



Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 12:25 PM EDT

PDB ID : 5VVR
EMDB ID : EMD-8735
Title : Ternary complex of RNA Pol II, transcription scaffold and Rad26
Authors : Lahiri, I.; Leschziner, A.E.
Deposited on : 2017-05-19
Resolution : 5.80 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

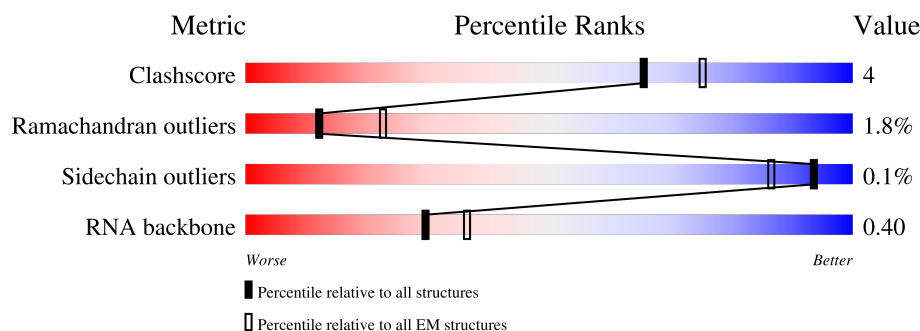
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	
4	D	221	
5	E	215	
6	F	155	
7	G	171	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	146	<div><div><div></div><div></div><div></div></div><div>87%11%</div><div></div></div>
9	I	122	<div><div><div></div><div></div><div></div></div><div>8%90%9%</div><div></div></div>
10	J	70	<div><div><div></div><div></div><div></div></div><div>89%11%</div><div></div></div>
11	K	120	<div><div><div></div><div></div><div></div></div><div>85%8%8%</div><div></div></div>
12	L	70	<div><div><div></div><div></div><div></div></div><div>53%11%34%</div><div></div></div>
13	M	1085	<div><div><div></div><div></div><div></div></div><div>24%43%54%</div><div></div></div>
14	N	47	<div><div><div></div><div></div><div></div></div><div>9%62%36%</div><div></div></div>
15	R	10	<div><div><div></div><div></div><div></div></div><div>80%20%</div><div></div></div>
16	T	47	<div><div><div></div><div></div><div></div></div><div>9%51%45%</div><div></div></div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1448	Total	C	N	O	S	0	0
			11385	7168	1988	2167	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1207	Total	C	N	O	S	0	0
			9608	6062	1678	1812	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1409	870	251	286	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	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	N	O	S	0	0
			657	419	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	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			997	613	182	191	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			4087	2620	726	722	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			965	460	176	282	47		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called DNA (TS).

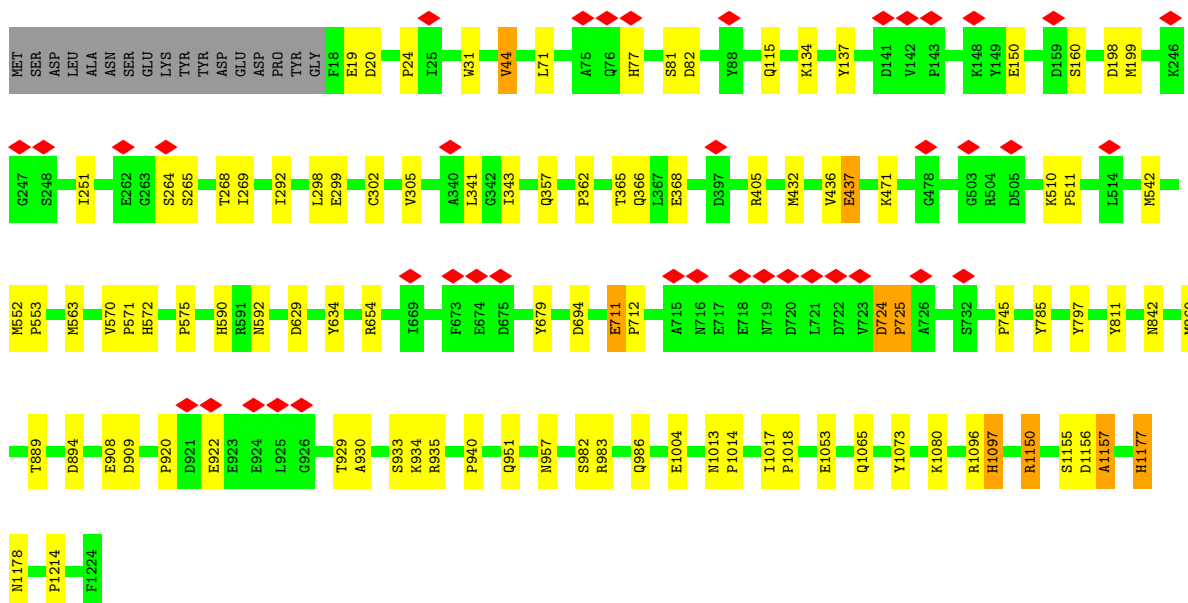
Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

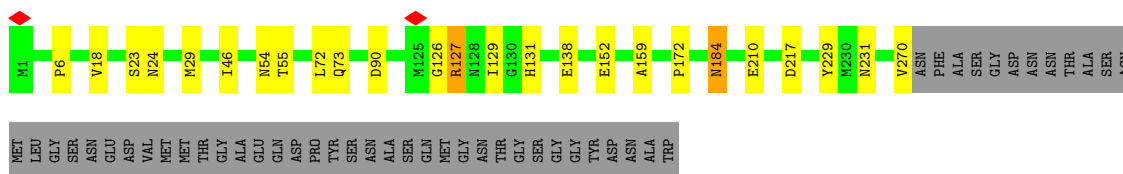
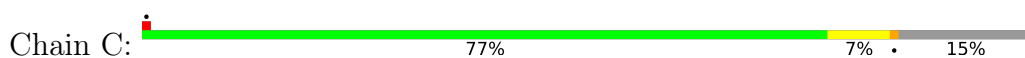
Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

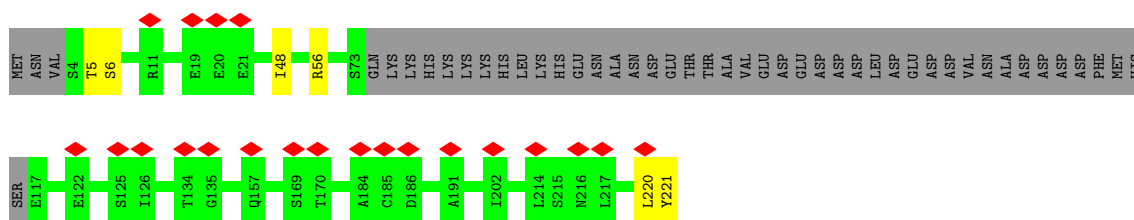
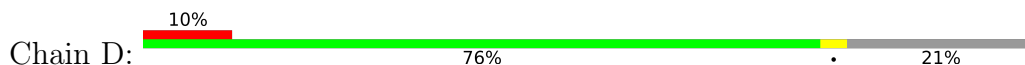
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



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



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



MET SER ASP TYR GLU ALA PHE ASN ASP GLY GLU ASN PHE GLU PHE ASP PHE ASP VAL HIS PHE SER ASP GLU GLU TYR THR GLU LYS PRO PHE GLN LYS ASP GLY GLU THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLN ASP PRO GLU ASP PHE GLN

HIS GLN TLE ARG LYS THR LEU LYS GLU LYS ALA TLE P75 F108 L111 D145 V153 D154 L155

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

Chain G: 5% 89% 11%

M1 T11 T12 L13 F17 G36 R58 G59 S67 A68 E69 F70 G84 V87 F99 M115 P116 N126 P127 Y130 Q131 E134 D135 T143 I147 K164 E165 D166 I171

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

Chain H: 87% 11%

M1 D7 R18 G19 R40 F47 T58 I59 A60 S61 S62 L63 E66 D67 T68 P69 A70 N71 D72 S73 A75 W79 A101 E105 Y115 Y116 L143 R146

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

Chain I: 8% 90% 9%

M1 R8 L14 E18 D19 K20 E21 F27 G39 T50 N51 G60 D61 G62 G63 S80 R81 F101 M116 K117 A118 T119 Q120 F121 S122

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

Chain J: 89% 11%

M1 L2 V3 P4 V5 R6 R38 E58 R69 D70

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

Chain K: 85% 8% 8%

M1 D5 K18 N29 F35 E49 R54 Y61 F71 T77 L111 GLN THR LEU ALA ALA ASP ASP ASP ALA PHE

- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 53% 11% 34%

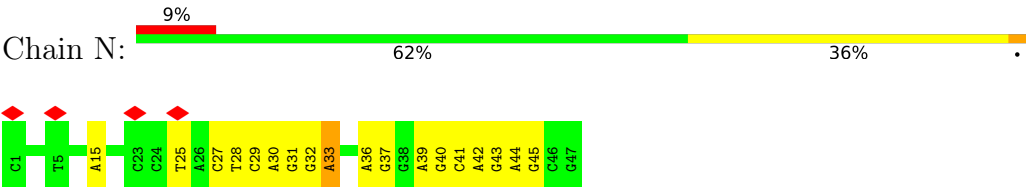
MET SER ARG GLU PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 D44 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 A69 R70

