



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 03:48 AM JST

PDB ID : 8YFQ / pdb\_00008yfq  
EMDB ID : EMD-39226  
Title : Cryo EM structure of Komagataella phaffii RNAPII-Rat1-Rai1 pre-termination complex  
Authors : Murayama, Y.; Yanagisawa, T.; Ehara, H.; Sekine, S.  
Deposited on : 2024-02-25  
Resolution : 3.30 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

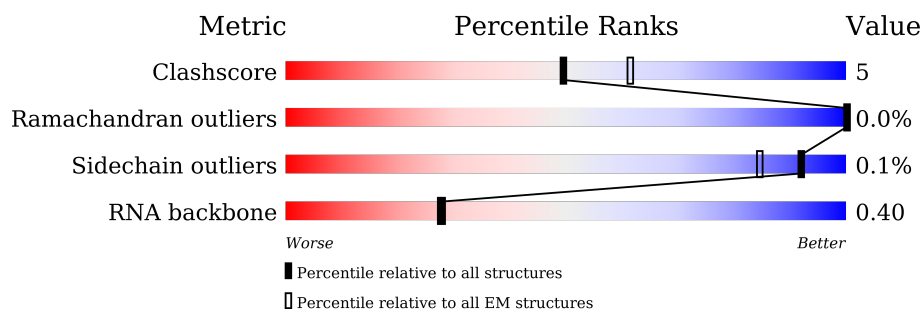
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*






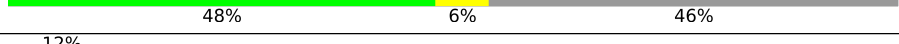

The reported resolution of this entry is 3.30 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	1743	
2	B	1227	
3	C	304	
4	D	186	
5	E	214	
6	F	155	
7	G	171	

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	N	90	
14	T	90	
15	P	22	
16	R	1006	
17	S	384	

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 42167 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			11027	6954	1923	2080	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1146	Total	C	N	O	S	0	0
			9139	5762	1611	1708	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	167	Total	C	N	O	S	0	0
			1302	803	236	261	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	212	Total	C	N	O	S	0	0
			1732	1089	311	322	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- 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	N	O	S	0	0
			1053	671	169	209	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a DNA chain called DNA (90-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	28	Total	C	N	O	P	0	0
			568	276	93	171	28		

- Molecule 14 is a DNA chain called DNA (90-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	38	Total	C	N	O	P	0	0
			786	376	146	226	38		

- Molecule 15 is a RNA chain called RNA (22-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	22	Total	C	N	O	P	0	0
			471	211	87	151	22		

- Molecule 16 is a protein called 5'-3' exoribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	746	Total	C	N	O	S	0	0
			6135	3927	1055	1131	22		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	203	GLN	GLU	engineered mutation	UNP F2QV79
R	205	GLN	GLU	engineered mutation	UNP F2QV79
R	233	ASN	ASP	engineered mutation	UNP F2QV79
R	235	ASN	ASP	engineered mutation	UNP F2QV79
R	330	ASN	ASP	engineered mutation	UNP F2QV79
R	995	SER	-	expression tag	UNP F2QV79
R	996	GLY	-	expression tag	UNP F2QV79
R	997	PRO	-	expression tag	UNP F2QV79
R	998	SER	-	expression tag	UNP F2QV79
R	999	SER	-	expression tag	UNP F2QV79
R	1000	GLY	-	expression tag	UNP F2QV79
R	1001	LEU	-	expression tag	UNP F2QV79
R	1002	GLU	-	expression tag	UNP F2QV79
R	1003	VAL	-	expression tag	UNP F2QV79
R	1004	LEU	-	expression tag	UNP F2QV79
R	1005	PHE	-	expression tag	UNP F2QV79
R	1006	GLN	-	expression tag	UNP F2QV79

- Molecule 17 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	377	Total	C	N	O	S	0	0
			3093	1979	523	578	13		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	GLY	-	expression tag	UNP F2QLF5
S	-1	PRO	-	expression tag	UNP F2QLF5
S	0	GLY	-	expression tag	UNP F2QLF5
S	213	ALA	GLU	engineered mutation	UNP F2QLF5
S	215	ALA	ASP	engineered mutation	UNP F2QLF5

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

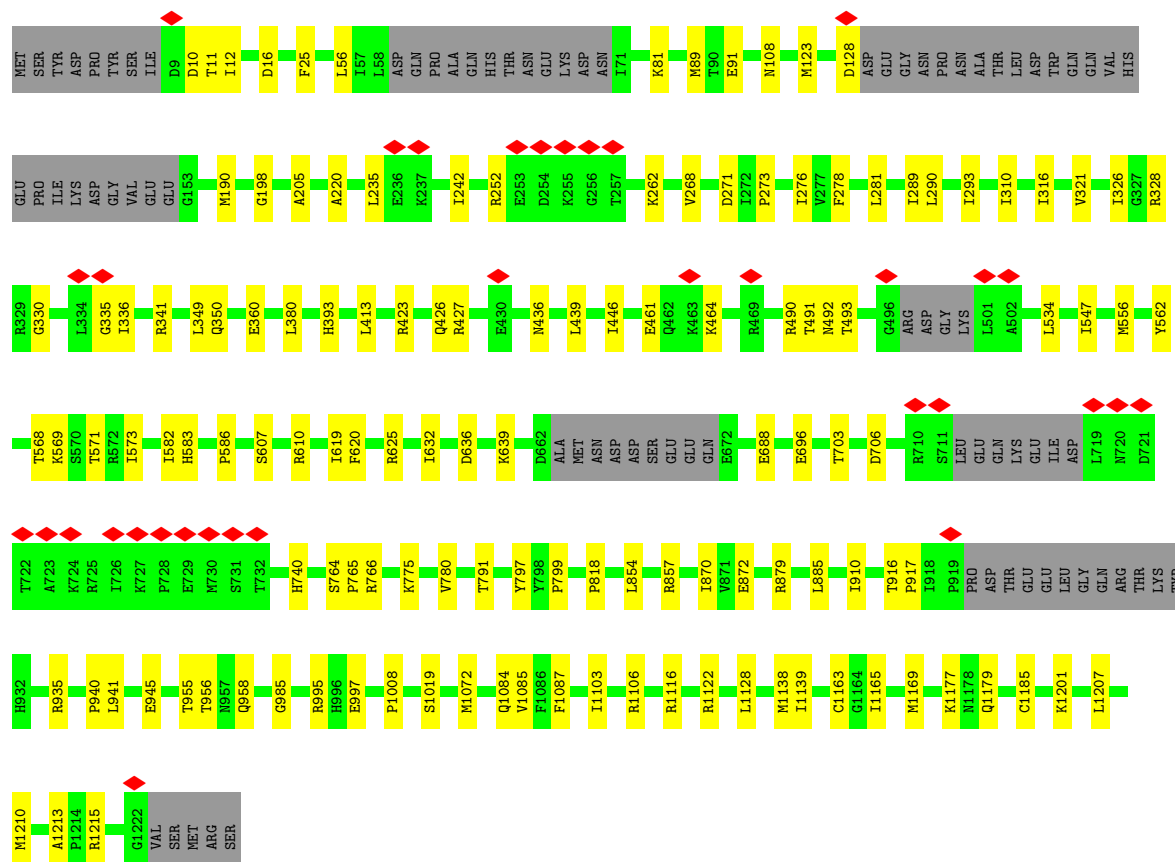
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	





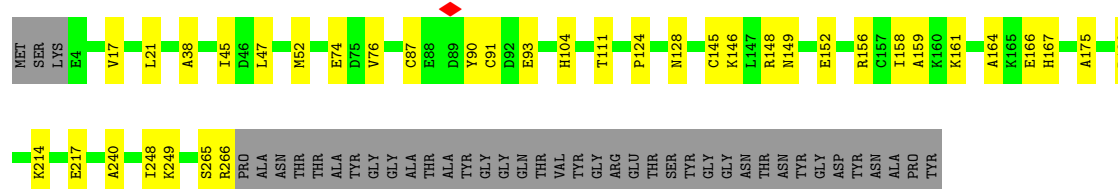
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:  83% 11% 7%



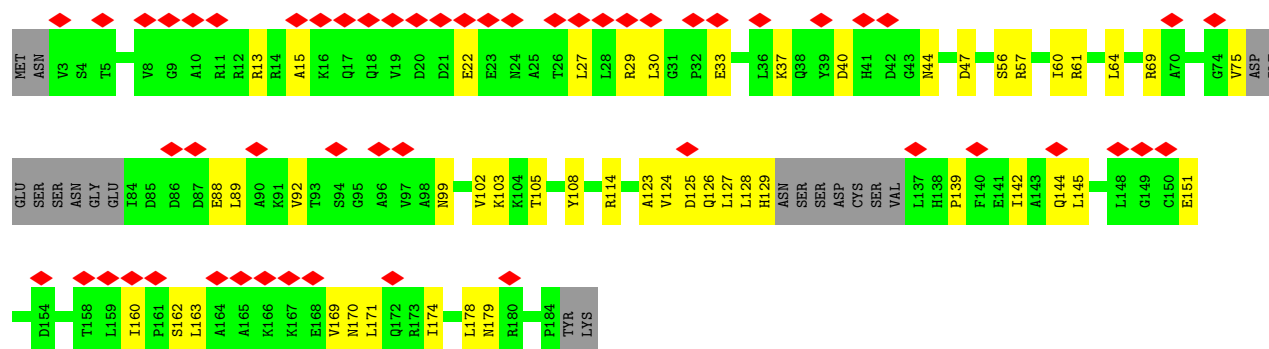
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:  74% 12% 13%



- Molecule 4: RNA polymerase II subunit B32

Chain D: 



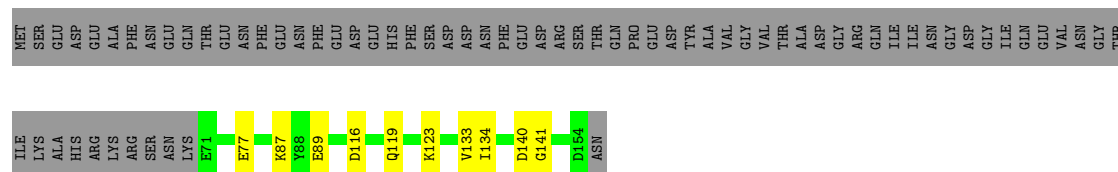
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 88% 11%



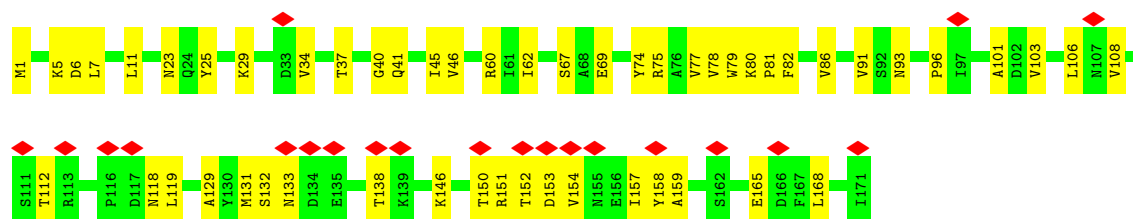
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F: 48% 6% 46%



