



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 08:15 AM UTC

PDB ID : 8YFR / pdb_00008yfr
EMDB ID : EMD-39227
Title : Cryo EM structure of Komagataella phaffii Rat1-Rai1 complex bound within the RNAPII cleft
Authors : Murayama, Y.; Yanagisawa, T.; Ehara, H.; Sekine, S.
Deposited on : 2024-02-25
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

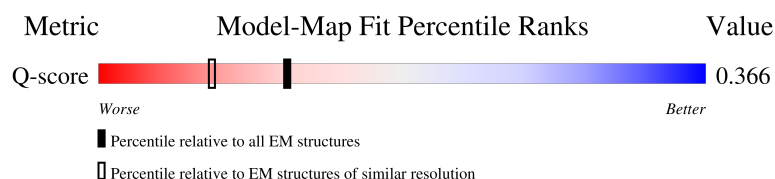
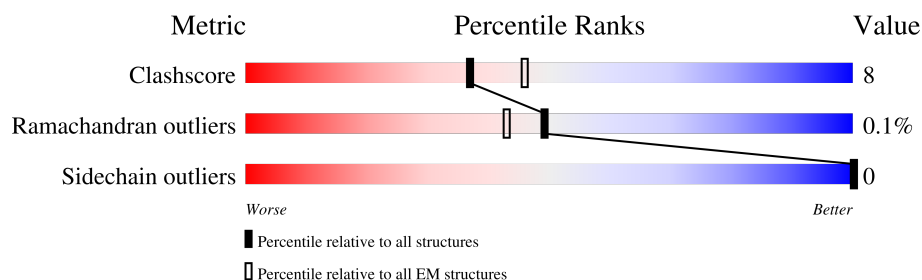
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



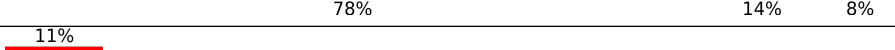
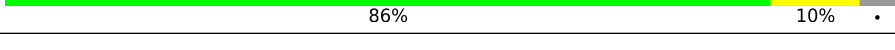
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1743	8% 66% 13% 21%
2	B	1227	5% 74% 18% 8%
3	C	304	79% 8% 13%
4	D	186	61% 49% 16% 34%

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Mol	Chain	Length	Quality of chain
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	R	1006	
14	S	384	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 39350 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	1384	Total	C	N	O	S	0	0
			10920	6895	1895	2060	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9031	5697	1586	1690	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	122	Total	C	N	O	S	0	0
			946	591	165	188	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	213	Total	C	N	O	S	0	0
			1740	1094	312	324	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
			1052	671	169	208	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 protein called 5'-3' exoribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	691	Total	C	N	O	S	0	0
			5698	3660	977	1039	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 14 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	378	Total	C	N	O	S	0	0
			3102	1984	524	581	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 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

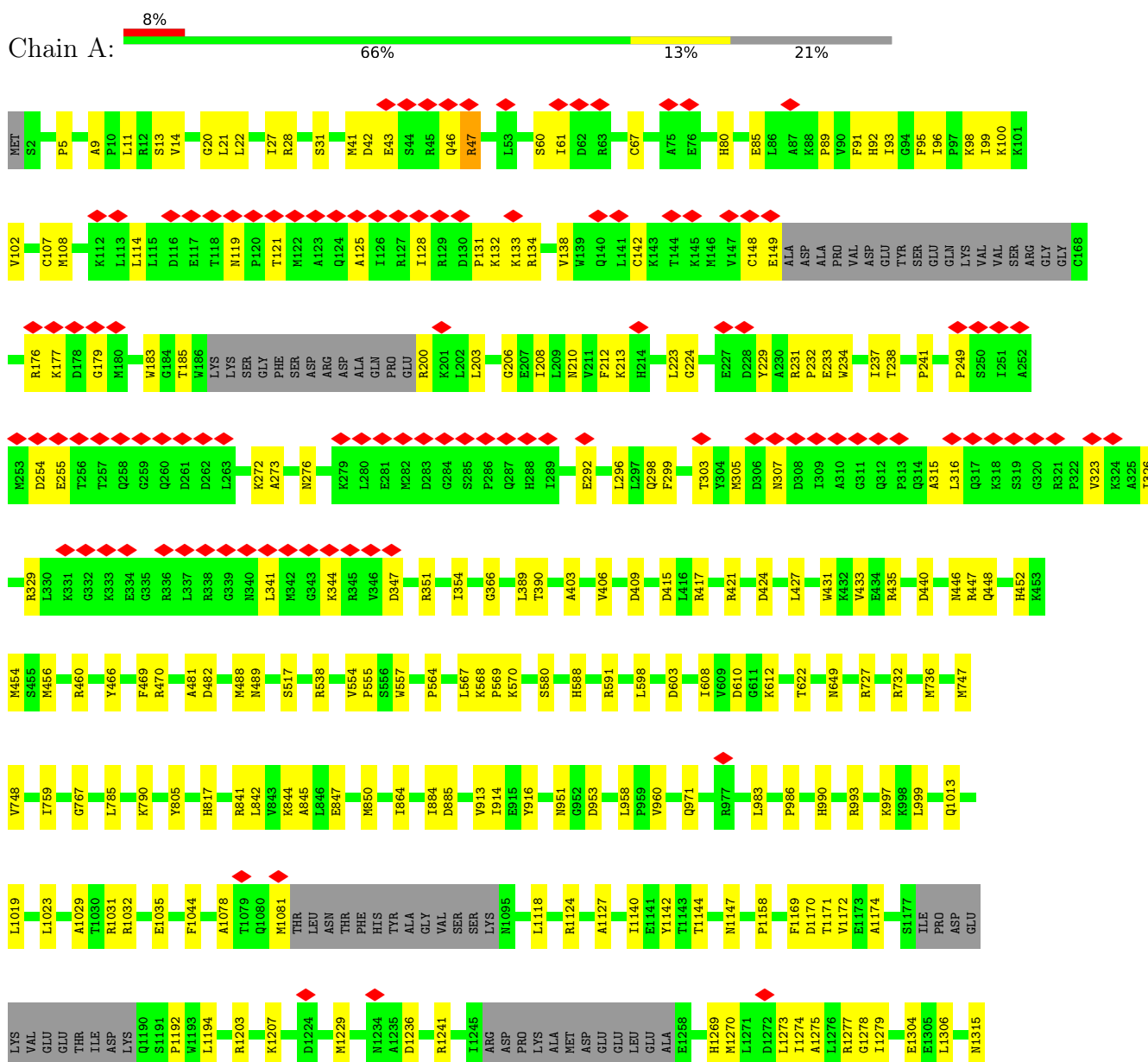
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

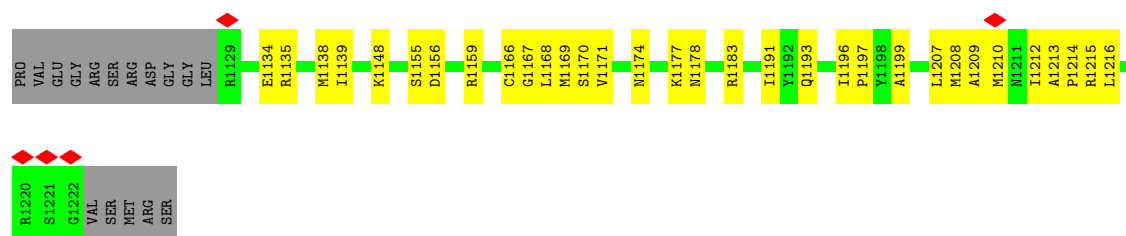
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total 1	Mg 1	0

3 Residue-property plots

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

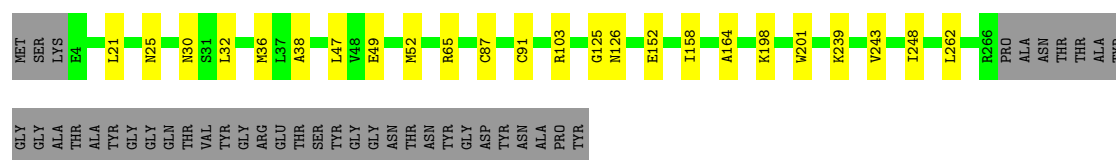
• Molecule 1: DNA-directed RNA polymerase subunit





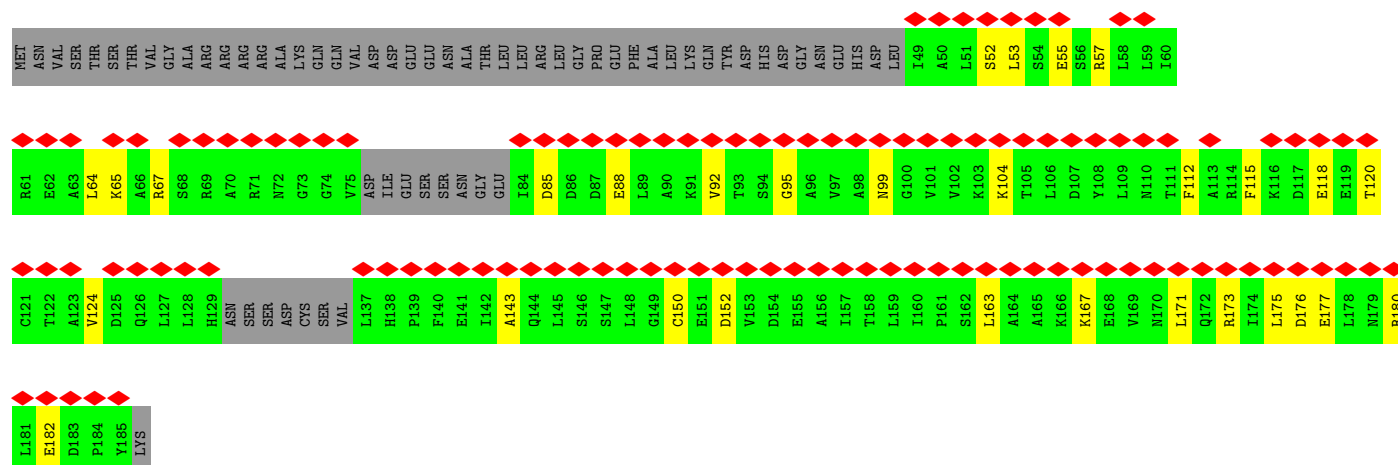
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C: 79% 8% 13%



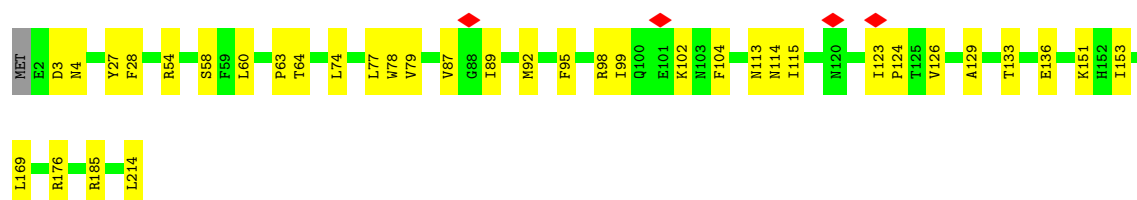
- Molecule 4: RNA polymerase II subunit B32

Chain D: 49% 16% 34%



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

Chain E: 83% 17%



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

Chain F: 50% 46%

MET SER GLU ASP GLU ALA PHE ASN GLU THR GLU ASN PHE GLU ASN PHE GLU ASP GLU HIS PHE SER ASP ASP ASN PHE GLU GLU ASP ARG ASP THR GLN PRO GLU ASP TVR ALA VAL GLY VAL THR THR ALA ASP GLY ARG GLN ILE ILE ASN GLY ASP GLY ILE GLN VAL ASN GLY THR

ILE LYS ALA HIS LYS ARG SER ASN LYS E71 R79 R97 A98 L99 M103 P131 E150 D154 ASN

• Molecule 7: RNA polymerase II subunit

Chain G: 

M1 F2 F3 L4 K5 D6 L13 H14 P15 Y25 L26 R27 A28 K29 L30 L31 L32 D33 V34 E35 C38 T39 G40 Q41 F42 G43 Y44 I45 L49 D50 G51 M52 N53 I54 D55 K73 Y74 R75 W79 K80 P81 F82 K83 G84 E85 V86 V87 D88 A89 I90 V91 S92 N93 V94

S95 P96 I97 G98 F99 F100 A101 D102 V103 G104 P105 L106 N107 V108 F109 V110 T111 T112 R113 L114 I115 P116 D117 N118 L119 V120 Y121 N122 P123 S124 N125 S126 D127 P128 A129 Y130 M131 S132 N133 D134 E135 L136 I137 T138 K139 G140 S141 K142 V143 L144 L145 K146 V147 V148 G149 T150 R151 T152 D153 V154

N155 E156 I157 Y158 A159 I160 G161 S162 T163 K164 E165 D166 F167 L168 G169 A170 I171

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

Chain H: 

MET SER S3 D8 I9 K22 R25 I36 D41 E45 M46 T56 L65 ASP GLU ASP GLU SER ALA ASN PHE SER K76 V100 Y101 K102 F103 E104 D107 E108 D109 Y114 V115 E125 K135 R144 R145

• Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 

MET ALA S3 F4 M13 L14 K17 E21 R24 L25 L26 C29 A38 K42 E45 M51 T52 G53 E54 T55 A56 V59 D60 T67 R70 S71 D72 D82 C83 V84 Q89 Q90 R91 F100 L104 K108 T109 E113 SER GLU

• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 

M1 I2 I3 C10 G11 D19 A20 R47 M48 T51 L55 E56 LYS LYS ASP PHE ASP SER

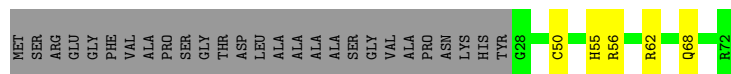
• Molecule 11: RNA polymerase II subunit B12.5

Chain K: 

M1 N2 A3 P4 D5 R6 F7 E8 L9 F10 I11 D14 D15 L45 L46 A47 E48 T57 Y61 Q76 L87 I94 L101 D102 H103 E107 N113 PHE SER LEU ASN ASP