Chain M:

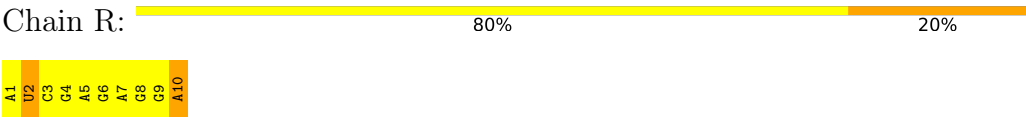


SER	SER	SER	SER	VAL	ILE	LEU	ASN	SER	ILE	GLY	VAL	SER	LEU	SER	ASP	LYS	GLU	ASP	VAL	ILE	LYS	VAL	ARG	ALA	LEU	LEU	LYS	THR	ILE	ALA	GLN	PHE	ASP	LYS	GLU	ARG	LYS	GLY	TRP	VAL	LEU	ASP	GLU	GLU	PHE	ARG	ASN	ASN	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

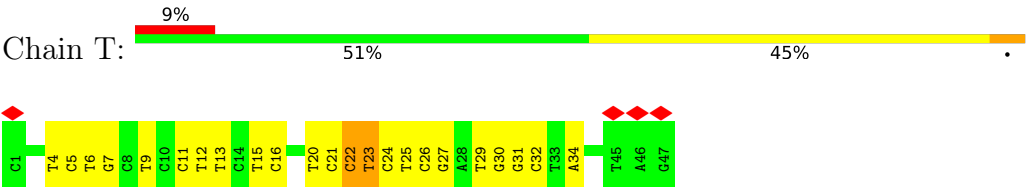
• Molecule 14: DNA (NTS)



• Molecule 15: RNA



• Molecule 16: DNA (TS)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19331	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 ($e^-/\text{\AA}^2$)	7.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0244	Depositor
Map size (\AA)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	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	0.83	0/11592	0.72	3/15682 (0.0%)
2	B	0.83	0/9799	0.75	5/13221 (0.0%)
3	C	0.87	0/2163	0.75	2/2930 (0.1%)
4	D	0.92	0/1419	0.68	1/1903 (0.1%)
5	E	0.87	0/1796	0.76	1/2416 (0.0%)
6	F	0.89	0/669	0.71	0/903
7	G	0.76	0/1368	0.82	2/1844 (0.1%)
8	H	0.82	0/1181	0.77	1/1602 (0.1%)
9	I	0.82	0/1016	0.75	0/1365
10	J	0.87	0/587	0.76	0/786
11	K	0.87	0/913	0.69	0/1232
12	L	0.78	0/366	0.91	1/485 (0.2%)
13	M	0.65	0/4180	0.71	2/5644 (0.0%)
14	N	0.59	1/1082 (0.1%)	0.82	1/1668 (0.1%)
15	R	0.59	0/247	0.80	0/384
16	T	0.72	0/1056	0.84	2/1624 (0.1%)
All	All	0.81	1/39434 (0.0%)	0.74	21/53689 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	33	DA	C3'-O3'	-5.45	1.36	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	56	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	1239	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	B	405	ARG	NE-CZ-NH2	-6.49	117.06	120.30
3	C	229	TYR	CB-CG-CD1	-6.15	117.31	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	130	TYR	CB-CG-CD2	-6.11	117.33	121.00
2	B	797	TYR	CB-CG-CD2	-5.88	117.47	121.00
16	T	23	DT	O4'-C4'-C3'	-5.73	102.21	104.50
13	M	677	ARG	NE-CZ-NH2	-5.71	117.45	120.30
7	G	58	ARG	NE-CZ-NH1	5.71	123.15	120.30
5	E	105	PHE	CB-CG-CD1	-5.69	116.82	120.80
13	M	564	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	1036	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	134	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	B	724	ASP	C-N-CD	-5.46	108.58	120.60
3	C	127	ARG	NE-CZ-NH2	-5.44	117.58	120.30
16	T	22	DC	O4'-C4'-C3'	-5.36	102.36	104.50
2	B	1150	ARG	NE-CZ-NH2	5.33	122.96	120.30
2	B	634	TYR	CB-CG-CD2	-5.25	117.85	121.00
14	N	31	DG	C3'-C2'-C1'	-5.12	96.36	102.50
8	H	115	TYR	CB-CG-CD1	-5.09	117.94	121.00
12	L	50	ASP	CB-CG-OD2	-5.06	113.74	118.30

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	A	11385	0	11443	57	0
2	B	9608	0	9577	60	0
3	C	2125	0	2091	15	0
4	D	1409	0	1423	4	0
5	E	1760	0	1788	12	0
6	F	657	0	673	7	0
7	G	1340	0	1357	9	0
8	H	1161	0	1124	12	0
9	I	997	0	961	7	0
10	J	578	0	591	6	0
11	K	895	0	903	7	0
12	L	364	0	389	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	4087	0	4145	18	0
14	N	965	0	531	29	0
15	R	220	0	110	26	0
16	T	947	0	532	41	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	38507	0	37638	294	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 4.

