Full wwPDB EM Validation Report

Feb 13, 2024 – 07:42 pm GMT

PDB ID	:	8POH
EMDB ID	:	EMD-17792
Title	:	Influenza A/H7N9 polymerase symmetric dimer bound to the promoter (PA K289A/C489R)
Authors	:	Arragain, B.; Cusack, S.
Deposited on	:	2023-07-04
Resolution	:	3.30 Å(reported)
Based on initial model	:	7Z4O

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 (i) 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 (i)) were used in the production of this report:

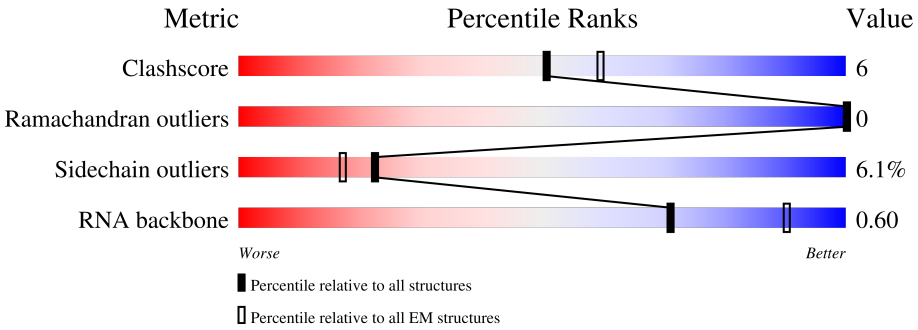
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	729	7% 60% 10% · 29%
1	E	729	29% 60% 9% · 29%
2	B	757	8% 71% 10% 18%
2	F	757	65% 66% 14% · 18%
3	C	788	9% 12% · 85%
3	G	788	6% 9% · 89%
4	R	51	10% 8% · 90%

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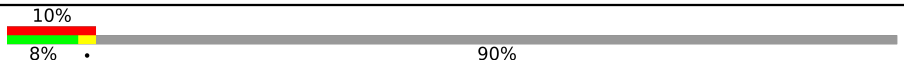
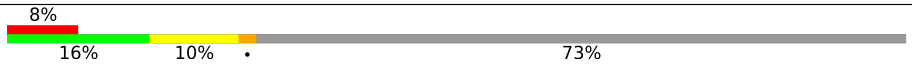
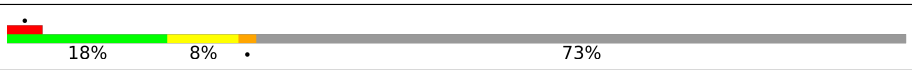
Mol	Chain	Length	Quality of chain
4	S	51	
4	U	51	
4	V	51	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20729 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total	C	N	O	S	1	0
			4155	2631	706	789	29		
1	E	515	Total	C	N	O	S	1	0
			4155	2631	706	789	29		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP M9TI86
A	-11	HIS	-	expression tag	UNP M9TI86
A	-10	HIS	-	expression tag	UNP M9TI86
A	-9	HIS	-	expression tag	UNP M9TI86
A	-8	HIS	-	expression tag	UNP M9TI86
A	-7	HIS	-	expression tag	UNP M9TI86
A	-6	HIS	-	expression tag	UNP M9TI86
A	-5	HIS	-	expression tag	UNP M9TI86
A	-4	HIS	-	expression tag	UNP M9TI86
A	-3	GLY	-	expression tag	UNP M9TI86
A	-2	SER	-	expression tag	UNP M9TI86
A	-1	GLY	-	expression tag	UNP M9TI86
A	0	SER	-	expression tag	UNP M9TI86
A	289	ALA	LYS	conflict	UNP M9TI86
A	489	ARG	CYS	engineered mutation	UNP M9TI86
E	-12	MET	-	initiating methionine	UNP M9TI86
E	-11	HIS	-	expression tag	UNP M9TI86
E	-10	HIS	-	expression tag	UNP M9TI86
E	-9	HIS	-	expression tag	UNP M9TI86
E	-8	HIS	-	expression tag	UNP M9TI86
E	-7	HIS	-	expression tag	UNP M9TI86
E	-6	HIS	-	expression tag	UNP M9TI86
E	-5	HIS	-	expression tag	UNP M9TI86
E	-4	HIS	-	expression tag	UNP M9TI86
E	-3	GLY	-	expression tag	UNP M9TI86
E	-2	SER	-	expression tag	UNP M9TI86

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP M9TI86
E	0	SER	-	expression tag	UNP M9TI86
E	289	ALA	LYS	conflict	UNP M9TI86
E	489	ARG	CYS	engineered mutation	UNP M9TI86

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	623	Total	C	N	O	S	0	0
			4954	3125	860	932	37		
2	F	623	Total	C	N	O	S	1	0
			4966	3134	861	934	37		

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			978	625	172	172	9		
3	G	84	Total	C	N	O	S	0	0
			694	442	122	123	7		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLY	-	expression tag	UNP X5F427
C	761	TRP	-	expression tag	UNP X5F427
C	762	SER	-	expression tag	UNP X5F427
C	763	HIS	-	expression tag	UNP X5F427
C	764	PRO	-	expression tag	UNP X5F427
C	765	GLN	-	expression tag	UNP X5F427
C	766	PHE	-	expression tag	UNP X5F427
C	767	GLU	-	expression tag	UNP X5F427
C	768	LYS	-	expression tag	UNP X5F427
C	769	GLY	-	expression tag	UNP X5F427
C	770	GLY	-	expression tag	UNP X5F427
C	771	GLY	-	expression tag	UNP X5F427
C	772	SER	-	expression tag	UNP X5F427
C	773	GLY	-	expression tag	UNP X5F427
C	774	GLY	-	expression tag	UNP X5F427
C	775	GLY	-	expression tag	UNP X5F427
C	776	SER	-	expression tag	UNP X5F427
C	777	GLY	-	expression tag	UNP X5F427

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	GLY	-	expression tag	UNP X5F427
C	779	SER	-	expression tag	UNP X5F427
C	780	ALA	-	expression tag	UNP X5F427
C	781	TRP	-	expression tag	UNP X5F427
C	782	SER	-	expression tag	UNP X5F427
C	783	HIS	-	expression tag	UNP X5F427
C	784	PRO	-	expression tag	UNP X5F427
C	785	GLN	-	expression tag	UNP X5F427
C	786	PHE	-	expression tag	UNP X5F427
C	787	GLU	-	expression tag	UNP X5F427
C	788	LYS	-	expression tag	UNP X5F427
G	760	GLY	-	expression tag	UNP X5F427
G	761	TRP	-	expression tag	UNP X5F427
G	762	SER	-	expression tag	UNP X5F427
G	763	HIS	-	expression tag	UNP X5F427
G	764	PRO	-	expression tag	UNP X5F427
G	765	GLN	-	expression tag	UNP X5F427
G	766	PHE	-	expression tag	UNP X5F427
G	767	GLU	-	expression tag	UNP X5F427
G	768	LYS	-	expression tag	UNP X5F427
G	769	GLY	-	expression tag	UNP X5F427
G	770	GLY	-	expression tag	UNP X5F427
G	771	GLY	-	expression tag	UNP X5F427
G	772	SER	-	expression tag	UNP X5F427
G	773	GLY	-	expression tag	UNP X5F427
G	774	GLY	-	expression tag	UNP X5F427
G	775	GLY	-	expression tag	UNP X5F427
G	776	SER	-	expression tag	UNP X5F427
G	777	GLY	-	expression tag	UNP X5F427
G	778	GLY	-	expression tag	UNP X5F427
G	779	SER	-	expression tag	UNP X5F427
G	780	ALA	-	expression tag	UNP X5F427
G	781	TRP	-	expression tag	UNP X5F427
G	782	SER	-	expression tag	UNP X5F427
G	783	HIS	-	expression tag	UNP X5F427
G	784	PRO	-	expression tag	UNP X5F427
G	785	GLN	-	expression tag	UNP X5F427
G	786	PHE	-	expression tag	UNP X5F427
G	787	GLU	-	expression tag	UNP X5F427
G	788	LYS	-	expression tag	UNP X5F427

- Molecule 4 is a RNA chain called 51-mer vRNA loop (v51_mut_S).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	5	Total	C	N	O	P	0	0
			103	46	16	36	5		
4	V	14	Total	C	N	O	P	0	0
			310	138	65	93	14		
4	S	5	Total	C	N	O	P	0	0
			103	46	16	36	5		
4	U	14	Total	C	N	O	P	0	0
			310	138	65	93	14		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

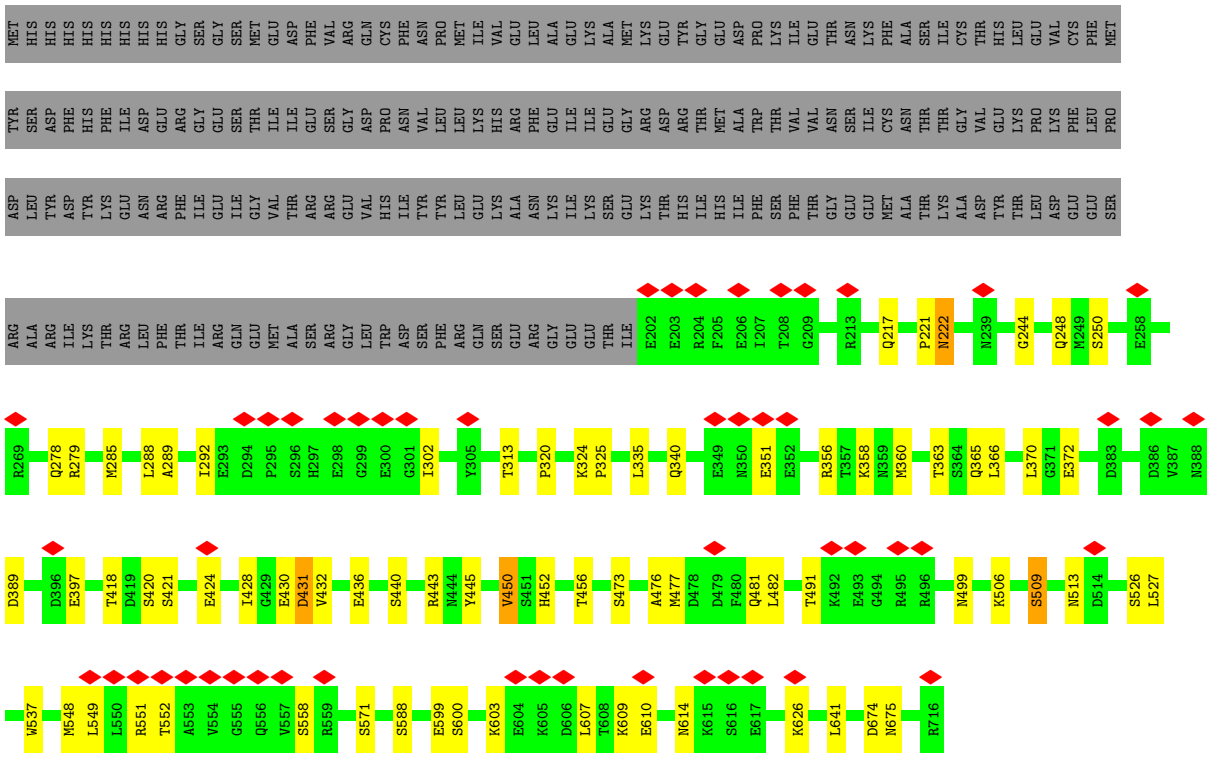
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