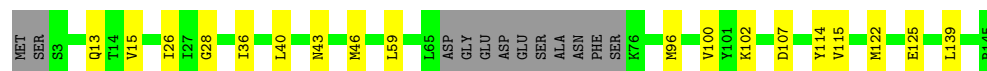
- Molecule 7: RNA polymerase II subunit

Chain G: 12% 69% 31%



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

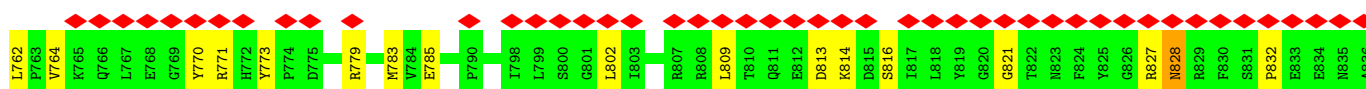
Chain H: 79% 12% 8%

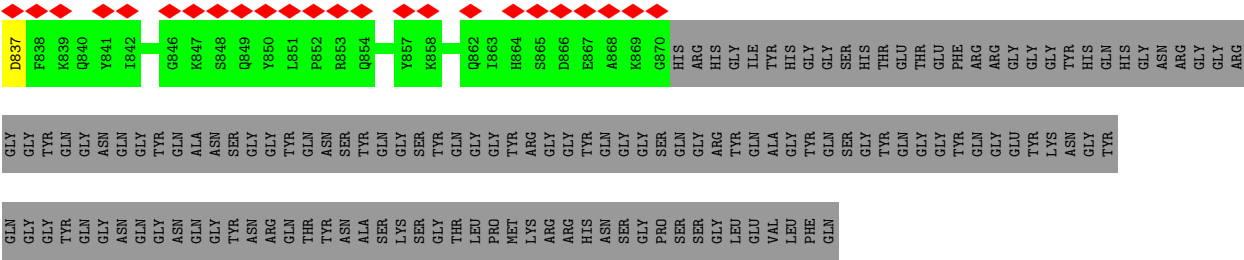


- Molecule 9: DNA-directed RNA polymerase subunit

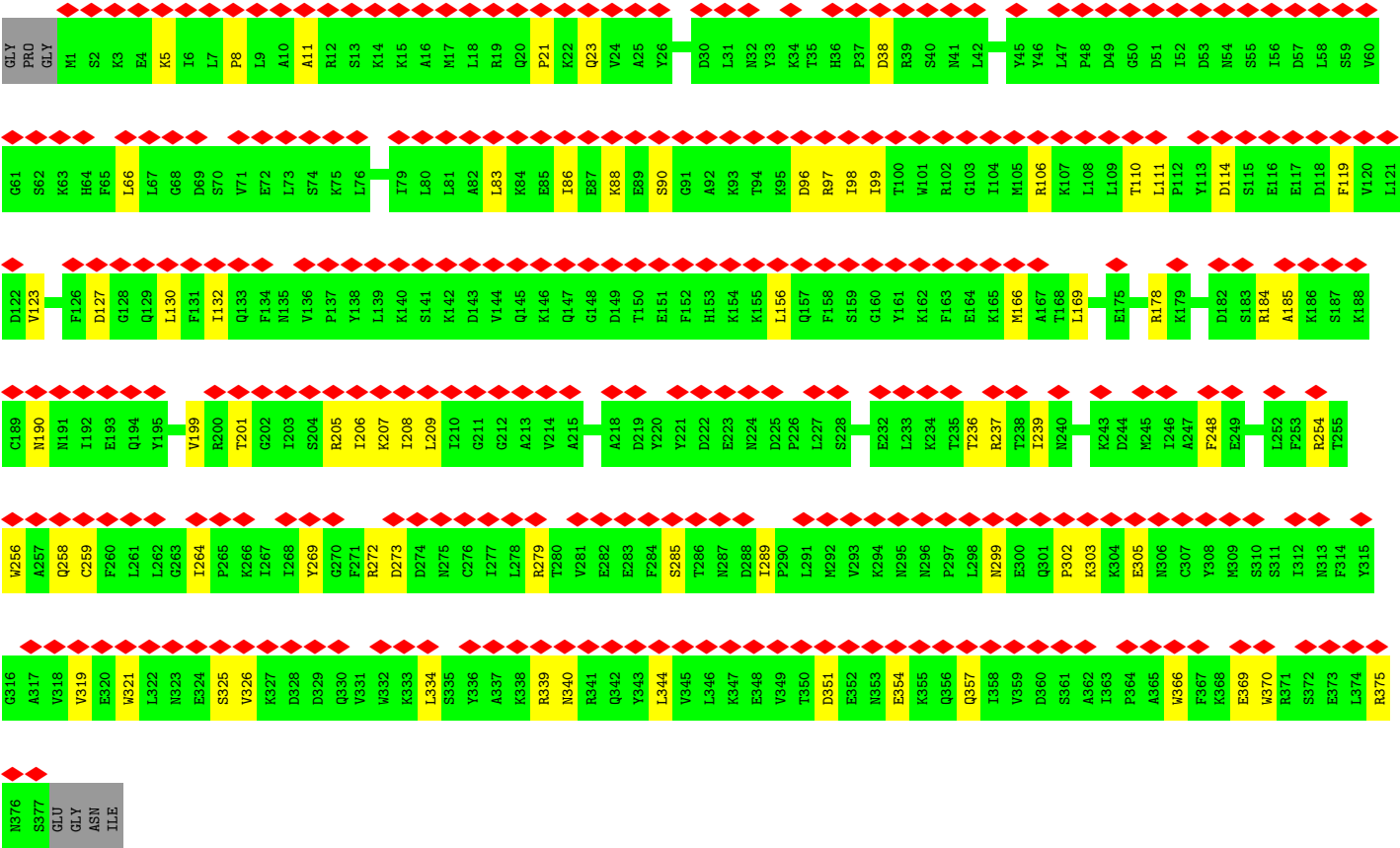
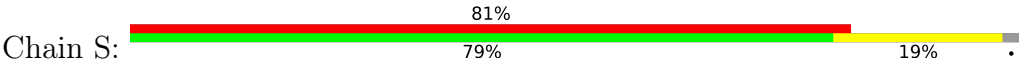
Chain I: 10% 83% 14%







• Molecule 17: Decapping nuclease



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44794	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.3	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0085	Depositor
Map size ( $\text{\AA}$ )	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83000004, 0.83000004, 0.83000004	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.10	0/11229	0.26	0/15169
2	B	0.11	0/9313	0.27	0/12555
3	C	0.09	0/2139	0.23	0/2895
4	D	0.14	0/1313	0.34	0/1770
5	E	0.11	0/1764	0.29	0/2373
6	F	0.09	0/687	0.22	0/931
7	G	0.11	0/1353	0.33	0/1837
8	H	0.09	0/1070	0.27	0/1444
9	I	0.11	0/934	0.35	0/1257
10	J	0.08	0/554	0.21	0/742
11	K	0.12	0/953	0.30	0/1291
12	L	0.08	0/365	0.26	0/484
13	N	0.20	0/633	0.42	0/971
14	T	0.16	0/883	0.35	0/1362
15	P	0.10	0/527	0.25	0/817
16	R	0.16	1/6297 (0.0%)	0.35	1/8518 (0.0%)
17	S	0.14	0/3159	0.35	0/4260
All	All	0.12	1/43173 (0.0%)	0.30	1/58676 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	828	ASN	C-N	-6.69	1.25	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	827	ARG	O-C-N	-5.04	116.49	122.63