All (294) 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)
15:R:5:A:H2'	15:R:6:G:C8	2.00	0.97
15:R:5:A:H2'	15:R:6:G:H8	1.37	0.89
11:K:49:GLU:OE1	11:K:49:GLU:HA	1.70	0.88
15:R:7:A:H2'	15:R:8:G:C8	2.09	0.88
13:M:345:LEU:O	13:M:345:LEU:HD23	1.74	0.86
1:A:26:GLU:N	1:A:26:GLU:OE1	2.11	0.83
14:N:39:DA:N6	16:T:9:DT:O4	2.13	0.81
2:B:343:ILE:HG22	2:B:343:ILE:O	1.78	0.81
15:R:10:A:H2	16:T:20:DT:H3	1.30	0.79
2:B:542:MET:O	2:B:542:MET:HG2	1.84	0.77
1:A:68:GLN:O	1:A:68:GLN:HG2	1.84	0.76
15:R:1:A:C2	16:T:30:DG:N2	2.54	0.75
10:J:70:ASP:OD1	10:J:70:ASP:O	2.05	0.74
1:A:226:GLU:OE1	1:A:226:GLU:N	2.19	0.71
5:E:203:GLU:OE1	5:E:203:GLU:N	2.24	0.70
2:B:982:SER:OG	2:B:983:ARG:N	2.25	0.69
13:M:461:VAL:HG12	13:M:461:VAL:O	1.93	0.68
2:B:44:VAL:HG12	2:B:44:VAL:O	1.95	0.65
16:T:29:DT:H2''	16:T:30:DG:C8	2.33	0.64
15:R:7:A:H2'	15:R:8:G:H8	1.62	0.63
1:A:1192:LEU:HD23	1:A:1192:LEU:O	1.98	0.62
16:T:24:DC:C4	16:T:25:DT:H73	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:172:GLU:OE1	5:E:172:GLU:N	2.28	0.61
15:R:1:A:H8	15:R:1:A:OP1	1.83	0.61
14:N:43:DG:N2	16:T:6:DT:O2	2.34	0.61
14:N:39:DA:N1	16:T:9:DT:N3	2.48	0.61
10:J:38:ARG:HA	10:J:38:ARG:NE	2.17	0.60
15:R:9:G:N2	16:T:21:DC:C2	2.71	0.59
2:B:115:GLN:OE1	2:B:115:GLN:N	2.26	0.59
16:T:21:DC:H2'	16:T:22:DC:C6	2.38	0.59
2:B:251:ILE:HG22	2:B:251:ILE:O	2.03	0.58
2:B:1177:HIS:O	2:B:1177:HIS:ND1	2.37	0.58
16:T:21:DC:H2'	16:T:22:DC:H6	1.69	0.58
11:K:49:GLU:OE1	11:K:49:GLU:CA	2.43	0.58
15:R:9:G:O2'	15:R:10:A:H5'	2.04	0.58
2:B:1177:HIS:O	2:B:1177:HIS:CG	2.57	0.57
14:N:33:DA:N6	16:T:16:DC:H42	2.02	0.57
1:A:535:THR:HG22	1:A:535:THR:O	2.03	0.57
3:C:72:LEU:HD12	3:C:72:LEU:O	2.04	0.57
3:C:55:THR:OG1	3:C:152:GLU:N	2.38	0.56
1:A:1454:MET:O	1:A:1454:MET:HG2	2.06	0.56
13:M:345:LEU:O	13:M:345:LEU:CD2	2.50	0.56
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.08	0.56
3:C:72:LEU:HD12	3:C:72:LEU:C	2.25	0.56
1:A:247:ARG:O	1:A:247:ARG:HG3	2.05	0.55
11:K:54:ARG:HA	11:K:54:ARG:NE	2.21	0.55
1:A:1192:LEU:O	1:A:1192:LEU:CD2	2.55	0.55
1:A:1329:THR:OG1	1:A:1330:ASN:N	2.40	0.54
6:F:155:LEU:HG	6:F:155:LEU:OXT	2.08	0.54
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.89	0.54
6:F:111:LEU:HD23	6:F:111:LEU:O	2.08	0.54
15:R:3:C:H2'	15:R:4:G:O4'	2.08	0.54
14:N:33:DA:H61	16:T:16:DC:H42	1.56	0.53
15:R:9:G:N2	16:T:21:DC:O2	2.41	0.53
14:N:15:DA:N6	16:T:34:DA:N1	2.55	0.53
1:A:264:PHE:N	1:A:264:PHE:CD1	2.76	0.53
7:G:131:GLN:O	7:G:131:GLN:HG2	2.09	0.53
15:R:9:G:N2	16:T:22:DC:C2	2.77	0.53
5:E:178:ILE:HG23	5:E:178:ILE:O	2.08	0.53
16:T:30:DG:H2'	16:T:31:DG:C8	2.44	0.53
14:N:39:DA:OP2	14:N:39:DA:H2'	2.09	0.53
2:B:510:LYS:N	2:B:511:PRO:O	2.42	0.53
14:N:33:DA:H61	16:T:16:DC:N4	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:CB	2:B:712:PRO:HD2	2.39	0.53
14:N:43:DG:H8	14:N:43:DG:OP2	1.92	0.52
2:B:20:ASP:C	2:B:20:ASP:OD1	2.44	0.52
1:A:1288:ASP:OD1	1:A:1288:ASP:C	2.48	0.52
1:A:471:ASN:O	1:A:472:LEU:CB	2.58	0.52
1:A:55:ASP:CG	1:A:55:ASP:O	2.47	0.52
1:A:1127:ASP:C	1:A:1127:ASP:OD1	2.48	0.52
2:B:724:ASP:HB3	2:B:725:PRO:HA	1.92	0.52
2:B:1053:GLU:OE1	2:B:1053:GLU:N	2.38	0.52
4:D:220:LEU:O	4:D:221:TYR:CB	2.58	0.51
1:A:185:TRP:O	1:A:197:PRO:HA	2.10	0.51
2:B:368:GLU:OE1	2:B:368:GLU:N	2.37	0.51
15:R:7:A:O5'	15:R:7:A:H8	1.93	0.51
14:N:40:DG:OP2	14:N:40:DG:H8	1.93	0.51
9:I:8:ARG:HA	9:I:8:ARG:NE	2.26	0.51
4:D:5:THR:OG1	4:D:6:SER:N	2.43	0.51
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.10	0.51
2:B:1150:ARG:HA	2:B:1150:ARG:NE	2.26	0.51
14:N:42:DA:H2'	14:N:42:DA:OP2	2.10	0.51
1:A:53:LEU:O	1:A:54:ASN:HB2	2.11	0.51
1:A:1342:GLU:OE1	1:A:1342:GLU:HA	2.11	0.51
16:T:6:DT:H2''	16:T:7:DG:C8	2.46	0.51
1:A:1192:LEU:HD23	1:A:1192:LEU:C	2.31	0.50
14:N:45:DG:N2	16:T:4:DT:O2	2.44	0.50
5:E:127:ILE:N	5:E:128:PRO:CD	2.75	0.50
11:K:29:ASN:ND2	11:K:77:THR:OG1	2.45	0.50
2:B:44:VAL:O	2:B:44:VAL:CG1	2.60	0.50
14:N:32:DG:O6	16:T:16:DC:C4	2.64	0.50
16:T:26:DC:C2	16:T:27:DG:N7	2.80	0.50
13:M:629:HIS:HB2	13:M:630:PRO:HA	1.92	0.50
16:T:12:DT:OP2	16:T:12:DT:H2'	2.12	0.49
1:A:55:ASP:N	1:A:56:PRO:CD	2.75	0.49
1:A:150:THR:HA	1:A:165:GLY:HA3	1.94	0.49
2:B:137:TYR:N	2:B:137:TYR:CD1	2.79	0.49
8:H:146:ARG:HG2	8:H:146:ARG:O	2.12	0.49
1:A:453:MET:O	1:A:454:SER:CB	2.60	0.49
13:M:561:ILE:HG22	13:M:561:ILE:O	2.12	0.49
16:T:7:DG:OP2	16:T:7:DG:H8	1.95	0.49
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.95	0.49
16:T:5:DC:OP2	16:T:5:DC:H2'	2.12	0.49
1:A:567:LYS:O	1:A:569:LYS:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:577:LEU:N	13:M:577:LEU:HD23	2.28	0.48
1:A:49:LYS:HB2	1:A:55:ASP:HB2	1.95	0.48
14:N:37:DG:H2'	14:N:37:DG:OP2	2.13	0.48
3:C:270:VAL:HG12	3:C:270:VAL:O	2.12	0.48
8:H:143:LEU:C	8:H:143:LEU:HD23	2.33	0.48
16:T:22:DC:H2'	16:T:23:DT:H6	1.78	0.48
5:E:56:LYS:O	5:E:57:MET:HB2	2.14	0.48
3:C:210:GLU:OE1	3:C:210:GLU:N	2.43	0.47
14:N:28:DT:H72	14:N:29:DC:H42	1.78	0.47
7:G:143:ILE:HG23	7:G:143:ILE:O	2.12	0.47
2:B:711:GLU:CB	2:B:712:PRO:CD	2.92	0.47
1:A:1312:ASN:OD1	1:A:1312:ASN:O	2.32	0.47
8:H:63:LEU:O	8:H:63:LEU:HG	2.13	0.47
2:B:894:ASP:OD1	2:B:894:ASP:C	2.53	0.47
16:T:6:DT:OP2	16:T:6:DT:H2'	2.14	0.47
1:A:507:VAL:HB	1:A:508:PRO:HD3	1.97	0.47
1:A:1046:LEU:HD23	1:A:1046:LEU:C	2.35	0.47
14:N:40:DG:OP2	14:N:40:DG:H2'	2.15	0.47
12:L:51:CYS:O	12:L:53:HIS:N	2.48	0.47
14:N:41:DC:OP2	14:N:41:DC:H2'	2.15	0.47
15:R:3:C:N4	16:T:27:DG:C6	2.79	0.47
15:R:8:G:H2'	15:R:9:G:C8	2.50	0.47
4:D:220:LEU:O	4:D:221:TYR:HB2	2.15	0.46
2:B:134:LYS:N	2:B:134:LYS:HD3	2.30	0.46
2:B:785:TYR:CD1	2:B:785:TYR:C	2.89	0.46
10:J:3:VAL:O	10:J:3:VAL:HG13	2.14	0.46
3:C:23:SER:OG	3:C:24:ASN:N	2.48	0.46
9:I:18:GLU:O	9:I:19:ASP:HB3	2.16	0.46
2:B:629:ASP:C	2:B:629:ASP:OD1	2.52	0.46
16:T:13:DT:H2'	16:T:13:DT:OP2	2.16	0.46
6:F:145:ASP:OD1	6:F:145:ASP:C	2.54	0.46
8:H:40:LEU:HD23	8:H:40:LEU:N	2.30	0.46
1:A:43:GLU:N	1:A:49:LYS:O	2.49	0.46
10:J:5:VAL:O	10:J:6:ARG:HB2	2.16	0.46
1:A:1004:ASN:C	1:A:1004:ASN:OD1	2.54	0.46
7:G:84:GLY:N	7:G:147:ILE:O	2.48	0.45
3:C:46:ILE:HA	3:C:159:ALA:HA	1.99	0.45
16:T:31:DG:H1'	16:T:32:DC:N3	2.30	0.45
10:J:58:GLU:OE1	10:J:58:GLU:N	2.44	0.45
2:B:542:MET:O	2:B:542:MET:CG	2.57	0.45
5:E:78:LEU:C	5:E:78:LEU:HD23	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:469:ASP:C	13:M:469:ASP:OD1	2.54	0.45
2:B:711:GLU:HB3	2:B:712:PRO:CD	2.47	0.45
14:N:33:DA:N6	16:T:15:DT:C4	2.84	0.45
2:B:19:GLU:OE1	2:B:19:GLU:N	2.40	0.45
2:B:343:ILE:O	2:B:343:ILE:CG2	2.50	0.45
3:C:73:GLN:N	3:C:131:HIS:O	2.42	0.45
3:C:184:ASN:OD1	3:C:184:ASN:O	2.35	0.45
14:N:44:DA:H8	14:N:44:DA:OP2	2.00	0.45
2:B:1177:HIS:O	2:B:1178:ASN:CB	2.64	0.44
2:B:570:VAL:HG23	2:B:570:VAL:O	2.18	0.44
5:E:197:LYS:HG3	5:E:209:ALA:HB1	1.99	0.44
16:T:24:DC:OP2	16:T:24:DC:H6	1.99	0.44
15:R:4:G:C6	16:T:27:DG:C6	3.05	0.44
1:A:414:ASP:C	1:A:414:ASP:OD1	2.55	0.44
1:A:851:HIS:ND1	1:A:852:TYR:N	2.66	0.44
2:B:563:MET:SD	2:B:590:HIS:HB2	2.57	0.44
2:B:1004:GLU:H	2:B:1004:GLU:CD	2.20	0.44
2:B:1156:ASP:O	2:B:1157:ALA:CB	2.65	0.44
6:F:153:VAL:HG12	6:F:153:VAL:O	2.17	0.44
15:R:3:C:H5'	15:R:3:C:H6	1.83	0.44
15:R:7:A:O5'	15:R:7:A:C8	2.70	0.44
1:A:596:THR:O	1:A:597:LEU:HB2	2.18	0.44
8:H:47:PHE:CD1	8:H:47:PHE:C	2.91	0.43
13:M:273:ARG:HB2	13:M:274:PRO:HD3	1.99	0.43
15:R:5:A:C2'	15:R:6:G:H8	2.20	0.43
1:A:1165:GLU:OE1	1:A:1165:GLU:N	2.39	0.43
3:C:29:MET:SD	3:C:29:MET:C	2.96	0.43
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.48	0.43
6:F:108:PHE:N	6:F:108:PHE:CD1	2.86	0.43
1:A:55:ASP:N	1:A:56:PRO:HD2	2.34	0.43
2:B:694:ASP:C	2:B:694:ASP:OD1	2.55	0.43
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.00	0.43
8:H:74:SER:HA	8:H:79:TRP:HA	2.00	0.43
2:B:357:GLN:O	2:B:365:THR:OG1	2.34	0.43
2:B:929:THR:OG1	2:B:930:ALA:N	2.52	0.43
5:E:40:GLU:OE1	5:E:40:GLU:N	2.33	0.43
14:N:33:DA:OP2	14:N:33:DA:H2'	2.19	0.43
1:A:1170:ILE:O	1:A:1174:PHE:N	2.51	0.43
7:G:11:ILE:HB	7:G:70:PHE:HB2	2.01	0.43
8:H:67:ASP:N	8:H:67:ASP:OD1	2.52	0.43
13:M:353:CYS:SG	13:M:358:MET:SD	3.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:469:ASP:O	13:M:470:GLU:C	2.57	0.43
9:I:50:THR:OG1	9:I:51:ASN:N	2.52	0.43
12:L:53:HIS:ND1	12:L:54:ARG:N	2.58	0.43
15:R:1:A:H2	16:T:30:DG:H21	1.60	0.43
15:R:4:G:N1	16:T:27:DG:C6	2.87	0.43
12:L:27:LEU:O	12:L:27:LEU:HG	2.19	0.43
2:B:150:GLU:OE1	2:B:150:GLU:N	2.39	0.43
7:G:126:ASN:HA	7:G:127:PRO:C	2.39	0.43
14:N:32:DG:H2''	14:N:33:DA:OP2	2.19	0.43
1:A:167:CYS:O	1:A:169:ASN:N	2.52	0.42
2:B:264:SER:OG	2:B:265:SER:N	2.52	0.42
16:T:22:DC:H2'	16:T:23:DT:C6	2.54	0.42
1:A:187:LYS:O	1:A:188:ASP:HB3	2.20	0.42
1:A:1186:ASP:O	1:A:1243:VAL:HA	2.18	0.42
2:B:71:LEU:HB3	2:B:432:MET:SD	2.59	0.42
2:B:341:LEU:N	2:B:341:LEU:HD12	2.34	0.42
2:B:365:THR:OG1	2:B:366:GLN:N	2.52	0.42
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.01	0.42
8:H:7:ASP:OD1	8:H:7:ASP:C	2.57	0.42
9:I:80:SER:OG	9:I:81:ARG:N	2.52	0.42
14:N:43:DG:OP2	14:N:43:DG:H2'	2.20	0.42
15:R:6:G:H2'	15:R:7:A:C8	2.54	0.42
1:A:170:THR:HB	1:A:186:LYS:HB3	2.01	0.42
7:G:164:LYS:O	7:G:164:LYS:HG2	2.18	0.42
2:B:592:ASN:OD1	2:B:592:ASN:C	2.57	0.42
9:I:101:PHE:CD1	9:I:101:PHE:N	2.87	0.42
8:H:105:GLU:O	8:H:105:GLU:HG2	2.20	0.42
1:A:50:ILE:HB	1:A:53:LEU:O	2.20	0.42
1:A:1248:LEU:O	1:A:1249:ASP:C	2.58	0.42
2:B:1004:GLU:CD	2:B:1004:GLU:N	2.73	0.42
12:L:58:LYS:O	12:L:59:ALA:HB3	2.20	0.42
2:B:842:ASN:OD1	2:B:842:ASN:C	2.58	0.42
14:N:29:DC:H1'	14:N:30:DA:H5'	2.01	0.42
2:B:436:VAL:O	2:B:437:GLU:HB2	2.20	0.42
2:B:711:GLU:HB2	2:B:712:PRO:HD2	2.02	0.42
12:L:56:LEU:N	12:L:56:LEU:HD12	2.34	0.42
1:A:832:ALA:O	1:A:834:THR:N	2.53	0.42
3:C:54:ASN:C	3:C:54:ASN:OD1	2.58	0.42
13:M:474:ILE:O	13:M:476:ASN:N	2.53	0.42
1:A:23:SER:HA	1:A:24:PRO:HD3	1.90	0.41
2:B:933:SER:O	2:B:935:ARG:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.20	0.41
15:R:5:A:C6	15:R:6:G:C6	3.08	0.41
1:A:465:TYR:O	1:A:466:SER:HB2	2.21	0.41
1:A:942:PHE:N	1:A:942:PHE:CD1	2.86	0.41
2:B:552:MET:HB3	2:B:553:PRO:HD3	2.01	0.41
6:F:108:PHE:N	6:F:108:PHE:HD1	2.17	0.41
14:N:25:DT:H2''	14:N:27:DC:C4	2.55	0.41
1:A:451:HIS:ND1	1:A:452:LYS:N	2.68	0.41
2:B:268:THR:OG1	2:B:269:ILE:N	2.54	0.41
6:F:111:LEU:HD23	6:F:111:LEU:C	2.41	0.41
1:A:184:SER:O	1:A:185:TRP:C	2.59	0.41
1:A:230:ARG:HA	1:A:231:PRO:HD3	1.96	0.41
1:A:644:LYS:HD3	1:A:644:LYS:HA	1.89	0.41
11:K:35:PHE:HB2	11:K:71:PHE:HB3	2.03	0.41
13:M:353:CYS:HB2	13:M:354:PRO:HD2	2.03	0.41
13:M:747:ILE:HB	13:M:777:ARG:HA	2.02	0.41
14:N:28:DT:H72	14:N:29:DC:N4	2.36	0.41
15:R:3:C:O2'	15:R:4:G:H5'	2.20	0.41
15:R:4:G:C6	16:T:27:DG:O6	2.74	0.41
1:A:596:THR:O	1:A:597:LEU:CB	2.68	0.41
5:E:68:SER:OG	5:E:69:ILE:N	2.53	0.41
13:M:737:VAL:HG12	13:M:739:LEU:HG	2.02	0.41
14:N:42:DA:OP2	14:N:42:DA:H8	2.04	0.41
16:T:15:DT:OP2	16:T:15:DT:H2'	2.21	0.41
16:T:24:DC:H2'	16:T:25:DT:C6	2.56	0.41
2:B:299:GLU:HB3	2:B:571:PRO:HG2	2.03	0.41
2:B:1156:ASP:O	2:B:1157:ALA:HB3	2.21	0.41
8:H:18:GLY:O	8:H:19:ARG:HB2	2.21	0.41
16:T:11:DC:H2''	16:T:12:DT:OP2	2.20	0.41
2:B:198:ASP:OD1	2:B:199:MET:N	2.54	0.41
2:B:298:LEU:O	2:B:302:CYS:N	2.54	0.41
3:C:129:ILE:O	3:C:129:ILE:HG23	2.19	0.41
5:E:131:THR:OG1	5:E:132:ILE:N	2.53	0.41
7:G:13:LEU:HB3	7:G:68:ALA:HB3	2.03	0.41
7:G:13:LEU:O	7:G:67:SER:HA	2.21	0.41
9:I:60:GLN:OE1	9:I:60:GLN:N	2.48	0.41
14:N:41:DC:H2''	14:N:42:DA:C8	2.56	0.41
1:A:406:ILE:HB	1:A:431:LYS:HB2	2.02	0.41
2:B:908:GLU:OE1	2:B:908:GLU:N	2.43	0.41
2:B:1013:ASN:HA	2:B:1014:PRO:HD3	1.94	0.41
13:M:370:PRO:N	13:M:371:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:31:DG:H1'	16:T:32:DC:C4	2.56	0.41
4:D:48:ILE:O	4:D:48:ILE:HG22	2.21	0.41
13:M:752:TRP:HB2	14:N:15:DA:H1'	2.02	0.41
1:A:187:LYS:O	1:A:188:ASP:CB	2.69	0.40
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.50	0.40
11:K:5:ASP:C	11:K:5:ASP:OD1	2.59	0.40
1:A:795:GLU:H	1:A:795:GLU:CD	2.23	0.40
2:B:889:THR:HB	2:B:909:ASP:HA	2.03	0.40
3:C:217:ASP:OD1	3:C:217:ASP:C	2.59	0.40
5:E:29:PHE:O	5:E:29:PHE:CD2	2.74	0.40
8:H:101:ALA:HA	8:H:116:TYR:HA	2.03	0.40
14:N:36:DA:H2''	14:N:37:DG:OP2	2.22	0.40
15:R:2:U:C5	15:R:2:U:OP2	2.74	0.40
2:B:957:ASN:C	2:B:957:ASN:OD1	2.58	0.40
13:M:562:SER:HB3	13:M:563:PRO:HD3	2.04	0.40
13:M:707:ASN:C	13:M:707:ASN:OD1	2.60	0.40
16:T:32:DC:H6	16:T:32:DC:H2'	1.74	0.40
2:B:31:TRP:O	2:B:811:TYR:OH	2.39	0.40
2:B:1073:TYR:CB	2:B:1080:LYS:HA	2.52	0.40
3:C:18:VAL:O	3:C:231:ASN:HA	2.22	0.40
3:C:126:GLY:O	3:C:127:ARG:HB3	2.21	0.40
1:A:567:LYS:HB2	1:A:567:LYS:HE2	1.89	0.40
2:B:134:LYS:HB2	2:B:160:SER:HB2	2.03	0.40
8:H:58:THR:OG1	8:H:59:ILE:N	2.55	0.40
10:J:3:VAL:HA	10:J:4:PRO:HD2	1.95	0.40
11:K:61:TYR:CD1	11:K:61:TYR:C	2.95	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	1446/1733 (83%)	1312 (91%)	109 (8%)	25 (2%)	9	42
2	B	1205/1224 (98%)	1092 (91%)	86 (7%)	27 (2%)	6	35
3	C	268/318 (84%)	238 (89%)	25 (9%)	5 (2%)	8	38
4	D	171/221 (77%)	157 (92%)	14 (8%)	0	100	100
5	E	213/215 (99%)	194 (91%)	14 (7%)	5 (2%)	6	33
6	F	79/155 (51%)	76 (96%)	2 (2%)	1 (1%)	12	48
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	25	66
8	H	144/146 (99%)	126 (88%)	14 (10%)	4 (3%)	5	30
9	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	9	42
10	J	68/70 (97%)	60 (88%)	7 (10%)	1 (2%)	10	45
11	K	109/120 (91%)	106 (97%)	2 (2%)	1 (1%)	17	56
12	L	44/70 (63%)	34 (77%)	8 (18%)	2 (4%)	2	21
13	M	497/1085 (46%)	460 (93%)	28 (6%)	9 (2%)	8	40
All	All	4533/5650 (80%)	4113 (91%)	337 (7%)	83 (2%)	12	40