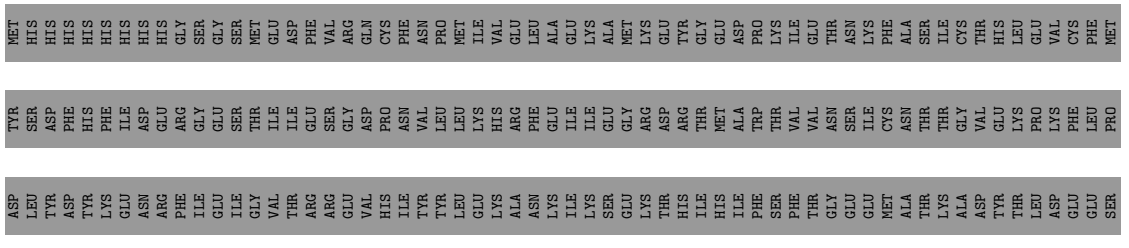
• Molecule 1: Polymerase acidic protein

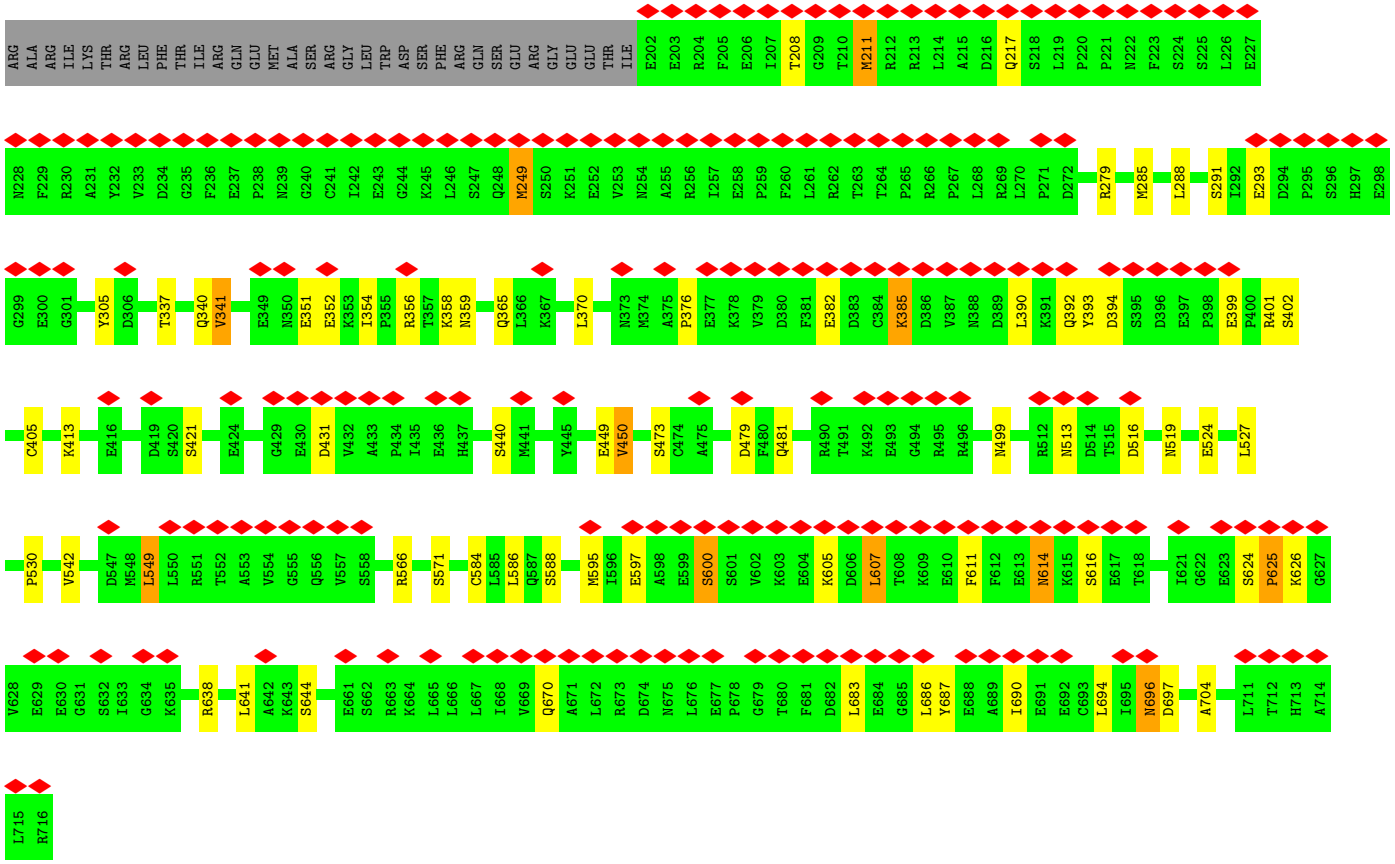
Chain A:



• Molecule 1: Polymerase acidic protein

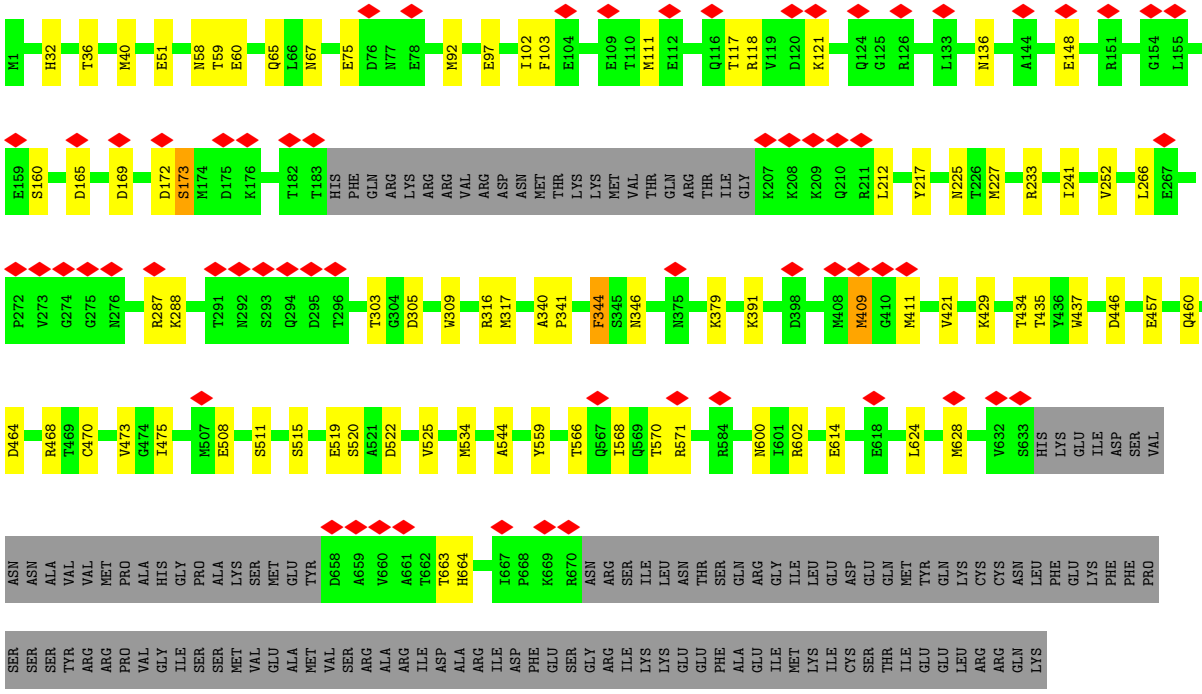
Chain E:





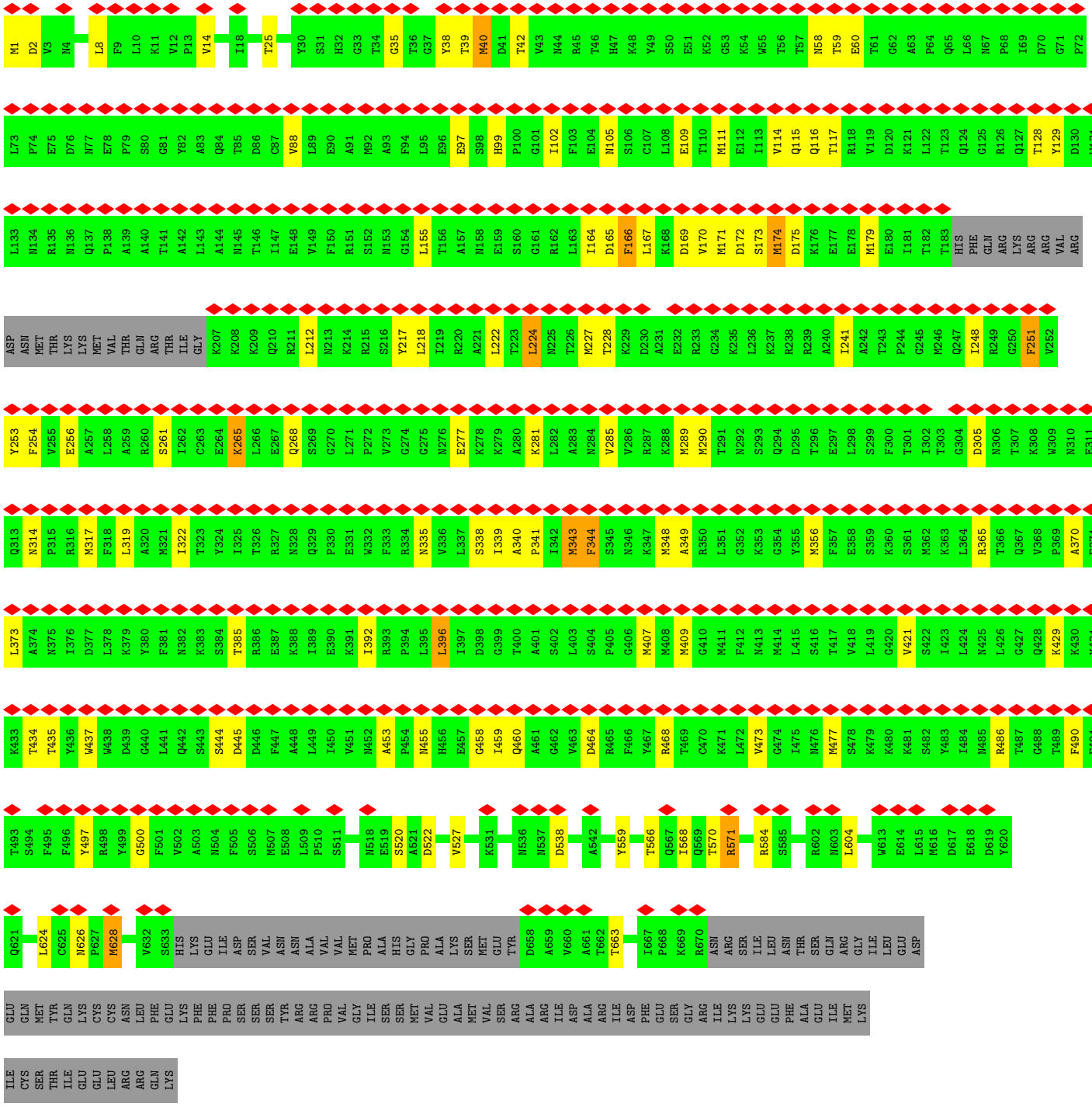
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain B:



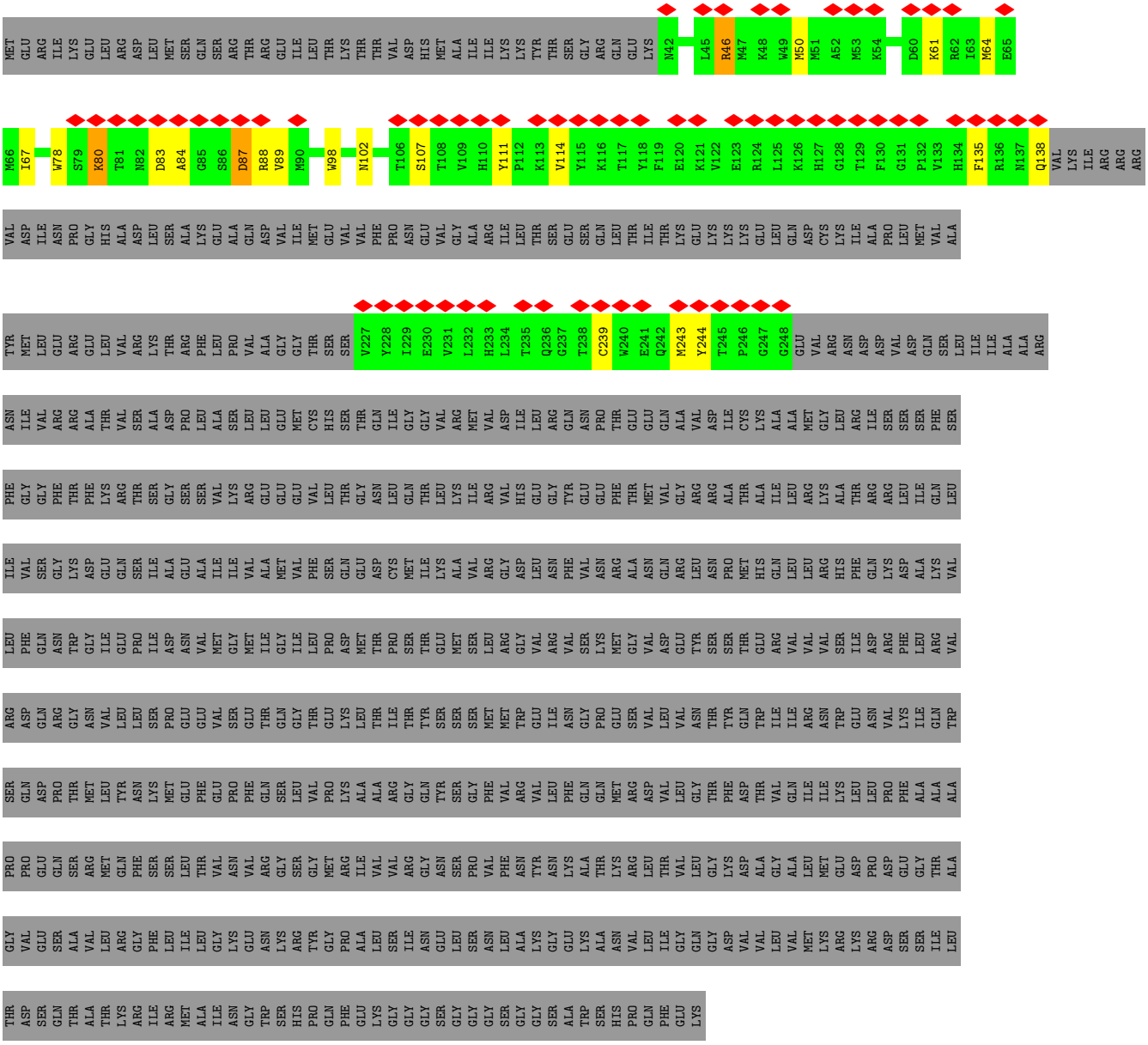
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain F:



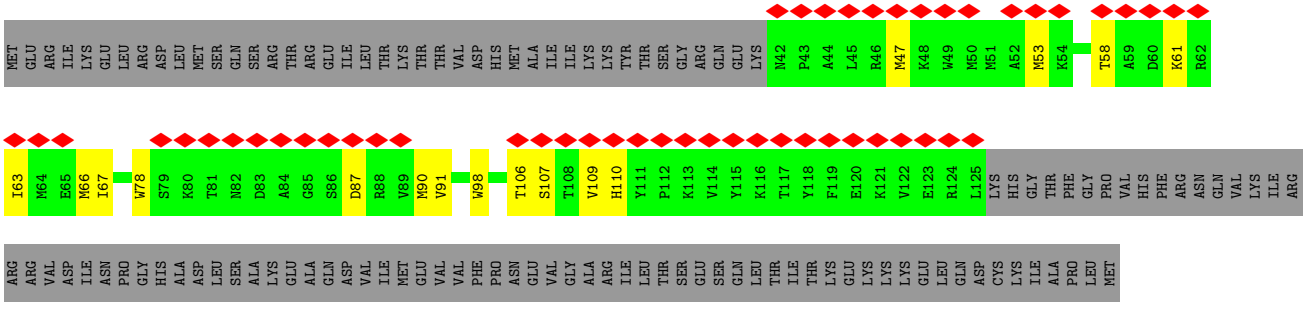
• Molecule 3: Polymerase basic protein 2

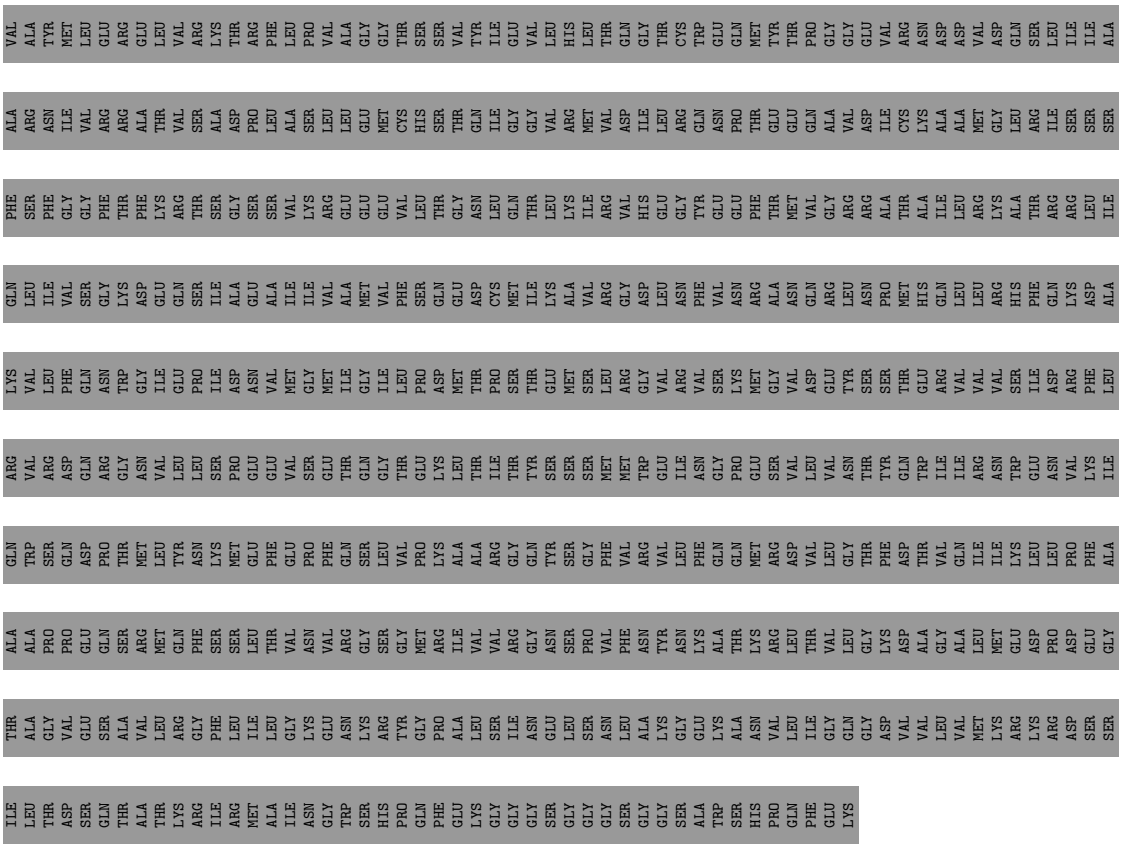
Chain C:



• Molecule 3: Polymerase basic protein 2

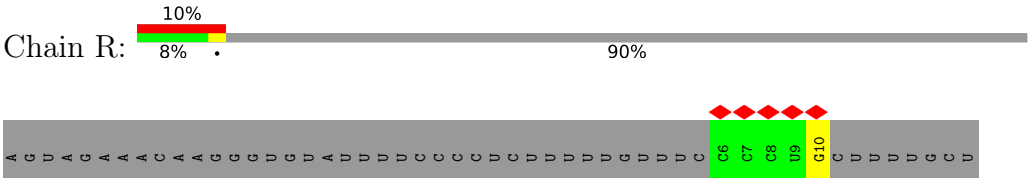
Chain G:





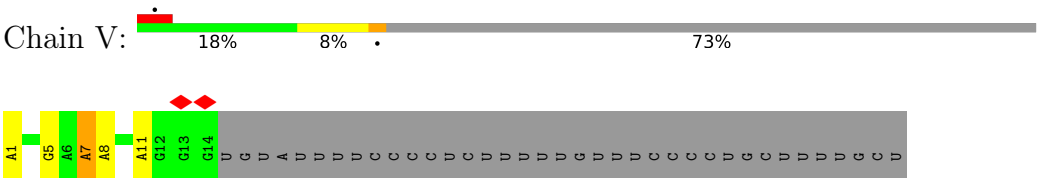
• Molecule 4: 51-mer vRNA loop (v51_mut_S)

Chain R:



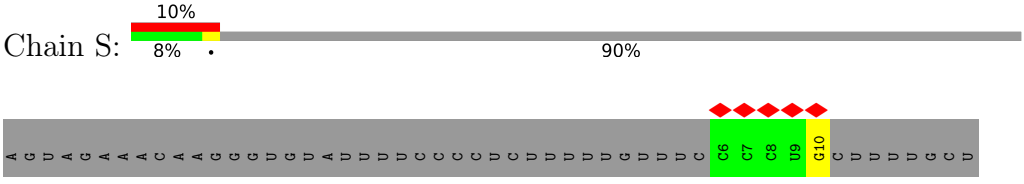
• Molecule 4: 51-mer vRNA loop (v51_mut_S)

Chain V:



• Molecule 4: 51-mer vRNA loop (v51_mut_S)

Chain S:



• Molecule 4: 51-mer vRNA loop (v51_mut_S)

Chain U:


A1
G2
U3
A4
G5
A6
A7
A8
A11
G12
G13
G14
U G U A U U U U C C C C U C U U U U U G U U U U C C C C C U G C U U U U G C U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.094	Depositor
Minimum map value	-2.612	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	308.38, 308.38, 308.38	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.907, 0.907, 0.907	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/4245	0.50	0/5732
1	E	0.29	1/4245 (0.0%)	0.52	2/5732 (0.0%)
2	B	0.26	0/5053	0.49	0/6823
2	F	0.26	0/5066	0.51	0/6841
3	C	0.25	0/1007	0.50	0/1365
3	G	0.25	0/713	0.51	0/966
4	R	0.11	0/113	0.69	0/173
4	S	0.10	0/113	0.68	0/173
4	U	0.60	1/349 (0.3%)	0.68	0/542
4	V	0.62	1/349 (0.3%)	0.70	0/542
All	All	0.28	3/21253 (0.0%)	0.52	2/28889 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-10.71	1.48	1.61
4	U	1	A	OP3-P	-10.66	1.48	1.61
1	E	625	PRO	N-CD	8.57	1.59	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	625	PRO	N-CD-CG	-7.38	92.13	103.20
1	E	625	PRO	CA-N-CD	-5.50	103.79	111.50

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	4155	0	4117	43	0
1	E	4155	0	4117	48	0
2	B	4954	0	4941	54	0
2	F	4966	0	4949	92	0
3	C	978	0	959	8	0
3	G	694	0	694	14	0
4	R	103	0	55	1	0
4	S	103	0	55	1	0
4	U	310	0	154	3	0
4	V	310	0	154	3	0
5	B	1	0	0	0	0
All	All	20729	0	20195	243	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 6.