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11027	0	11057	110	0
2	B	9139	0	9151	83	0
3	C	2098	0	2057	24	0
4	D	1302	0	1305	32	0
5	E	1732	0	1748	14	0
6	F	677	0	693	7	0
7	G	1324	0	1342	38	0
8	H	1053	0	1050	12	0
9	I	917	0	864	10	0
10	J	545	0	560	5	0
11	K	932	0	944	8	0
12	L	359	0	358	3	0
13	N	568	0	323	1	0
14	T	786	0	431	14	0
15	P	471	0	238	3	0
16	R	6135	0	6052	91	0
17	S	3093	0	3115	46	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	42167	0	41288	457	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 5.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:338:LEU:O	16:R:338:LEU:HD12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:ARG:HD2	16:R:28:ASP:HB3	1.70	0.74
1:A:255:GLU:HB3	2:B:935:ARG:HH12	1.54	0.71
16:R:72:THR:HG22	16:R:73:GLU:H	1.55	0.71
9:I:19:ASP:O	9:I:23:GLN:HA	1.91	0.70
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.75	0.69
16:R:335:LEU:HB2	16:R:338:LEU:HG	1.74	0.68
1:A:1118:LEU:HD11	1:A:1315:ASN:H	1.59	0.67
1:A:90:VAL:HG13	1:A:298:GLN:HG2	1.76	0.67
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.59	0.66
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.29	0.65
1:A:446:ASN:HB2	1:A:456:MET:HG3	1.78	0.65
2:B:571:THR:HG21	2:B:586:PRO:HB3	1.77	0.65
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.77	0.64
16:R:68:PRO:HB3	16:R:268:GLN:HA	1.80	0.64
2:B:632:ILE:HD11	2:B:688:GLU:HB3	1.80	0.64
7:G:152:THR:HG22	7:G:154:VAL:H	1.63	0.64
3:C:93:GLU:HA	3:C:124:PRO:HB3	1.78	0.64
9:I:47:GLU:HG3	9:I:50:THR:HB	1.80	0.64
17:S:156:LEU:HD22	17:S:272:ARG:HH21	1.61	0.64
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.71	0.63
7:G:11:LEU:HD22	7:G:29:LYS:HE3	1.81	0.63
2:B:268:VAL:HG23	2:B:330:GLY:HA2	1.81	0.63
7:G:81:PRO:HG2	7:G:157:ILE:HG21	1.80	0.63
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.79	0.63
8:H:36:ILE:HA	8:H:125:GLU:O	1.99	0.63
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.32	0.62
2:B:879:ARG:HE	2:B:885:LEU:HD22	1.64	0.62
1:A:1201:ARG:HG2	1:A:1238:LEU:HD11	1.81	0.62
16:R:749:ILE:HB	16:R:785:GLU:HB3	1.82	0.62
16:R:623:GLU:HG2	16:R:689:VAL:HG11	1.82	0.61
7:G:1:MET:N	7:G:80:LYS:O	2.33	0.61
17:S:8:PRO:HG2	17:S:11:ALA:HB2	1.83	0.61
4:D:126:GLN:HA	4:D:129:HIS:CD2	2.34	0.61
17:S:321:TRP:O	17:S:325:SER:HB2	2.01	0.61
4:D:30:LEU:HG	7:G:82:PHE:HE2	1.65	0.61
1:A:1447:MET:HB2	6:F:133:VAL:HB	1.83	0.60
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.84	0.60
1:A:243:PRO:O	1:A:248:ARG:NH1	2.32	0.60
5:E:92:MET:HG3	5:E:119:ALA:HB1	1.83	0.60
5:E:126:VAL:HG21	5:E:131:ILE:HG12	1.82	0.60
17:S:97:ARG:HG3	17:S:98:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:VAL:HG22	1:A:1031:ARG:HH11	1.67	0.60
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.83	0.60
3:C:248:ILE:HG21	11:K:102:ASP:HB2	1.84	0.59
4:D:64:LEU:HB3	4:D:89:LEU:HD22	1.84	0.59
2:B:436:ASN:HD21	2:B:439:LEU:HG	1.67	0.59
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.84	0.59
16:R:402:ASN:HB3	16:R:406:ARG:HH21	1.67	0.59
1:A:333:LYS:NZ	14:T:2:DG:OP2	2.35	0.59
16:R:603:PHE:HB3	16:R:606:LEU:HD11	1.85	0.59
2:B:220:ALA:O	2:B:252:ARG:NH2	2.35	0.59
1:A:326:ILE:HA	1:A:329:ARG:HD3	1.83	0.59
4:D:69:ARG:NH2	4:D:75:VAL:O	2.36	0.59
8:H:40:LEU:HB2	8:H:122:MET:HG3	1.85	0.58
15:P:1:A:OP1	16:R:117:ARG:NH2	2.36	0.58
1:A:421:ARG:HH22	16:R:821:GLY:HA3	1.68	0.58
1:A:1450:GLU:OE2	7:G:23:ASN:ND2	2.31	0.58
4:D:27:LEU:HD12	4:D:29:ARG:HH21	1.69	0.58
17:S:110:THR:HG21	17:S:254:ARG:HG3	1.86	0.58
17:S:321:TRP:O	17:S:325:SER:CB	2.52	0.58
17:S:83:LEU:HD11	17:S:99:ILE:HD13	1.85	0.57
6:F:89:GLU:HG2	6:F:134:ILE:HD12	1.85	0.57
4:D:145:LEU:HD21	4:D:163:LEU:HD11	1.87	0.57
17:S:236:THR:HG22	17:S:237:ARG:N	2.18	0.57
3:C:167:HIS:NE2	12:L:72:ARG:OXT	2.36	0.57
17:S:303:LYS:HG2	17:S:305:GLU:H	1.69	0.57
16:R:79:ASP:OD2	16:R:280:LYS:NZ	2.38	0.56
7:G:86:VAL:HG12	7:G:146:LYS:HB2	1.85	0.56
16:R:256:PHE:HD2	16:R:832:PRO:HD3	1.70	0.56
16:R:232:LEU:O	16:R:252:ARG:NH2	2.38	0.56
4:D:57:ARG:HE	4:D:61:ARG:HD2	1.69	0.56
1:A:215:ILE:O	1:A:231:ARG:NH2	2.39	0.56
3:C:104:HIS:ND1	3:C:111:THR:OG1	2.37	0.56
1:A:468:THR:O	1:A:470:ARG:NH1	2.39	0.56
3:C:47:LEU:HB3	3:C:158:ILE:HB	1.88	0.56
16:R:117:ARG:NH1	16:R:161:THR:OG1	2.39	0.56
2:B:607:SER:OG	2:B:625:ARG:NH1	2.39	0.56
1:A:885:ASP:OD2	1:A:1032:ARG:NH1	2.37	0.55
1:A:1243:ARG:HD3	1:A:1246:ARG:HH12	1.70	0.55
17:S:339:ARG:NH1	17:S:340:ASN:OD1	2.40	0.55
17:S:351:ASP:HB3	17:S:354:GLU:HB3	1.88	0.55
1:A:1429:GLU:HA	1:A:1432:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:11:DT:H2"	14:T:12:DT:C5	2.41	0.55
4:D:22:GLU:OE2	4:D:29:ARG:NH2	2.29	0.55
16:R:135:LEU:HD22	16:R:145:ILE:HD13	1.89	0.55
16:R:120:SER:OG	16:R:157:SER:OG	2.25	0.55
7:G:96:PRO:O	7:G:112:THR:OG1	2.23	0.54
16:R:111:ASN:OD1	16:R:112:GLN:N	2.40	0.54
17:S:21:PRO:HB3	17:S:201:THR:HG22	1.89	0.54
17:S:110:THR:HG22	17:S:114:ASP:HB3	1.89	0.54
16:R:771:ARG:NH2	16:R:773:TYR:OH	2.40	0.54
16:R:119:ARG:O	16:R:119:ARG:HD3	2.07	0.54
1:A:92:HIS:HD2	1:A:237:ILE:HD11	1.72	0.54
2:B:1177:LYS:HG3	2:B:1179:GLN:HG3	1.89	0.54
16:R:363:LEU:HD21	16:R:377:LEU:HD22	1.88	0.54
16:R:622:TYR:OH	16:R:700:GLU:OE1	2.26	0.54
1:A:545:GLU:HA	1:A:548:MET:HE2	1.89	0.54
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.89	0.53
6:F:140:ASP:OD1	6:F:141:GLY:N	2.41	0.53
1:A:1415:ALA:HA	1:A:1420:GLU:HG3	1.91	0.53
16:R:58:VAL:HG23	16:R:80:VAL:HG21	1.90	0.53
17:S:114:ASP:OD2	17:S:254:ARG:NE	2.41	0.53
1:A:1412:LEU:HD13	2:B:1207:LEU:HD21	1.90	0.53
2:B:607:SER:HB2	2:B:620:PHE:HB2	1.90	0.53
3:C:214:LYS:HB2	3:C:217:GLU:HG3	1.89	0.53
1:A:927:GLN:NE2	1:A:931:ASN:OD1	2.40	0.53
1:A:1424:CYS:HA	1:A:1429:GLU:HG3	1.91	0.53
2:B:89:MET:HE3	2:B:91:GLU:HG2	1.91	0.53
16:R:347:THR:O	16:R:350:THR:OG1	2.24	0.53
17:S:127:ASP:OD2	17:S:375:ARG:NH1	2.41	0.53
16:R:720:TYR:OH	16:R:756:ARG:NH2	2.41	0.53
2:B:393:HIS:NE2	2:B:696:GLU:OE2	2.38	0.53
4:D:99:ASN:O	4:D:103:LYS:HG2	2.09	0.53
4:D:171:LEU:HA	4:D:174:ILE:HG12	1.90	0.53
16:R:338:LEU:HB2	16:R:344:SER:HB2	1.89	0.53
8:H:13:GLN:HG3	8:H:28:GLY:HA2	1.91	0.53
1:A:970:GLN:HG2	1:A:975:LEU:HD12	1.91	0.53
4:D:40:ASP:OD1	4:D:44:ASN:N	2.42	0.53
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.91	0.53
4:D:169:VAL:HG23	4:D:170:ASN:H	1.74	0.52
17:S:86:ILE:O	17:S:90:SER:HB3	2.10	0.52
2:B:413:LEU:HD13	2:B:446:ILE:HA	1.90	0.52
1:A:1237:LYS:HB3	1:A:1239:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:NH2	2:B:985:GLY:O	2.43	0.52
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.91	0.52
1:A:447:ARG:HD2	1:A:481:ALA:HB2	1.92	0.52
5:E:27:TYR:HA	5:E:63:PRO:HA	1.92	0.52
1:A:1347:THR:HG21	1:A:1384:LEU:HD21	1.92	0.52
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.92	0.52
1:A:1447:MET:HE1	7:G:60:ARG:HD2	1.92	0.51
2:B:1169:MET:HE1	2:B:1201:LYS:HG2	1.92	0.51
16:R:663:ASP:HB3	16:R:674:ILE:HB	1.92	0.51
16:R:637:LEU:HD21	16:R:641:PHE:HB2	1.91	0.51
2:B:278:PHE:HB3	2:B:289:ILE:HD12	1.92	0.51
4:D:124:VAL:O	4:D:128:LEU:HG	2.11	0.51
2:B:870:ILE:HG23	2:B:917:PRO:HG2	1.91	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
16:R:6:LEU:HA	16:R:342:ASP:OD2	2.10	0.51
17:S:236:THR:HG1	17:S:269:TYR:HE1	1.58	0.51
16:R:813:ASP:HA	16:R:816:SER:HB3	1.93	0.51
16:R:213:ARG:NH1	16:R:582:TYR:O	2.44	0.51
1:A:91:PHE:HZ	1:A:208:ILE:HD12	1.76	0.50
1:A:1111:LYS:H	1:A:1111:LYS:HD2	1.76	0.50
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.45	0.50
2:B:316:ILE:HG23	2:B:321:VAL:HG13	1.94	0.50
4:D:160:ILE:HG22	4:D:162:SER:H	1.76	0.50
7:G:6:ASP:OD1	7:G:75:ARG:NE	2.44	0.50
16:R:145:ILE:HB	16:R:150:LYS:HE3	1.93	0.50
16:R:762:LEU:HG	16:R:764:VAL:H	1.76	0.50
1:A:347:ASP:OD1	2:B:1106:ARG:NE	2.38	0.50
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.50
1:A:665:ILE:HD11	1:A:744:VAL:HG22	1.92	0.50
9:I:19:ASP:O	9:I:23:GLN:CA	2.58	0.50
9:I:98:THR:OG1	9:I:111:ARG:NH2	2.44	0.50
1:A:251:ILE:O	1:A:259:GLY:N	2.44	0.50
4:D:37:LYS:NZ	4:D:47:ASP:OD1	2.44	0.50
16:R:188:TRP:HA	16:R:191:ILE:HD12	1.93	0.50
1:A:74:MET:O	2:B:1116:ARG:NH2	2.44	0.50
2:B:857:ARG:NE	2:B:945:GLU:OE1	2.41	0.50
7:G:25:TYR:HE1	7:G:29:LYS:HD2	1.77	0.50
16:R:192:GLU:HB3	16:R:711:LEU:HD11	1.93	0.50
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.94	0.50
1:A:1126:ILE:HG21	1:A:1136:ILE:HD12	1.94	0.50
13:N:13:DT:H4'	13:N:14:DT:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:106:ARG:HG3	17:S:258:GLN:HB2	1.94	0.50
1:A:1033:ILE:HD13	1:A:1037:PHE:HD2	1.76	0.49
9:I:74:GLU:OE1	9:I:81:ARG:NH2	2.45	0.49
3:C:166:GLU:HG2	12:L:72:ARG:HH12	1.78	0.49
1:A:151:ASP:HA	1:A:164:SER:HB2	1.94	0.49
16:R:3:VAL:HG12	16:R:255:VAL:HG12	1.93	0.49
1:A:409:ASP:OD1	1:A:410:ASN:N	2.45	0.49
9:I:103:CYS:SG	9:I:104:LEU:N	2.84	0.49
16:R:33:SER:OG	16:R:34:ARG:N	2.45	0.49
1:A:327:ARG:HE	1:A:1409:VAL:HG21	1.77	0.49
7:G:79:TRP:HZ3	7:G:81:PRO:HG3	1.76	0.49
1:A:1236:ASP:N	1:A:1236:ASP:OD1	2.46	0.49
8:H:107:ASP:N	8:H:107:ASP:OD1	2.44	0.49
16:R:18:ILE:HG22	16:R:832:PRO:HB3	1.94	0.49
2:B:1165:ILE:HG22	4:D:13:ARG:N	2.28	0.49
17:S:123:VAL:HG22	17:S:132:ILE:HD12	1.94	0.49
3:C:90:TYR:OH	3:C:156:ARG:NH2	2.46	0.49
7:G:153:ASP:HB2	7:G:158:TYR:HE2	1.77	0.49
2:B:636:ASP:HB3	2:B:639:LYS:HG2	1.94	0.48
7:G:45:ILE:HG12	7:G:78:VAL:HG12	1.96	0.48
1:A:1344:ILE:HD11	1:A:1379:THR:HB	1.95	0.48
16:R:55:ASN:HA	16:R:58:VAL:HG12	1.95	0.48
1:A:216:SER:OG	1:A:219:ASP:OD1	2.28	0.48
3:C:76:VAL:HG22	3:C:161:LYS:HD2	1.94	0.48
1:A:228:ASP:OD1	4:D:15:ALA:N	2.47	0.48
17:S:169:LEU:HD21	17:S:184:ARG:HH11	1.78	0.48
1:A:1338:ILE:HG23	1:A:1342:LEU:HD12	1.96	0.48
2:B:328:ARG:NH2	2:B:341:ARG:HD3	2.29	0.48
2:B:910:ILE:HD13	2:B:940:PRO:HB3	1.96	0.48
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.44	0.48
4:D:151:GLU:OE1	4:D:179:ASN:ND2	2.46	0.48
1:A:204:THR:HG23	1:A:207:GLU:H	1.77	0.48
17:S:5:LYS:HB3	17:S:321:TRP:HZ2	1.78	0.48
3:C:52:MET:HE2	3:C:152:GLU:HB3	1.96	0.48
17:S:130:LEU:HD11	17:S:326:VAL:HG11	1.96	0.48
7:G:81:PRO:HB2	7:G:150:THR:HG21	1.95	0.47
1:A:1165:ILE:HG13	1:A:1167:GLU:H	1.78	0.47
1:A:926:LEU:HD22	1:A:986:PRO:HD3	1.97	0.47
2:B:205:ALA:HB3	2:B:491:THR:HG22	1.96	0.47
2:B:271:ASP:N	2:B:271:ASP:OD1	2.47	0.47
1:A:1156:TYR:OH	9:I:23:GLN:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:O	7:G:37:THR:OG1	2.28	0.47
2:B:1072:MET:HG3	2:B:1085:VAL:HB	1.97	0.47
6:F:123:LYS:HB2	6:F:123:LYS:HE2	1.65	0.47
9:I:42:LYS:NZ	9:I:45:ARG:HB2	2.30	0.47
16:R:712:VAL:HG22	16:R:783:MET:HG2	1.95	0.47
17:S:23:GLN:HA	17:S:199:VAL:HG22	1.96	0.47
1:A:41:MET:HE3	1:A:41:MET:HA	1.95	0.47
1:A:608:ILE:HG12	1:A:613:VAL:HG22	1.95	0.47
4:D:144:GLN:HE22	4:D:162:SER:HB2	1.79	0.47
6:F:77:GLU:CD	6:F:77:GLU:H	2.23	0.47
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.79	0.47
16:R:23:GLN:NE2	16:R:284:THR:O	2.48	0.47
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.45	0.47
9:I:6:PHE:HA	9:I:13:MET:HA	1.97	0.47
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.80	0.46
14:T:17:DG:H2''	14:T:18:DT:H5'	1.98	0.46
16:R:651:GLU:HG2	16:R:652:ILE:HG23	1.97	0.46
1:A:456:MET:HE3	2:B:1138:MET:HE3	1.97	0.46
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.96	0.46
16:R:641:PHE:HD1	16:R:644:LEU:HD12	1.80	0.46
17:S:236:THR:CG2	17:S:237:ARG:N	2.79	0.46