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	SER
1	A	472	LEU
1	A	568	PRO
1	A	597	LEU
2	B	44	VAL
2	B	572	HIS
2	B	711	GLU
2	B	725	PRO
2	B	934	LYS
2	B	1214	PRO
3	C	172	PRO
3	C	184	ASN
7	G	59	GLY
8	H	61	SER
12	L	52	GLY
13	M	379	SER
13	M	475	ARG
13	M	629	HIS
1	A	54	ASN
1	A	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	GLU
1	A	164	ARG
1	A	168	GLY
1	A	593	GLU
1	A	833	GLU
1	A	1087	ALA
1	A	1249	ASP
2	B	77	HIS
2	B	82	ASP
2	B	471	LYS
2	B	1157	ALA
5	E	6	GLU
5	E	141	VAL
8	H	63	LEU
8	H	67	ASP
9	I	19	ASP
9	I	62	ILE
11	K	18	LYS
13	M	610	GLN
1	A	66	LYS
1	A	308	ILE
1	A	441	PRO
1	A	525	GLN
2	B	575	PRO
2	B	920	PRO
2	B	922	GLU
2	B	986	GLN
2	B	1065	GLN
2	B	1155	SER
10	J	2	ILE
13	M	277	ASN
1	A	35	ILE
1	A	752	LYS
2	B	437	GLU
2	B	951	GLN
2	B	1177	HIS
3	C	138	GLU
13	M	454	HIS
1	A	188	ASP
1	A	424	ILE
1	A	627	GLY
1	A	1403	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	81	SER
2	B	1097	HIS
3	C	6	PRO
3	C	90	ASP
5	E	29	PHE
6	F	154	ASP
12	L	56	LEU
13	M	469	ASP
2	B	362	PRO
2	B	940	PRO
5	E	86	PRO
1	A	55	ASP
1	A	673	GLY
13	M	461	VAL
2	B	745	PRO
13	M	500	PRO
2	B	24	PRO
2	B	292	ILE
2	B	305	VAL
5	E	127	ILE
8	H	69	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1264/1520 (83%)	1263 (100%)	1 (0%)	93	96
2	B	1046/1061 (99%)	1043 (100%)	3 (0%)	92	94
3	C	238/274 (87%)	238 (100%)	0	100	100
4	D	157/200 (78%)	157 (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	152/152 (100%)	151 (99%)	1 (1%)	84	90
8	H	128/128 (100%)	127 (99%)	1 (1%)	81	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	116/116 (100%)	116 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
11	K	96/102 (94%)	96 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	449/978 (46%)	449 (100%)	0	100	100
All	All	4020/4987 (81%)	4014 (100%)	6 (0%)	93	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	ARG
2	B	654	ARG
2	B	679	TYR
2	B	860	MET
7	G	17	PHE
8	H	47	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	358	ASN
7	G	117	GLN
12	L	66	GLN
13	M	664	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	2	U
15	R	10	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