All (243) 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)
1:A:610:GLU:OE2	1:A:614:ASN:ND2	2.00	0.94
1:A:397:GLU:N	1:A:397:GLU:OE2	2.02	0.93
2:B:409:MET:CE	2:B:411:MET:HG3	2.01	0.91
1:A:351:GLU:O	1:E:356:ARG:NH1	2.10	0.85
2:F:224:LEU:CD1	2:F:349:ALA:HA	2.07	0.84
4:U:5:G:OP2	4:U:5:G:N2	2.10	0.84
2:B:252:VAL:HG11	2:B:411:MET:HE3	1.61	0.81
2:B:429:LYS:NZ	2:B:434:THR:O	2.13	0.81
2:F:224:LEU:HD12	2:F:224:LEU:O	1.80	0.81
2:F:114:VAL:HG22	2:F:164:ILE:HD11	1.63	0.81
4:V:5:G:OP2	4:V:5:G:N2	2.11	0.80
1:A:356:ARG:NH1	1:E:351:GLU:O	2.14	0.80
1:E:352:GLU:N	1:E:352:GLU:OE1	2.16	0.79
2:F:224:LEU:HD11	2:F:349:ALA:HA	1.67	0.77
1:E:305:TYR:OH	1:E:354:ILE:HD13	1.84	0.76
2:B:409:MET:HE2	2:B:411:MET:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:429:LYS:NZ	2:F:434:THR:O	2.18	0.75
1:A:431:ASP:OD2	1:A:440:SER:OG	2.02	0.75
4:V:7:A:O2'	4:V:8:A:OP2	2.02	0.74
2:F:88:VAL:HG22	2:F:473:VAL:HG13	1.69	0.74
1:A:250:SER:O	2:B:468:ARG:NH2	2.21	0.73
2:F:114:VAL:HG23	2:F:254:PHE:CZ	2.25	0.72
4:U:7:A:O2'	4:U:8:A:OP2	2.07	0.70
1:E:211:MET:SD	1:E:211:MET:N	2.65	0.69
1:A:436:GLU:OE1	2:B:600:ASN:ND2	2.25	0.69
2:F:444:SER:OG	2:F:445:ASP:N	2.27	0.68
1:A:217:GLN:OE1	2:B:58:ASN:ND2	2.27	0.68
3:G:67:ILE:O	3:G:67:ILE:HD12	1.93	0.68
1:A:476:ALA:O	1:A:506:LYS:NZ	2.26	0.68
1:A:430:GLU:OE1	1:A:431:ASP:N	2.27	0.68
2:F:224:LEU:HD11	2:F:349:ALA:CB	2.24	0.68
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.76	0.68
2:B:252:VAL:HG21	2:B:411:MET:CE	2.24	0.67
1:E:524:GLU:N	1:E:524:GLU:OE1	2.27	0.67
2:F:224:LEU:HD12	2:F:349:ALA:HA	1.77	0.66
1:E:431:ASP:OD2	1:E:440:SER:OG	2.11	0.66
3:G:58:THR:HG22	3:G:90:MET:CE	2.26	0.66
2:B:67:ASN:OD1	2:B:316:ARG:NH1	2.29	0.66
2:B:59:THR:OG1	2:B:60:GLU:OE1	2.14	0.66
2:F:174:MET:HE3	2:F:175:ASP:N	2.11	0.65
1:A:288:LEU:HD13	1:A:527:LEU:HD13	1.79	0.65
2:F:251:PHE:CD2	2:F:339:ILE:HG21	2.31	0.65
3:C:83:ASP:OD2	3:C:88:ARG:NH1	2.30	0.65
1:A:289:ALA:HB1	1:A:499:ASN:HB3	1.79	0.64
1:A:445:TYR:OH	1:A:609:LYS:NZ	2.31	0.64
2:F:38:TYR:O	2:F:42:THR:HG23	1.97	0.63
1:E:208:THR:OG1	1:E:211:MET:SD	2.57	0.63
1:E:549:LEU:HD12	1:E:549:LEU:O	1.98	0.63
2:F:251:PHE:CE2	2:F:339:ILE:HG21	2.33	0.63
1:A:599:GLU:HG3	1:A:607:LEU:HD12	1.79	0.62
2:B:75:GLU:OE2	2:B:75:GLU:C	2.38	0.62
2:F:224:LEU:HD11	2:F:349:ALA:CA	2.29	0.62
1:A:302:ILE:HD12	1:A:302:ILE:H	1.64	0.62
1:E:449:GLU:O	1:E:638:ARG:NH1	2.33	0.62
4:R:10:G:OP2	4:R:10:G:N2	2.32	0.61
2:B:409:MET:HE3	2:B:411:MET:HG3	1.78	0.61
2:F:171:MET:HE3	2:F:171:MET:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:GLU:OE1	2:B:614:GLU:O	2.19	0.60
4:S:10:G:OP2	4:S:10:G:N2	2.26	0.60
3:G:90:MET:CE	3:G:90:MET:HA	2.32	0.60
2:B:160:SER:OG	2:B:165:ASP:OD2	2.14	0.60
3:G:58:THR:HG22	3:G:90:MET:HE3	1.83	0.60
2:F:114:VAL:O	2:F:117:THR:HG22	2.02	0.59
3:G:109:VAL:HG12	3:G:109:VAL:O	2.02	0.59
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.35	0.59
1:A:420:SER:O	1:A:452:HIS:ND1	2.35	0.58
1:E:584:CYS:SG	2:F:25:THR:HG21	2.43	0.58
2:F:111:MET:HE2	2:F:115:GLN:HG3	1.84	0.58
1:E:566:ARG:NH2	4:U:3:U:OP1	2.37	0.58
1:A:424:GLU:OE1	1:A:424:GLU:HA	2.03	0.57
2:F:335:ASN:O	2:F:339:ILE:HG13	2.05	0.57
1:E:337:THR:O	1:E:341:VAL:HG12	2.05	0.57
2:F:256:GLU:OE2	2:F:256:GLU:HA	2.05	0.57
2:F:261:SER:O	2:F:265:LYS:NZ	2.38	0.57
1:A:610:GLU:OE2	1:A:614:ASN:CG	2.42	0.57
2:B:624:LEU:O	2:B:663:THR:OG1	2.23	0.56
2:F:343:MET:HA	2:F:343:MET:CE	2.34	0.56
2:F:453:ALA:HB3	2:F:459:ILE:HG23	1.86	0.56
2:B:252:VAL:HG11	2:B:411:MET:CE	2.33	0.56
1:A:603:LYS:HE2	1:A:603:LYS:HA	1.87	0.55
2:B:519:GLU:OE1	2:B:664:HIS:ND1	2.39	0.55
2:B:434:THR:HG22	2:B:435:THR:H	1.71	0.55
3:G:78:TRP:HB3	3:G:91:VAL:HG12	1.89	0.55
1:E:614:ASN:OD1	1:E:616:SER:N	2.38	0.55
1:A:302:ILE:HD12	1:A:302:ILE:N	2.22	0.54
3:G:61:LYS:N	3:G:61:LYS:HD2	2.22	0.54
2:F:527:VAL:HG13	2:F:604:LEU:HD22	1.90	0.54
1:A:397:GLU:H	1:A:397:GLU:CD	2.06	0.54
1:A:340:GLN:OE1	1:A:365:GLN:NE2	2.42	0.53
2:F:624:LEU:O	2:F:663:THR:OG1	2.26	0.53
1:E:211:MET:SD	2:F:174:MET:HE2	2.48	0.53
1:E:217:GLN:OE1	2:F:58:ASN:ND2	2.39	0.52
2:B:460:GLN:NE2	2:B:464:ASP:OD1	2.43	0.52
2:F:166:PHE:HD1	2:F:166:PHE:O	1.91	0.52
2:B:252:VAL:HG21	2:B:411:MET:HE1	1.91	0.52
2:F:344:PHE:CD2	2:F:407:MET:SD	3.03	0.52
2:F:372:MET:O	2:F:372:MET:SD	2.68	0.51
2:F:522:ASP:OD2	2:F:559:TYR:OH	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLU:C	2:B:148:GLU:OE2	2.49	0.51
1:E:394:ASP:C	1:E:394:ASP:OD1	2.49	0.51
2:F:570:THR:HG22	2:F:571:ARG:H	1.76	0.51
2:F:99:HIS:HB2	2:F:102:ILE:HD13	1.92	0.50
1:A:600:SER:HG	3:C:135:PHE:HD2	1.58	0.50
1:E:600:SER:OG	1:E:605:LYS:O	2.26	0.50
3:G:67:ILE:HG22	3:G:98:TRP:CE3	2.47	0.50
1:E:211:MET:CG	2:F:171:MET:HE1	2.42	0.50
1:A:509:SER:O	1:A:509:SER:OG	2.25	0.50
1:A:526:SER:C	1:A:527:LEU:HD12	2.31	0.49
2:F:455:ASN:OD1	2:F:458:GLY:N	2.38	0.49
1:E:340:GLN:OE1	1:E:365:GLN:NE2	2.40	0.49
2:F:1:MET:SD	2:F:2:ASP:N	2.86	0.49
2:B:36:THR:O	2:B:40:MET:HG3	2.13	0.49
2:F:212:LEU:HD21	2:F:217:TYR:N	2.28	0.49
1:E:211:MET:HG3	2:F:171:MET:HE1	1.94	0.49
1:E:624:SER:OG	1:E:625:PRO:CD	2.60	0.49
2:F:497:TYR:HE1	2:F:500:GLY:H	1.61	0.49
2:B:60:GLU:OE1	2:B:60:GLU:N	2.46	0.48
2:F:224:LEU:CD1	2:F:224:LEU:O	2.57	0.48
2:B:309:TRP:HZ3	2:B:475:ILE:HG23	1.78	0.48
1:E:211:MET:HG2	2:F:171:MET:CE	2.44	0.48
2:F:59:THR:OG1	2:F:60:GLU:OE1	2.30	0.48
1:E:683:LEU:C	1:E:683:LEU:HD23	2.34	0.48
1:A:428:ILE:HD11	1:A:443:ARG:NH2	2.28	0.47
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.26	0.47
2:F:167:LEU:O	2:F:170:VAL:HG22	2.14	0.47
1:E:249:MET:CE	2:F:468:ARG:NH2	2.77	0.47
2:F:174:MET:HE1	2:F:175:ASP:HA	1.94	0.47
1:E:211:MET:HE2	2:F:171:MET:CE	2.44	0.47
2:F:128:THR:OG1	2:F:129:TYR:N	2.47	0.47
2:B:534:MET:CE	2:B:544:ALA:CB	2.92	0.47
3:C:64:MET:SD	3:C:80:LYS:NZ	2.87	0.47
2:B:473:VAL:HG12	2:B:473:VAL:O	2.15	0.47
1:E:686:LEU:O	1:E:690:ILE:HD12	2.14	0.47
2:B:534:MET:HE2	2:B:544:ALA:HB2	1.96	0.47
2:F:566:THR:HG22	2:F:568:ILE:H	1.79	0.47
1:A:288:LEU:HD13	1:A:527:LEU:CD1	2.43	0.47
2:F:319:LEU:HB2	2:F:341:PRO:HB3	1.97	0.47
2:F:459:ILE:HD12	2:F:460:GLN:N	2.29	0.47
1:E:291:SER:OG	1:E:499:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:ILE:HD13	3:G:91:VAL:HG11	1.97	0.47
2:F:344:PHE:HD2	2:F:407:MET:SD	2.39	0.46
2:B:241:ILE:HD12	2:B:241:ILE:O	2.15	0.46
1:E:450:VAL:HG22	1:E:641:LEU:HD22	1.96	0.46
3:C:87:ASP:OD1	3:C:87:ASP:C	2.52	0.46
1:E:399:GLU:O	1:E:696:ASN:ND2	2.41	0.46
1:E:211:MET:HE1	2:F:174:MET:CE	2.46	0.46
2:F:241:ILE:O	2:F:241:ILE:HD12	2.15	0.46
2:F:277:GLU:OE1	2:F:277:GLU:N	2.49	0.46
3:C:98:TRP:O	3:C:102:ASN:N	2.47	0.46
2:F:396:LEU:HD12	2:F:396:LEU:O	2.16	0.46
3:C:67:ILE:HD11	3:C:78:TRP:HD1	1.81	0.46
2:F:628:MET:N	2:F:628:MET:SD	2.89	0.46
2:F:105:ASN:O	2:F:109:GLU:HG2	2.16	0.46
1:E:305:TYR:CE1	1:E:354:ILE:HG21	2.52	0.45
1:A:418:THR:OG1	1:A:452:HIS:O	2.27	0.45
1:E:393:TYR:OH	2:F:356:MET:HG2	2.16	0.45
1:A:244:GLY:O	1:A:248:GLN:OE1	2.34	0.45
1:A:526:SER:OG	1:A:527:LEU:N	2.50	0.45
2:F:1:MET:HA	2:F:1:MET:HE2	1.98	0.45
2:F:222:LEU:O	2:F:348:MET:N	2.46	0.45
1:A:360:MET:HE3	1:A:482:LEU:HD22	1.98	0.45
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.98	0.45
2:F:251:PHE:CD2	2:F:339:ILE:CG2	2.98	0.45
2:F:40:MET:SD	2:F:392:ILE:HG21	2.57	0.45
2:F:179:MET:HA	2:F:179:MET:CE	2.47	0.45
2:B:566:THR:HG22	2:B:568:ILE:H	1.82	0.45
3:G:58:THR:HA	3:G:90:MET:HE1	1.98	0.45
1:E:670:GLN:HG2	2:F:14:VAL:HG12	1.99	0.45
1:E:211:MET:HG2	2:F:171:MET:HE2	1.99	0.44
2:B:252:VAL:CG1	2:B:411:MET:HE3	2.40	0.44
2:B:409:MET:HE2	2:B:411:MET:CG	2.42	0.44
2:B:570:THR:HG22	2:B:571:ARG:H	1.83	0.44
1:E:211:MET:CE	2:F:174:MET:HE2	2.47	0.44
2:F:340:ALA:HB3	2:F:341:PRO:CD	2.47	0.44
1:A:292:ILE:HG22	1:A:313:THR:HG21	1.99	0.44
1:A:360:MET:CE	1:A:482:LEU:HD22	2.48	0.44
3:C:83:ASP:OD1	3:C:84:ALA:N	2.50	0.44
2:F:174:MET:CE	2:F:175:ASP:HA	2.48	0.44
2:F:218:LEU:O	2:F:222:LEU:HG	2.18	0.44
1:A:320:PRO:HG2	1:A:335:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:GLN:HB2	2:F:421:VAL:HG23	2.00	0.44
1:A:221:PRO:O	1:A:222:ASN:OD1	2.36	0.44
2:B:317:MET:HA	2:B:317:MET:CE	2.48	0.44
1:E:683:LEU:HD21	1:E:687:TYR:CD2	2.52	0.44
2:B:305:ASP:OD1	2:B:305:ASP:N	2.51	0.43
2:B:117:THR:OG1	2:B:118:ARG:N	2.51	0.43
2:B:409:MET:CE	2:B:411:MET:CG	2.86	0.43
2:B:534:MET:HE1	2:B:544:ALA:CB	2.48	0.43
1:E:607:LEU:HD13	1:E:611:PHE:CZ	2.53	0.43
2:F:35:GLY:O	2:F:39:THR:HG23	2.18	0.43
2:F:322:ILE:HD11	2:F:338:SER:CB	2.47	0.43
2:B:515:SER:OG	2:B:525:VAL:HG11	2.17	0.43
2:F:319:LEU:HB2	2:F:341:PRO:CB	2.48	0.43
1:A:366:LEU:O	1:A:370:LEU:HD12	2.18	0.43
2:F:253:TYR:CD1	2:F:253:TYR:C	2.92	0.43
4:V:7:A:HO2'	4:V:8:A:P	2.30	0.43
1:E:288:LEU:HD13	1:E:527:LEU:HG	2.01	0.43
2:F:626:ASN:OD1	2:F:628:MET:SD	2.76	0.43
3:G:61:LYS:HD2	3:G:61:LYS:H	1.84	0.43
3:G:67:ILE:HG22	3:G:98:TRP:CZ3	2.54	0.43
2:F:464:ASP:O	2:F:468:ARG:HG3	2.19	0.43
1:A:288:LEU:HD22	1:A:527:LEU:CD1	2.49	0.42
2:F:155:LEU:HD23	2:F:155:LEU:HA	1.93	0.42
2:B:457:GLU:OE1	2:B:457:GLU:N	2.44	0.42
1:E:694:LEU:HD21	1:E:704:ALA:HB2	2.00	0.42
2:B:65:GLN:NE2	2:B:346:ASN:OD1	2.50	0.42
2:F:174:MET:SD	2:F:174:MET:C	2.97	0.42
2:B:173:SER:HG	2:B:217:TYR:HH	1.65	0.42
2:F:343:MET:HA	2:F:343:MET:HE2	2.01	0.42
1:A:432:VAL:HG22	2:B:602:ARG:NE	2.34	0.42
2:B:317:MET:HA	2:B:317:MET:HE2	2.01	0.42
1:A:324:LYS:NZ	1:A:537:TRP:O	2.52	0.42
1:E:413:LYS:HD2	1:E:413:LYS:O	2.20	0.42
1:E:211:MET:HE1	2:F:174:MET:HE3	2.01	0.42
2:F:434:THR:HG22	2:F:435:THR:H	1.83	0.42
2:F:570:THR:HG22	2:F:571:ARG:N	2.35	0.42
2:F:281:LYS:O	2:F:285:VAL:HG12	2.19	0.41
2:B:344:PHE:HZ	2:B:411:MET:HE2	1.86	0.41
2:B:434:THR:HG22	2:B:435:THR:N	2.34	0.41
1:A:674:ASP:O	1:A:675:ASN:OD1	2.38	0.41
2:F:167:LEU:HD22	2:F:251:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD22	1:A:527:LEU:HD11	2.02	0.41
3:G:58:THR:HG22	3:G:90:MET:HE1	2.01	0.41
1:E:376:PRO:O	2:F:365:ARG:NE	2.47	0.41
3:C:46:ARG:HG3	3:C:46:ARG:HH11	1.86	0.41
1:E:382:GLU:HA	1:E:385:LYS:HZ2	1.86	0.41
2:F:222:LEU:CD2	2:F:343:MET:SD	3.09	0.41
3:G:106:THR:HG22	3:G:107:SER:N	2.35	0.41
1:A:551:ARG:CZ	1:A:551:ARG:HB2	2.51	0.41
2:B:233:ARG:NH2	2:B:508:GLU:OE2	2.54	0.41
2:B:287:ARG:HG3	2:B:288:LYS:N	2.36	0.41
2:B:473:VAL:O	2:B:473:VAL:CG1	2.69	0.41
1:E:305:TYR:HE1	1:E:354:ILE:HG21	1.86	0.41
1:E:359:ASN:OD1	1:E:479:ASP:HB3	2.22	0.41
2:F:117:THR:HG21	2:F:254:PHE:HZ	1.86	0.40
2:F:224:LEU:HD11	2:F:349:ALA:HB2	2.03	0.40
2:F:370:ALA:HA	2:F:373:LEU:HD23	2.03	0.40
1:E:530:PRO:HG3	1:E:542:VAL:HG11	2.03	0.40
1:E:595:MET:CE	2:F:8:LEU:HD21	2.51	0.40
2:B:102:ILE:HG23	2:B:103:PHE:N	2.36	0.40
2:B:534:MET:HE2	2:B:544:ALA:CB	2.52	0.40
2:F:490:PHE:CE2	2:F:497:TYR:HD2	2.39	0.40
1:A:450:VAL:HG22	1:A:641:LEU:HD22	2.03	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	514/729 (70%)	498 (97%)	16 (3%)	0	100	100
1	E	514/729 (70%)	503 (98%)	11 (2%)	0	100	100
2	B	617/757 (82%)	594 (96%)	23 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	618/757 (82%)	596 (96%)	22 (4%)	0	100	100
3	C	115/788 (15%)	113 (98%)	2 (2%)	0	100	100
3	G	82/788 (10%)	80 (98%)	2 (2%)	0	100	100
All	All	2460/4548 (54%)	2384 (97%)	76 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	462/655 (70%)	436 (94%)	26 (6%)	21	52
1	E	462/655 (70%)	429 (93%)	33 (7%)	14	42
2	B	545/668 (82%)	523 (96%)	22 (4%)	31	61
2	F	546/668 (82%)	512 (94%)	34 (6%)	18	47
3	C	106/685 (16%)	93 (88%)	13 (12%)	4	20
3	G	76/685 (11%)	71 (93%)	5 (7%)	16	46
All	All	2197/4016 (55%)	2064 (94%)	133 (6%)	22	48