1:A:599:LEU:HD22	8:H:114:TYR:HE2	1.80	0.46
2:B:10:ASP:OD1	2:B:11:THR:N	2.46	0.46
14:T:5:DT:H2'	14:T:6:DG:C8	2.50	0.46
1:A:420:LYS:HG3	1:A:421:ARG:HD3	1.96	0.46
2:B:12:ILE:HG23	2:B:16:ASP:HB2	1.97	0.46
1:A:1127:ALA:HB1	1:A:1306:LEU:HB3	1.98	0.46
11:K:84:LYS:O	11:K:88:GLU:HG3	2.15	0.46
16:R:348:LEU:HD21	16:R:381:LEU:HD22	1.97	0.46
1:A:1247:ASP:OD1	1:A:1247:ASP:N	2.47	0.46
1:A:1439:MET:HE1	2:B:1139:ILE:HA	1.97	0.46
4:D:124:VAL:O	4:D:125:ASP:C	2.57	0.46
16:R:21:VAL:HG11	16:R:286:PHE:HB2	1.96	0.46
17:S:273:ASP:OD2	17:S:279:ARG:NH2	2.47	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HB3	1.80	0.46
8:H:102:LYS:HB3	8:H:114:TYR:HB2	1.98	0.46
16:R:537:LEU:HD13	16:R:542:TYR:HB2	1.96	0.46
1:A:557:TRP:O	11:K:26:ARG:NH1	2.49	0.46
16:R:637:LEU:HD13	16:R:645:MET:HE1	1.98	0.46
4:D:56:SER:O	4:D:60:ILE:HG12	2.16	0.45
17:S:256:TRP:HD1	17:S:289:ILE:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:CYS:SG	3:C:93:GLU:HG2	2.56	0.45
16:R:394:GLU:OE2	16:R:398:ARG:NH1	2.49	0.45
16:R:669:VAL:HB	16:R:672:GLN:HB2	1.97	0.45
1:A:982:ASP:OD1	1:A:982:ASP:N	2.46	0.45
2:B:423:ARG:O	2:B:426:GLN:HG3	2.16	0.45
2:B:568:THR:HG23	2:B:569:LYS:HG2	1.98	0.45
2:B:190:MET:SD	2:B:190:MET:N	2.86	0.45
2:B:328:ARG:HH21	2:B:341:ARG:HH11	1.64	0.45
3:C:265:SER:OG	3:C:266:ARG:NH2	2.50	0.45
16:R:124:ALA:O	16:R:128:ASN:ND2	2.49	0.45
1:A:580:SER:HB3	1:A:612:LYS:HA	1.98	0.45
2:B:123:MET:HE3	2:B:123:MET:O	2.17	0.45
2:B:281:LEU:HD22	2:B:349:LEU:HD13	1.98	0.45
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.45
4:D:33:GLU:OE2	7:G:5:LYS:NZ	2.44	0.45
1:A:1343:GLY:O	1:A:1347:THR:OG1	2.25	0.45
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.43	0.45
7:G:7:LEU:HB2	7:G:74:TYR:CZ	2.51	0.45
16:R:164:THR:HG23	16:R:167:MET:H	1.82	0.45
16:R:571:ILE:HG13	16:R:606:LEU:HD22	1.99	0.45
1:A:92:HIS:CD2	1:A:237:ILE:HD11	2.52	0.45
4:D:103:LYS:HE3	4:D:103:LYS:HB3	1.84	0.45
4:D:123:ALA:O	4:D:127:LEU:HG	2.17	0.45
16:R:54:MET:HE3	16:R:99:ILE:HG23	1.99	0.45
16:R:733:ASP:OD1	16:R:733:ASP:N	2.50	0.45
1:A:445:PHE:HE2	1:A:471:LEU:HD11	1.81	0.45
2:B:556:MET:HG3	2:B:573:ILE:HD12	1.99	0.45
7:G:1:MET:HA	7:G:79:TRP:CE2	2.51	0.45
7:G:40:GLY:HA2	7:G:152:THR:HG21	1.98	0.45
16:R:125:LYS:HA	16:R:128:ASN:HD21	1.81	0.45
16:R:389:PHE:HD1	16:R:392:ARG:HE	1.65	0.45
1:A:226:ASN:HB3	1:A:230:ALA:H	1.82	0.44
1:A:369:ILE:HD13	1:A:463:VAL:HG12	1.98	0.44
5:E:47:ASP:OD1	5:E:51:ASN:N	2.50	0.44
5:E:92:MET:HE3	5:E:92:MET:HB3	1.82	0.44
1:A:529:LEU:O	1:A:532:VAL:HG12	2.18	0.44
1:A:912:ASP:OD1	1:A:912:ASP:N	2.50	0.44
16:R:382:ALA:HB1	16:R:601:ALA:HB2	1.97	0.44
16:R:713:LEU:HD21	16:R:720:TYR:HA	1.99	0.44
17:S:285:SER:O	17:S:289:ILE:HG13	2.17	0.44
1:A:1339:LEU:HD22	1:A:1384:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLN:HE21	2:B:360:GLU:HA	1.82	0.44
16:R:246:PRO:HG2	16:R:802:LEU:HD21	1.99	0.44
16:R:300:ILE:HD13	16:R:814:LYS:HG3	1.98	0.44
16:R:663:ASP:HB2	16:R:676:LEU:HD11	1.99	0.44
1:A:753:LYS:HD2	2:B:1019:SER:HB2	1.99	0.44
2:B:290:LEU:HD21	2:B:310:ILE:HD11	2.00	0.44
2:B:780:VAL:HG21	10:J:55:LEU:HD13	2.00	0.44
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.98	0.44
7:G:118:ASN:OD1	7:G:119:LEU:N	2.50	0.44
9:I:7:CYS:N	9:I:12:ASN:O	2.49	0.44
17:S:178:ARG:HA	17:S:178:ARG:HD2	1.85	0.44
5:E:71:TYR:OH	5:E:154:ARG:O	2.35	0.44
7:G:103:VAL:HG23	7:G:106:LEU:HB3	2.00	0.44
14:T:12:DT:H2"	14:T:13:DA:N7	2.33	0.44
17:S:96:ASP:HA	17:S:207:LYS:HB2	1.99	0.44
17:S:366:TRP:O	17:S:369:GLU:HG3	2.18	0.44
2:B:81:LYS:HB3	2:B:81:LYS:HE2	1.81	0.44
3:C:148:ARG:HG2	3:C:149:ASN:H	1.82	0.44
17:S:83:LEU:HA	17:S:86:ILE:HG22	1.99	0.44
17:S:86:ILE:O	17:S:90:SER:CB	2.66	0.44
1:A:276:ASN:HA	1:A:279:LYS:HG2	1.99	0.44
16:R:135:LEU:HD23	16:R:138:MET:HE3	2.00	0.44
16:R:626:MET:HE3	16:R:626:MET:HA	2.00	0.44
17:S:38:ASP:OD1	17:S:38:ASP:N	2.50	0.44
2:B:703:THR:HG23	2:B:706:ASP:H	1.83	0.44
16:R:226:THR:HG22	16:R:247:HIS:HB3	1.99	0.44
16:R:626:MET:HE1	16:R:645:MET:HE2	1.99	0.44
1:A:828:THR:O	1:A:832:THR:HG23	2.18	0.44
17:S:98:ILE:HA	17:S:130:LEU:HB2	2.00	0.44
17:S:299:ASN:HD21	17:S:302:PRO:HB3	1.83	0.43
1:A:330:LEU:HD11	2:B:1210:MET:HE1	2.00	0.43
1:A:1388:THR:HG23	1:A:1390:HIS:H	1.82	0.43
2:B:492:ASN:OD1	2:B:493:THR:N	2.51	0.43
7:G:131:MET:HE3	7:G:131:MET:HB2	1.78	0.43
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.99	0.43
2:B:427:ARG:NH1	14:T:14:DC:OP1	2.45	0.43
4:D:114:ARG:NH2	4:D:178:LEU:HD21	2.33	0.43
16:R:180:TYR:O	16:R:184:THR:HG22	2.18	0.43
16:R:362:TYR:O	16:R:370:ASN:ND2	2.51	0.43
16:R:837:ASP:OD1	16:R:837:ASP:N	2.48	0.43
17:S:88:LYS:HE3	17:S:370:TRP:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ARG:NE	1:A:1387:ILE:O	2.46	0.43
17:S:239:ILE:HD11	17:S:248:PHE:HB2	2.01	0.43
1:A:1285:VAL:HG13	1:A:1311:THR:HG22	2.00	0.43
2:B:490:ARG:HH22	2:B:775:LYS:HE2	1.83	0.43
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.01	0.43
16:R:809:LEU:HD12	16:R:813:ASP:HB2	2.01	0.43
1:A:35:ILE:HG21	1:A:53:LEU:HD23	1.99	0.43
6:F:116:ASP:HB3	6:F:119:GLN:HG2	2.00	0.43
16:R:21:VAL:HG23	16:R:288:TRP:NE1	2.34	0.43
1:A:482:ASP:OD1	1:A:482:ASP:N	2.52	0.43
14:T:9:DC:N3	15:P:13:A:N6	2.67	0.43
1:A:554:VAL:HB	1:A:557:TRP:HB2	2.01	0.43
16:R:17:ILE:HG22	16:R:293:ILE:HB	2.00	0.43
1:A:26:GLU:OE1	2:B:1215:ARG:NH2	2.52	0.43
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.45	0.43
7:G:46:VAL:HB	7:G:77:VAL:HG13	2.00	0.43
7:G:62:ILE:HD12	7:G:67:SER:HB2	2.01	0.43
4:D:33:GLU:OE1	7:G:41:GLN:NE2	2.51	0.42
16:R:568:GLN:HA	16:R:609:LEU:HD13	2.01	0.42
17:S:205:ARG:H	17:S:206:ILE:HD12	1.84	0.42
3:C:87:CYS:SG	3:C:91:CYS:HB3	2.58	0.42
4:D:114:ARG:NH1	4:D:145:LEU:O	2.50	0.42
7:G:129:ALA:HB2	7:G:138:THR:HG22	2.00	0.42
1:A:568:LYS:HG3	1:A:569:PRO:HA	2.01	0.42
7:G:93:ASN:OD1	16:R:37:ARG:NH1	2.50	0.42
1:A:555:PRO:HD2	1:A:649:ASN:ND2	2.34	0.42
2:B:262:LYS:HA	2:B:273:PRO:HA	2.02	0.42
2:B:278:PHE:CZ	2:B:293:ILE:HD11	2.53	0.42
1:A:904:ASP:O	1:A:908:SER:OG	2.38	0.42
1:A:1209:LEU:HD21	1:A:1277:ARG:HD3	2.00	0.42
16:R:72:THR:HG22	16:R:73:GLU:N	2.30	0.42
16:R:828:ASN:OD1	16:R:828:ASN:O	2.38	0.42
17:S:66:LEU:HB3	17:S:190:ASN:HB3	2.02	0.42
1:A:544:TYR:O	1:A:548:MET:HG3	2.20	0.42
1:A:1427:VAL:O	1:A:1431:VAL:HG23	2.20	0.42
4:D:108:TYR:CE1	7:G:103:VAL:HA	2.55	0.42
16:R:757:SER:HB3	16:R:779:ARG:HH21	1.83	0.42
2:B:791:THR:HG21	14:T:6:DG:H5"	2.01	0.42
2:B:955:THR:OG1	2:B:956:THR:N	2.53	0.42
3:C:21:LEU:HD22	11:K:101:LEU:HD11	2.01	0.42
3:C:74:GLU:OE1	3:C:128:ASN:ND2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:3:DC:H2'	14:T:4:DC:H6	1.85	0.42
17:S:354:GLU:O	17:S:357:GLN:HG3	2.20	0.42
1:A:533:ARG:HD3	1:A:750:ALA:HB2	2.01	0.42
2:B:872:GLU:HG2	2:B:916:THR:HB	2.01	0.42
5:E:61:ALA:HB3	5:E:77:LEU:HD23	2.00	0.42
17:S:166:MET:HE1	17:S:185:ALA:HB2	2.02	0.42
1:A:219:ASP:HA	1:A:222:ARG:HG2	2.02	0.42
2:B:128:ASP:OD1	2:B:128:ASP:N	2.52	0.42
2:B:235:LEU:HD22	2:B:242:ILE:HD11	2.01	0.42
2:B:573:ILE:HD11	2:B:583:HIS:HB2	2.02	0.42
2:B:941:LEU:HD12	2:B:941:LEU:HA	1.93	0.42
3:C:175:ALA:HB2	10:J:10:CYS:HB2	2.02	0.42
1:A:363:ASP:HB3	1:A:509:PRO:HD3	2.01	0.42
1:A:1061:HIS:ND1	6:F:87:LYS:HG2	2.35	0.42
10:J:48:MET:HE3	10:J:48:MET:HB3	1.85	0.42
16:R:644:LEU:HD13	16:R:652:ILE:HD11	2.02	0.42
1:A:1381:ARG:NH2	1:A:1385:MET:SD	2.93	0.41
2:B:461:GLU:HG2	2:B:464:LYS:H	1.84	0.41
4:D:102:VAL:HA	4:D:105:THR:HG22	2.02	0.41
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.86	0.41
2:B:336:ILE:O	2:B:336:ILE:HG22	2.20	0.41
5:E:99:ILE:HD13	5:E:104:PHE:HD2	1.85	0.41
14:T:4:DC:H2'	14:T:5:DT:C6	2.55	0.41
16:R:644:LEU:HB3	16:R:652:ILE:HD11	2.02	0.41
1:A:394:ARG:NH1	1:A:423:GLY:O	2.53	0.41
1:A:424:ASP:OD1	1:A:424:ASP:N	2.53	0.41
3:C:249:LYS:HE3	3:C:249:LYS:HB3	1.73	0.41
7:G:60:ARG:HB2	7:G:69:GLU:HB2	2.02	0.41
8:H:43:ASN:HB3	8:H:46:MET:HB2	2.01	0.41
14:T:4:DC:H2'	14:T:5:DT:H6	1.83	0.41
2:B:89:MET:HE1	2:B:958:GLN:OE1	2.20	0.41
4:D:99:ASN:HB3	4:D:103:LYS:NZ	2.35	0.41
5:E:58:SER:HA	5:E:79:VAL:O	2.21	0.41
8:H:40:LEU:HD11	8:H:96:MET:HE1	2.03	0.41
10:J:4:PRO:HG2	10:J:48:MET:HE1	2.02	0.41
16:R:296:GLU:HG2	16:R:809:LEU:HD23	2.01	0.41
16:R:375:GLU:HA	16:R:606:LEU:HD12	2.02	0.41
14:T:18:DT:H6	14:T:18:DT:H2'	1.64	0.41
16:R:545:ARG:O	16:R:549:THR:OG1	2.32	0.41
5:E:3:ASP:OD1	5:E:4:ASN:N	2.54	0.41
11:K:20:LYS:HA	11:K:20:LYS:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:62:SER:HB2	16:R:155:TRP:CZ3	2.56	0.41
1:A:17:VAL:HB	1:A:1422:ASP:HB3	2.03	0.41
2:B:56:LEU:HD12	2:B:56:LEU:HA	1.89	0.41
2:B:108:ASN:HA	2:B:198:GLY:HA3	2.02	0.41
5:E:167:TYR:HB3	5:E:169:LEU:HG	2.02	0.41
12:L:51:LYS:HD3	12:L:51:LYS:HA	1.82	0.41
15:P:6:U:H3	16:R:668:LYS:HB2	1.86	0.41
1:A:452:HIS:CD2	1:A:454:MET:HB2	2.55	0.41
1:A:1195:LEU:O	1:A:1241:ARG:HA	2.20	0.41
2:B:328:ARG:HH12	2:B:335:GLY:H	1.68	0.41
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.85	0.41
3:C:45:ILE:HA	3:C:159:ALA:HA	2.03	0.41
7:G:25:TYR:CE1	7:G:29:LYS:HD2	2.54	0.41
7:G:46:VAL:H	7:G:78:VAL:HA	1.86	0.41
16:R:228:CYS:HA	16:R:249:LYS:O	2.21	0.41
16:R:628:VAL:HG23	16:R:629:LEU:HD22	2.03	0.41
17:S:208:ILE:HD11	17:S:319:VAL:HG21	2.03	0.41
1:A:290:ILE:HD12	1:A:290:ILE:H	1.86	0.41
1:A:1320:MET:HE2	5:E:141:VAL:HG11	2.02	0.41
2:B:326:ILE:O	2:B:330:GLY:N	2.54	0.41
4:D:88:GLU:O	4:D:92:VAL:HG23	2.21	0.41
8:H:59:LEU:HD23	8:H:139:LEU:HD13	2.02	0.41
16:R:156:ASP:OD2	16:R:635:HIS:NE2	2.53	0.41
1:A:266:LYS:HA	1:A:266:LYS:HD3	1.95	0.40
1:A:1209:LEU:HD21	1:A:1277:ARG:HH11	1.85	0.40
1:A:128:ILE:HB	1:A:134:ARG:HB2	2.02	0.40
2:B:380:LEU:HD23	2:B:380:LEU:HA	1.96	0.40
2:B:562:TYR:HD1	2:B:582:ILE:HD13	1.86	0.40
7:G:132:SER:OG	7:G:133:ASN:N	2.54	0.40
16:R:329:ASN:HD21	16:R:332:LEU:HB2	1.86	0.40
16:R:668:LYS:HA	16:R:668:LYS:HD3	1.96	0.40
17:S:334:LEU:HD12	17:S:344:LEU:HD21	2.02	0.40
7:G:91:VAL:HA	7:G:101:ALA:HA	2.03	0.40
14:T:6:DG:H2''	14:T:7:DG:H5'	2.02	0.40
16:R:340:VAL:HB	16:R:343:ASN:ND2	2.37	0.40
1:A:1221:VAL:HG11	1:A:1274:ILE:HD12	2.02	0.40
2:B:764:SER:OG	2:B:765:PRO:HD3	2.22	0.40
5:E:122:MET:O	5:E:125:THR:OG1	2.34	0.40
17:S:99:ILE:HG23	17:S:209:LEU:HD23	2.03	0.40
17:S:259:CYS:SG	17:S:264:ILE:HB	2.61	0.40
2:B:586:PRO:HG2	2:B:610:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:139:PRO:HA	4:D:142:ILE:HG12	2.02	0.40
14:T:15:DT:H2''	14:T:16:DA:C8	2.57	0.40
16:R:343:ASN:O	16:R:346:THR:HB	2.22	0.40
16:R:390:ARG:HA	16:R:390:ARG:CZ	2.51	0.40
17:S:111:LEU:HD13	17:S:119:PHE:HE1	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1386/1743 (80%)	1351 (98%)	34 (2%)	1 (0%)	48	76
2	B	1132/1227 (92%)	1104 (98%)	28 (2%)	0	100	100
3	C	261/304 (86%)	256 (98%)	5 (2%)	0	100	100
4	D	161/186 (87%)	155 (96%)	6 (4%)	0	100	100
5	E	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
6	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	129/145 (89%)	128 (99%)	1 (1%)	0	100	100
9	I	109/115 (95%)	104 (95%)	5 (5%)	0	100	100
10	J	64/72 (89%)	63 (98%)	1 (2%)	0	100	100
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	1 (2%)	0	100	100
16	R	742/1006 (74%)	700 (94%)	42 (6%)	0	100	100
17	S	375/384 (98%)	360 (96%)	15 (4%)	0	100	100
All	All	4974/5912 (84%)	4821 (97%)	152 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