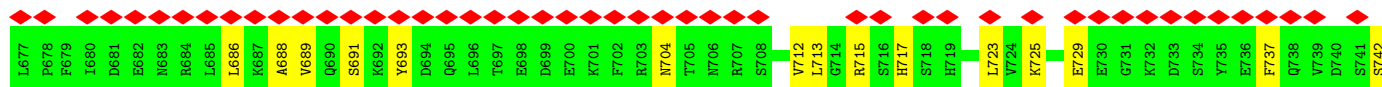
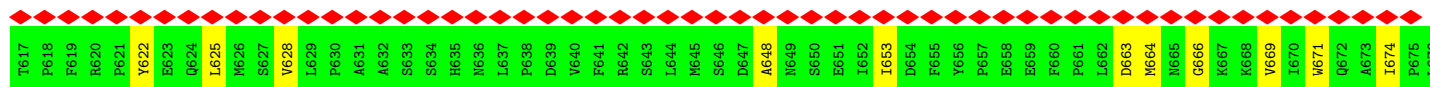
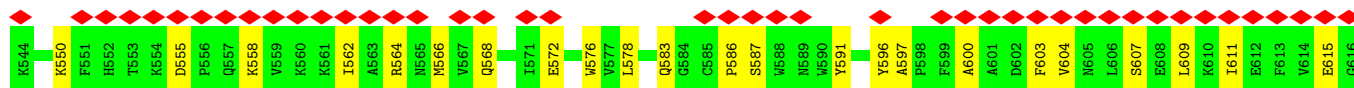
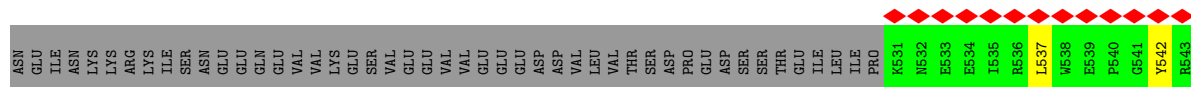
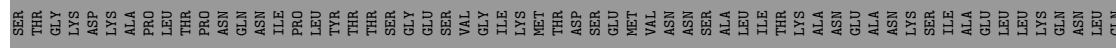
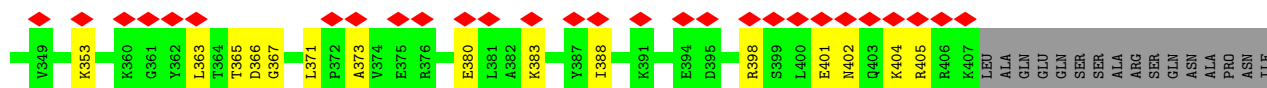
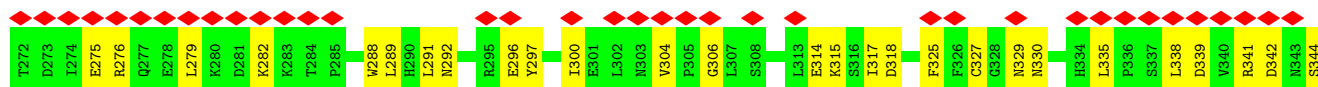
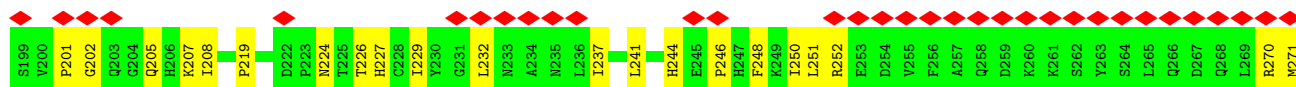
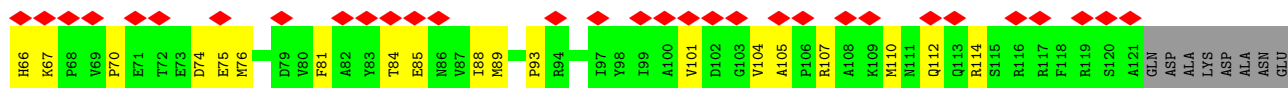
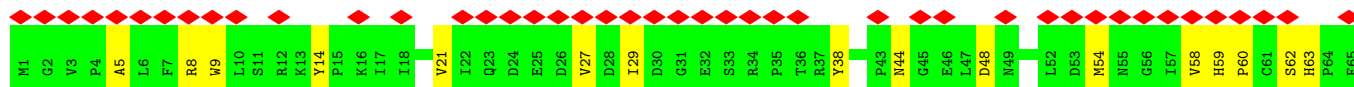
• Molecule 12: RNA polymerase subunit ABC10-alpha

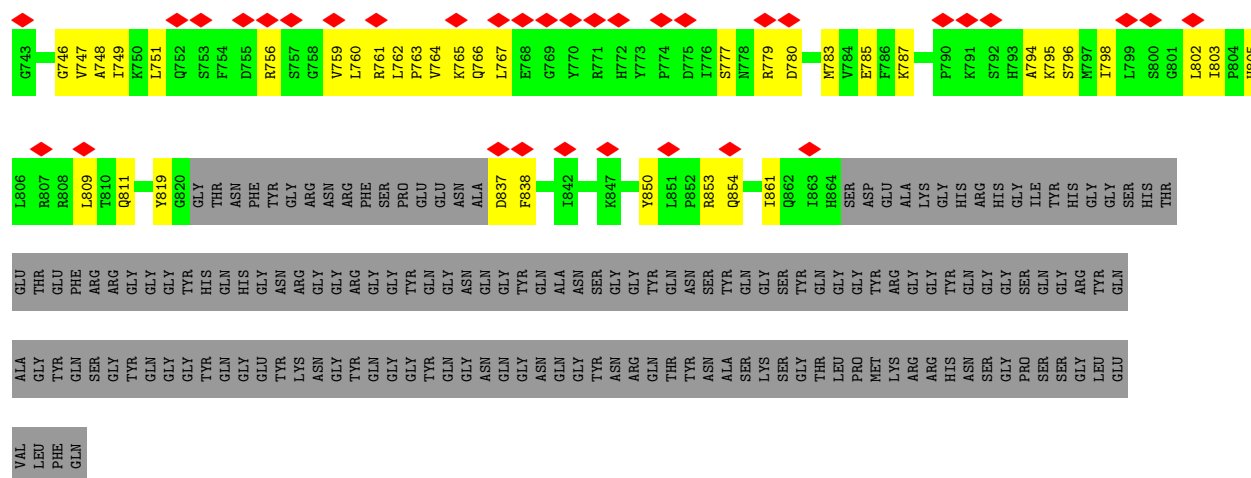
Chain L:  56% 7% 38%



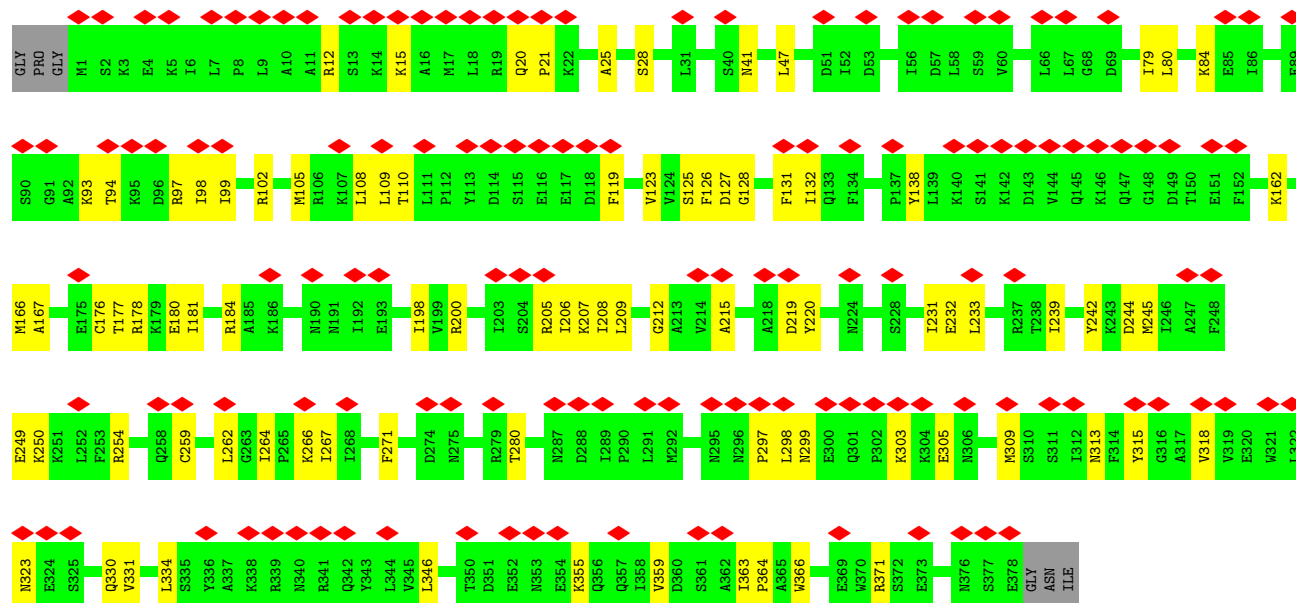
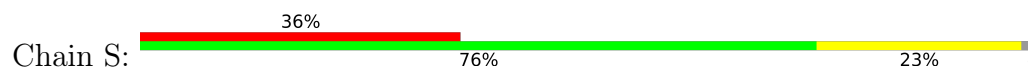
• Molecule 13: 5'-3' exoribonuclease

Chain R:  49% 38% 20% 31%





• Molecule 14: Decapping nuclease



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35181	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	0.041	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	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: 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	0.12	0/11121	0.29	0/15027
2	B	0.12	0/9207	0.29	0/12415
3	C	0.13	0/2139	0.26	0/2895
4	D	0.14	0/953	0.35	0/1285
5	E	0.11	0/1772	0.29	0/2385
6	F	0.11	0/687	0.23	0/931
7	G	0.11	0/1353	0.34	0/1837
8	H	0.12	0/1069	0.29	0/1444
9	I	0.12	0/934	0.36	0/1257
10	J	0.13	0/554	0.25	0/742
11	K	0.15	0/953	0.32	0/1291
12	L	0.10	0/365	0.27	0/484
13	R	0.13	0/5852	0.33	0/7922
14	S	0.11	0/3168	0.28	0/4272
All	All	0.12	0/40127	0.30	0/54187

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10920	0	10948	163	0
2	B	9031	0	9028	156	0
3	C	2098	0	2057	20	0
4	D	946	0	962	24	0
5	E	1740	0	1754	25	0
6	F	677	0	693	5	0
7	G	1324	0	1342	21	0
8	H	1052	0	1050	14	0
9	I	917	0	864	20	0
10	J	545	0	560	7	0
11	K	932	0	944	9	0
12	L	359	0	358	5	0
13	R	5698	0	5632	135	0
14	S	3102	0	3121	57	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	39350	0	39313	600	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 8.