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	278	GLN
1	A	279	ARG
1	A	285	MET
1	A	325	PRO
1	A	358	LYS
1	A	363	THR
1	A	372	GLU
1	A	389	ASP
1	A	421	SER

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Mol	Chain	Res	Type
1	A	431	ASP
1	A	450	VAL
1	A	456	THR
1	A	473	SER
1	A	477	MET
1	A	481	GLN
1	A	491	THR
1	A	509	SER
1	A	513	ASN
1	A	548	MET
1	A	549	LEU
1	A	552	THR
1	A	558	SER
1	A	571	SER
1	A	588	SER
1	A	626	LYS
2	B	32	HIS
2	B	51	GLU
2	B	92	MET
2	B	97	GLU
2	B	111	MET
2	B	121	LYS
2	B	169	ASP
2	B	172	ASP
2	B	173	SER
2	B	212	LEU
2	B	227	MET
2	B	303	THR
2	B	344	PHE
2	B	379	LYS
2	B	391	LYS
2	B	409	MET
2	B	437	TRP
2	B	446	ASP
2	B	470	CYS
2	B	511	SER
2	B	520	SER
2	B	628	MET
3	C	46	ARG
3	C	50	MET
3	C	61	LYS
3	C	80	LYS

Continued on next page...

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Mol	Chain	Res	Type
3	C	87	ASP
3	C	89	VAL
3	C	107	SER
3	C	111	TYR
3	C	114	VAL
3	C	138	GLN
3	C	239	CYS
3	C	243	MET
3	C	244	TYR
1	E	211	MET
1	E	249	MET
1	E	279	ARG
1	E	285	MET
1	E	293	GLU
1	E	341	VAL
1	E	358	LYS
1	E	370	LEU
1	E	385	LYS
1	E	390	LEU
1	E	392	GLN
1	E	401	ARG
1	E	402	SER
1	E	405	CYS
1	E	421	SER
1	E	450	VAL
1	E	473	SER
1	E	481	GLN
1	E	513	ASN
1	E	516	ASP
1	E	519	ASN
1	E	549	LEU
1	E	571	SER
1	E	586	LEU
1	E	588	SER
1	E	597	GLU
1	E	600	SER
1	E	607	LEU
1	E	614	ASN
1	E	626	LYS
1	E	644	SER
1	E	696	ASN
1	E	697	ASP

Continued on next page...

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Mol	Chain	Res	Type
2	F	40	MET
2	F	97	GLU
2	F	116	GLN
2	F	165	ASP
2	F	166	PHE
2	F	169	ASP
2	F	172	ASP
2	F	173	SER
2	F	174	MET
2	F	224	LEU
2	F	227	MET
2	F	228	THR
2	F	248	ILE
2	F	251	PHE
2	F	265	LYS
2	F	289	MET
2	F	290	MET
2	F	305	ASP
2	F	312	ASN
2	F	314	ASN
2	F	317	MET
2	F	343	MET
2	F	344	PHE
2	F	385	THR
2	F	396	LEU
2	F	409	MET
2	F	437	TRP
2	F	477	MET
2	F	486	ARG
2	F	520	SER
2	F	538	ASP
2	F	571	ARG
2	F	584	ARG
2	F	628	MET
3	G	47	MET
3	G	53	MET
3	G	66	MET
3	G	87	ASP
3	G	110	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	4/51 (7%)	0	0
4	S	4/51 (7%)	0	0
4	U	13/51 (25%)	2 (15%)	0
4	V	13/51 (25%)	2 (15%)	0
All	All	34/204 (16%)	4 (11%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	7	A
4	V	11	A
4	U	7	A
4	U	11	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

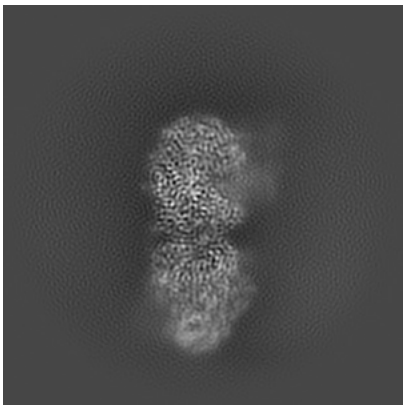
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17792. These allow visual inspection of the internal detail of the map and identification of artifacts.

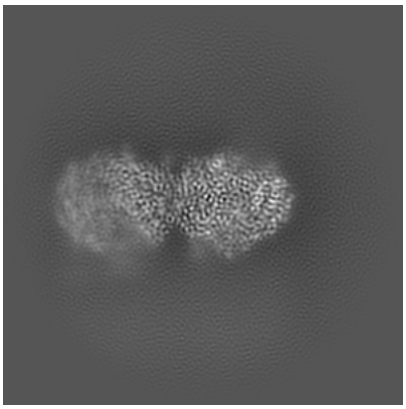
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

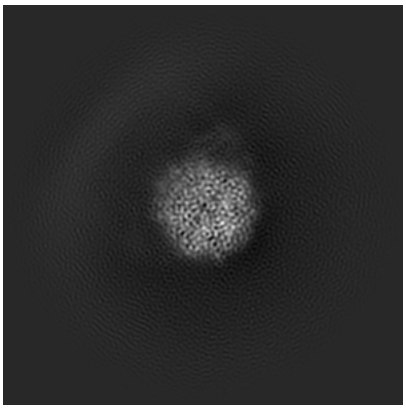
6.1.1 Primary map



X

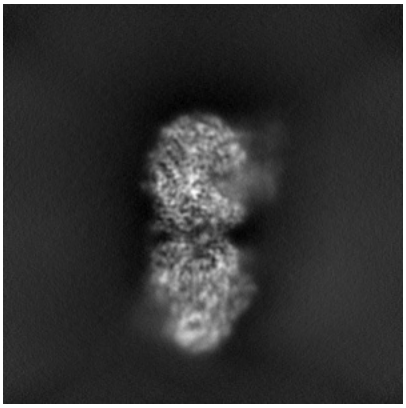


Y

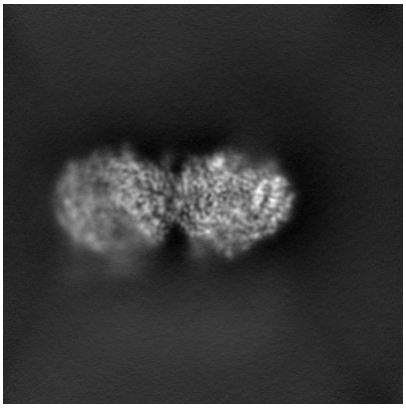


Z

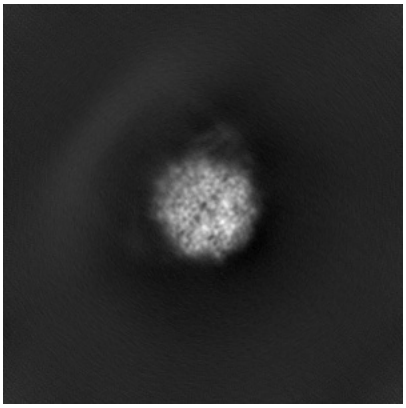
6.1.2 Raw map



X



Y

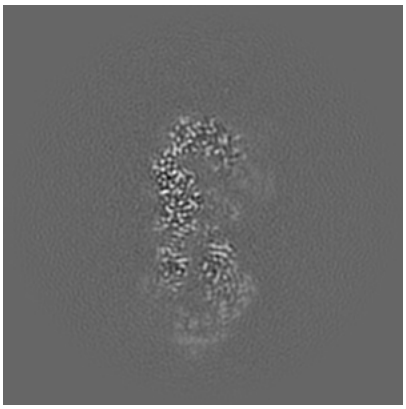


Z

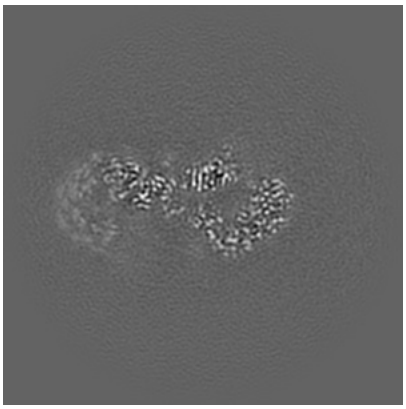
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

