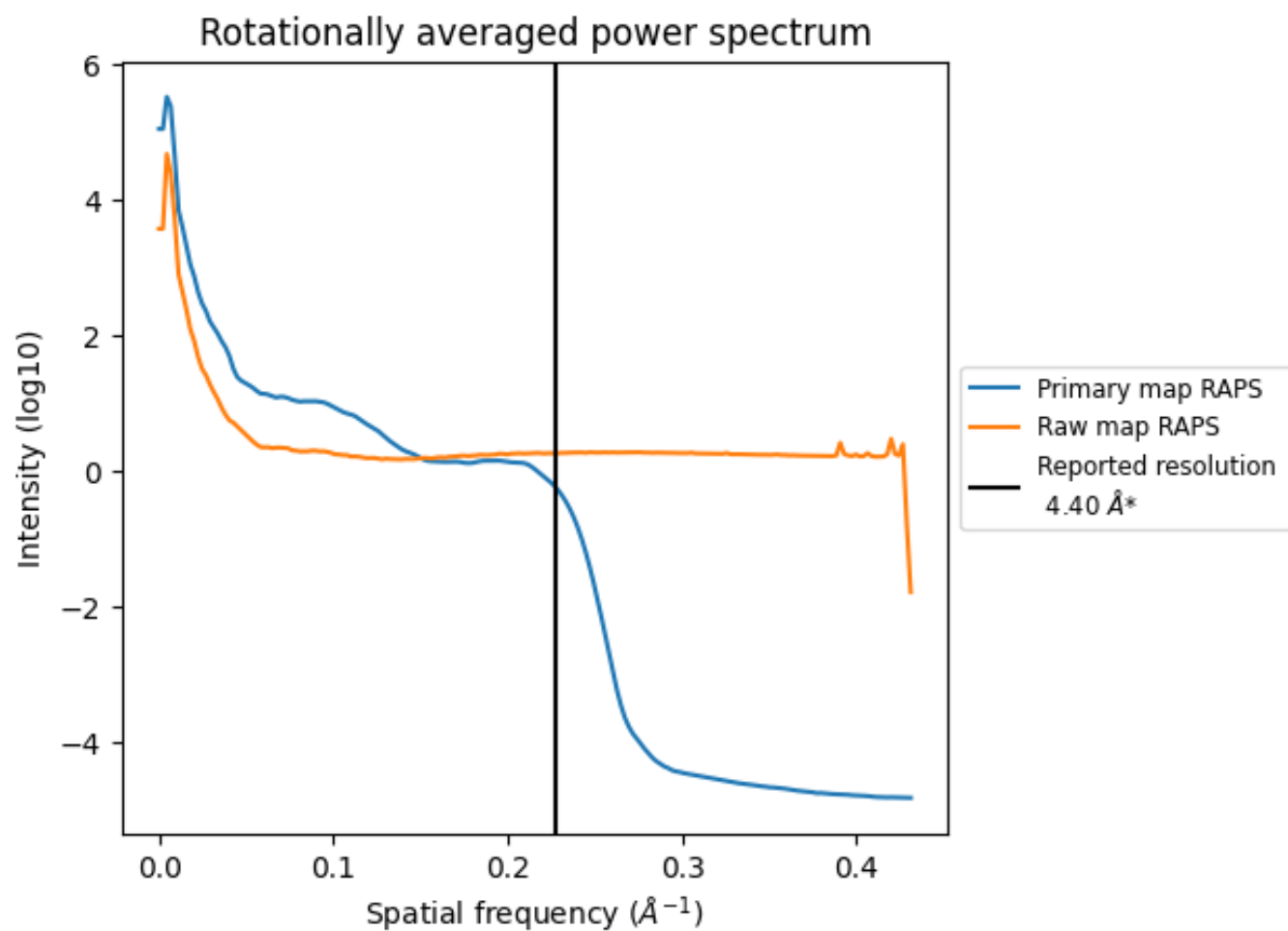
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 652 nm³; this corresponds to an approximate mass of 589 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 [i](#)