All (600) 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)
4:D:57:ARG:NH2	4:D:112:PHE:O	2.19	0.76
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.67	0.75
1:A:452:HIS:ND1	1:A:454:MET:SD	2.59	0.74
13:R:59:HIS:HD2	13:R:62:SER:HB3	1.51	0.74
1:A:203:LEU:HB3	1:A:208:ILE:HD11	1.71	0.72
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.54	0.72
4:D:120:THR:HG21	4:D:182:GLU:HG3	1.71	0.72
13:R:178:ALA:HB1	13:R:193:VAL:HG21	1.72	0.70
8:H:36:ILE:HA	8:H:125:GLU:O	1.90	0.70
13:R:749:ILE:HB	13:R:785:GLU:HB3	1.74	0.70
1:A:13:SER:HB3	1:A:1433:LEU:HD13	1.74	0.69
3:C:87:CYS:SG	3:C:91:CYS:HB3	2.32	0.69
2:B:490:ARG:HE	2:B:531:ASN:HD21	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LEU:HD11	11:K:101:LEU:HD11	1.75	0.68
3:C:52:MET:HE1	3:C:152:GLU:HB3	1.74	0.68
4:D:53:LEU:HD23	4:D:57:ARG:HH22	1.58	0.68
13:R:583:GLN:NE2	13:R:794:ALA:O	2.26	0.68
13:R:101:VAL:O	13:R:207:LYS:NZ	2.25	0.68
1:A:1118:LEU:HD11	1:A:1315:ASN:H	1.58	0.68
13:R:104:VAL:H	13:R:201:PRO:HA	1.58	0.67
13:R:237:ILE:HD13	13:R:250:ILE:HD12	1.75	0.67
2:B:336:ILE:HB	2:B:341:ARG:HE	1.59	0.66
13:R:160:ILE:HA	13:R:167:MET:HE3	1.76	0.66
1:A:14:VAL:HG12	1:A:1433:LEU:HD21	1.76	0.66
1:A:307:ASN:ND2	1:A:323:VAL:O	2.30	0.65
2:B:456:THR:HG23	2:B:458:ASN:H	1.58	0.65
8:H:22:LYS:NZ	8:H:45:GLU:OE2	2.27	0.65
14:S:206:ILE:HG12	14:S:323:ASN:HD22	1.62	0.65
13:R:237:ILE:HD11	13:R:289:LEU:HD13	1.78	0.65
13:R:192:GLU:OE2	13:R:717:HIS:NE2	2.30	0.65
1:A:249:PRO:HD2	1:A:329:ARG:HH22	1.61	0.64
2:B:704:PRO:HA	2:B:707:LEU:HD23	1.79	0.64
1:A:841:ARG:HG3	1:A:1387:ILE:HG22	1.78	0.64
1:A:299:PHE:HB3	14:S:15:LYS:HZ2	1.62	0.64
1:A:148:CYS:SG	1:A:149:GLU:N	2.71	0.64
1:A:134:ARG:HH21	1:A:224:GLY:HA2	1.61	0.64
13:R:756:ARG:HB3	13:R:779:ARG:HH12	1.64	0.62
13:R:74:ASP:OD1	13:R:169:ARG:NH2	2.33	0.62
2:B:972:LYS:HE3	2:B:1098:MET:HE2	1.80	0.62
1:A:1407:GLU:HG2	1:A:1410:GLU:HB2	1.81	0.62
5:E:113:ASN:OD1	5:E:114:ASN:N	2.32	0.61
1:A:255:GLU:HB2	2:B:883:LEU:HD12	1.81	0.61
13:R:747:VAL:HB	13:R:787:LYS:HB2	1.80	0.61
1:A:131:PRO:HB2	1:A:1418:ALA:HB1	1.81	0.61
14:S:125:SER:HB3	14:S:330:GLN:H	1.66	0.61
2:B:175:LEU:HB3	2:B:179:ASP:HB2	1.83	0.61
2:B:613:ARG:NH1	9:I:89:GLN:OE1	2.34	0.61
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.66	0.61
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.34	0.61
1:A:128:ILE:HG21	1:A:133:LYS:HB3	1.83	0.60
13:R:327:CYS:SG	13:R:344:SER:OG	2.56	0.60
13:R:766:GLN:NE2	13:R:767:LEU:O	2.33	0.60
13:R:5:ALA:HA	13:R:8:ARG:HB2	1.83	0.60
9:I:24:ARG:NH2	9:I:38:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:NH1	1:A:424:ASP:O	2.34	0.60
13:R:114:ARG:HA	13:R:628:VAL:HG23	1.84	0.60
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.84	0.60
14:S:242:TYR:HA	14:S:245:MET:HE2	1.82	0.60
1:A:95:PHE:HD1	1:A:98:LYS:HD3	1.66	0.60
13:R:276:ARG:HB2	13:R:282:LYS:HB2	1.84	0.59
2:B:264:THR:OG1	2:B:271:ASP:OD1	2.17	0.59
2:B:270:GLN:HE22	13:R:811:GLN:HG2	1.67	0.59
9:I:108:LYS:NZ	9:I:109:THR:O	2.29	0.59
1:A:22:LEU:HD11	2:B:1208:MET:HE3	1.83	0.59
1:A:951:ASN:ND2	1:A:953:ASP:OD2	2.35	0.59
3:C:103:ARG:HB3	3:C:152:GLU:HG3	1.83	0.59
1:A:1078:ALA:HA	1:A:1081:MET:HG2	1.84	0.59
1:A:255:GLU:HG3	2:B:884:ARG:H	1.67	0.59
2:B:220:ALA:O	2:B:252:ARG:NH2	2.34	0.59
1:A:1127:ALA:HB1	1:A:1306:LEU:HB3	1.82	0.59
13:R:401:GLU:OE1	13:R:405:ARG:NH1	2.35	0.59
2:B:254:ASP:H	2:B:259:ARG:HH21	1.51	0.59
13:R:737:PHE:HB2	13:R:746:GLY:H	1.68	0.59
1:A:95:PHE:O	1:A:99:ILE:N	2.35	0.59
13:R:715:ARG:HD2	13:R:780:ASP:HA	1.85	0.59
13:R:564:ARG:NH1	13:R:604:VAL:O	2.31	0.58
2:B:22:SER:HG	2:B:811:TYR:HH	1.52	0.58
9:I:13:MET:HE3	9:I:14:LEU:H	1.67	0.58
1:A:446:ASN:HB2	1:A:456:MET:HE3	1.84	0.58
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.58
13:R:325:PHE:O	13:R:329:ASN:ND2	2.36	0.58
1:A:98:LYS:HE2	1:A:1417:ALA:HA	1.85	0.58
9:I:51:ASN:C	9:I:51:ASN:HD22	2.11	0.58
2:B:650:GLU:OE1	2:B:653:ARG:NH1	2.37	0.58
13:R:339:ASP:OD1	13:R:341:ARG:NH1	2.36	0.58
2:B:1169:MET:HE3	2:B:1169:MET:HA	1.86	0.58
14:S:242:TYR:OH	14:S:299:ASN:ND2	2.36	0.58
13:R:398:ARG:O	13:R:402:ASN:ND2	2.37	0.58
13:R:837:ASP:OD1	13:R:838:PHE:N	2.36	0.58
2:B:979:LYS:HG2	2:B:989:THR:HG22	1.85	0.58
13:R:759:VAL:HA	13:R:777:SER:HA	1.86	0.58
3:C:36:MET:HG2	3:C:243:VAL:HG12	1.85	0.57
13:R:669:VAL:HG12	13:R:671:TRP:H	1.68	0.57
2:B:262:LYS:HB3	2:B:271:ASP:HB3	1.87	0.57
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:246:PRO:HG2	13:R:802:LEU:HD21	1.87	0.57
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.37	0.57
4:D:53:LEU:HB3	4:D:57:ARG:HH12	1.69	0.57
7:G:122:ASN:O	7:G:128:PRO:HA	2.05	0.57
1:A:176:ARG:NH1	1:A:185:THR:OG1	2.38	0.57
14:S:127:ASP:OD2	14:S:371:ARG:NH1	2.38	0.56
5:E:58:SER:HA	5:E:79:VAL:O	2.06	0.56
5:E:87:VAL:HG11	5:E:115:ILE:HG12	1.88	0.56
13:R:550:LYS:NZ	13:R:663:ASP:OD2	2.37	0.56
1:A:580:SER:HB3	1:A:612:LYS:HA	1.87	0.56
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.39	0.56
2:B:653:ARG:NH2	2:B:661:ASP:OD2	2.38	0.56
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.86	0.56
1:A:21:LEU:HD23	2:B:1212:ILE:HG22	1.86	0.56
2:B:106:LEU:HD12	2:B:953:LEU:HD22	1.88	0.56
4:D:176:ASP:O	4:D:180:ARG:CB	2.54	0.56
2:B:257:THR:OG1	2:B:258:GLY:N	2.37	0.55
13:R:315:LYS:HE3	13:R:365:THR:HG23	1.86	0.55
2:B:269:LYS:HE2	2:B:331:SER:HA	1.88	0.55
2:B:254:ASP:OD1	2:B:259:ARG:NH2	2.39	0.55
2:B:55:ARG:NH1	2:B:76:GLU:OE2	2.39	0.55
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.89	0.55
1:A:31:SER:O	2:B:1183:ARG:NH2	2.39	0.55
3:C:49:GLU:OE2	12:L:68:GLN:NE2	2.37	0.55
7:G:49:LEU:HD12	7:G:75:ARG:HG2	1.88	0.55
13:R:241:LEU:HD23	13:R:317:ILE:HG23	1.87	0.55
4:D:176:ASP:O	4:D:180:ARG:HB2	2.07	0.55
13:R:107:ARG:HG3	13:R:591:TYR:HB3	1.89	0.55
10:J:19:ASP:OD1	10:J:20:ALA:N	2.39	0.55
3:C:103:ARG:NH1	3:C:152:GLU:OE1	2.41	0.54
5:E:78:TRP:HD1	5:E:95:PHE:HE1	1.55	0.54
13:R:366:ASP:OD2	14:S:178:ARG:NH1	2.38	0.54
13:R:572:GLU:HG2	13:R:611:ILE:HG23	1.88	0.54
14:S:166:MET:HA	14:S:184:ARG:HE	1.72	0.54
1:A:390:THR:HG22	1:A:427:LEU:HD12	1.89	0.54
1:A:448:GLN:OE1	1:A:489:ASN:ND2	2.40	0.54
1:A:1347:THR:HG21	1:A:1384:LEU:HD21	1.89	0.54
4:D:53:LEU:HB3	4:D:57:ARG:NH1	2.22	0.54
13:R:85:GLU:OE2	13:R:177:TRP:NE1	2.39	0.54
13:R:105:ALA:H	13:R:110:MET:HE3	1.73	0.54
1:A:28:ARG:NE	1:A:85:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:OG	1:A:61:ILE:N	2.41	0.54
5:E:54:ARG:NH1	5:E:136:GLU:OE1	2.40	0.54
1:A:296:LEU:O	14:S:15:LYS:NZ	2.41	0.54
1:A:406:VAL:HG22	1:A:433:VAL:HG22	1.90	0.54
1:A:983:LEU:HD11	1:A:1044:PHE:HB2	1.90	0.54
1:A:389:LEU:HD21	1:A:433:VAL:HG21	1.90	0.54
1:A:1434:GLY:O	2:B:1148:LYS:NZ	2.36	0.53
8:H:102:LYS:NZ	8:H:104:GLU:OE2	2.36	0.53
13:R:338:LEU:HD22	13:R:344:SER:HB2	1.91	0.53
5:E:89:ILE:HD13	13:R:270:ARG:O	2.09	0.53
14:S:231:ILE:HD13	14:S:266:LYS:HB3	1.90	0.53
1:A:440:ASP:OD1	1:A:460:ARG:NH1	2.38	0.53
1:A:727:ARG:HD3	1:A:767:GLY:HA3	1.89	0.53
1:A:125:ALA:HA	1:A:128:ILE:HD12	1.91	0.53
13:R:112:GLN:HG2	13:R:330:ASN:HB2	1.90	0.53
13:R:271:MET:HG3	13:R:275:GLU:HB3	1.91	0.53
14:S:123:VAL:HG13	14:S:132:ILE:HG22	1.90	0.53
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.35	0.53
10:J:10:CYS:SG	10:J:11:GLY:N	2.81	0.53
13:R:244:HIS:NE2	13:R:318:ASP:OD1	2.38	0.53
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.74	0.53
1:A:1147:ASN:O	1:A:1203:ARG:NH1	2.42	0.53
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.91	0.53
7:G:4:LEU:HD22	7:G:49:LEU:HD11	1.90	0.53
13:R:70:PRO:HB3	13:R:75:GLU:HB2	1.90	0.52
1:A:231:ARG:HD2	1:A:232:PRO:HD2	1.90	0.52
2:B:74:ARG:HB2	2:B:124:PHE:HB3	1.92	0.52
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.43	0.52
4:D:67:ARG:HH22	4:D:92:VAL:HB	1.73	0.52
13:R:366:ASP:OD1	13:R:796:SER:OG	2.24	0.52
2:B:233:SER:OG	2:B:356:HIS:ND1	2.36	0.52
1:A:1194:LEU:HD21	1:A:1241:ARG:HG2	1.91	0.52
2:B:273:PRO:HB2	2:B:276:ILE:HG12	1.92	0.52
2:B:607:SER:OG	2:B:625:ARG:NH1	2.43	0.52
13:R:227:HIS:HB2	13:R:248:PHE:HD1	1.75	0.52
2:B:223:SER:O	2:B:252:ARG:NH2	2.34	0.52
2:B:942:ARG:HE	2:B:943:SER:H	1.57	0.52
13:R:14:TYR:HB3	13:R:297:TYR:CE2	2.45	0.52
13:R:587:SER:HA	13:R:615:GLU:HA	1.92	0.52
1:A:1171:THR:HG22	1:A:1229:MET:HE1	1.92	0.52
2:B:413:LEU:HD13	2:B:446:ILE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.91	0.52
1:A:538:ARG:NH2	1:A:603:ASP:OD1	2.43	0.52
2:B:901:PRO:HG2	12:L:62:ARG:HA	1.90	0.52
10:J:47:ARG:O	10:J:51:THR:OG1	2.25	0.52
13:R:314:GLU:OE2	13:R:798:ILE:HG12	2.10	0.52
2:B:102:GLN:HG2	2:B:184:LYS:HB2	1.91	0.52
13:R:190:GLY:HA2	13:R:717:HIS:HD2	1.75	0.51
1:A:210:ASN:OD1	1:A:213:LYS:NZ	2.26	0.51
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.91	0.51
4:D:52:SER:N	4:D:55:GLU:OE2	2.44	0.51
4:D:163:LEU:HD22	4:D:171:LEU:HD11	1.92	0.51
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.43	0.51
9:I:4:PHE:CD2	9:I:13:MET:HE1	2.45	0.51
13:R:297:TYR:O	13:R:300:ILE:N	2.43	0.51
13:R:762:LEU:HG	13:R:764:VAL:H	1.75	0.51
13:R:765:LYS:NZ	13:R:766:GLN:O	2.42	0.51
1:A:92:HIS:O	1:A:96:ILE:HG13	2.10	0.51
1:A:447:ARG:HB2	1:A:488:MET:HE1	1.92	0.51
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.93	0.51
2:B:179:ASP:HA	2:B:182:LYS:HB2	1.92	0.51
2:B:207:GLU:HB3	2:B:493:THR:HA	1.92	0.51
7:G:25:TYR:O	7:G:28:GLU:HG3	2.11	0.51
14:S:126:PHE:HB3	14:S:131:PHE:HE2	1.75	0.51
1:A:102:VAL:HG13	1:A:223:LEU:HD21	1.92	0.51
2:B:957:ASN:OD1	2:B:961:LEU:N	2.43	0.51
13:R:88:ILE:HD12	13:R:188:TRP:HZ2	1.76	0.51
9:I:70:ARG:HG2	9:I:84:VAL:HG12	1.92	0.50
1:A:296:LEU:HG	14:S:15:LYS:HE3	1.92	0.50
1:A:409:ASP:OD1	1:A:409:ASP:N	2.42	0.50
2:B:128:ASP:OD1	2:B:128:ASP:N	2.45	0.50
6:F:103:MET:HE3	7:G:15:PRO:HG3	1.92	0.50
13:R:54:MET:HA	13:R:54:MET:HE3	1.93	0.50
1:A:241:PRO:HG2	2:B:1209:ALA:HA	1.94	0.50
13:R:688:ALA:O	13:R:691:SER:OG	2.28	0.50
14:S:215:ALA:HB3	14:S:232:GLU:HA	1.94	0.50