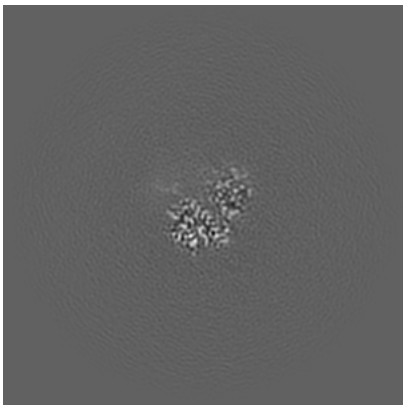
6.2.1 Primary map



X Index: 170

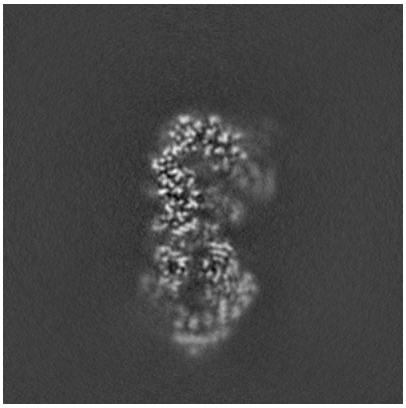


Y Index: 170

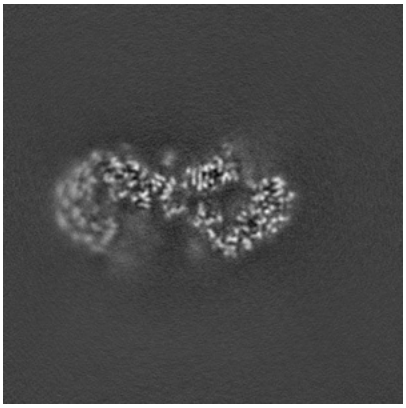


Z Index: 170

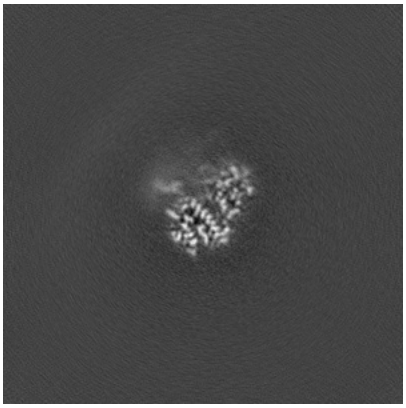
6.2.2 Raw map



X Index: 170



Y Index: 170

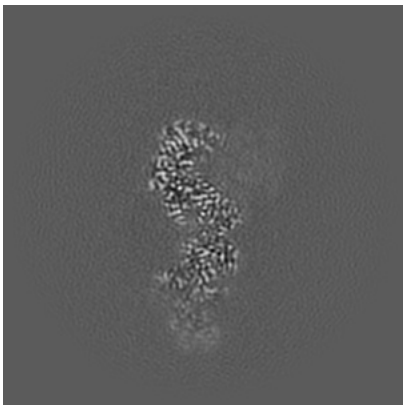


Z Index: 170

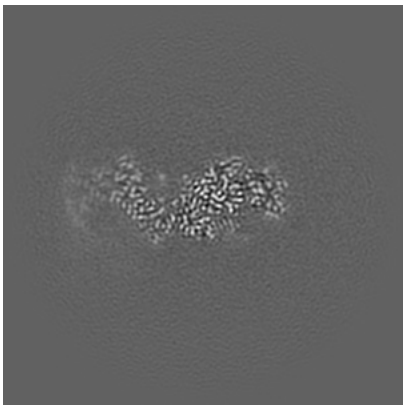
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

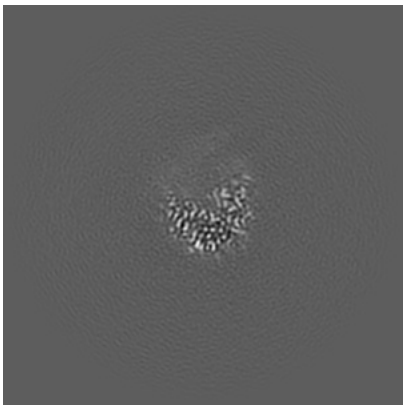
6.3.1 Primary map



X Index: 188

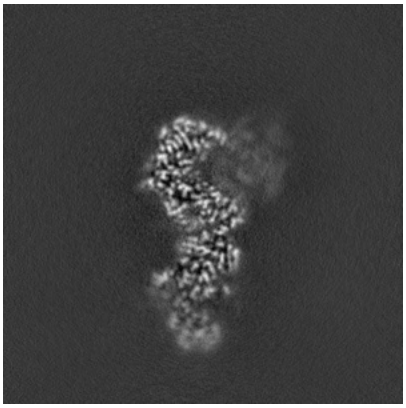


Y Index: 148

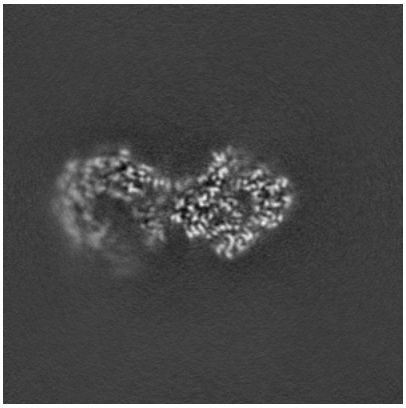


Z Index: 178

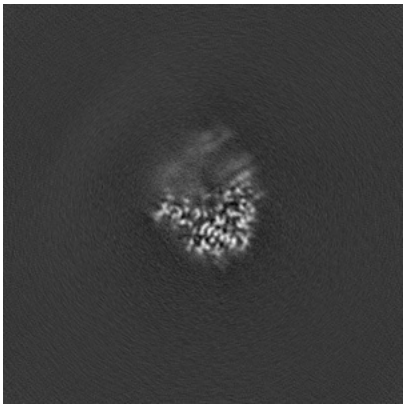
6.3.2 Raw map



X Index: 187



Y Index: 158

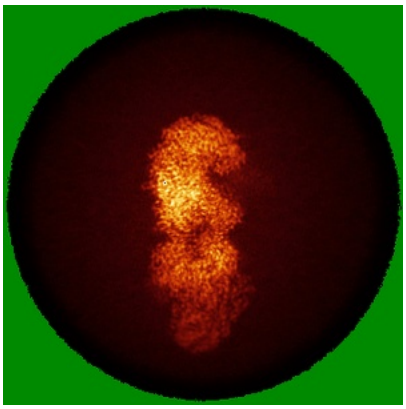


Z Index: 181

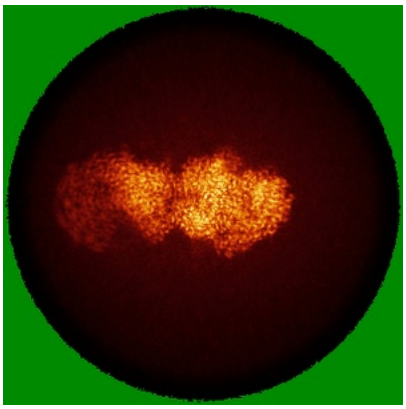
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

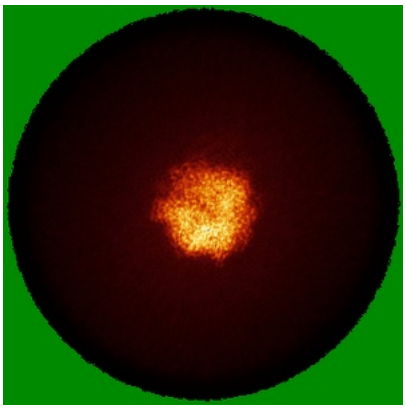
6.4.1 Primary map



X

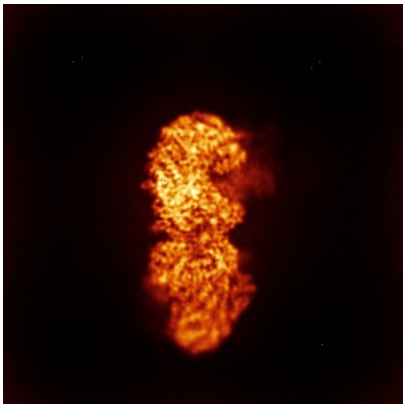


Y

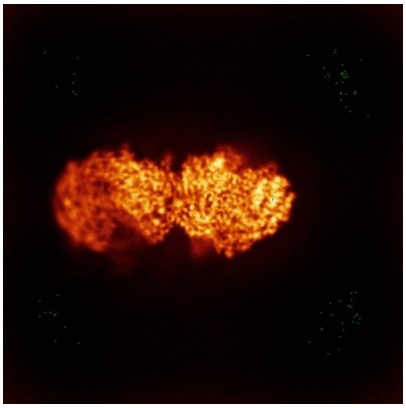


Z

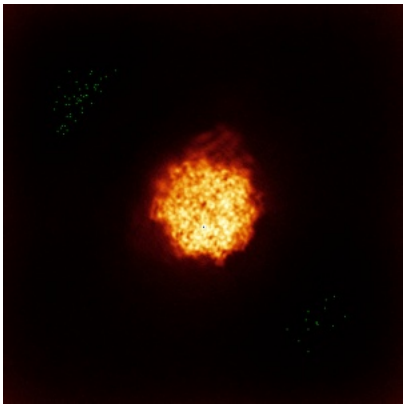
6.4.2 Raw map



X



Y

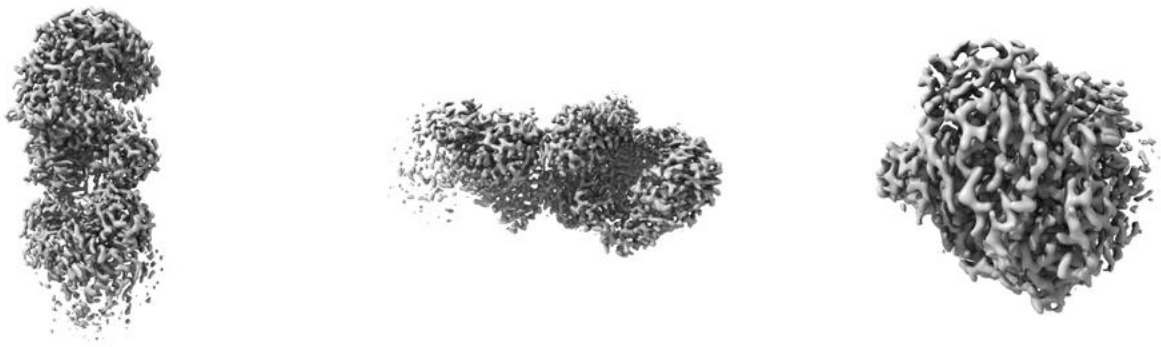


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

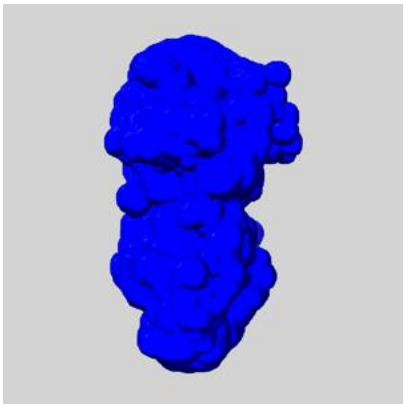
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