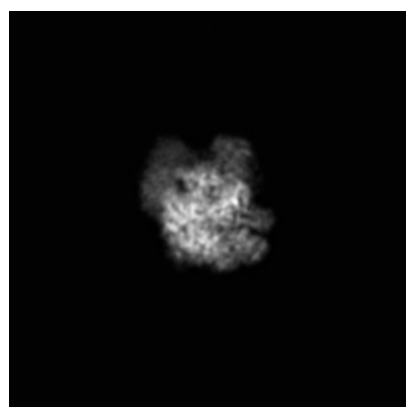
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8735. These allow visual inspection of the internal detail of the map and identification of artifacts.

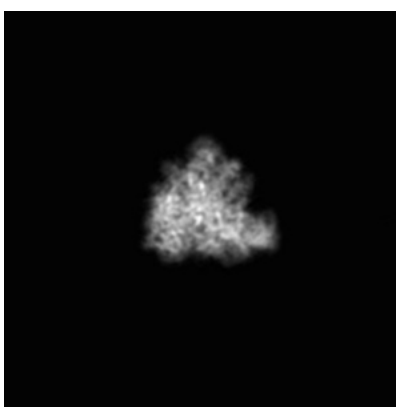
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

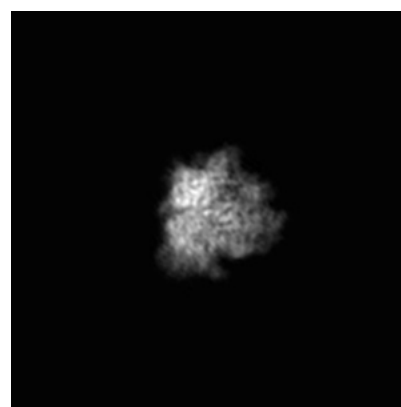
6.1.1 Primary map



X



Y

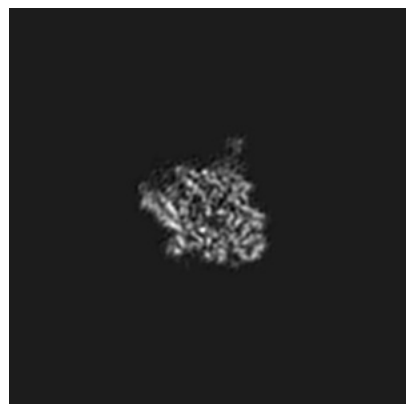


Z

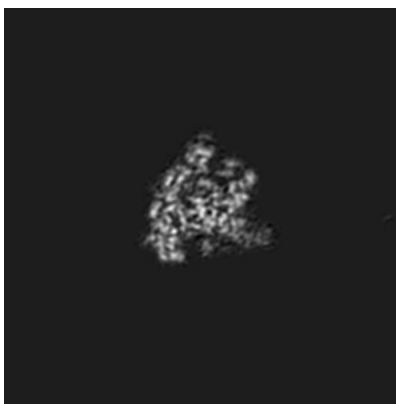
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