1:A:303:THR:HB	1:A:315:ALA:HB2	1.93	0.50
1:A:1453:LEU:HD23	1:A:1456:LEU:HD12	1.94	0.50
2:B:190:MET:SD	2:B:190:MET:N	2.84	0.50
13:R:292:ASN:HB2	13:R:805:HIS:CE1	2.46	0.50
13:R:568:GLN:HB2	13:R:609:LEU:HD22	1.91	0.50
13:R:38:TYR:HA	13:R:89:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:363:LEU:HD23	13:R:373:ALA:HB1	1.94	0.50
13:R:555:ASP:HB3	13:R:558:LYS:HB2	1.94	0.50
1:A:108:MET:SD	1:A:108:MET:N	2.84	0.50
1:A:183:TRP:HE3	1:A:200:ARG:HH22	1.58	0.50
5:E:27:TYR:HA	5:E:63:PRO:HA	1.93	0.50
2:B:1171:VAL:HG13	2:B:1191:ILE:HD13	1.93	0.50
9:I:4:PHE:HD2	9:I:13:MET:HE1	1.77	0.50
13:R:837:ASP:CG	13:R:838:PHE:H	2.18	0.50
2:B:337:ARG:HH12	13:R:306:GLY:H	1.60	0.50
2:B:755:ILE:HA	2:B:809:MET:HE2	1.94	0.50
1:A:132:LYS:NZ	1:A:1414:GLU:O	2.45	0.50
2:B:357:ILE:HD11	2:B:366:ARG:HG2	1.92	0.50
7:G:26:LEU:HA	7:G:29:LYS:HZ3	1.77	0.49
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.93	0.49
9:I:84:VAL:HG13	9:I:104:LEU:HD11	1.94	0.49
1:A:885:ASP:OD2	1:A:1032:ARG:NH1	2.39	0.49
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.49
13:R:104:VAL:O	13:R:202:GLY:N	2.45	0.49
1:A:986:PRO:O	1:A:990:HIS:ND1	2.43	0.49
13:R:81:PHE:O	13:R:84:THR:OG1	2.25	0.49
1:A:22:LEU:HD23	1:A:27:ILE:HG12	1.94	0.49
1:A:1144:THR:HA	1:A:1275:ALA:HA	1.94	0.49
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.34	0.49
2:B:1170:SER:HB2	2:B:1183:ARG:HG2	1.94	0.49
9:I:24:ARG:CZ	9:I:25:LEU:H	2.26	0.49
13:R:70:PRO:HG2	13:R:76:MET:SD	2.52	0.49
13:R:339:ASP:HB3	13:R:342:ASP:HB2	1.93	0.49
1:A:231:ARG:HG3	1:A:233:GLU:HG2	1.94	0.49
2:B:89:MET:HG3	2:B:109:LEU:HD13	1.95	0.49
1:A:92:HIS:CE1	1:A:305:MET:HE1	2.47	0.49
2:B:415:ARG:HD2	2:B:416:LYS:N	2.27	0.49
2:B:505:ARG:NH1	2:B:526:CYS:O	2.45	0.49
13:R:48:ASP:H	13:R:226:THR:HG23	1.78	0.49
13:R:401:GLU:HA	13:R:404:LYS:HE2	1.94	0.49
1:A:916:TYR:OH	1:A:983:LEU:O	2.14	0.49
2:B:632:ILE:HD11	2:B:688:GLU:HB3	1.94	0.49
13:R:648:ALA:HA	13:R:653:ILE:HG12	1.94	0.49
2:B:154:ASN:CG	2:B:155:LYS:H	2.20	0.49
2:B:865:ARG:HA	2:B:871:VAL:HG12	1.95	0.49
1:A:447:ARG:HD2	1:A:481:ALA:HB2	1.94	0.49
1:A:517:SER:OG	1:A:1365:TYR:O	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD11	14:S:309:MET:HE1	1.94	0.48
1:A:1207:LYS:O	1:A:1277:ARG:NH1	2.45	0.48
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.77	0.48
1:A:42:ASP:OD1	1:A:43:GLU:N	2.44	0.48
2:B:252:ARG:HB3	2:B:255:LYS:HB3	1.95	0.48
8:H:108:GLU:CD	8:H:109:ASP:H	2.20	0.48
1:A:91:PHE:O	1:A:298:GLN:NE2	2.46	0.48
1:A:847:GLU:OE2	2:B:1135:ARG:NH2	2.46	0.48
13:R:712:VAL:HG22	13:R:783:MET:HG2	1.96	0.48
2:B:337:ARG:O	2:B:341:ARG:HB2	2.13	0.48
2:B:1207:LEU:HG	2:B:1214:PRO:HD3	1.93	0.48
4:D:150:CYS:HB2	4:D:175:LEU:HD21	1.94	0.48
2:B:59:ASP:OD1	2:B:59:ASP:N	2.46	0.48
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.45	0.48
4:D:112:PHE:HE2	7:G:88:ASP:HB2	1.77	0.48
5:E:89:ILE:HA	5:E:92:MET:SD	2.54	0.48
8:H:102:LYS:HB3	8:H:114:TYR:HB2	1.96	0.48
13:R:296:GLU:O	13:R:300:ILE:HG12	2.14	0.48
14:S:303:LYS:HG2	14:S:305:GLU:H	1.77	0.48
1:A:732:ARG:O	1:A:736:MET:HG2	2.14	0.48
1:A:993:ARG:HG2	1:A:997:LYS:HE3	1.96	0.48
2:B:1174:ASN:HB3	2:B:1177:LYS:HB2	1.96	0.48
2:B:1174:ASN:O	2:B:1178:ASN:N	2.47	0.48
1:A:93:ILE:HD12	1:A:96:ILE:HD12	1.95	0.48
1:A:206:GLY:O	1:A:210:ASN:ND2	2.47	0.48
1:A:884:ILE:HD13	1:A:1023:LEU:HD13	1.96	0.48
2:B:102:GLN:NE2	2:B:184:LYS:O	2.47	0.48
2:B:316:ILE:HG23	2:B:321:VAL:HG13	1.95	0.48
5:E:78:TRP:CD1	5:E:95:PHE:HE1	2.32	0.48
7:G:13:LEU:HD22	7:G:26:LEU:HD21	1.95	0.48
2:B:911:ILE:HG13	2:B:912:ILE:HD12	1.95	0.48
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.78	0.48
14:S:105:MET:HE3	14:S:315:TYR:CE1	2.49	0.48
1:A:20:GLY:N	2:B:1213:ALA:O	2.33	0.47
1:A:1270:MET:HA	1:A:1274:ILE:HG12	1.96	0.47
2:B:489:ARG:NH2	2:B:533:SER:O	2.47	0.47
13:R:27:VAL:HG12	13:R:29:ILE:HG13	1.95	0.47
1:A:95:PHE:CD1	1:A:98:LYS:HD3	2.48	0.47
1:A:254:ASP:HA	2:B:884:ARG:HB2	1.96	0.47
2:B:413:LEU:HB3	2:B:446:ILE:HG12	1.96	0.47
13:R:600:ALA:HA	13:R:603:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HD22	2:B:1199:ALA:HB2	1.97	0.47
1:A:554:VAL:HB	1:A:557:TRP:HB2	1.95	0.47
2:B:612:ILE:HG13	9:I:59:VAL:HG11	1.96	0.47
2:B:760:ASP:OD1	2:B:760:ASP:N	2.43	0.47
9:I:54:GLU:HB3	9:I:100:PHE:CZ	2.49	0.47
2:B:27:GLU:OE2	2:B:679:SER:OG	2.32	0.47
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.48	0.47
14:S:162:LYS:HG3	14:S:166:MET:HE3	1.97	0.47
1:A:1029:ALA:HB3	1:A:1032:ARG:HG3	1.95	0.47
2:B:391:ARG:HD2	2:B:503:LYS:NZ	2.29	0.47
14:S:331:VAL:HG21	14:S:355:LYS:HG3	1.96	0.47
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.42	0.47
13:R:224:ASN:HD21	13:R:803:ILE:HB	1.80	0.47
14:S:166:MET:O	14:S:184:ARG:NH2	2.47	0.47
14:S:79:ILE:HG21	14:S:99:ILE:HG23	1.97	0.47
1:A:351:ARG:NH1	1:A:489:ASN:OD1	2.42	0.47
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47
8:H:107:ASP:N	8:H:107:ASP:OD1	2.48	0.47
13:R:219:PRO:HB2	14:S:220:TYR:HB3	1.97	0.47
14:S:80:LEU:HD12	14:S:364:PRO:HD2	1.96	0.47
2:B:235:LEU:HG	2:B:242:ILE:HG13	1.97	0.46
13:R:60:PRO:HA	13:R:63:HIS:CE1	2.51	0.46
13:R:861:ILE:HD12	14:S:297:PRO:HD2	1.97	0.46
1:A:212:PHE:O	1:A:231:ARG:NH2	2.31	0.46
1:A:415:ASP:OD2	1:A:417:ARG:NH2	2.41	0.46
1:A:421:ARG:HG2	1:A:424:ASP:HB3	1.96	0.46
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.96	0.46
2:B:205:ALA:HB3	2:B:491:THR:HG22	1.96	0.46
9:I:70:ARG:NH1	9:I:82:ASP:OD2	2.49	0.46
12:L:50:CYS:HB3	12:L:55:HIS:H	1.80	0.46
14:S:28:SER:HB3	14:S:41:ASN:HB2	1.98	0.46
1:A:177:LYS:NZ	1:A:179:GLY:O	2.34	0.46
5:E:92:MET:HA	5:E:95:PHE:HB2	1.98	0.46
9:I:54:GLU:HB3	9:I:100:PHE:HZ	1.80	0.46
13:R:583:GLN:OE1	13:R:794:ALA:N	2.37	0.46
13:R:861:ILE:HD13	14:S:298:LEU:HD13	1.96	0.46
1:A:305:MET:HG2	1:A:326:ILE:HD11	1.98	0.46
8:H:56:THR:HB	8:H:144:ARG:HB3	1.97	0.46
13:R:737:PHE:CZ	13:R:748:ALA:HB2	2.50	0.46
14:S:109:LEU:HG	14:S:315:TYR:HB2	1.98	0.46
1:A:5:PRO:O	2:B:1159:ARG:NH1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:ILE:HG21	11:K:102:ASP:HB2	1.98	0.46
13:R:38:TYR:OH	13:R:93:PRO:O	2.34	0.46
1:A:1279:ILE:HD12	1:A:1318:GLU:HB3	1.97	0.46
4:D:85:ASP:N	4:D:88:GLU:OE2	2.49	0.46
4:D:104:LYS:HB3	7:G:105:PRO:HA	1.98	0.46
14:S:102:ARG:HG2	14:S:212:GLY:HA2	1.98	0.46
1:A:1170:ASP:O	1:A:1174:ALA:N	2.45	0.46
2:B:249:LEU:HD13	2:B:261:ILE:HG12	1.97	0.46
5:E:98:ARG:O	5:E:102:LYS:HG2	2.15	0.46
13:R:713:LEU:HD11	13:R:717:HIS:ND1	2.31	0.46
14:S:12:ARG:HD2	14:S:313:ASN:HB2	1.98	0.46
14:S:84:LYS:HD3	14:S:366:TRP:HZ3	1.80	0.46
13:R:622:TYR:N	13:R:704:ASN:OD1	2.41	0.46
1:A:366:GLY:HA3	1:A:470:ARG:HB2	1.98	0.45
1:A:1169:PHE:O	1:A:1172:VAL:HG22	2.16	0.45
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.97	0.45
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.32	0.45
13:R:188:TRP:CG	13:R:191:ILE:HD12	2.50	0.45
14:S:181:ILE:HG23	14:S:184:ARG:HH12	1.81	0.45
1:A:805:TYR:OH	1:A:817:HIS:NE2	2.47	0.45
7:G:41:GLN:C	7:G:80:LYS:HZ3	2.25	0.45
1:A:273:ALA:HA	1:A:276:ASN:HD21	1.80	0.45
1:A:1439:MET:HE1	2:B:1139:ILE:HA	1.97	0.45
14:S:108:LEU:HD12	14:S:318:VAL:HG11	1.99	0.45
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	1.99	0.45
1:A:1343:GLY:O	1:A:1347:THR:OG1	2.27	0.45
2:B:279:ARG:HD3	2:B:284:VAL:HA	1.98	0.45
2:B:879:ARG:HA	2:B:885:LEU:HD11	1.98	0.45
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.45
1:A:292:GLU:HG2	14:S:205:ARG:HG2	1.98	0.45
4:D:88:GLU:O	4:D:92:VAL:HG23	2.16	0.45
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.99	0.45
7:G:121:TYR:HB2	7:G:130:TYR:CE2	2.52	0.45
13:R:380:GLU:HA	13:R:383:LYS:HE2	1.99	0.45
14:S:93:LYS:NZ	14:S:94:THR:O	2.49	0.45
14:S:167:ALA:HB3	14:S:233:LEU:HD13	1.99	0.45
1:A:344:LYS:HD3	1:A:344:LYS:HA	1.78	0.45
4:D:65:LYS:HE2	4:D:65:LYS:HB3	1.78	0.45
13:R:850:TYR:OH	14:S:47:LEU:O	2.29	0.45
1:A:11:LEU:HA	2:B:1193:GLN:HG3	1.99	0.45
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:NH1	1:A:622:THR:OG1	2.37	0.45
2:B:179:ASP:O	2:B:183:MET:HG2	2.17	0.45
1:A:845:ALA:HB2	1:A:1387:ILE:HG23	1.98	0.45
2:B:186:CYS:SG	2:B:783:THR:OG1	2.61	0.45
1:A:1229:MET:SD	1:A:1241:ARG:HB2	2.57	0.45
13:R:88:ILE:HD12	13:R:188:TRP:CZ2	2.52	0.45
13:R:761:ARG:HH21	13:R:763:PRO:HA	1.82	0.45
2:B:547:ILE:HG21	2:B:619:ILE:HG21	2.00	0.44
7:G:38:CYS:HB2	7:G:44:TYR:CD1	2.52	0.44
1:A:114:LEU:HA	1:A:148:CYS:HA	1.99	0.44
1:A:213:LYS:HA	1:A:231:ARG:NH2	2.32	0.44
3:C:49:GLU:HG2	12:L:68:GLN:HG2	1.99	0.44
4:D:167:LYS:HA	4:D:167:LYS:HD3	1.70	0.44
2:B:289:ILE:O	2:B:293:ILE:HG12	2.17	0.44
3:C:25:ASN:HB3	11:K:48:GLU:OE1	2.17	0.44
4:D:118:GLU:OE1	4:D:118:GLU:N	2.49	0.44
13:R:576:TRP:CD1	13:R:586:PRO:HG2	2.52	0.44
14:S:259:CYS:HB3	14:S:264:ILE:HB	1.99	0.44
1:A:958:LEU:HD21	1:A:1019:LEU:HD23	2.00	0.44
7:G:30:LEU:O	7:G:34:VAL:HB	2.17	0.44
13:R:664:MET:HG2	13:R:666:GLY:H	1.82	0.44
14:S:200:ARG:HD2	14:S:207:LYS:HB3	1.99	0.44
5:E:126:VAL:HG12	5:E:129:ALA:HB3	2.00	0.44
13:R:67:LYS:HD2	13:R:67:LYS:O	2.18	0.44
13:R:176:TYR:HD1	13:R:760:LEU:HG	1.83	0.44
13:R:205:GLN:HA	13:R:208:ILE:HD13	2.00	0.44
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.82	0.44
7:G:6:ASP:OD1	7:G:75:ARG:NE	2.51	0.44
14:S:359:VAL:O	14:S:363:ILE:N	2.37	0.44
2:B:315:VAL:HB	13:R:819:TYR:HB3	1.98	0.44
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.99	0.44
13:R:229:ILE:HD12	13:R:248:PHE:HZ	1.82	0.44
13:R:304:VAL:HG11	13:R:353:LYS:HA	2.00	0.44
2:B:49:LEU:HD23	2:B:410:PHE:HD2	1.81	0.44
2:B:58:LEU:HD23	2:B:58:LEU:HA	1.80	0.44
13:R:576:TRP:HE1	13:R:587:SER:HB3	1.82	0.44
1:A:254:ASP:HB2	2:B:883:LEU:HG	2.00	0.44
13:R:562:ILE:O	13:R:566:MET:HG2	2.18	0.44
14:S:97:ARG:NH1	14:S:128:GLY:O	2.50	0.44
14:S:98:ILE:HB	14:S:208:ILE:HG23	1.98	0.44
1:A:92:HIS:NE2	1:A:305:MET:HE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:HIS:HB3	9:I:70:ARG:NH2	2.33	0.43
2:B:1210:MET:HB3	2:B:1212:ILE:HG12	2.00	0.43