### 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	1215/1528 (80%)	1215 (100%)	0	100	100
2	B	1003/1077 (93%)	1001 (100%)	2 (0%)	92	95
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	142/160 (89%)	142 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	102 (98%)	2 (2%)	52	72
12	L	38/56 (68%)	38 (100%)	0	100	100
16	R	672/881 (76%)	670 (100%)	2 (0%)	91	94
17	S	344/348 (99%)	344 (100%)	0	100	100
All	All	4458/5210 (86%)	4452 (100%)	6 (0%)	92	96

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

Mol	Chain	Res	Type
2	B	1163	CYS
2	B	1185	CYS
11	K	112	LYS
11	K	113	ASN
16	R	112	GLN

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Mol	Chain	Res	Type
16	R	770	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	649	ASN
1	A	742	ASN
1	A	743	ASN
1	A	866	GLN
1	A	961	ASN
1	A	1095	ASN
1	A	1390	HIS
2	B	215	GLN
2	B	531	ASN
2	B	657	GLN
2	B	794	ASN
2	B	1195	HIS
2	B	1205	GLN
3	C	126	ASN
5	E	53	GLN
7	G	41	GLN
16	R	66	HIS
16	R	290	HIS
16	R	329	ASN
16	R	557	GLN
16	R	793	HIS
17	S	64	HIS
17	S	224	ASN
17	S	295	ASN
17	S	296	ASN
17	S	299	ASN
17	S	342	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	21/22 (95%)	9 (42%)	1 (4%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	3	A
15	P	4	U
15	P	6	U
15	P	7	G
15	P	8	C
15	P	9	A
15	P	10	U
15	P	11	A
15	P	13	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	9	A

## 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 ⓘ

There are no chain breaks in this entry.



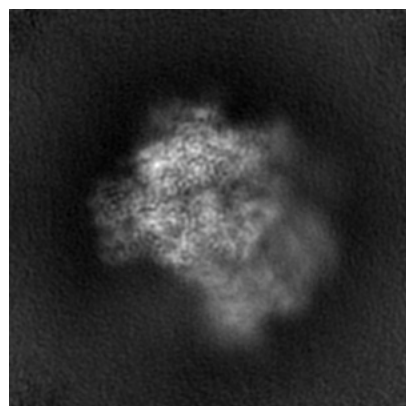
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39226. These allow visual inspection of the internal detail of the map and identification of artifacts.

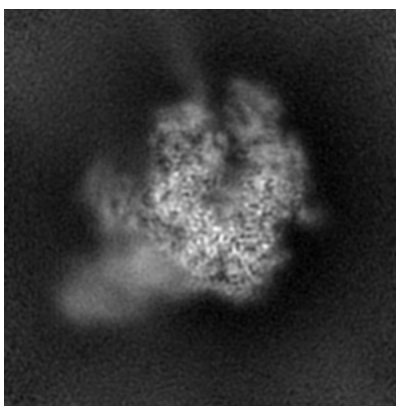
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

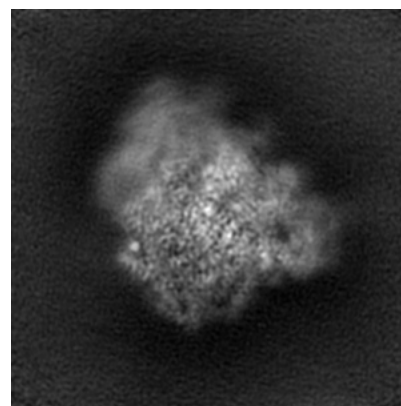
#### 6.1.1 Primary map



X

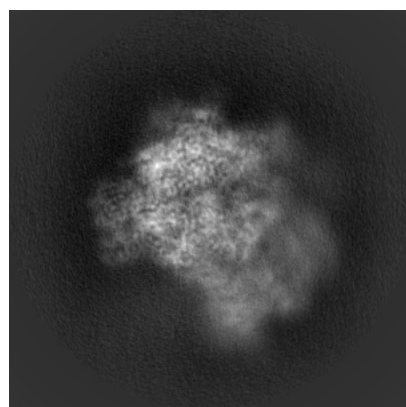


Y

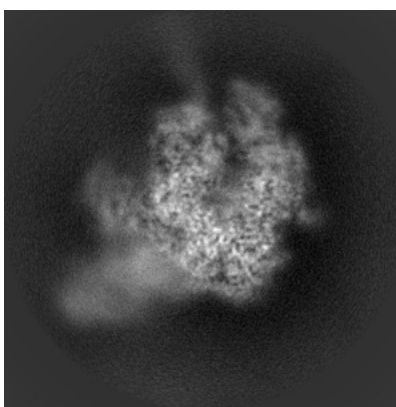


Z

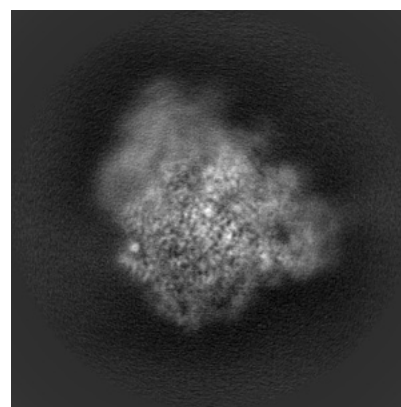
#### 6.1.2 Raw map



X



Y

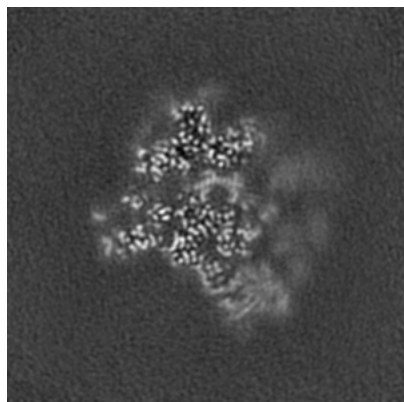


Z

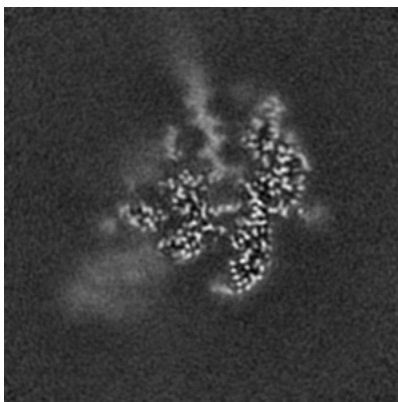
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