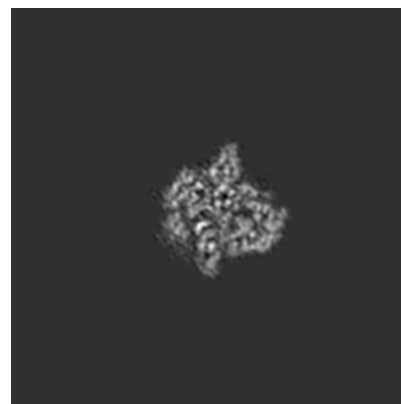
6.2.1 Primary map



X Index: 192



Y Index: 192

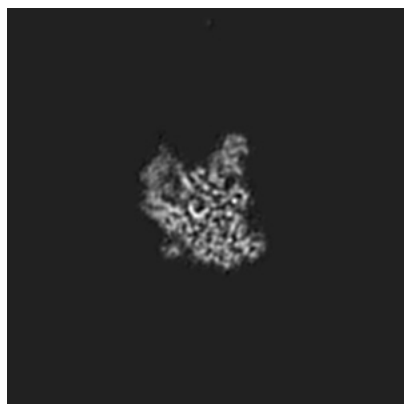


Z Index: 192

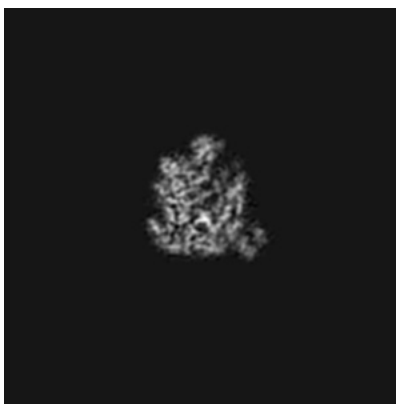
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 184



Y Index: 175

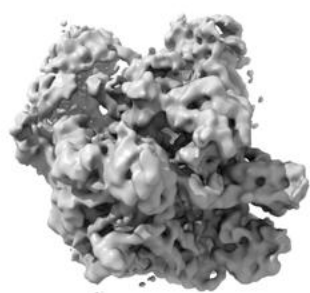


Z Index: 187

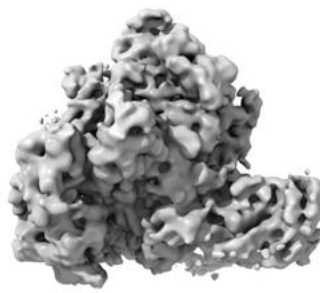
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

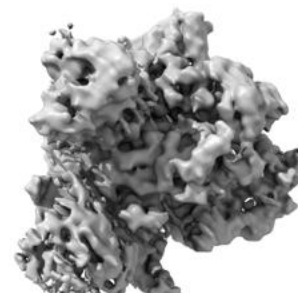
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0244. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

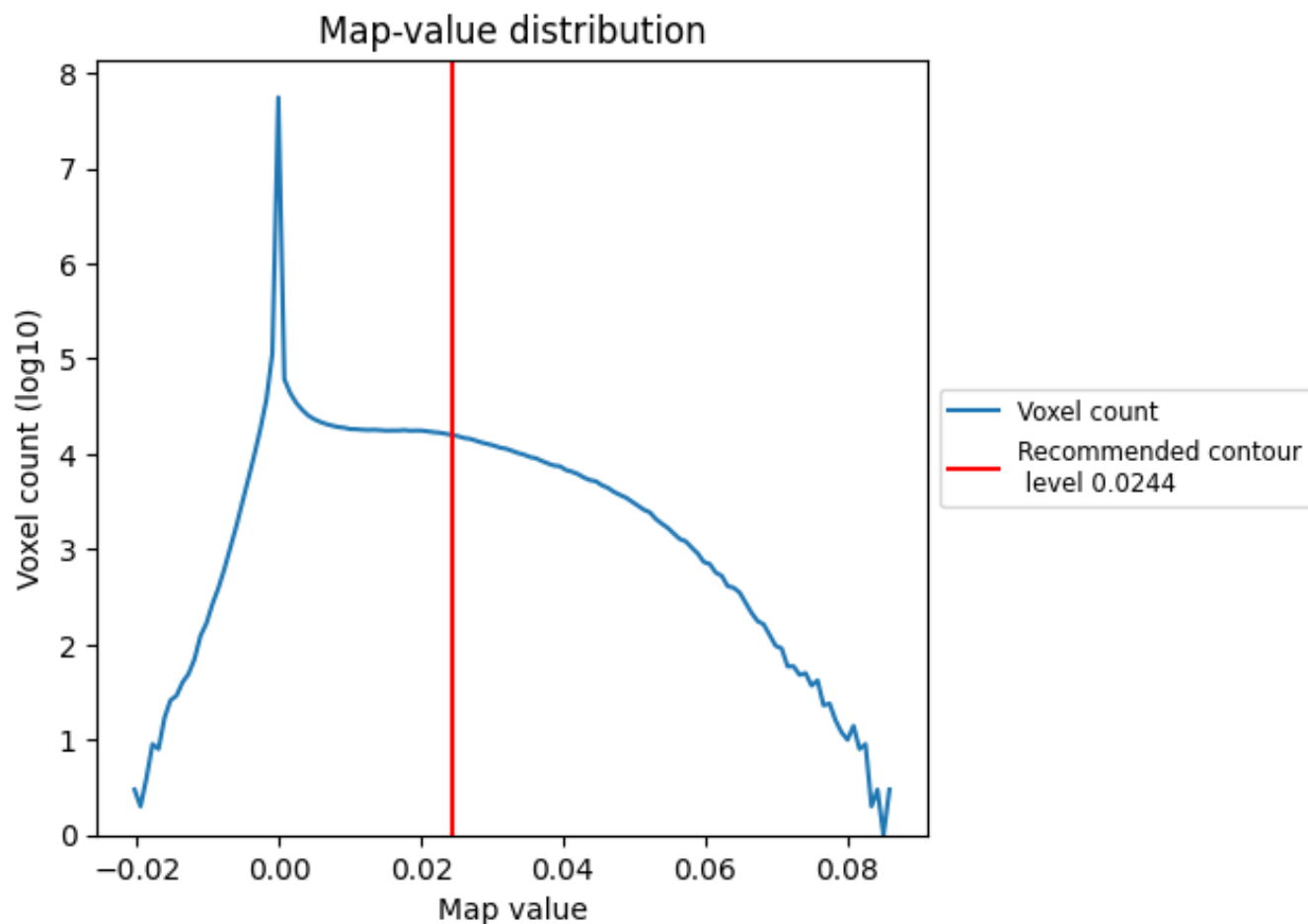
6.5 Mask visualisation

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

7 Map analysis [i](#)

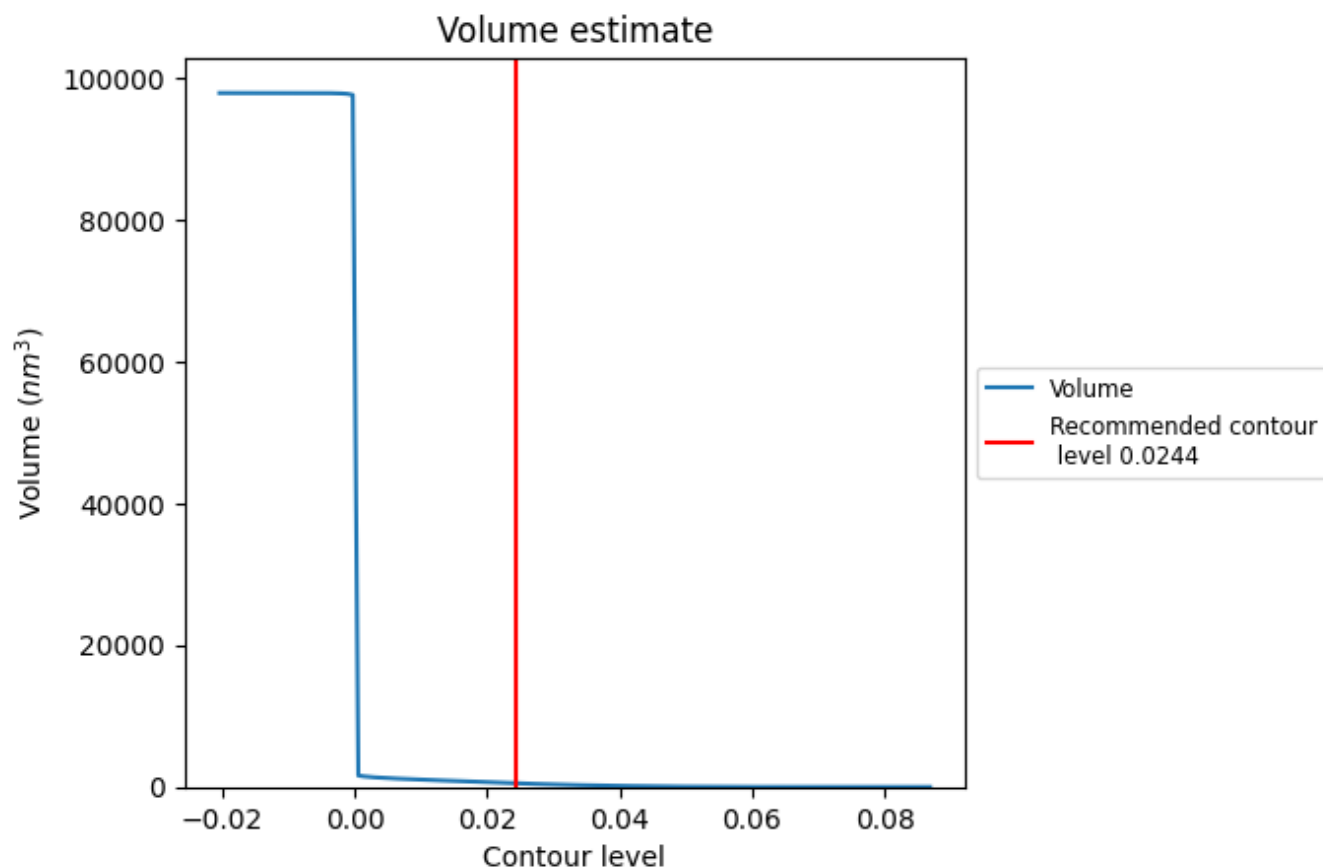
This section contains the results of statistical analysis of the map.