13:R:163:GLY:HA3	13:R:625:LEU:HD11	2.00	0.43
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.83	0.43
9:I:17:LYS:NZ	9:I:26:LEU:HD12	2.34	0.43
1:A:272:LYS:O	1:A:276:ASN:ND2	2.51	0.43
2:B:376:ASN:O	2:B:380:LEU:HD23	2.19	0.43
9:I:14:LEU:HD23	9:I:29:CYS:HB2	1.99	0.43
10:J:1:MET:HA	10:J:55:LEU:HB2	2.01	0.43
1:A:92:HIS:CD2	1:A:237:ILE:HD11	2.53	0.43
2:B:733:SER:OG	2:B:735:HIS:O	2.35	0.43
4:D:52:SER:HB3	4:D:143:ALA:HA	1.99	0.43
1:A:351:ARG:HA	1:A:488:MET:O	2.18	0.43
2:B:91:GLU:OE1	12:L:56:ARG:NH1	2.51	0.43
5:E:99:ILE:HD12	5:E:104:PHE:HB2	2.01	0.43
13:R:232:LEU:O	13:R:252:ARG:NH1	2.52	0.43
13:R:596:TYR:OH	13:R:663:ASP:OD2	2.34	0.43
1:A:67:CYS:SG	1:A:80:HIS:HD2	2.29	0.43
2:B:9:ASP:HB3	2:B:10:ASP:H	1.53	0.43
2:B:327:GLY:O	2:B:341:ARG:NH1	2.38	0.43
2:B:957:ASN:ND2	2:B:959:GLU:OE2	2.51	0.43
2:B:1168:LEU:HD11	2:B:1213:ALA:HB1	2.00	0.43
6:F:99:LEU:HG	6:F:103:MET:HE2	2.01	0.43
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.36	0.43
13:R:169:ARG:HH21	13:R:764:VAL:HA	1.83	0.43
1:A:482:ASP:OD1	1:A:482:ASP:N	2.50	0.43
1:A:555:PRO:HD2	1:A:649:ASN:ND2	2.33	0.43
2:B:37:SER:O	2:B:40:GLU:HG3	2.18	0.43
13:R:693:TYR:HE1	13:R:704:ASN:HD22	1.65	0.43
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.01	0.43
1:A:41:MET:HE3	1:A:42:ASP:OD1	2.18	0.43
1:A:568:LYS:HG3	1:A:569:PRO:HA	2.01	0.43
2:B:534:LEU:HD23	2:B:747:MET:SD	2.59	0.43
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.84	0.43
13:R:686:LEU:HA	13:R:689:VAL:HG22	2.01	0.43
13:R:795:LYS:NZ	14:S:176:CYS:O	2.39	0.43
1:A:1124:ARG:NH1	1:A:1304:GLU:OE2	2.51	0.42
1:A:1269:HIS:NE2	1:A:1273:LEU:HD13	2.34	0.42
5:E:95:PHE:O	5:E:99:ILE:HG12	2.18	0.42
5:E:123:ILE:N	5:E:124:PRO:HD2	2.34	0.42
2:B:660:ASP:OD1	2:B:661:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1196:ILE:HD12	2:B:1197:PRO:HD2	1.99	0.42
4:D:95:GLY:O	4:D:99:ASN:N	2.38	0.42
13:R:44:ASN:HB3	13:R:288:TRP:CH2	2.54	0.42
13:R:367:GLY:HA2	13:R:578:LEU:HG	2.01	0.42
14:S:177:THR:HG23	14:S:180:GLU:H	1.84	0.42
14:S:219:ASP:N	14:S:219:ASP:OD1	2.52	0.42
1:A:958:LEU:HD23	1:A:958:LEU:HA	1.87	0.42
13:R:568:GLN:HA	13:R:609:LEU:HD13	2.00	0.42
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.54	0.42
5:E:89:ILE:HG13	5:E:92:MET:SD	2.59	0.42
13:R:371:LEU:HD13	13:R:607:SER:HA	2.01	0.42
14:S:198:ILE:HG22	14:S:209:LEU:HD11	2.00	0.42
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.78	0.42
13:R:162:PRO:HB3	13:R:198:ALA:HB1	2.02	0.42
13:R:251:LEU:HD13	13:R:288:TRP:NE1	2.34	0.42
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	2.01	0.42
7:G:119:LEU:HD11	7:G:130:TYR:O	2.19	0.42
2:B:319:LYS:HE2	2:B:323:LEU:HD11	2.02	0.42
13:R:251:LEU:HD13	13:R:288:TRP:HE1	1.84	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.91	0.42
1:A:913:VAL:HG23	1:A:914:ILE:HG23	2.01	0.42
2:B:101:PRO:HG2	2:B:172:LEU:HD11	2.01	0.42
2:B:333:ALA:HB2	13:R:854:GLN:H	1.85	0.42
3:C:47:LEU:HB3	3:C:158:ILE:HB	2.01	0.42
5:E:151:LYS:HE2	5:E:153:ILE:HD11	2.01	0.42
14:S:242:TYR:HA	14:S:245:MET:CE	2.49	0.42
14:S:271:PHE:HB2	14:S:280:THR:H	1.85	0.42
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.43	0.42
1:A:119:ASN:ND2	1:A:121:THR:OG1	2.52	0.42
1:A:448:GLN:NE2	2:B:1134:GLU:OE2	2.46	0.42
1:A:1335:PHE:HA	1:A:1338:ILE:HB	2.01	0.42
2:B:634:GLU:OE2	2:B:635:ASP:N	2.52	0.42
2:B:1207:LEU:O	2:B:1210:MET:HB2	2.19	0.42
5:E:74:LEU:HD12	5:E:74:LEU:HA	1.91	0.42
14:S:262:LEU:HD23	14:S:264:ILE:HD11	2.01	0.42
1:A:1207:LYS:HA	1:A:1207:LYS:HD3	1.79	0.41
9:I:71:SER:OG	9:I:72:ASP:N	2.53	0.41
14:S:25:ALA:HB3	14:S:198:ILE:HB	2.01	0.41
1:A:790:LYS:NZ	9:I:67:THR:OG1	2.49	0.41
2:B:864:LYS:HE3	2:B:872:GLU:OE1	2.20	0.41
4:D:173:ARG:O	4:D:177:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:MET:HE2	1:A:850:MET:HB3	1.96	0.41
2:B:40:GLU:HG2	2:B:540:ILE:HG23	2.03	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.55	0.41
5:E:60:LEU:HD12	5:E:77:LEU:O	2.21	0.41
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.88	0.41
13:R:297:TYR:CE1	13:R:809:LEU:HD21	2.56	0.41
13:R:388:ILE:HD13	13:R:388:ILE:HA	1.94	0.41
14:S:206:ILE:HG12	14:S:323:ASN:ND2	2.33	0.41
2:B:371:LEU:HD12	2:B:371:LEU:HA	1.90	0.41
13:R:182:LEU:HD12	13:R:188:TRP:HE3	1.85	0.41
2:B:608:ILE:HG23	2:B:617:PHE:HE1	1.85	0.41
3:C:125:GLY:HA2	3:C:126:ASN:HA	1.80	0.41
13:R:335:LEU:HD23	13:R:338:LEU:HG	2.03	0.41
14:S:20:GLN:HA	14:S:21:PRO:HD3	1.93	0.41
1:A:427:LEU:HD23	1:A:431:TRP:HE3	1.85	0.41
1:A:569:PRO:HD2	8:H:46:MET:HE3	2.02	0.41
1:A:1236:ASP:OD1	1:A:1236:ASP:N	2.51	0.41
2:B:640:ASP:OD1	2:B:640:ASP:N	2.53	0.41
11:K:47:ARG:NH2	11:K:48:GLU:HB2	2.35	0.41
13:R:192:GLU:OE2	13:R:742:SER:OG	2.37	0.41
1:A:107:CYS:HB2	1:A:148:CYS:SG	2.60	0.41
1:A:588:HIS:HA	1:A:608:ILE:O	2.21	0.41
2:B:308:PRO:HA	2:B:311:GLU:HG3	2.01	0.41
2:B:336:ILE:HD12	2:B:336:ILE:H	1.86	0.41
5:E:133:THR:O	5:E:185:ARG:NH2	2.54	0.41
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.46	0.41
1:A:46:GLN:O	1:A:47:ARG:HG2	2.21	0.41
1:A:456:MET:SD	2:B:1138:MET:HE3	2.61	0.41
1:A:748:VAL:HG21	1:A:759:ILE:HD11	2.02	0.41
2:B:108:ASN:HA	2:B:198:GLY:HA3	2.03	0.41
2:B:183:MET:HE2	2:B:183:MET:HB3	1.87	0.41
2:B:609:ILE:HD13	2:B:693:GLU:HG3	2.03	0.41
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.37	0.41
13:R:746:GLY:HA3	13:R:787:LYS:O	2.20	0.41
1:A:138:VAL:O	1:A:142:CYS:HB2	2.21	0.41
1:A:347:ASP:N	1:A:347:ASP:OD1	2.53	0.41
1:A:610:ASP:OD1	1:A:971:GLN:NE2	2.54	0.41
1:A:747:MET:SD	2:B:1018:PRO:HG3	2.61	0.41
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.89	0.41
2:B:557:GLU:HA	2:B:558:PRO:HD3	1.97	0.41
4:D:152:ASP:N	4:D:152:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:VAL:HG12	5:E:126:VAL:O	2.21	0.41
7:G:55:ASP:OD1	7:G:55:ASP:N	2.48	0.41
8:H:101:TYR:CZ	8:H:114:TYR:HB3	2.55	0.41
13:R:58:VAL:HG13	13:R:58:VAL:O	2.21	0.41
13:R:248:PHE:HD2	13:R:291:LEU:HD12	1.84	0.41
13:R:401:GLU:HB3	13:R:405:ARG:HH12	1.85	0.41
13:R:663:ASP:HB3	13:R:674:ILE:HB	2.02	0.41
13:R:723:LEU:HD23	13:R:723:LEU:HA	1.90	0.41
13:R:725:LYS:O	13:R:729:GLU:HB2	2.21	0.41
13:R:751:LEU:HD23	13:R:751:LEU:HA	1.90	0.41
14:S:249:GLU:OE2	14:S:250:LYS:HE3	2.20	0.41
14:S:334:LEU:HD13	14:S:346:LEU:HD13	2.03	0.41
1:A:89:PRO:HB3	1:A:238:THR:HG22	2.03	0.41
1:A:785:LEU:HD23	1:A:785:LEU:HA	1.94	0.41
1:A:1031:ARG:NE	1:A:1035:GLU:OE1	2.54	0.41
2:B:219:LYS:HD2	2:B:219:LYS:HA	1.88	0.41
2:B:291:GLN:HG2	2:B:564:PRO:HG2	2.03	0.41
2:B:1166:CYS:SG	2:B:1167:GLY:N	2.93	0.41
4:D:64:LEU:HD23	4:D:67:ARG:HE	1.85	0.41
5:E:176:ARG:HD3	5:E:214:LEU:HD21	2.03	0.41
8:H:135:LYS:HB2	8:H:135:LYS:HE3	1.78	0.41
9:I:42:LYS:NZ	9:I:45:ARG:HB2	2.36	0.41
10:J:48:MET:HB3	10:J:48:MET:HE3	1.75	0.41
13:R:5:ALA:O	13:R:9:TRP:N	2.44	0.41
13:R:66:HIS:HB3	13:R:279:LEU:HB3	2.02	0.41
13:R:105:ALA:HB3	13:R:110:MET:HE3	2.03	0.41
13:R:335:LEU:HD12	13:R:597:ALA:HB1	2.02	0.41
1:A:21:LEU:HD13	1:A:234:TRP:HB2	2.02	0.40
2:B:333:ALA:HB2	13:R:854:GLN:N	2.35	0.40
2:B:452:TYR:O	2:B:456:THR:HG22	2.20	0.40
2:B:1155:SER:OG	2:B:1156:ASP:N	2.54	0.40
3:C:65:ARG:NH1	10:J:3:ILE:O	2.45	0.40
3:C:239:LYS:HB2	3:C:239:LYS:HE3	1.95	0.40
4:D:115:PHE:HE2	4:D:124:VAL:HG21	1.87	0.40
7:G:153:ASP:O	7:G:155:ASN:N	2.53	0.40
14:S:239:ILE:HA	14:S:244:ASP:HB3	2.02	0.40
2:B:480:THR:HG23	2:B:483:SER:H	1.86	0.40
3:C:32:LEU:HG	3:C:36:MET:CE	2.51	0.40
5:E:3:ASP:OD1	5:E:4:ASN:N	2.53	0.40
10:J:1:MET:HE3	10:J:1:MET:HB2	1.82	0.40
14:S:110:THR:HG21	14:S:254:ARG:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ALA:HB1	13:R:853:ARG:HB2	2.03	0.40
2:B:1076:HIS:O	3:C:30:ASN:ND2	2.54	0.40
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.21	0.40
3:C:198:LYS:HE2	3:C:198:LYS:HB2	1.94	0.40
13:R:193:VAL:CG2	13:R:712:VAL:HB	2.51	0.40
14:S:119:PHE:HA	14:S:138:TYR:CE2	2.57	0.40
14:S:232:GLU:OE2	14:S:267:ILE:HG23	2.21	0.40
1:A:100:LYS:HD3	1:A:177:LYS:HB2	2.03	0.40
1:A:229:TYR:HB3	2:B:1215:ARG:NH1	2.37	0.40
13:R:537:LEU:HD13	13:R:542:TYR:HB2	2.04	0.40
1:A:403:ALA:HA	1:A:435:ARG:HA	2.03	0.40
1:A:1140:ILE:HD11	1:A:1319:VAL:HG22	2.03	0.40
2:B:841:MET:HE3	2:B:1010:LEU:HD21	2.03	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	1370/1743 (79%)	1320 (96%)	48 (4%)	2 (0%)	48	78
2	B	1119/1227 (91%)	1081 (97%)	37 (3%)	1 (0%)	48	78
3	C	261/304 (86%)	255 (98%)	6 (2%)	0	100	100
4	D	116/186 (62%)	110 (95%)	6 (5%)	0	100	100
5	E	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
6	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
8	H	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
9	I	109/115 (95%)	102 (94%)	7 (6%)	0	100	100
10	J	64/72 (89%)	62 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
13	R	683/1006 (68%)	650 (95%)	32 (5%)	1 (0%)	48	78
14	S	376/384 (98%)	370 (98%)	6 (2%)	0	100	100
All	All	4843/5912 (82%)	4670 (96%)	169 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	501	LEU
1	A	960	VAL
13	R	21	VAL
1	A	47	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1205/1528 (79%)	1205 (100%)	0	100	100
2	B	992/1077 (92%)	992 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	104/160 (65%)	104 (100%)	0	100	100
5	E	196/197 (100%)	196 (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%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	R	628/881 (71%)	628 (100%)	0	100	100
14	S	345/348 (99%)	345 (100%)	0	100	100
All	All	4357/5210 (84%)	4357 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
1	A	119	ASN
1	A	274	ASN
1	A	276	ASN
1	A	577	GLN
1	A	649	ASN
1	A	692	GLN
1	A	737	ASN
1	A	936	GLN
1	A	1021	GLN
1	A	1213	GLN
2	B	270	GLN
2	B	298	ASN
2	B	317	GLN
2	B	343	GLN
2	B	458	ASN
2	B	506	GLN
2	B	770	GLN
2	B	946	ASN
2	B	986	GLN
2	B	1179	GLN
3	C	167	HIS
4	D	144	GLN
5	E	4	ASN
5	E	53	GLN
5	E	120	ASN
6	F	127	GLN
7	G	53	ASN
8	H	13	GLN
8	H	136	GLN
9	I	31	ASN
13	R	49	ASN
13	R	111	ASN