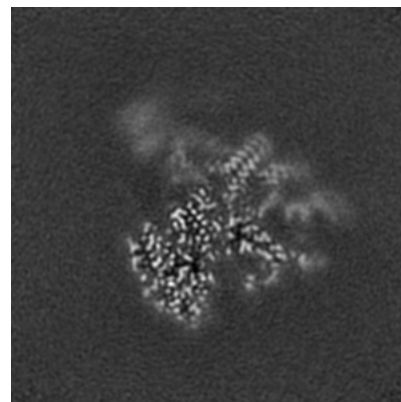
### 6.2.1 Primary map



X Index: 160

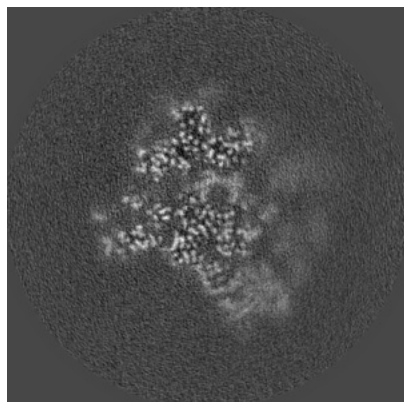


Y Index: 160

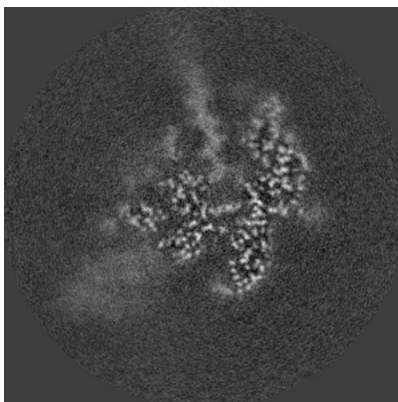


Z Index: 160

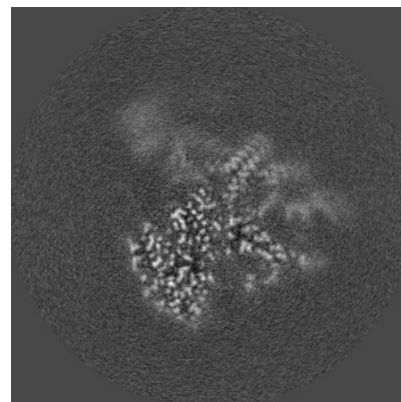
### 6.2.2 Raw map



X Index: 160



Y Index: 160

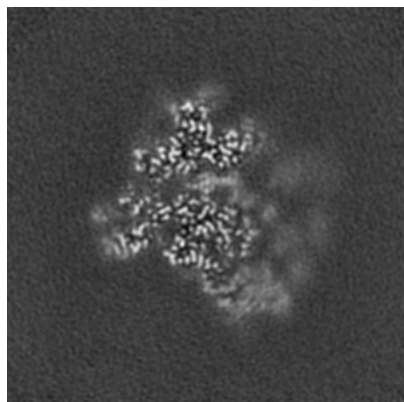


Z Index: 160

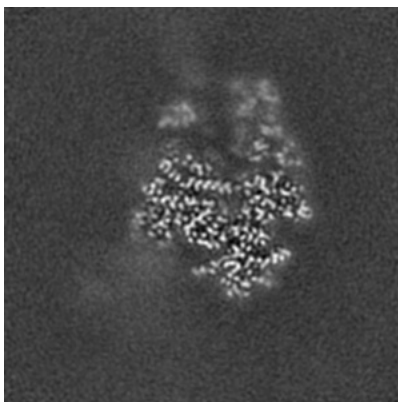
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

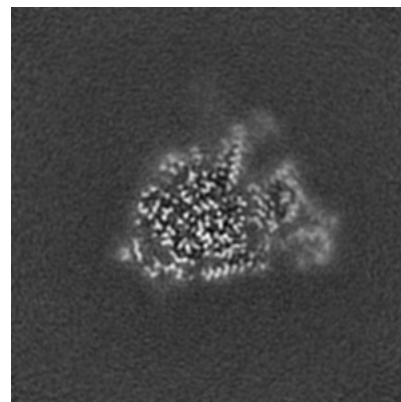
### 6.3.1 Primary map



X Index: 158

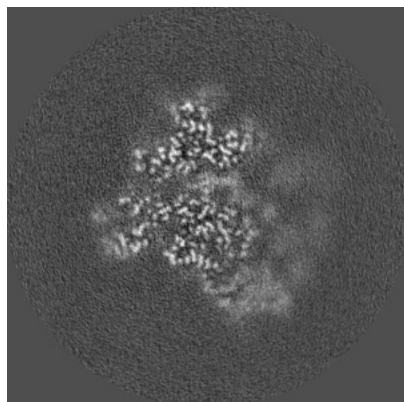


Y Index: 146

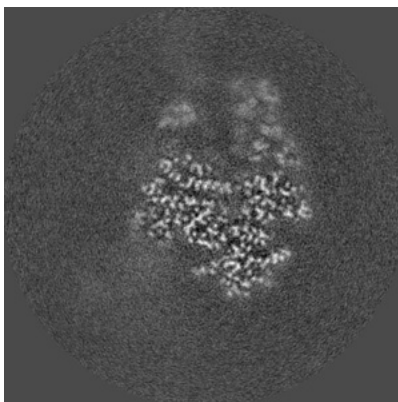


Z Index: 203

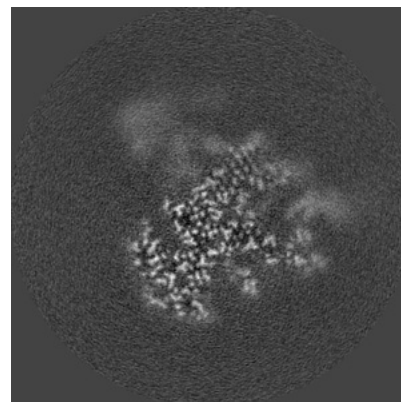
### 6.3.2 Raw map



X Index: 158



Y Index: 146

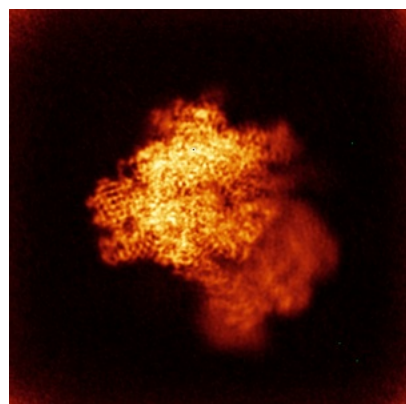


Z Index: 155

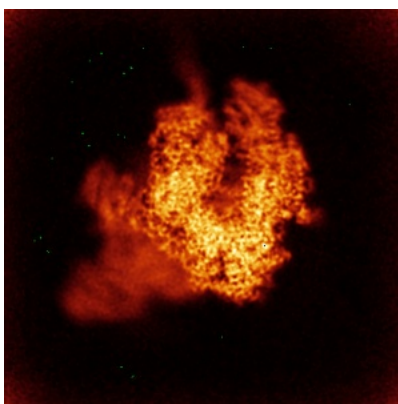
The images above show the largest variance slices of the map in three orthogonal directions.

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

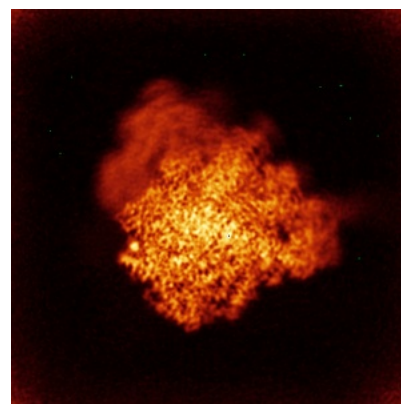
### 6.4.1 Primary map



X

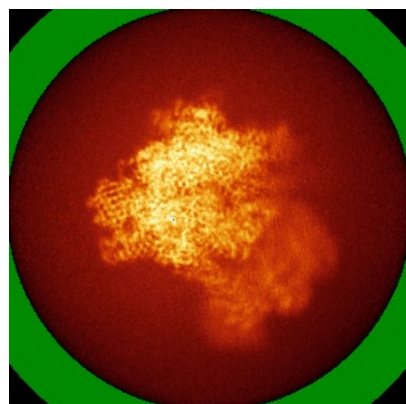


Y

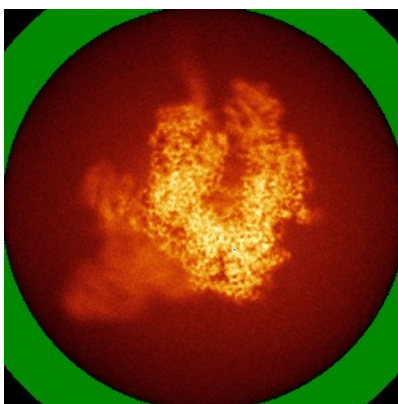


Z

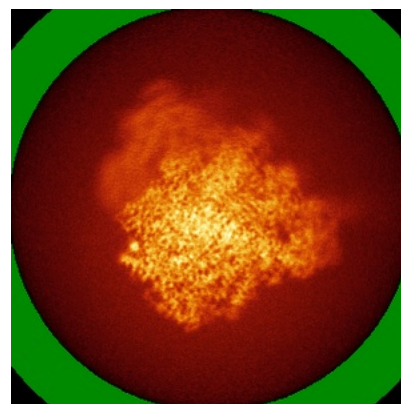
### 6.4.2 Raw map



X



Y



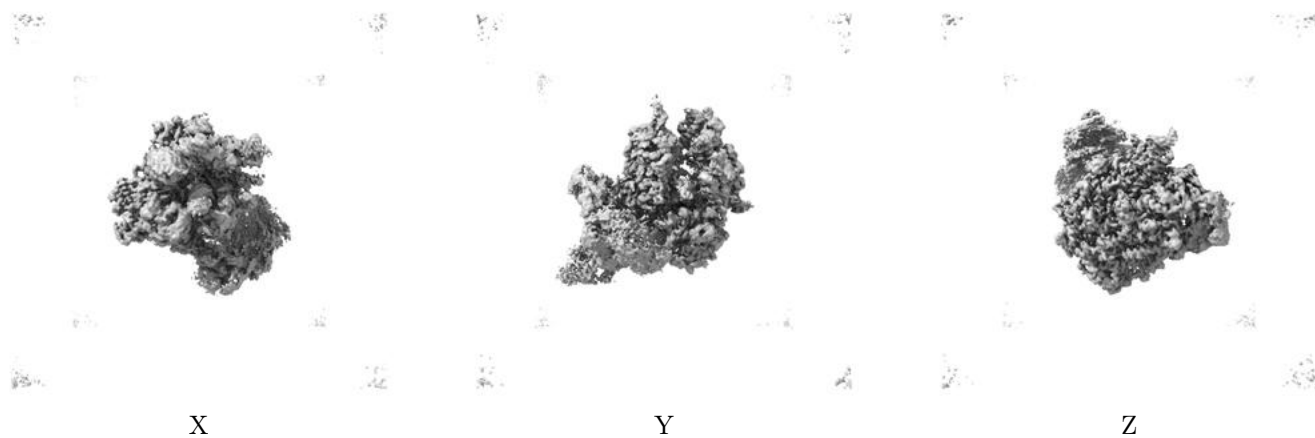
Z

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



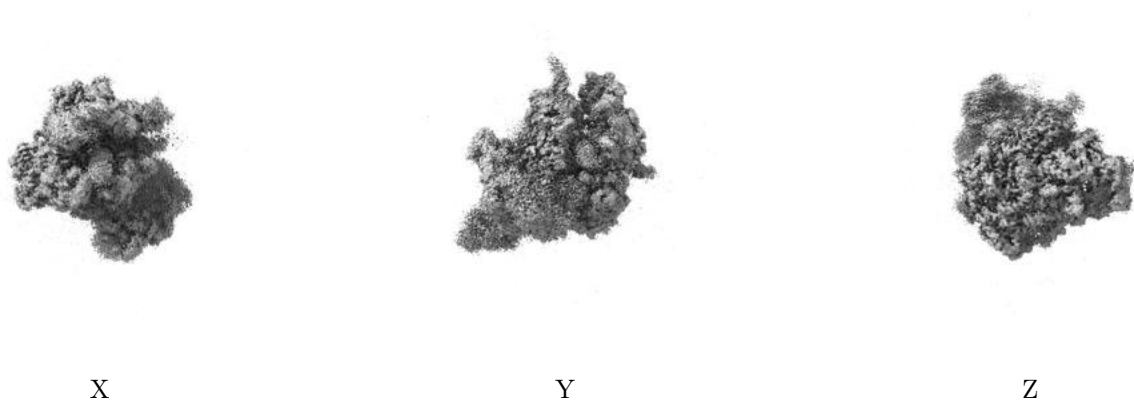
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