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.

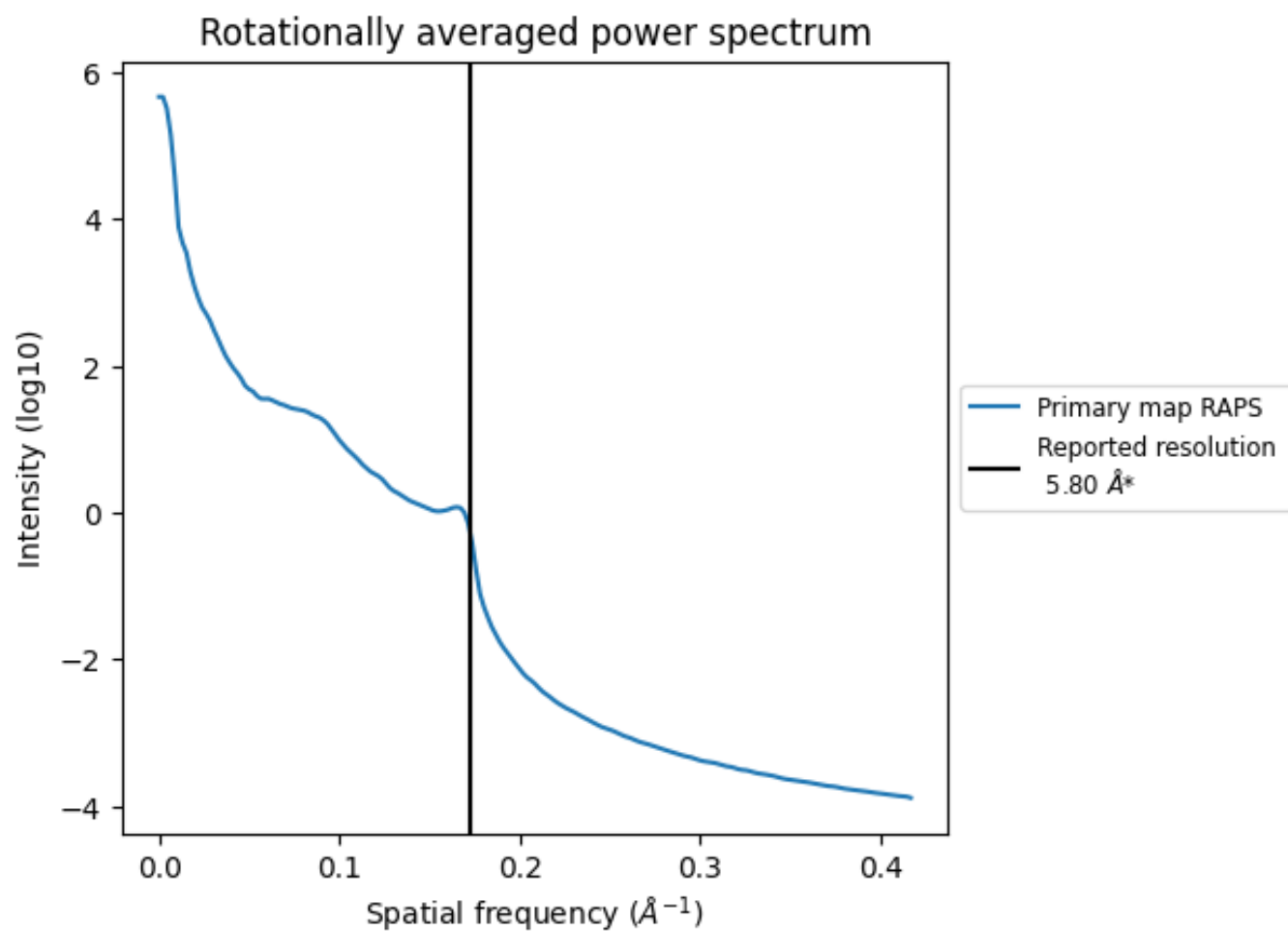
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm^3 ; this corresponds to an approximate mass of 467 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 ⓘ

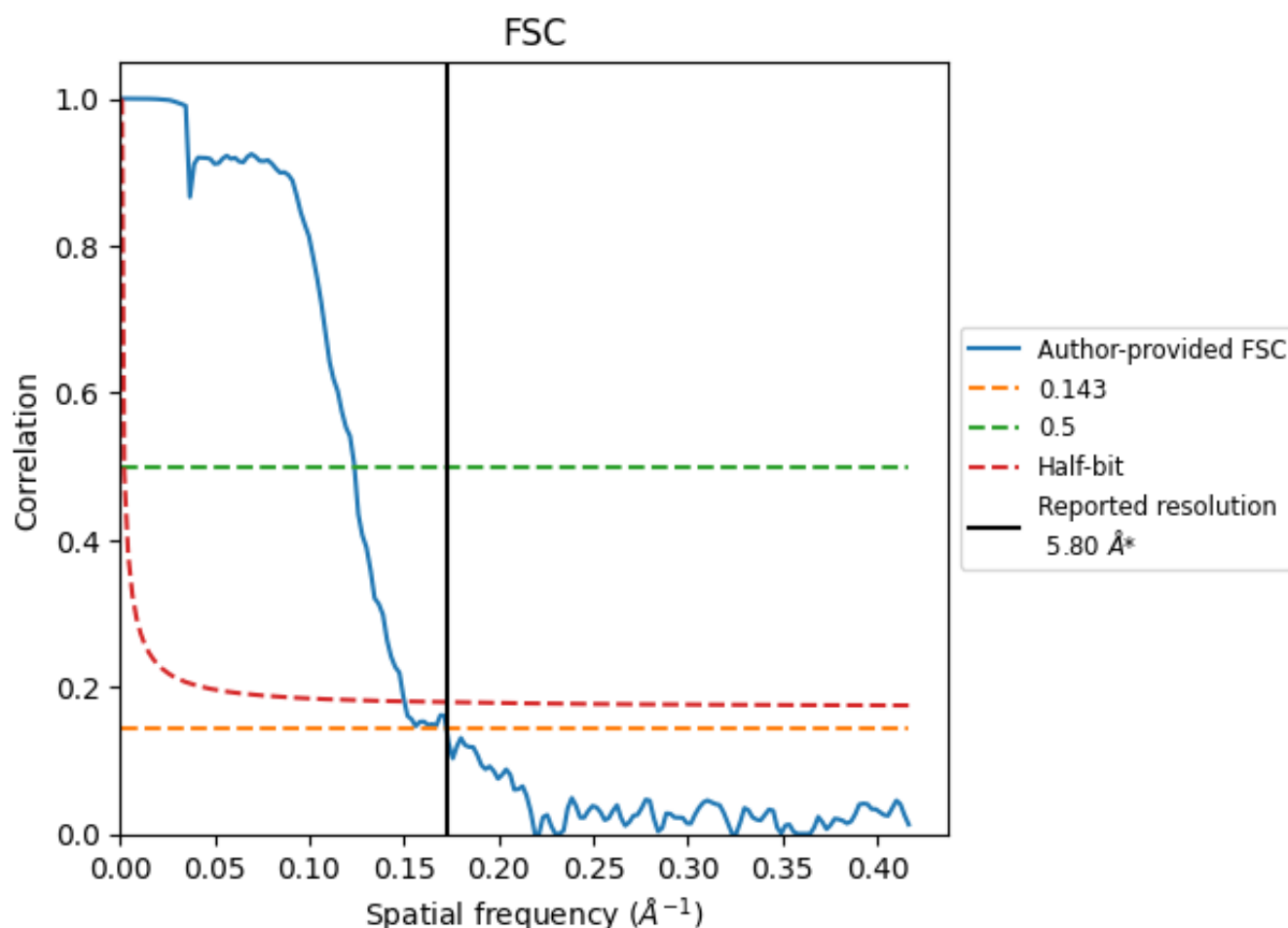


*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

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 0.172 Å⁻¹

8.2 Resolution estimates [i](#)

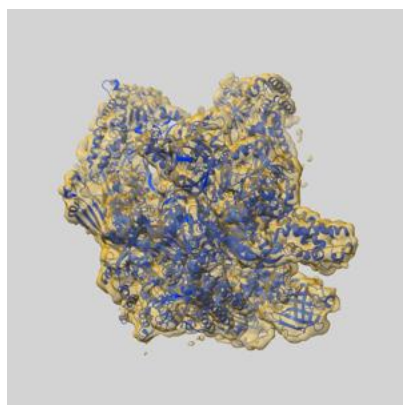
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.80	8.08	6.65
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