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Mol	Chain	Res	Type
13	R	235	ASN
13	R	624	GLN
13	R	719	HIS
13	R	811	GLN
14	S	299	ASN
14	S	301	GLN
14	S	340	ASN
14	S	356	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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.

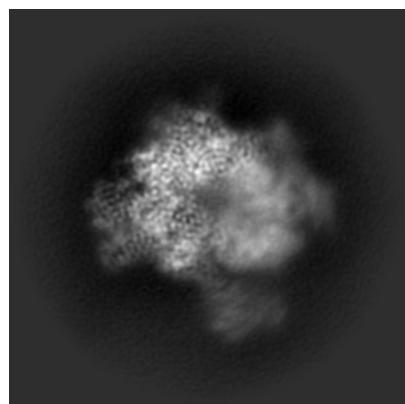
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39227. These allow visual inspection of the internal detail of the map and identification of artifacts.

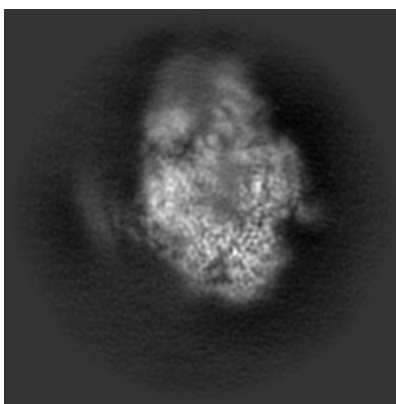
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

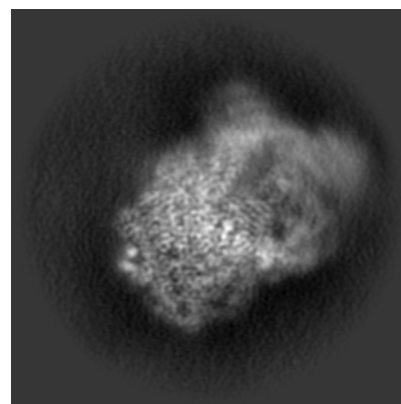
6.1.1 Primary map



X

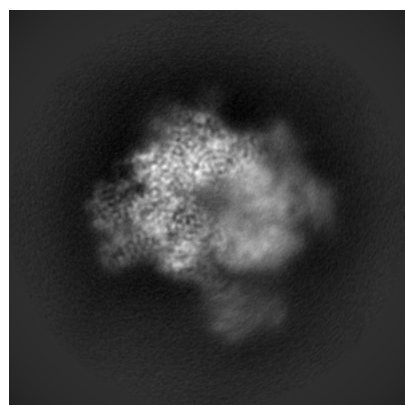


Y

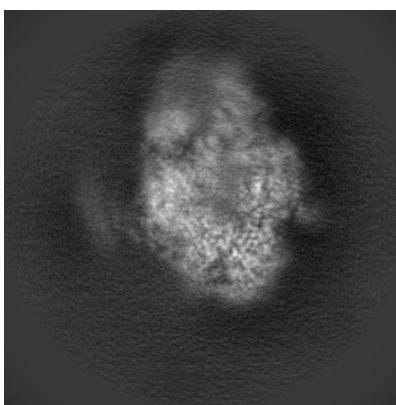


Z

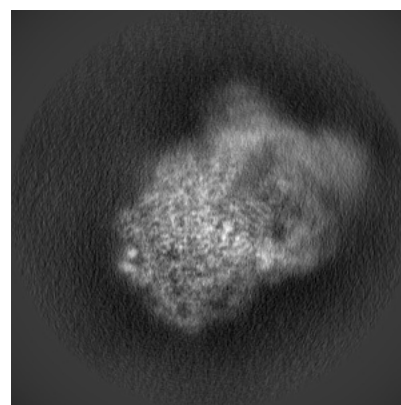
6.1.2 Raw map



X



Y

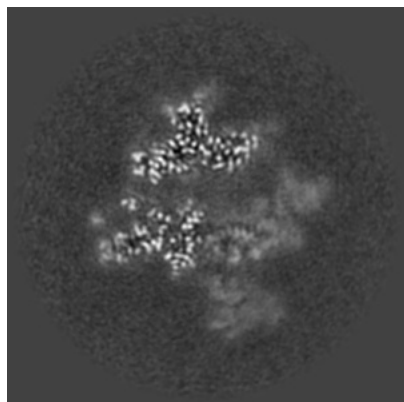


Z

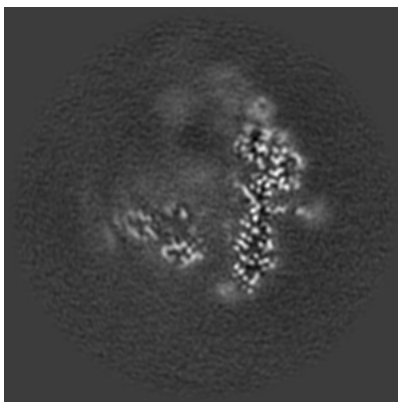
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

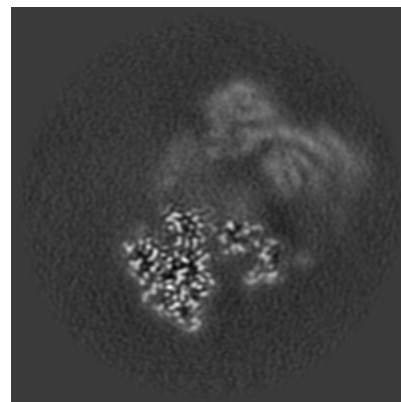
6.2.1 Primary map



X Index: 160

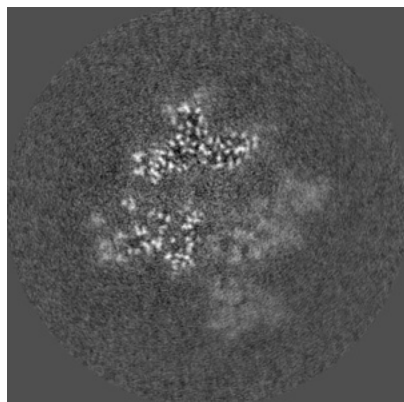


Y Index: 160

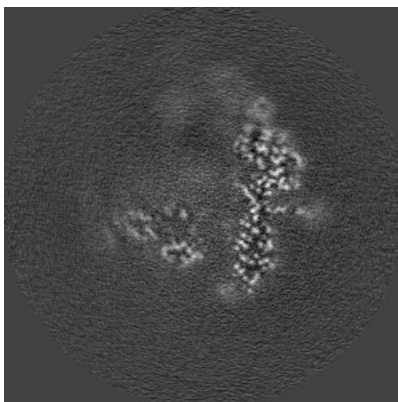


Z Index: 160

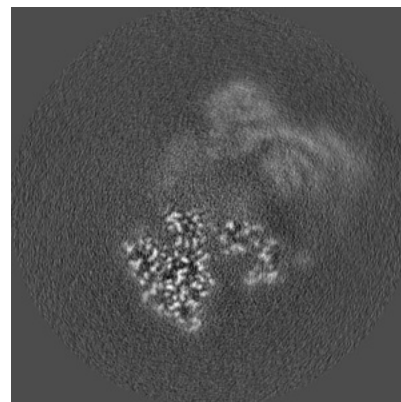
6.2.2 Raw map



X Index: 160



Y Index: 160

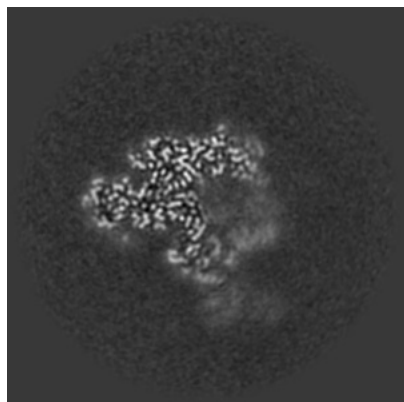


Z Index: 160

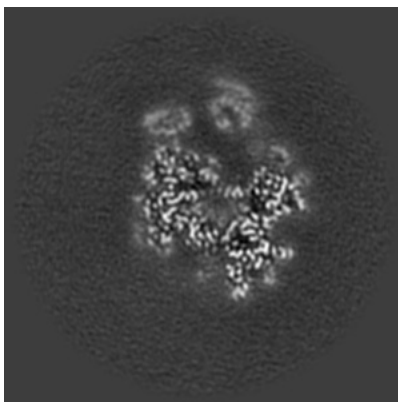
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

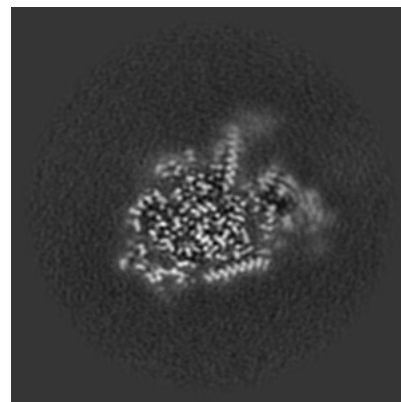
6.3.1 Primary map



X Index: 140

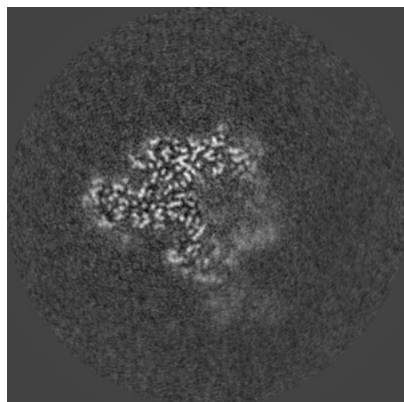


Y Index: 139

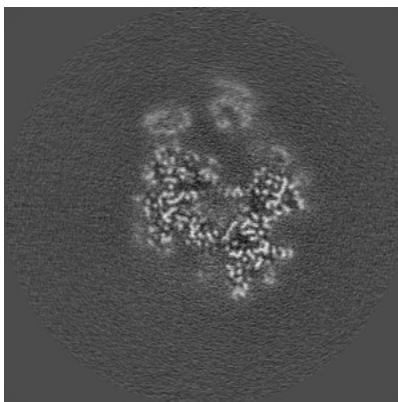


Z Index: 202

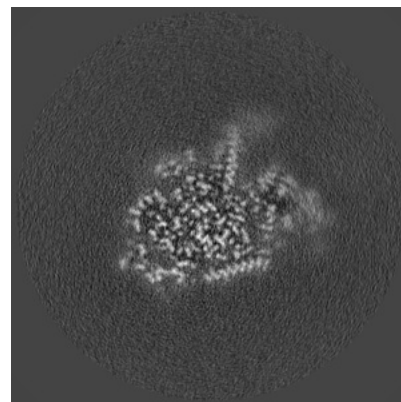
6.3.2 Raw map



X Index: 140



Y Index: 139

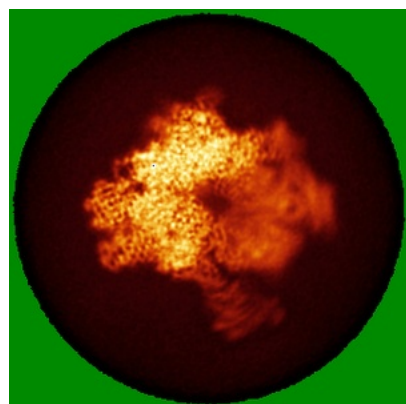


Z Index: 202

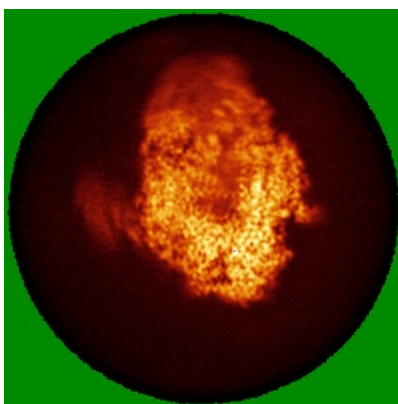
The images above show the largest variance slices of the map in three orthogonal directions.