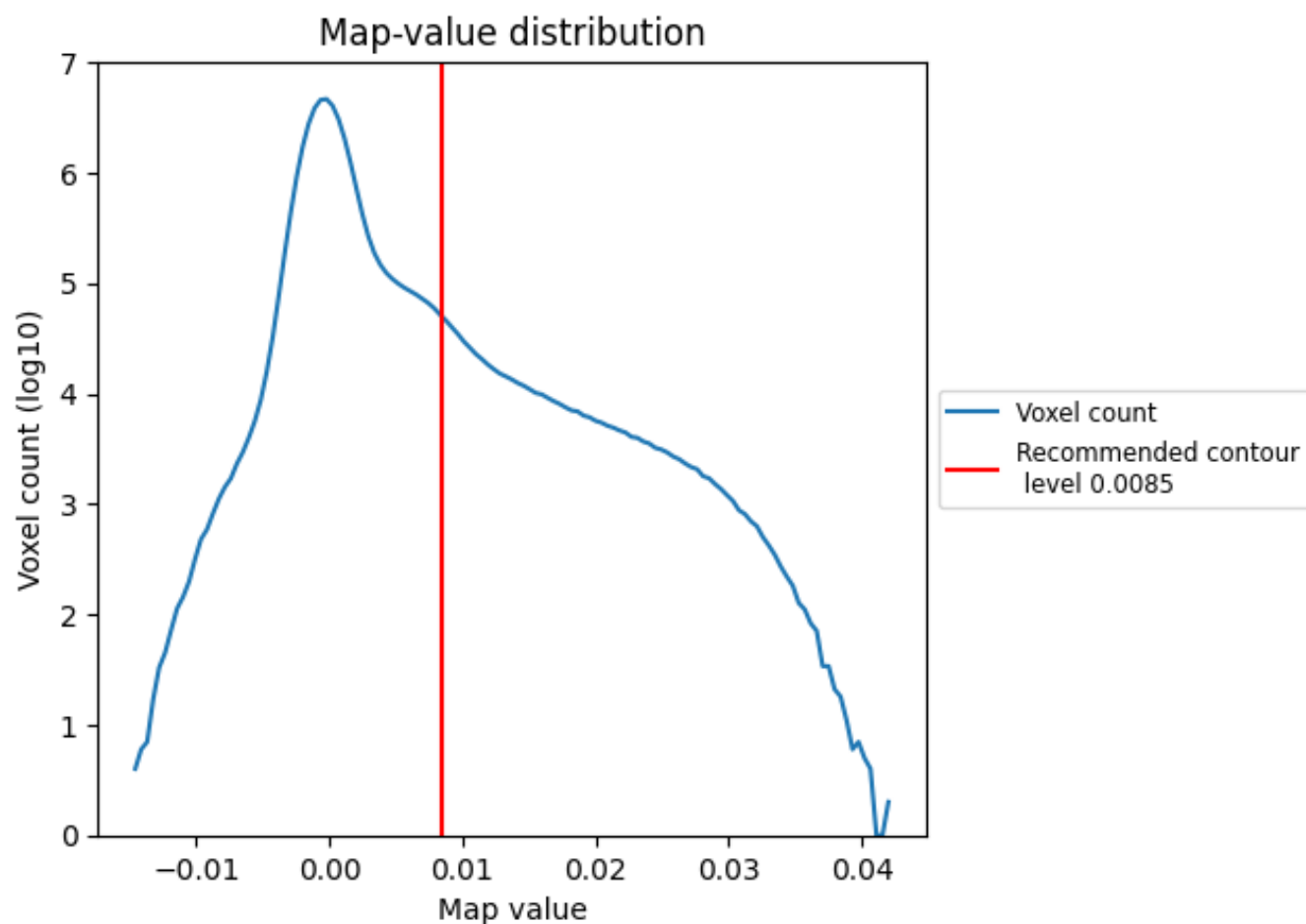
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

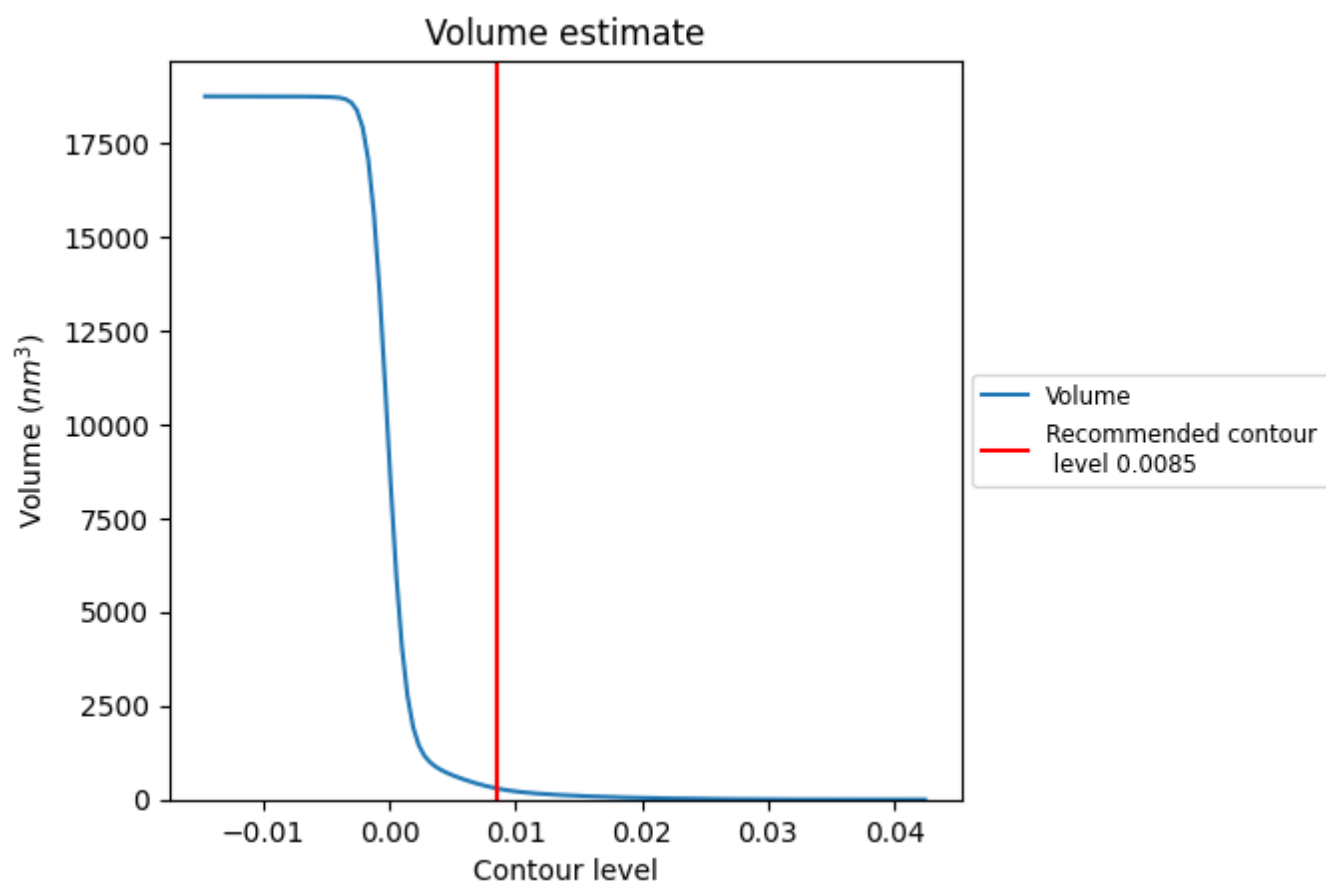
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

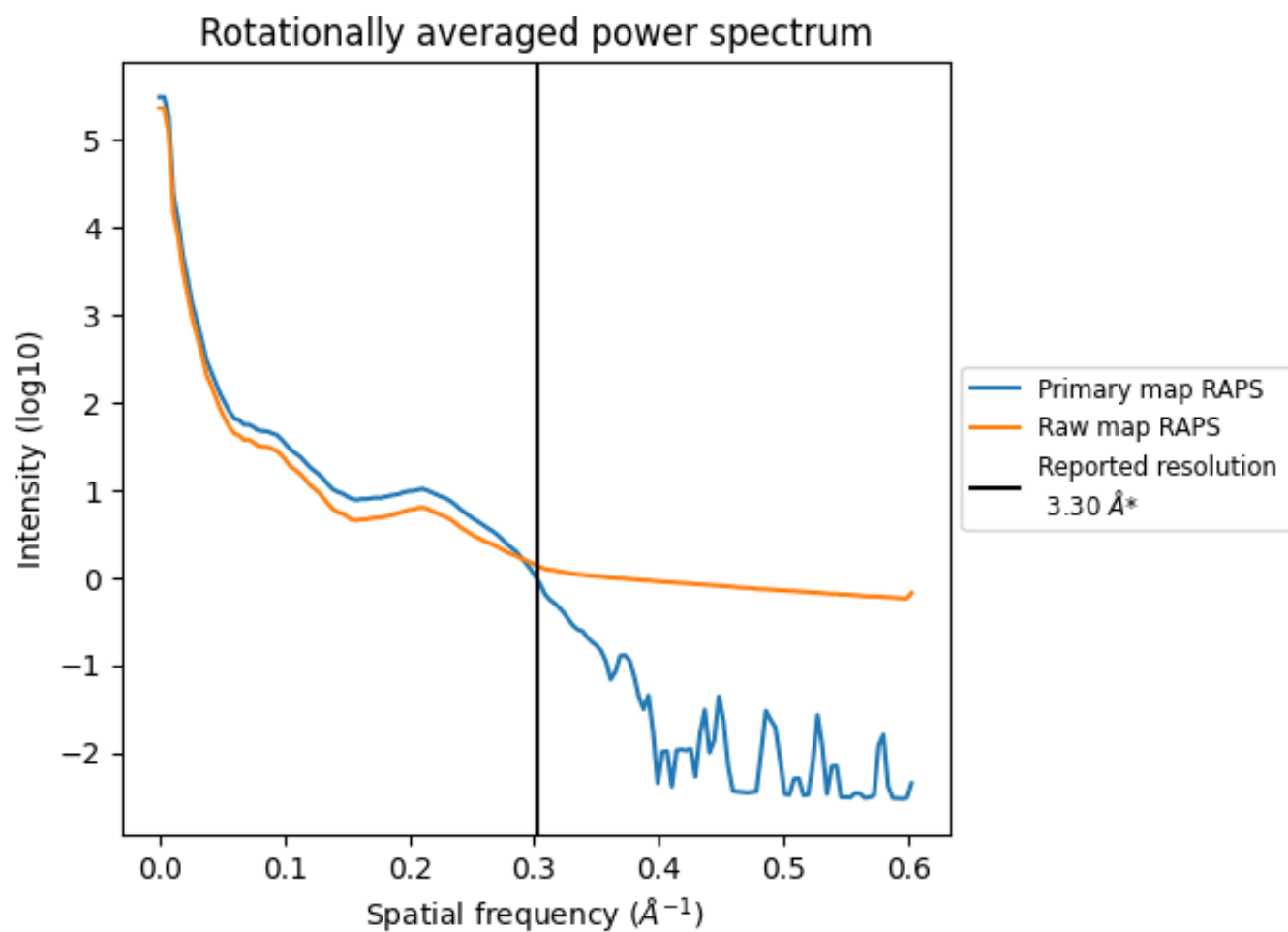
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm<sup>3</sup>; this corresponds to an approximate mass of 270 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 ⓘ