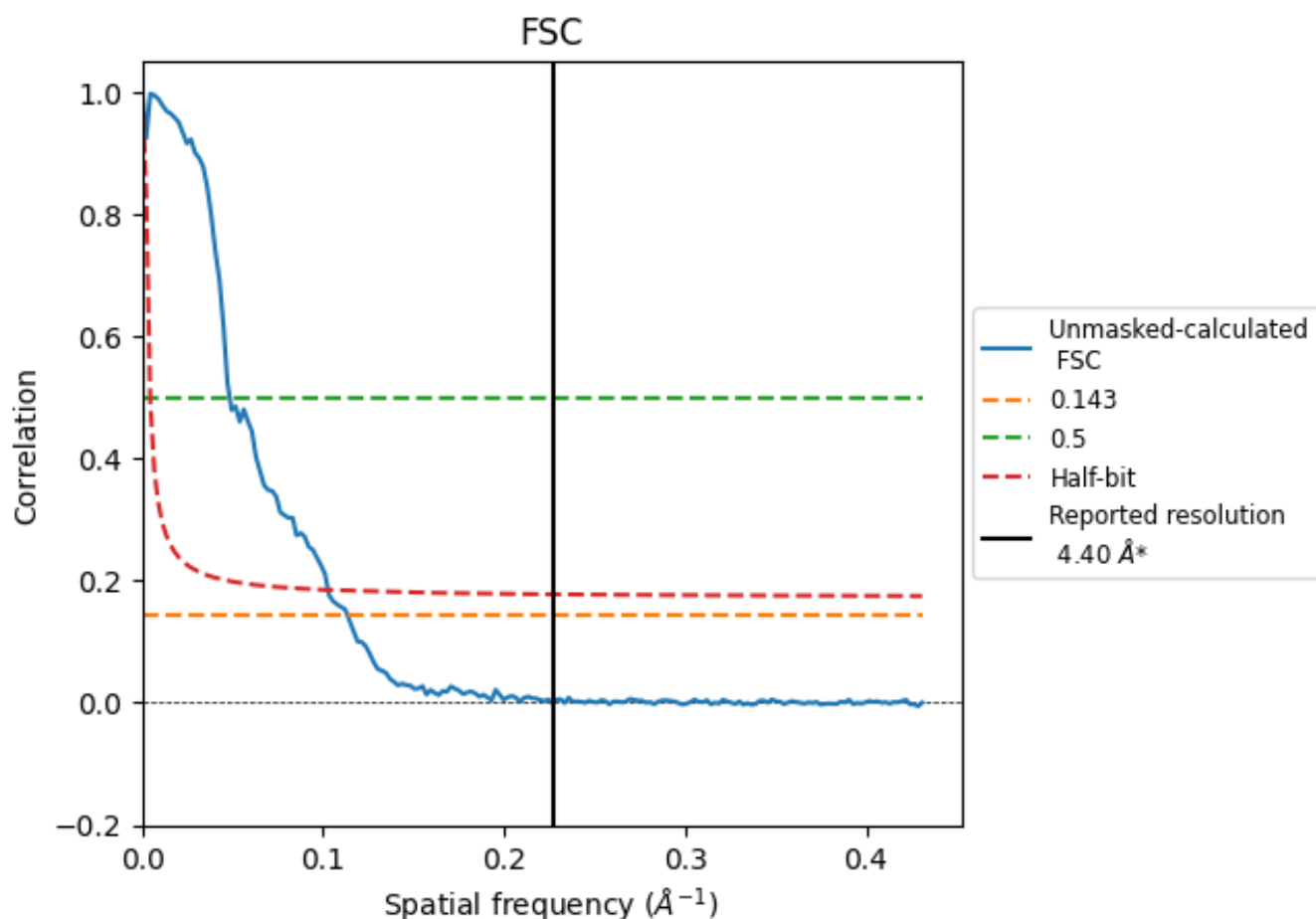


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

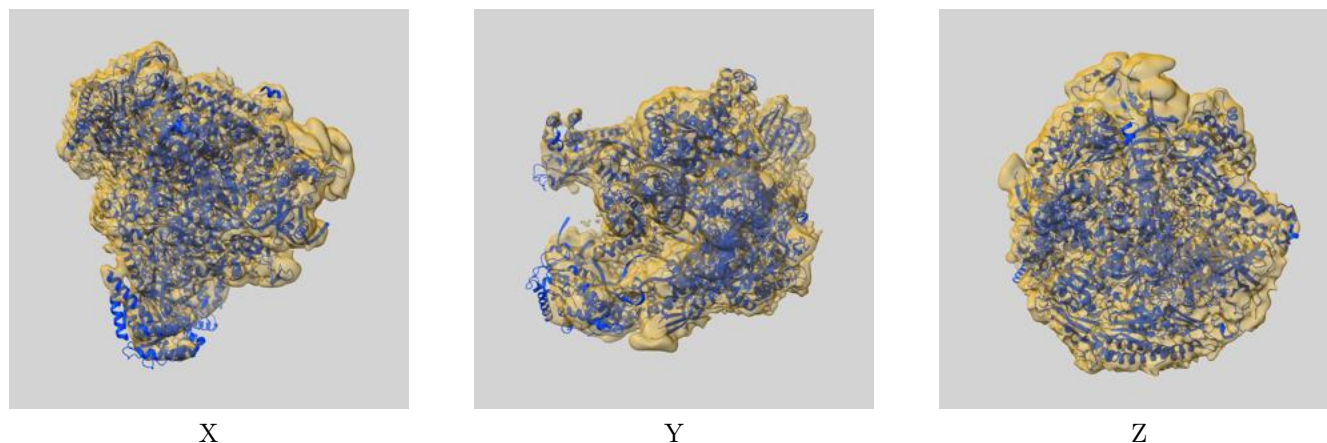
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.81	20.70	9.74