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

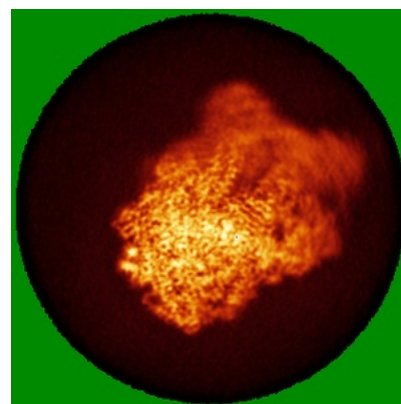
6.4.1 Primary map



X

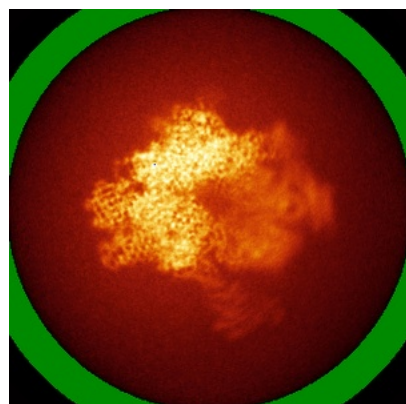


Y

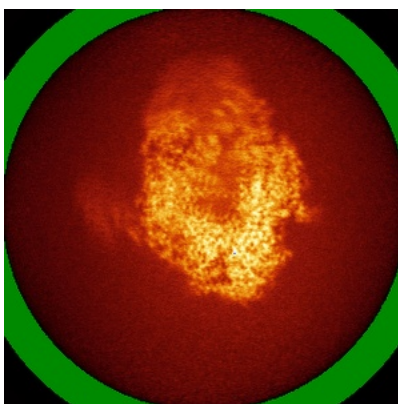


Z

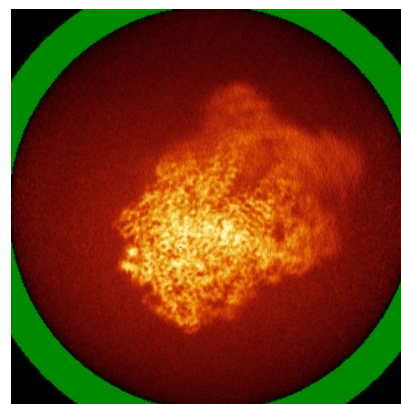
6.4.2 Raw map



X



Y

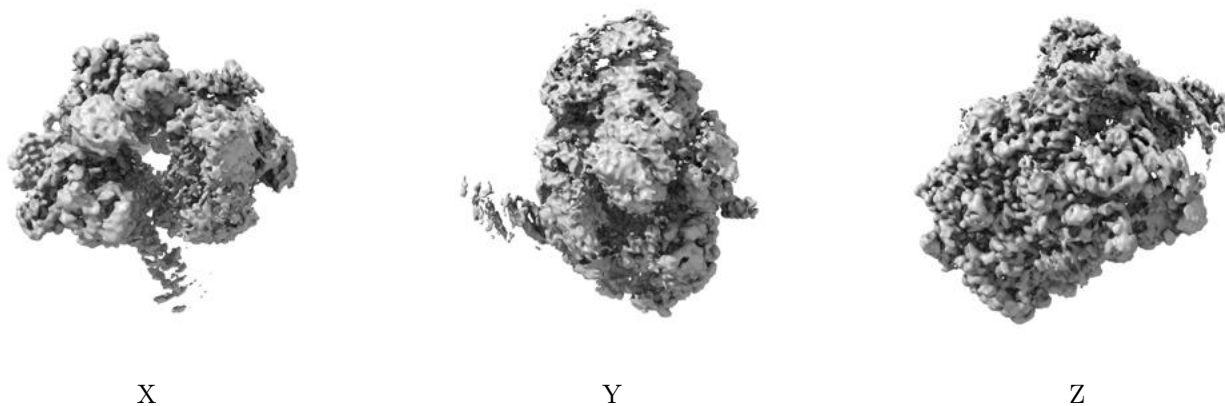


Z

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.

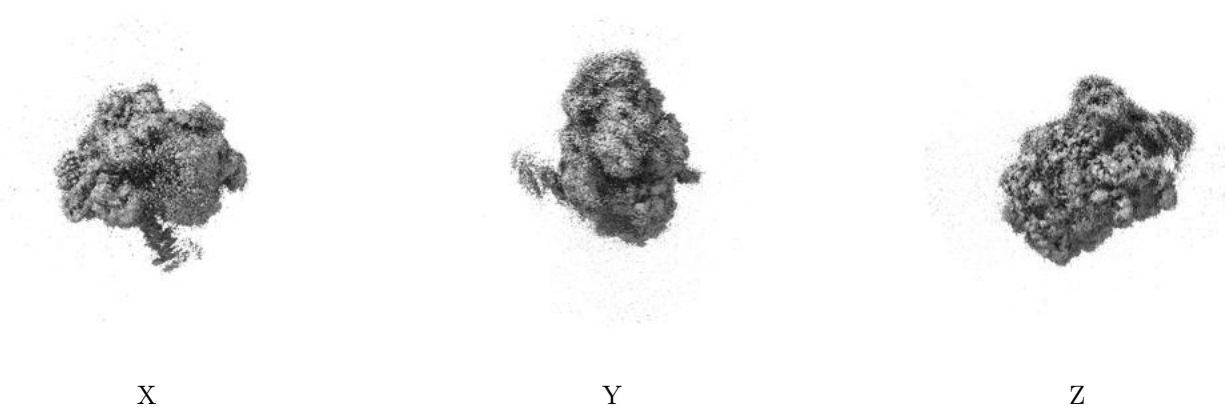
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

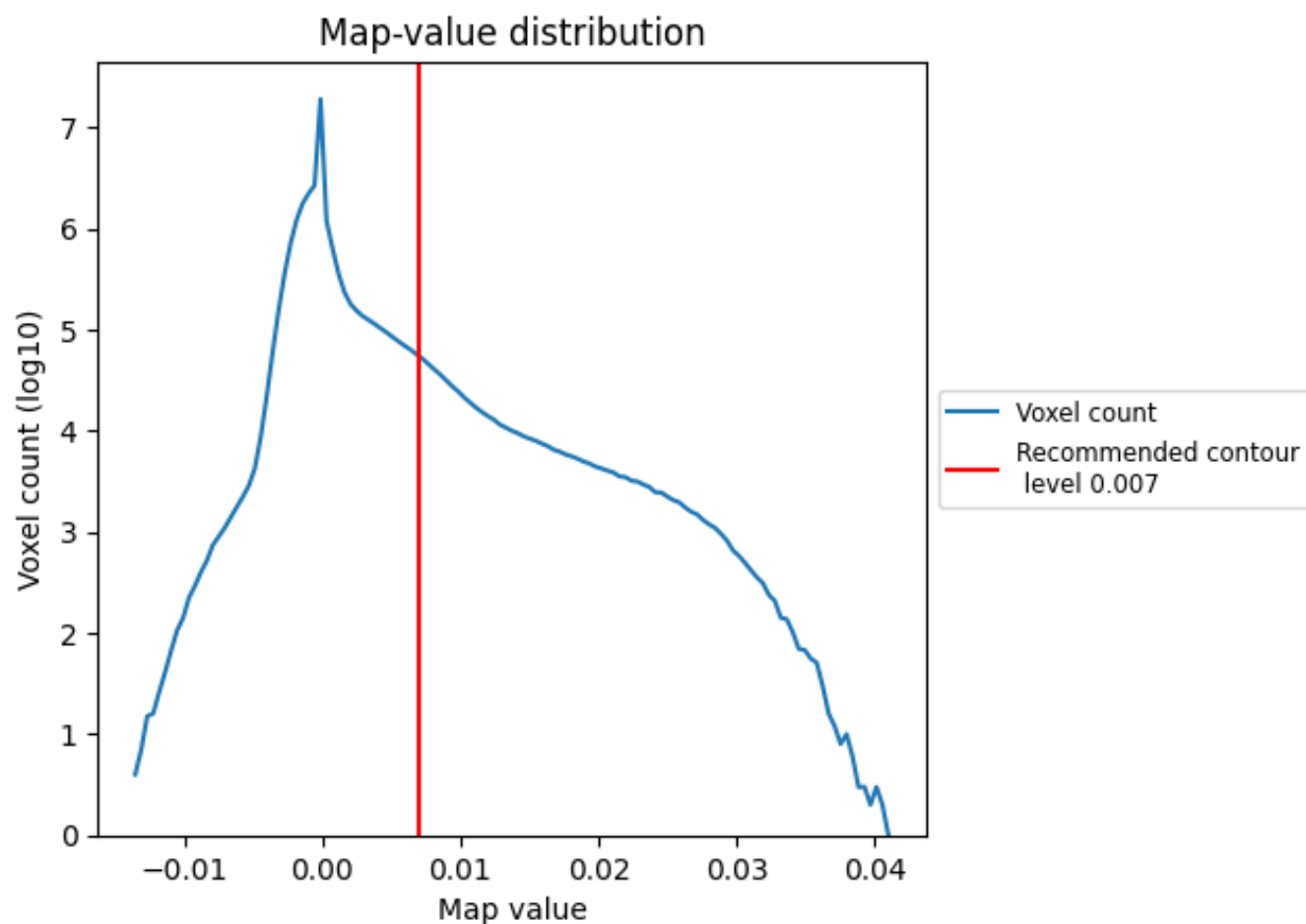
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

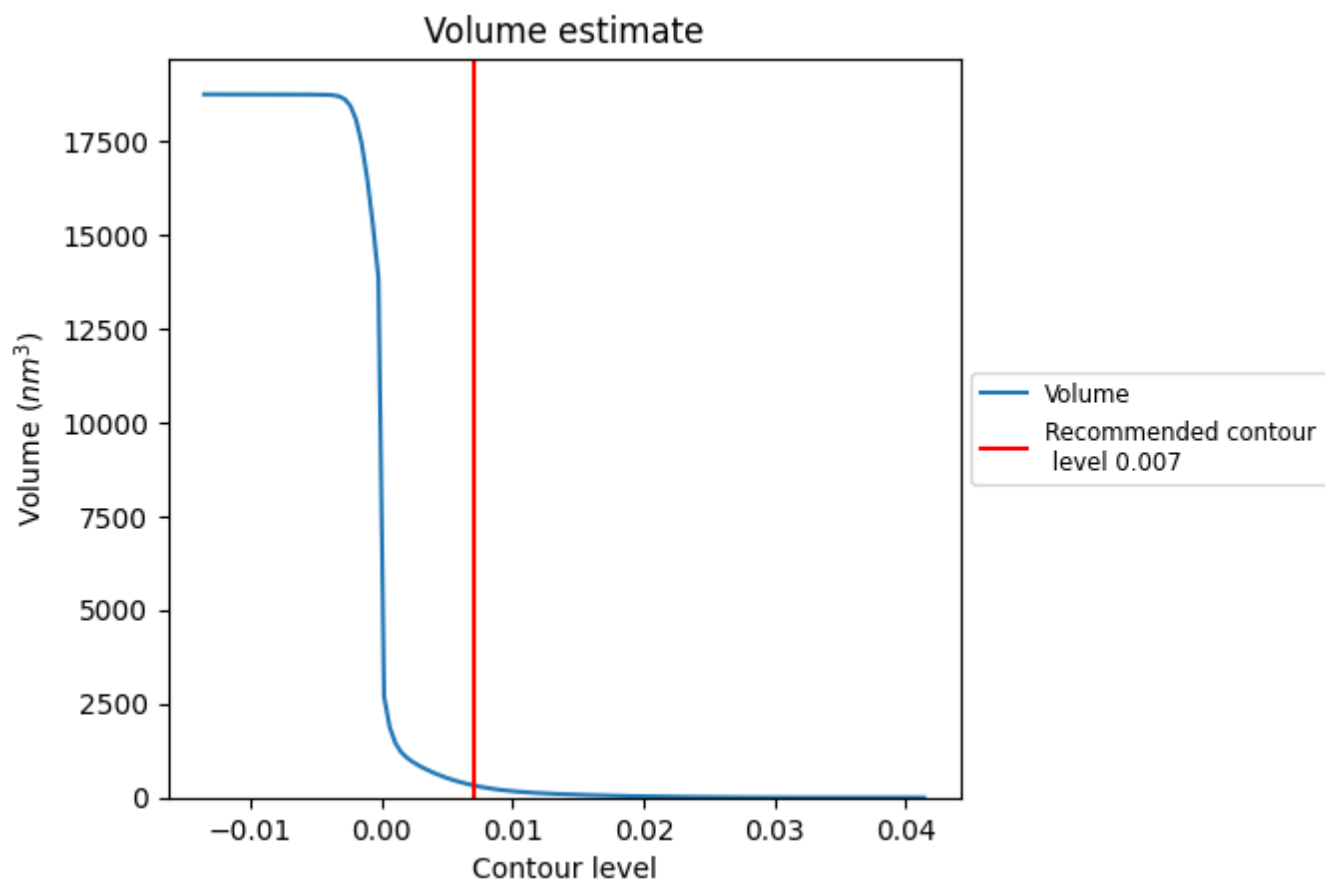
This section contains the results of statistical analysis of the map.

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.

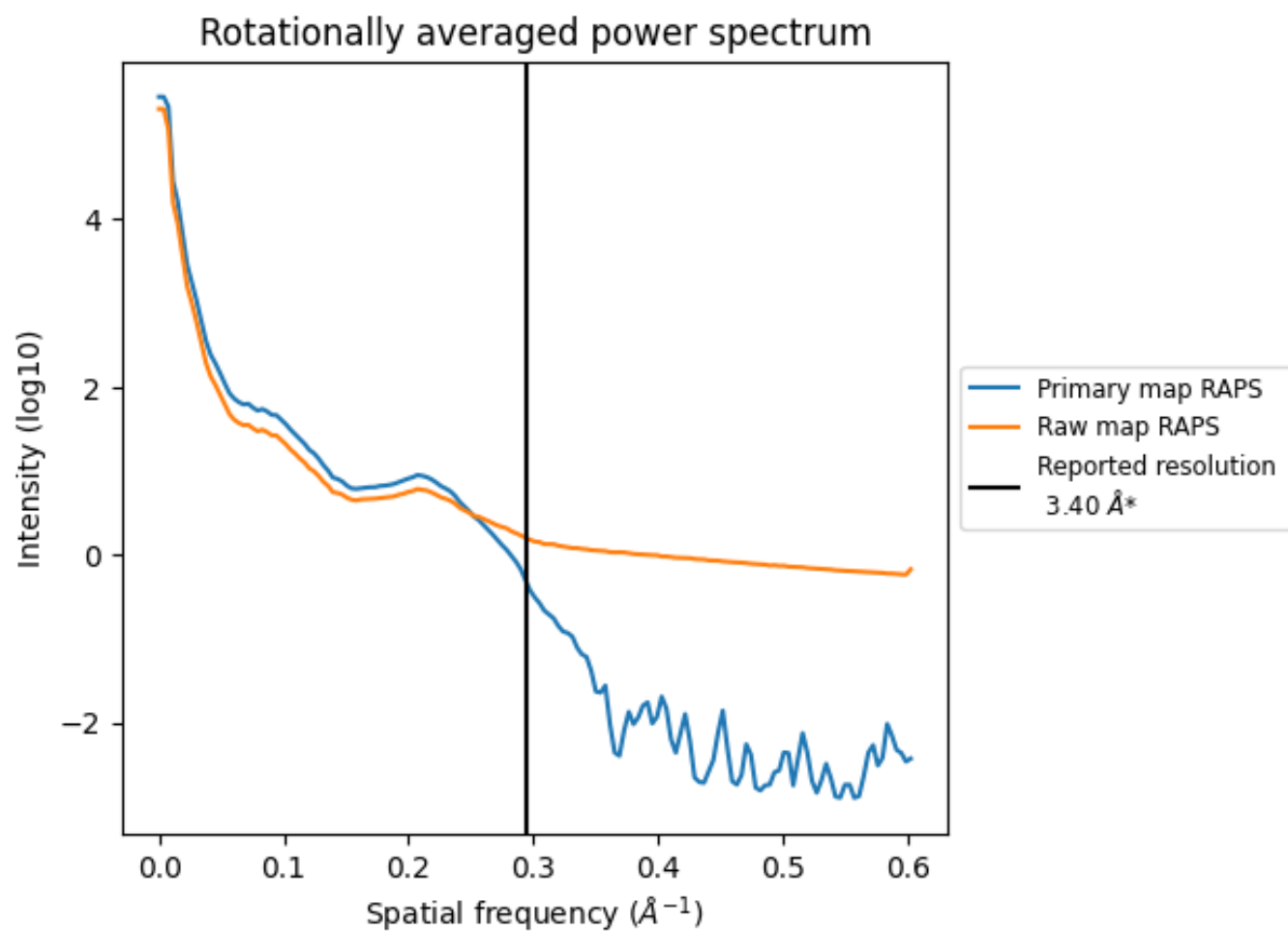
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 295 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 ⓘ