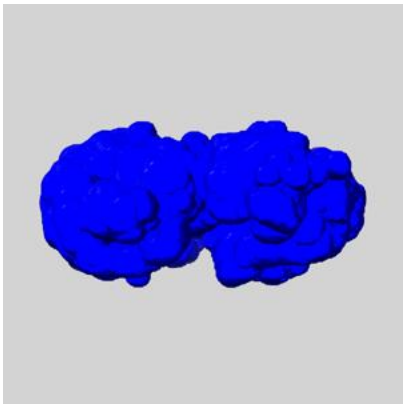
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

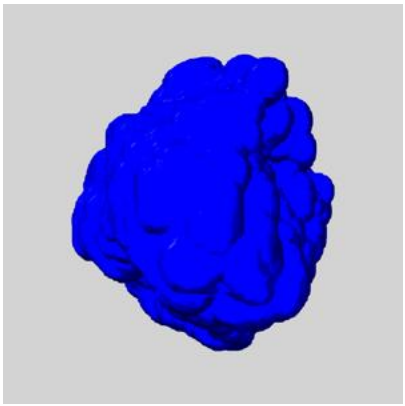
6.6.1 emd_17792_msk_1.map (i)



X



Y

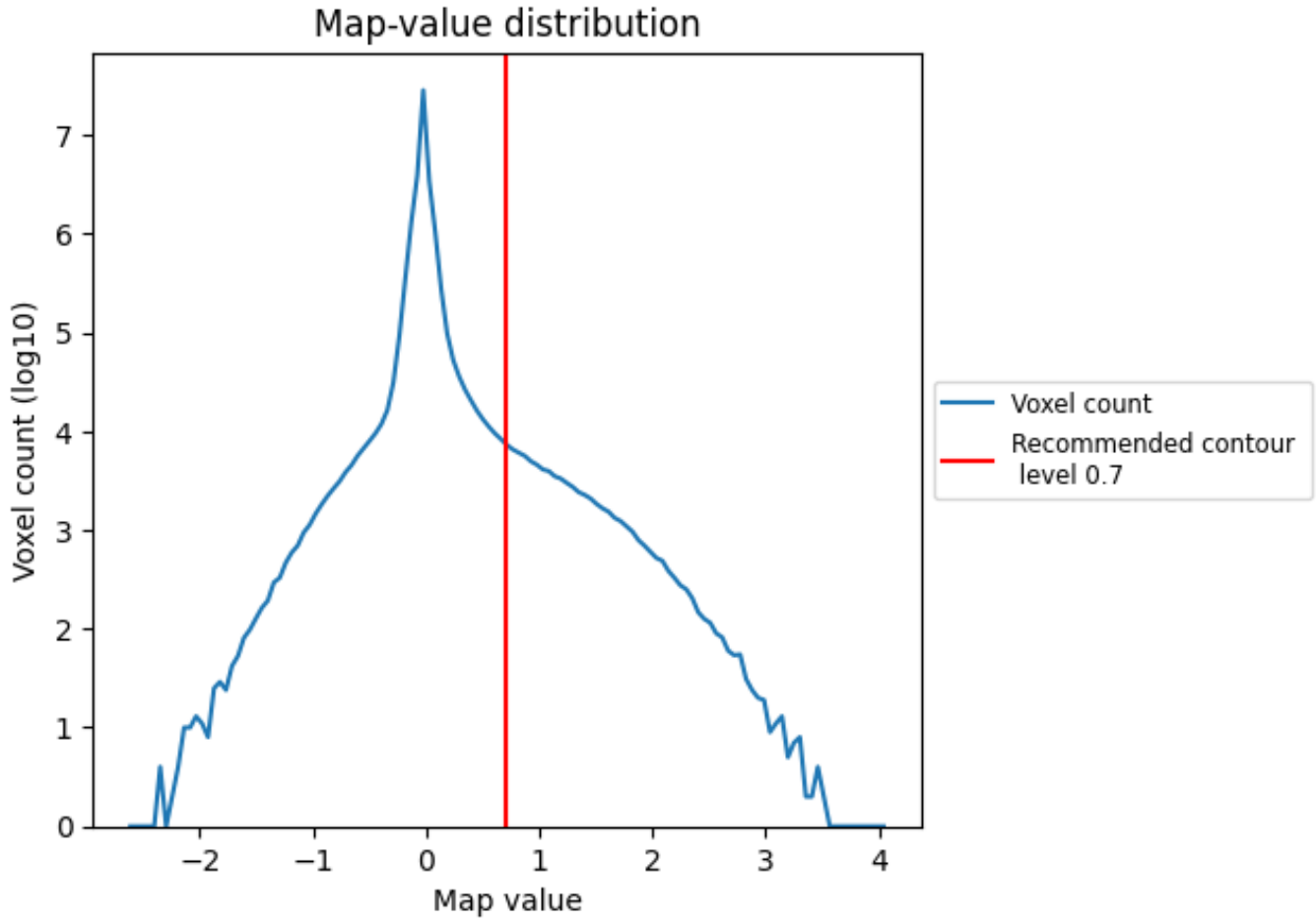


Z

7 Map analysis

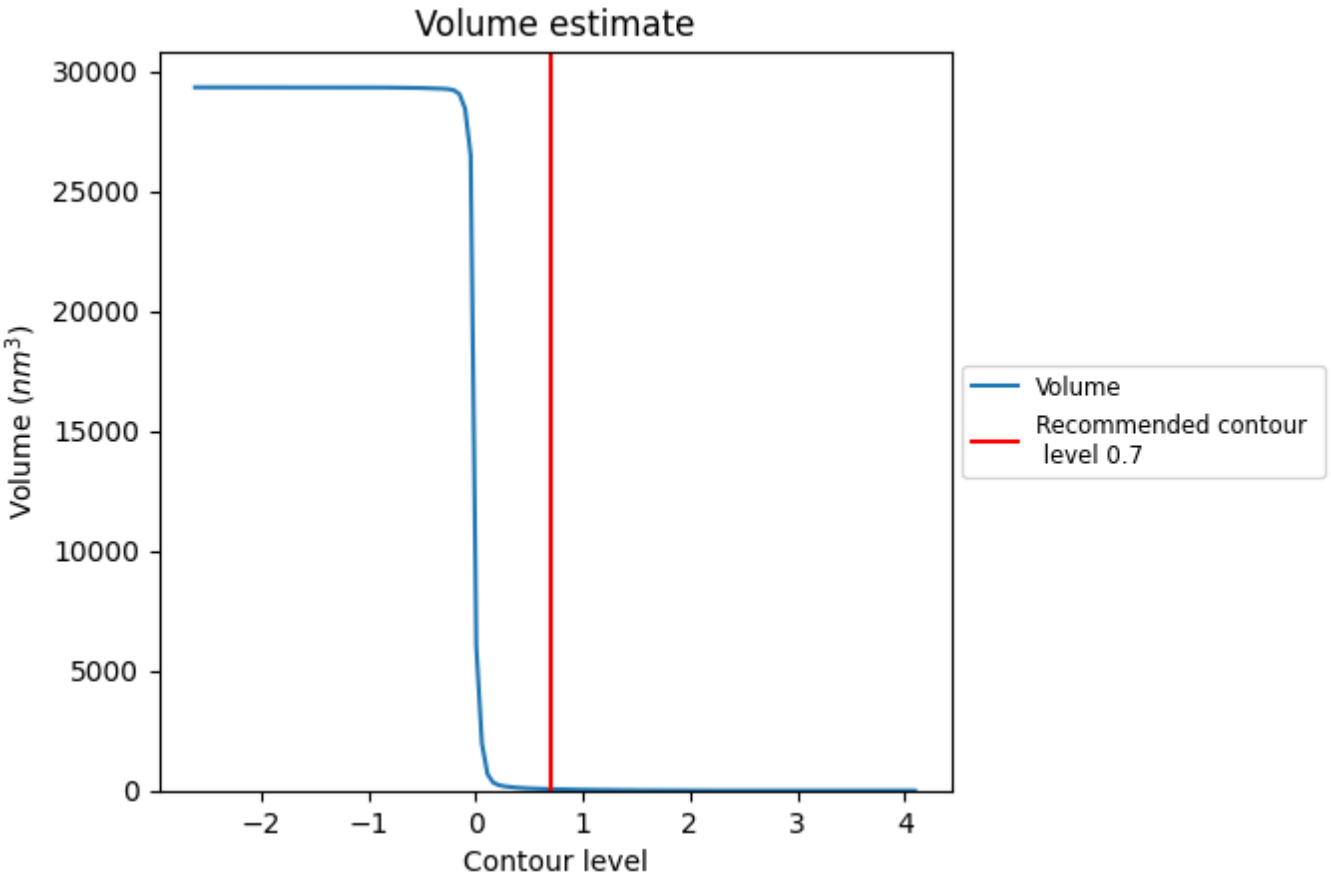
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