*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 8.81 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

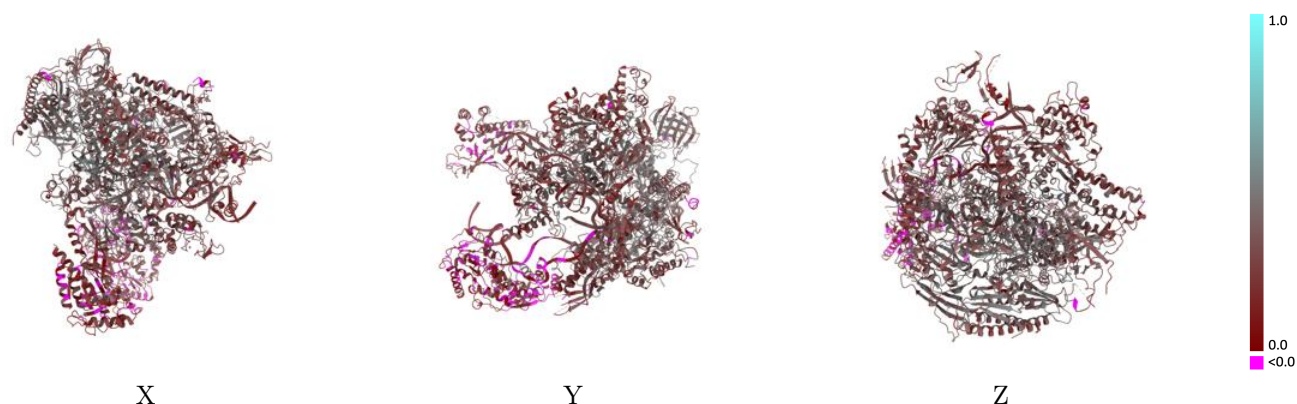
This section contains information regarding the fit between EMDB map EMD-41650 and PDB model 8TVS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



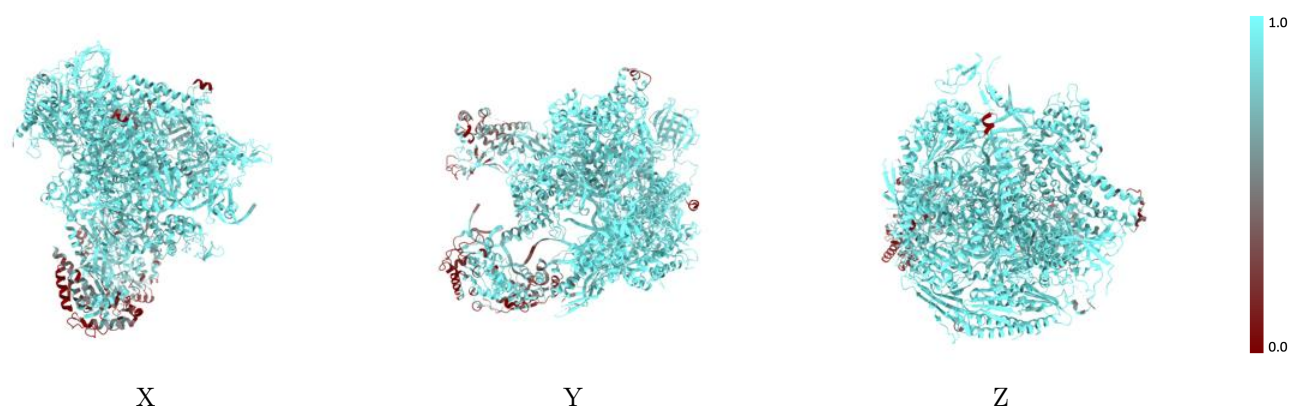
The images above show the 3D surface view of the map at the recommended contour level 1.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