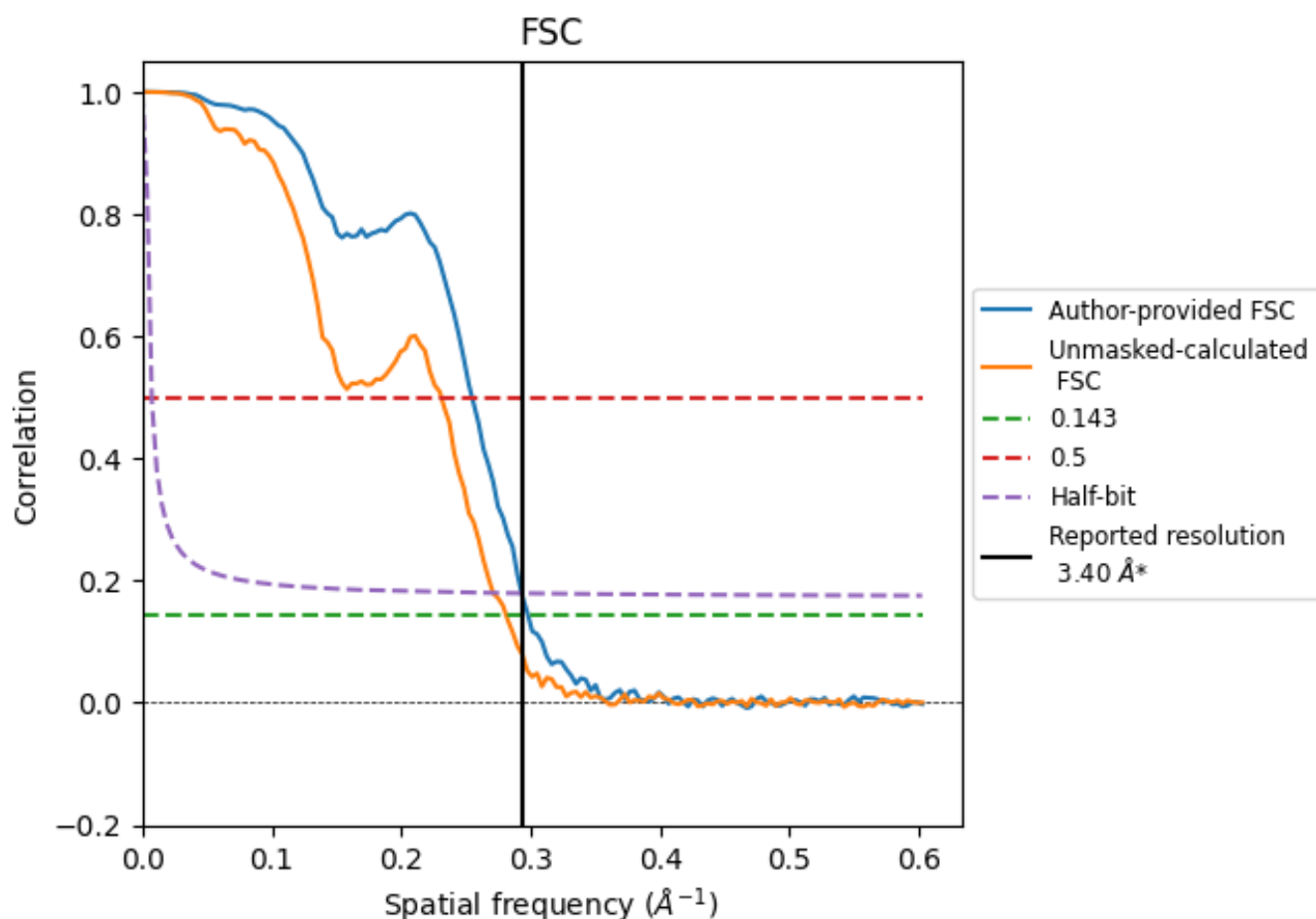


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

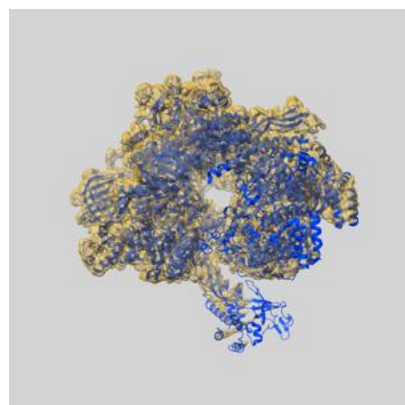
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.93	3.41
Unmasked-calculated*	3.56	4.33	3.69

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

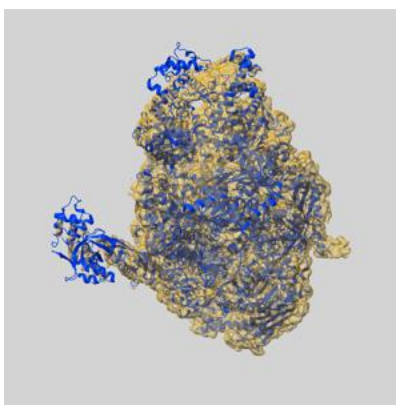
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39227 and PDB model 8YFR. Per-residue inclusion information can be found in section 3 on page 8.

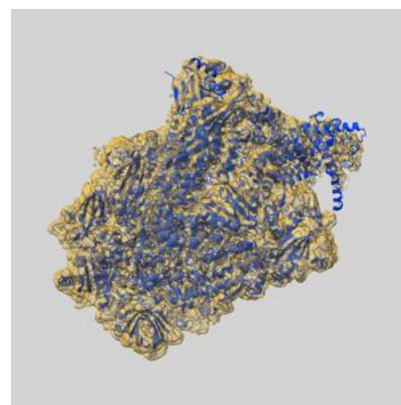
9.1 Map-model overlay [i](#)



X



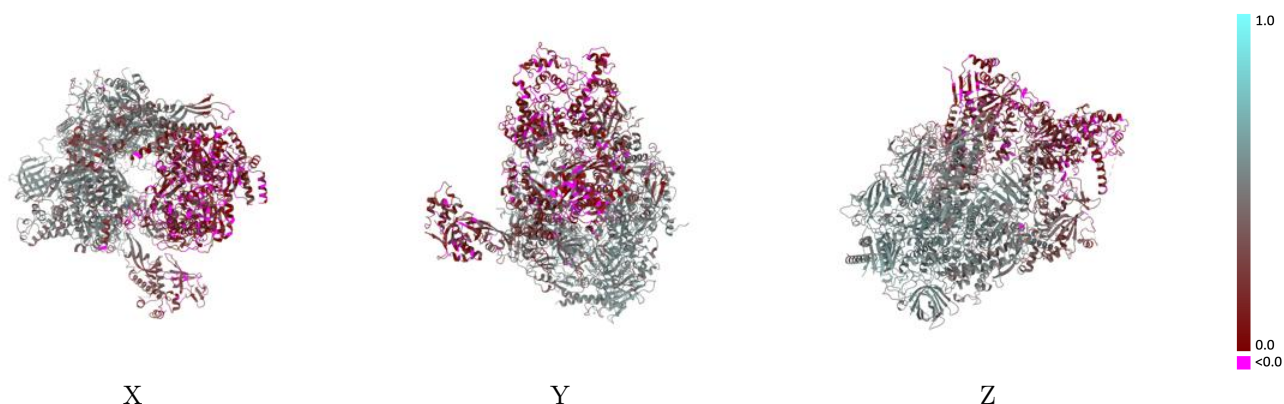
Y



Z

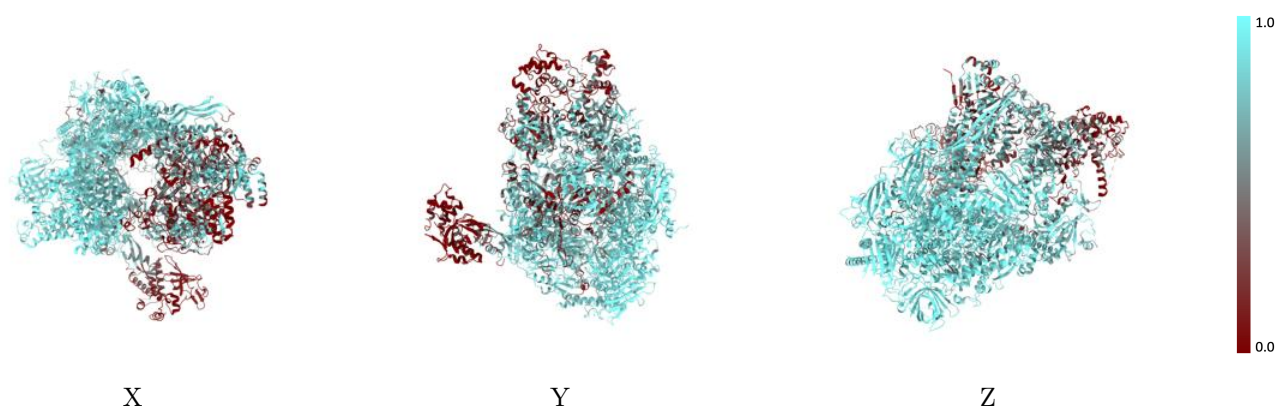
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



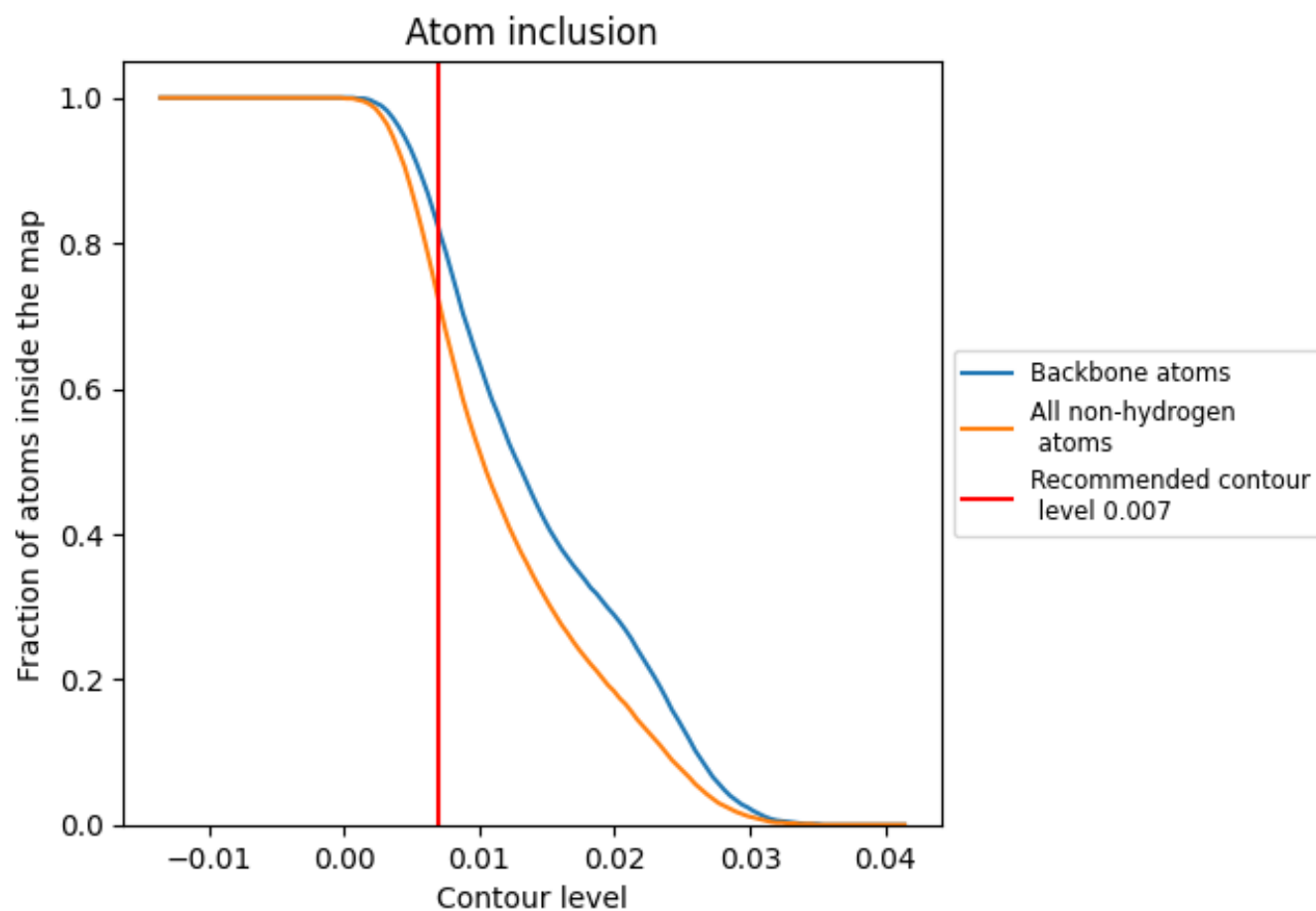
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.3660
A	 0.8010	 0.4170
B	 0.8650	 0.4760
C	 0.9360	 0.5310
D	 0.0970	 0.1920
E	 0.8770	 0.4400
F	 0.9360	 0.5220
G	 0.2740	 0.2480
H	 0.9570	 0.5160
I	 0.7990	 0.3850
J	 0.9660	 0.5450
K	 0.8440	 0.5070
L	 0.9430	 0.4710
R	 0.3690	 0.1060
S	 0.5480	 0.1180