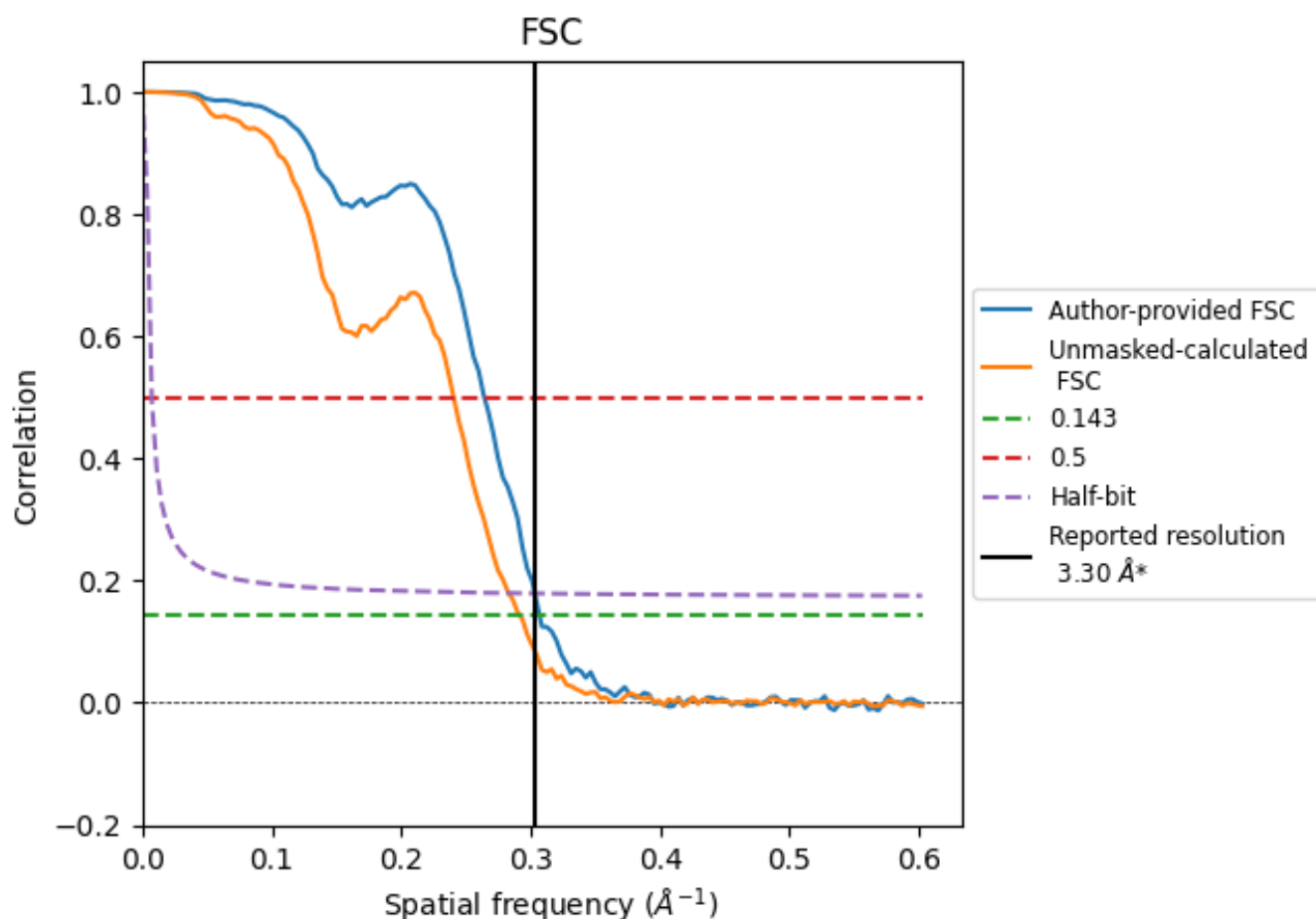
\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$



## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

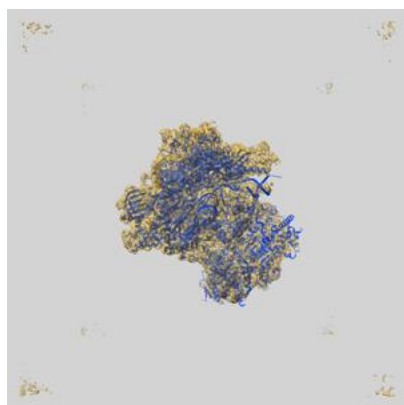
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.79	3.30
Unmasked-calculated*	3.43	4.16	3.53

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

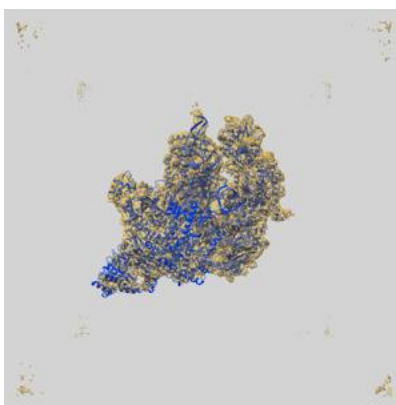
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39226 and PDB model 8YFQ. Per-residue inclusion information can be found in section 3 on page 8.

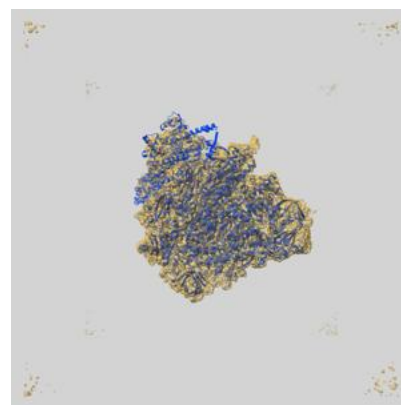
### 9.1 Map-model overlay [i](#)



X



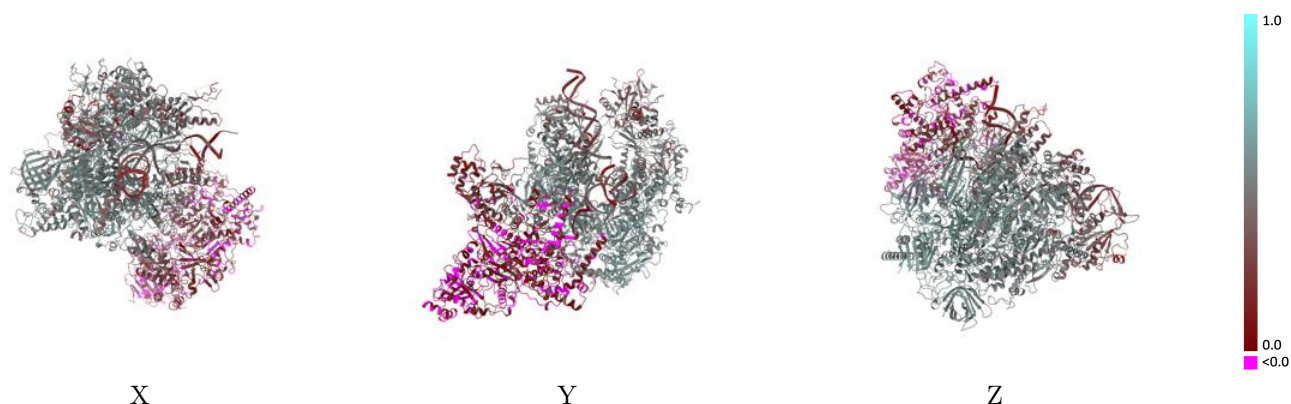
Y



Z

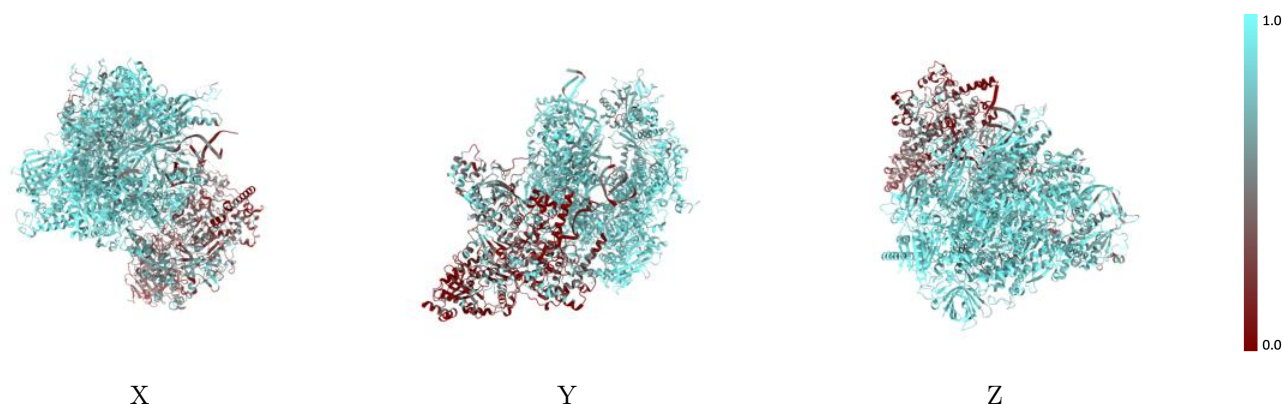
The images above show the 3D surface view of the map at the recommended contour level 0.0085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



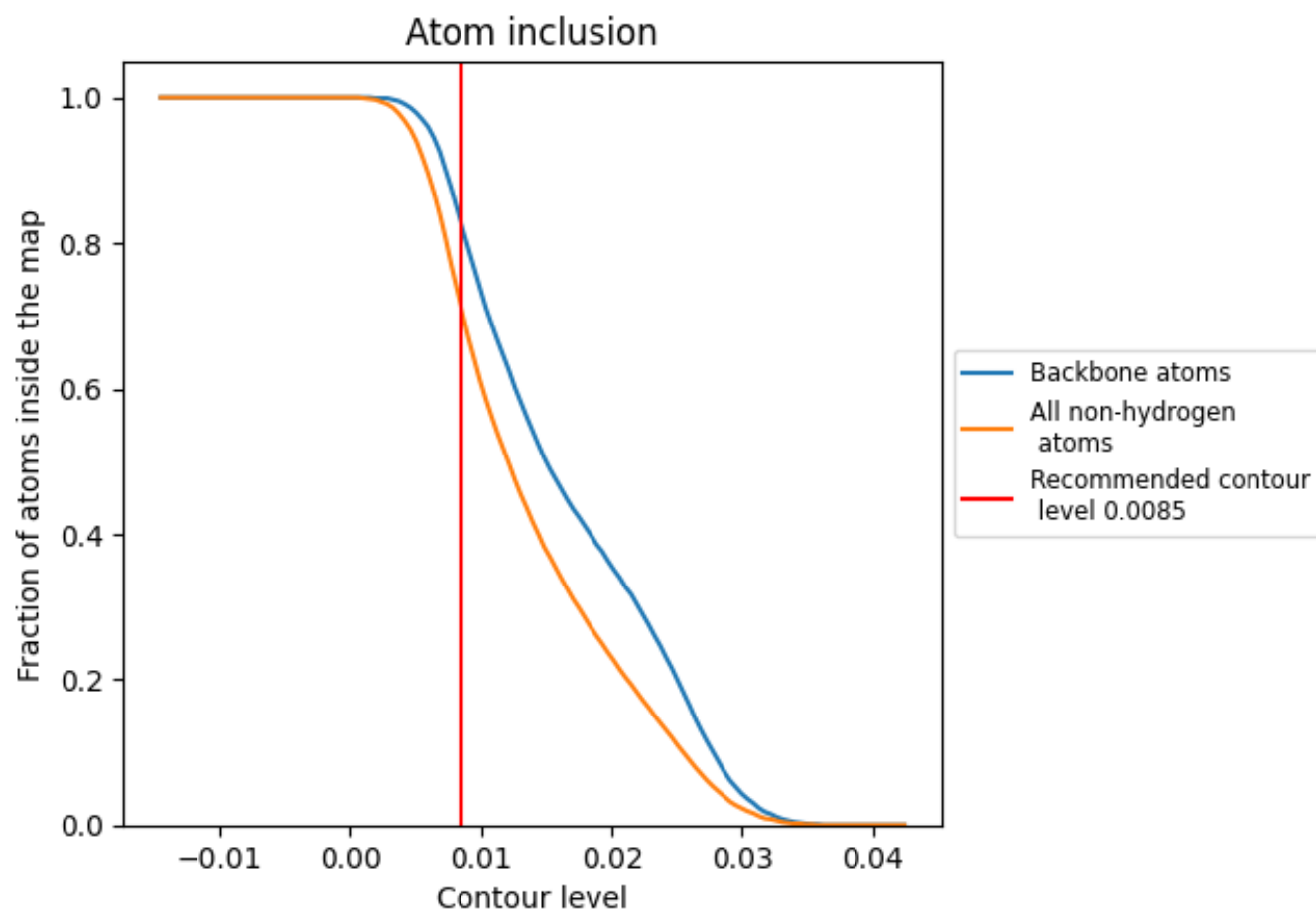
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0085).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 71% 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 (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.3930
A	 0.8530	 0.5030
B	 0.8610	 0.5150
C	 0.9150	 0.5460
D	 0.5150	 0.2470
E	 0.8870	 0.4940
F	 0.9220	 0.5510
G	 0.6610	 0.3060
H	 0.9110	 0.5290
I	 0.7490	 0.4120
J	 0.9110	 0.5580
K	 0.9250	 0.5550
L	 0.8940	 0.5020
N	 0.5950	 0.2450
P	 0.4650	 0.2400
R	 0.3200	 0.1040
S	 0.1820	 0.0440
T	 0.7000	 0.3060