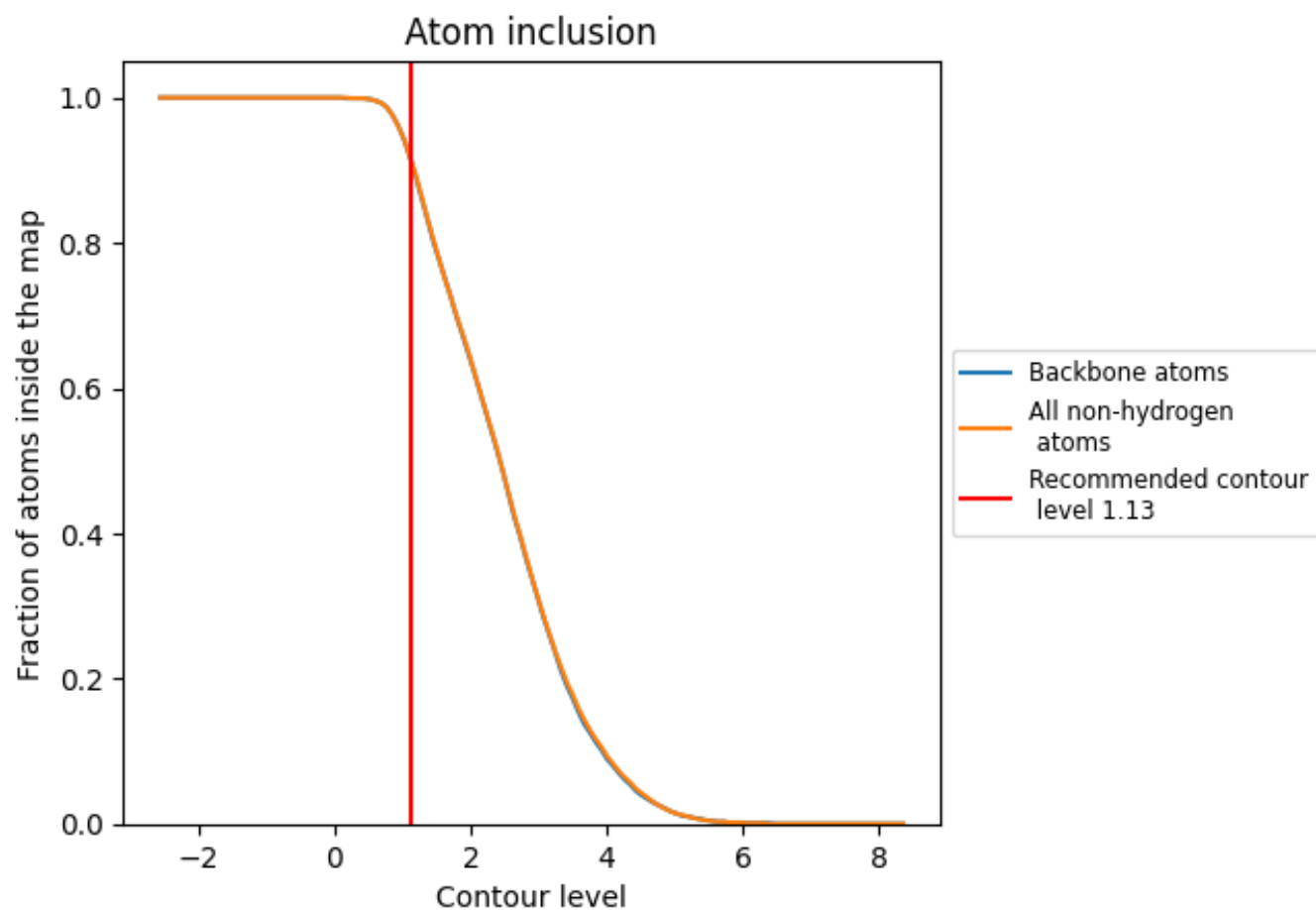
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (1.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.3050
A	 0.9590	 0.3450
B	 0.9750	 0.3550
C	 0.9740	 0.3800
D	 0.4710	 0.1730
E	 0.9700	 0.2840
F	 0.9750	 0.3530
G	 0.7370	 0.2060
H	 0.9520	 0.3350
I	 0.9350	 0.2810
J	 0.9870	 0.3830
K	 0.9590	 0.3560
L	 0.9800	 0.3010
M	 0.6100	 0.0790
N	 0.8280	 0.1230
R	 0.9920	 0.2780
T	 0.8630	 0.1620