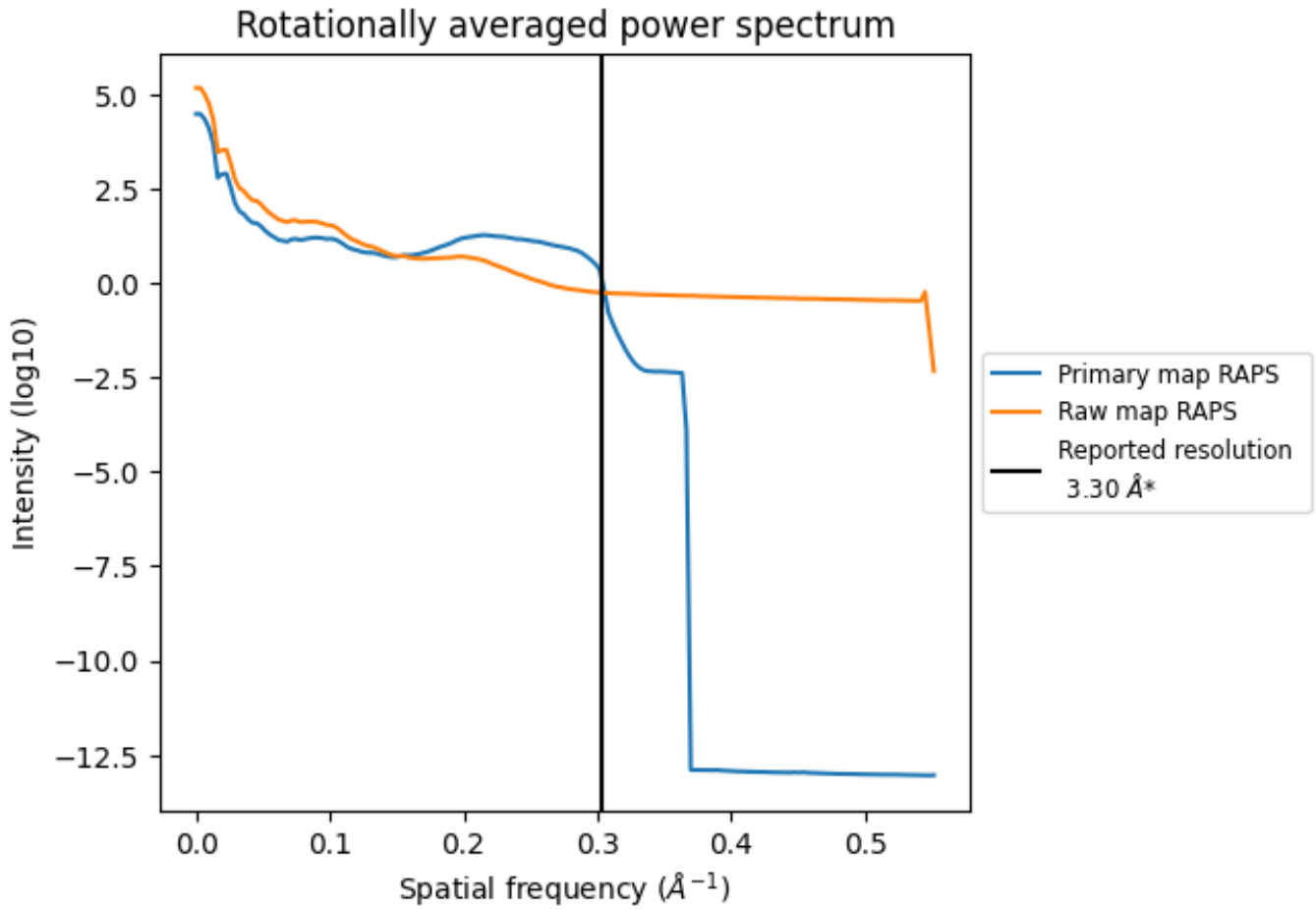
7.2 Volume estimate



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

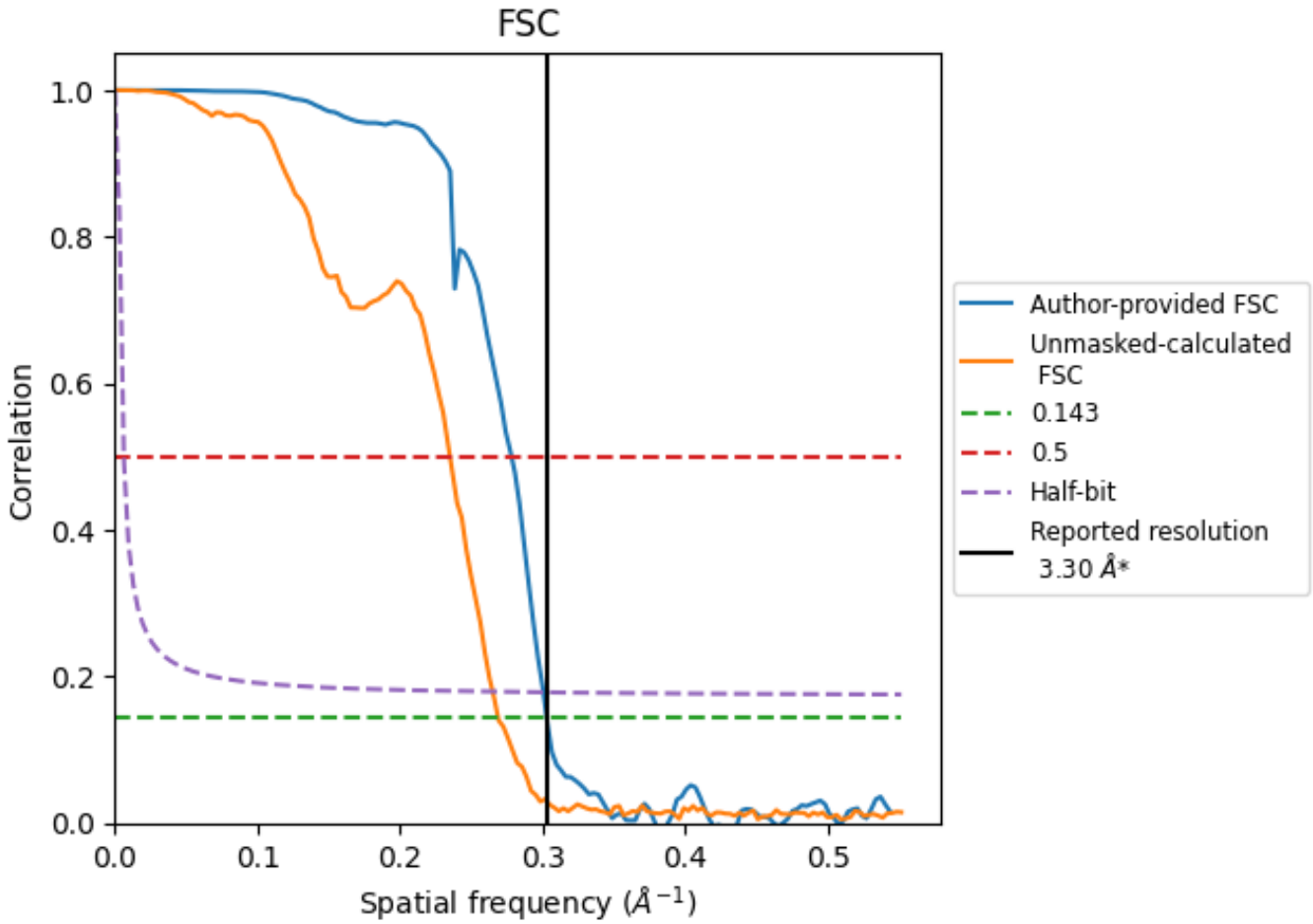


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

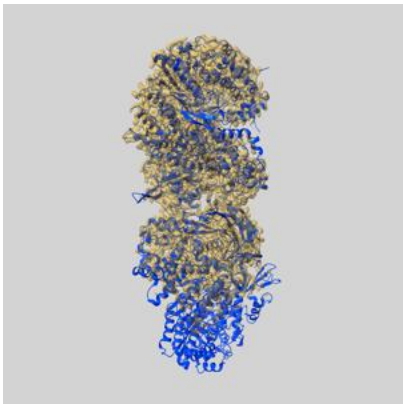
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.60	3.33
Unmasked-calculated*	3.72	4.26	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 3.3 by more than 10 %

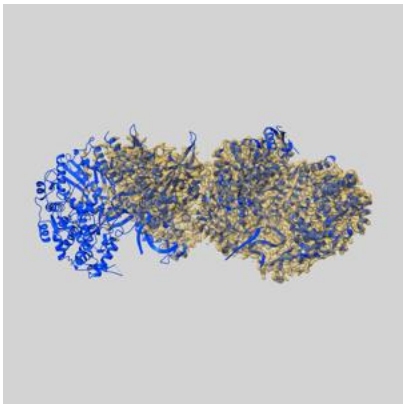
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17792 and PDB model 8POH. Per-residue inclusion information can be found in section 3 on page 8.

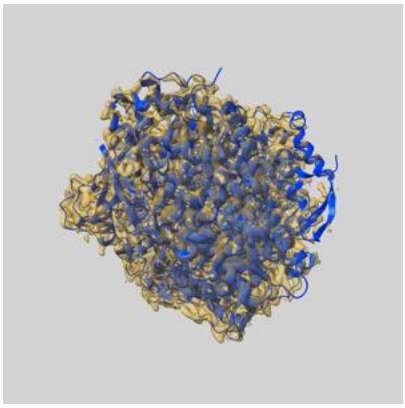
9.1 Map-model overlay



X



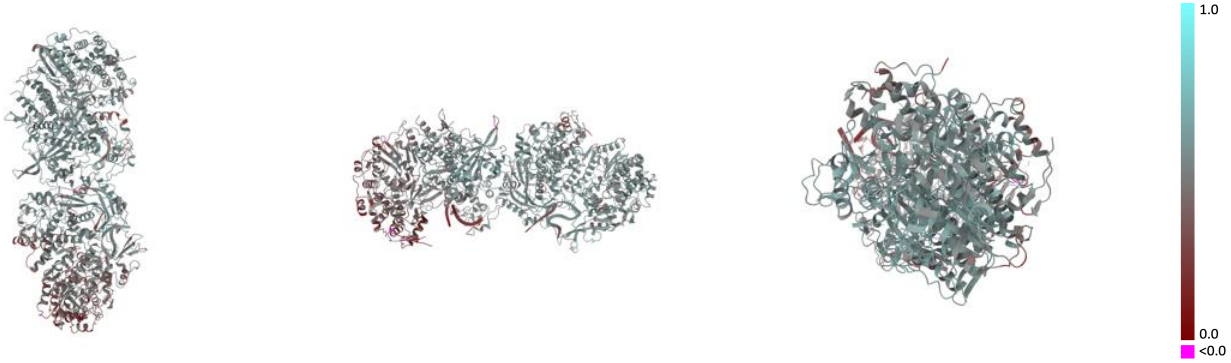
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

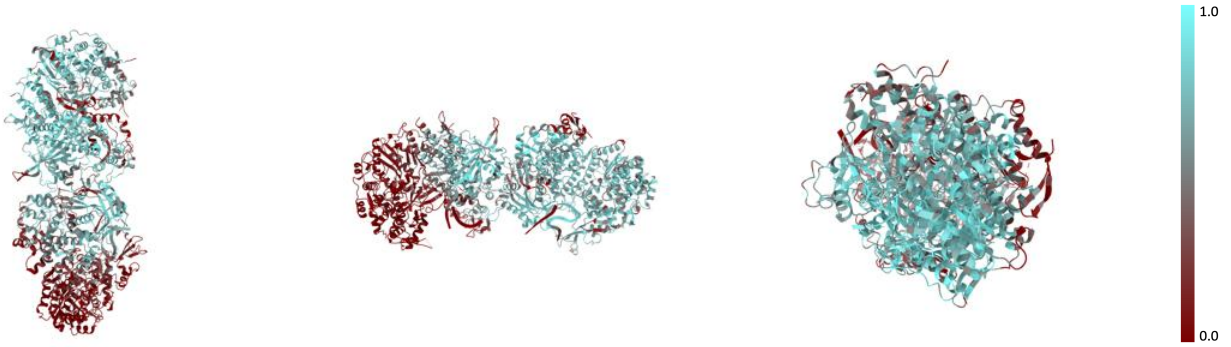
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

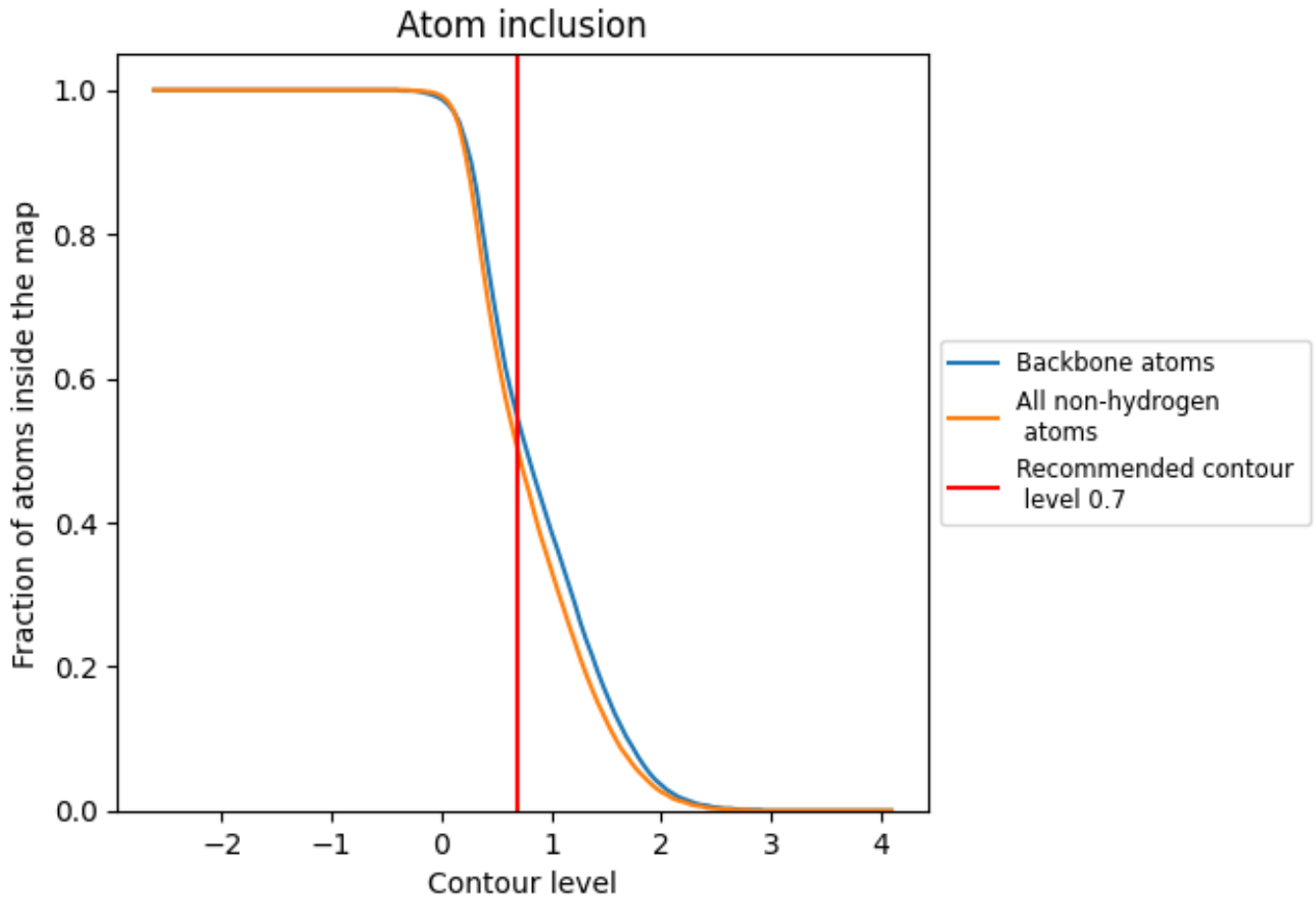
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 50% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4970	0.4970
A	0.7250	0.5510
B	0.7130	0.5460
C	0.3530	0.4870
E	0.4620	0.4880
F	0.1790	0.4260
G	0.3290	0.4550
R	0.0190	0.3180
S	0.0000	0.2010
U	0.4610	0.4670
V	0.7360	0.5350