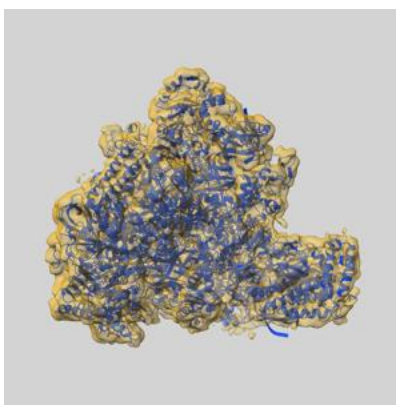
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8735 and PDB model 5VVR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

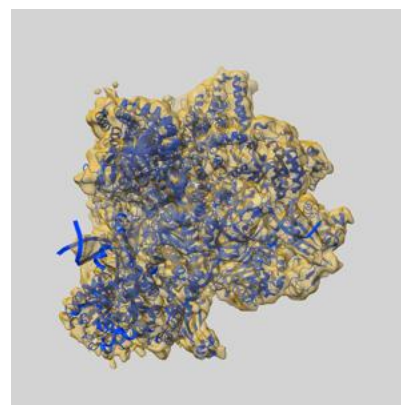
9.1 Map-model overlay [i](#)



X



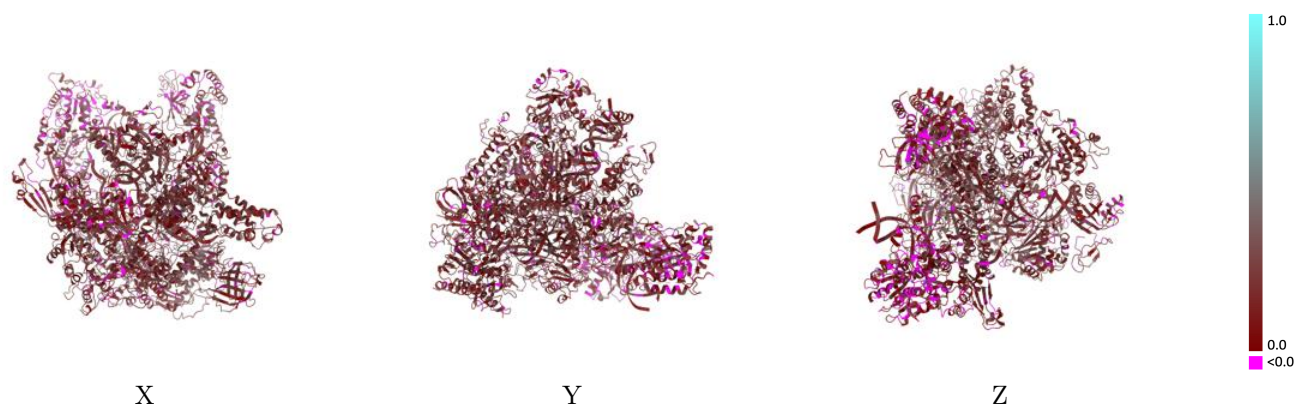
Y



Z

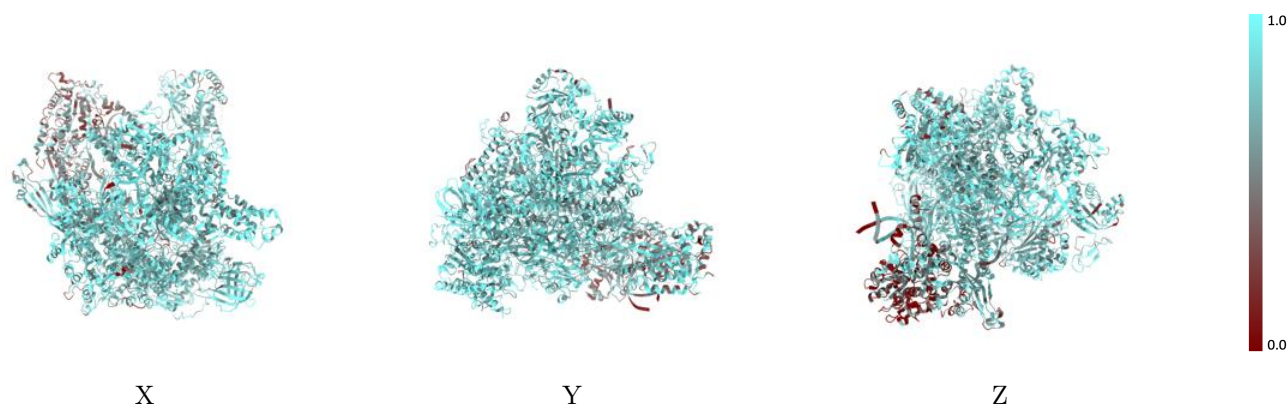
The images above show the 3D surface view of the map at the recommended contour level 0.0244 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



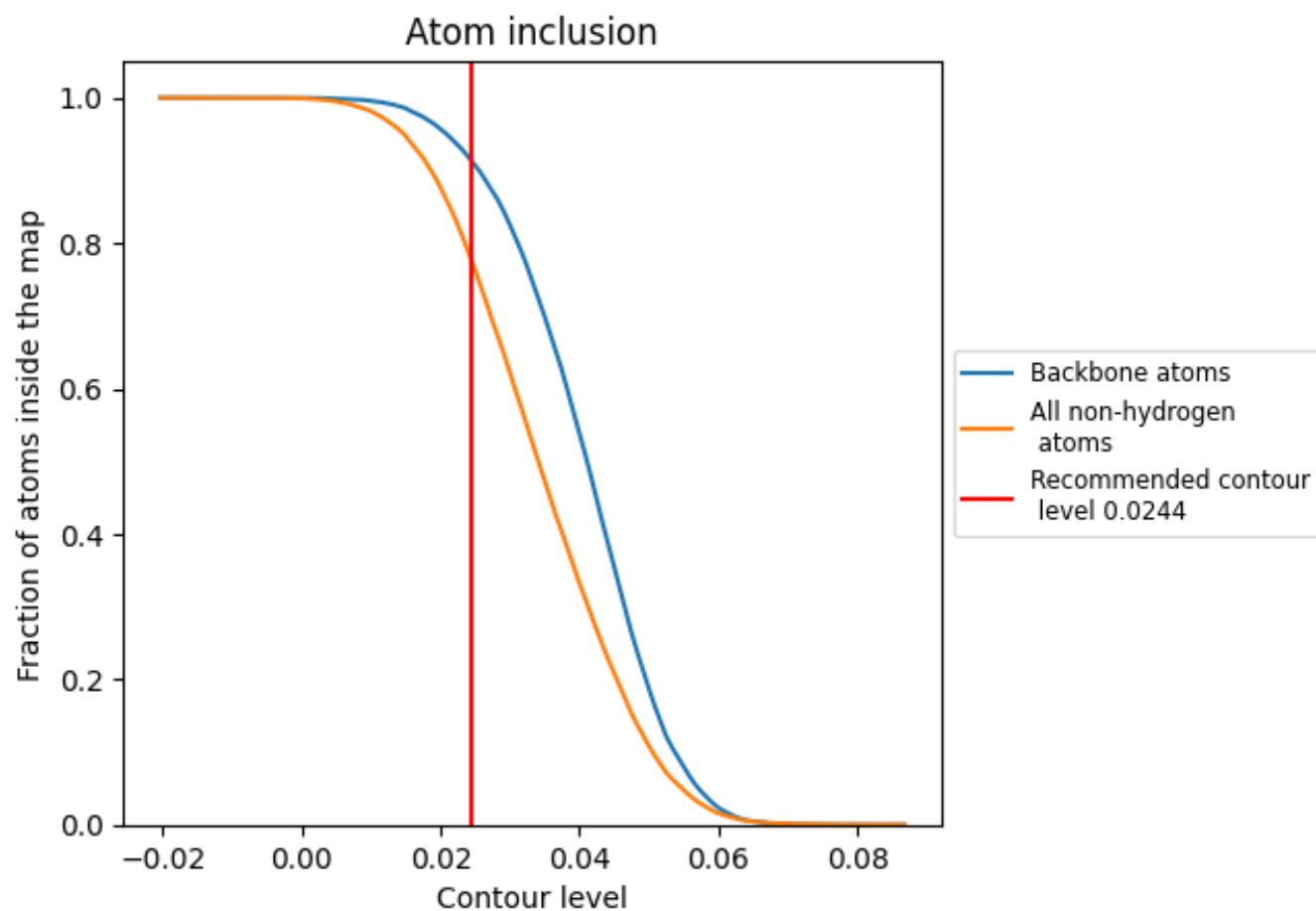
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0244).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.0244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7774	 0.1740
A	 0.8180	 0.1930
B	 0.8120	 0.1860
C	 0.8551	 0.1950
D	 0.7386	 0.1410
E	 0.8480	 0.1930
F	 0.8388	 0.2010
G	 0.8094	 0.1400
H	 0.8332	 0.1750
I	 0.8241	 0.1640
J	 0.8610	 0.1710
K	 0.8628	 0.1970
L	 0.8466	 0.1820
M	 0.4214	 0.0790
N	 0.7565	 0.1860
R	 0.9864	 0.2630
T	 0.8310	 0.1950

