



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:42 AM UTC

PDB ID : 8RMR / pdb_00008rmr
EMDB ID : EMD-19368
Title : Influenza polymerase A/H7N9-4M replication complex, an asymmetric polymerase dimer bound to human ANP32A
Authors : Arragain, B.; Cusack, S.
Deposited on : 2024-01-08
Resolution : 3.25 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

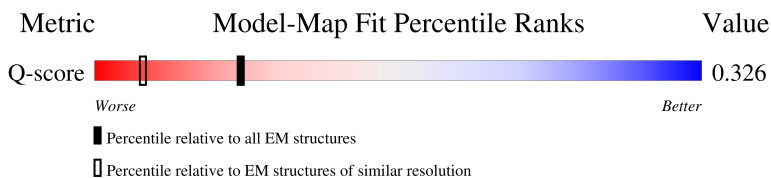
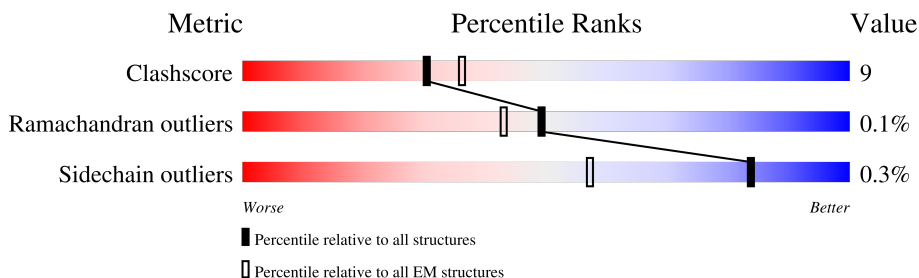
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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	716	21% 79% 19% .
1	D	716	30% 84% 15% .
2	B	757	12% 75% 19% 6%
2	E	757	65% 16% 19%

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Mol	Chain	Length	Quality of chain
3	C	788	27% 76% 20%
3	F	788	35% 60% 18% 22%
4	G	275	15% 44% 13% 43%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 68466 atoms, of which 34252 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	708	Total	C	H	N	O	S	0	0
			11437	3641	5689	976	1090	41		
1	D	707	Total	C	H	N	O	S	0	0
			11417	3635	5678	975	1088	41		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	LYS	GLU	engineered mutation	UNP M9TI86
A	490	ILE	ARG	engineered mutation	UNP M9TI86
D	349	LYS	GLU	engineered mutation	UNP M9TI86
D	490	ILE	ARG	engineered mutation	UNP M9TI86

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	714	Total	C	H	N	O	S	0	0
			11376	3591	5673	993	1074	45		
2	E	613	Total	C	H	N	O	S	0	0
			9700	3076	4830	836	921	37		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	GLY	LYS	engineered mutation	UNP S5ME50
E	577	GLY	LYS	engineered mutation	UNP S5ME50

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	759	Total	C	H	N	O	S	0	0
			12186	3779	6163	1087	1116	41		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	615	Total	C	H	N	O	S	0	0
			9821	3069	4945	874	900	33		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	ARG	GLY	engineered mutation	UNP X5F427
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
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
F	74	ARG	GLY	engineered mutation	UNP X5F427
F	760	GLY	-	expression tag	UNP X5F427
F	761	TRP	-	expression tag	UNP X5F427
F	762	SER	-	expression tag	UNP X5F427
F	763	HIS	-	expression tag	UNP X5F427
F	764	PRO	-	expression tag	UNP X5F427

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

- Molecule 4 is a protein called Acidic leucine-rich nuclear phosphoprotein 32 family member A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	157	Total	C	H	N	O	S	0	0
			2528	783	1274	215	252	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-25	MET	-	initiating methionine	UNP P39687
G	-24	LYS	-	expression tag	UNP P39687
G	-23	HIS	-	expression tag	UNP P39687
G	-22	HIS	-	expression tag	UNP P39687
G	-21	HIS	-	expression tag	UNP P39687
G	-20	HIS	-	expression tag	UNP P39687
G	-19	HIS	-	expression tag	UNP P39687

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	HIS	-	expression tag	UNP P39687
G	-17	PRO	-	expression tag	UNP P39687
G	-16	MET	-	expression tag	UNP P39687
G	-15	SER	-	expression tag	UNP P39687
G	-14	ASP	-	expression tag	UNP P39687
G	-13	TYR	-	expression tag	UNP P39687
G	-12	ASP	-	expression tag	UNP P39687
G	-11	ILE	-	expression tag	UNP P39687
G	-10	PRO	-	expression tag	UNP P39687
G	-9	THR	-	expression tag	UNP P39687
G	-8	THR	-	expression tag	UNP P39687
G	-7	GLU	-	expression tag	UNP P39687
G	-6	ASN	-	expression tag	UNP P39687
G	-5	LEU	-	expression tag	UNP P39687
G	-4	TYR	-	expression tag	UNP P39687
G	-3	PHE	-	expression tag	UNP P39687
G	-2	GLN	-	expression tag	UNP P39687
G	-1	GLY	-	expression tag	UNP P39687
G	0	ALA	-	expression tag	UNP P39687

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

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

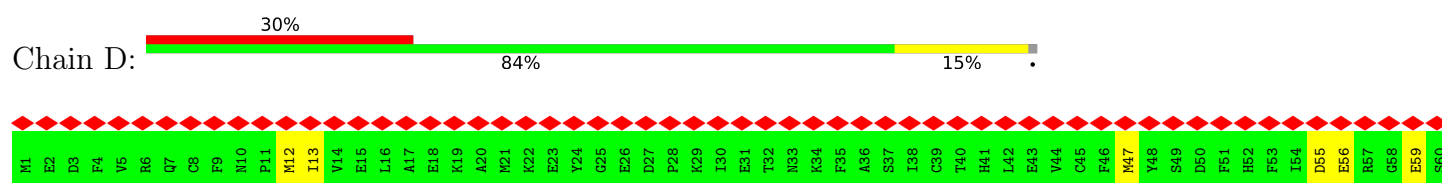
3 Residue-property plots

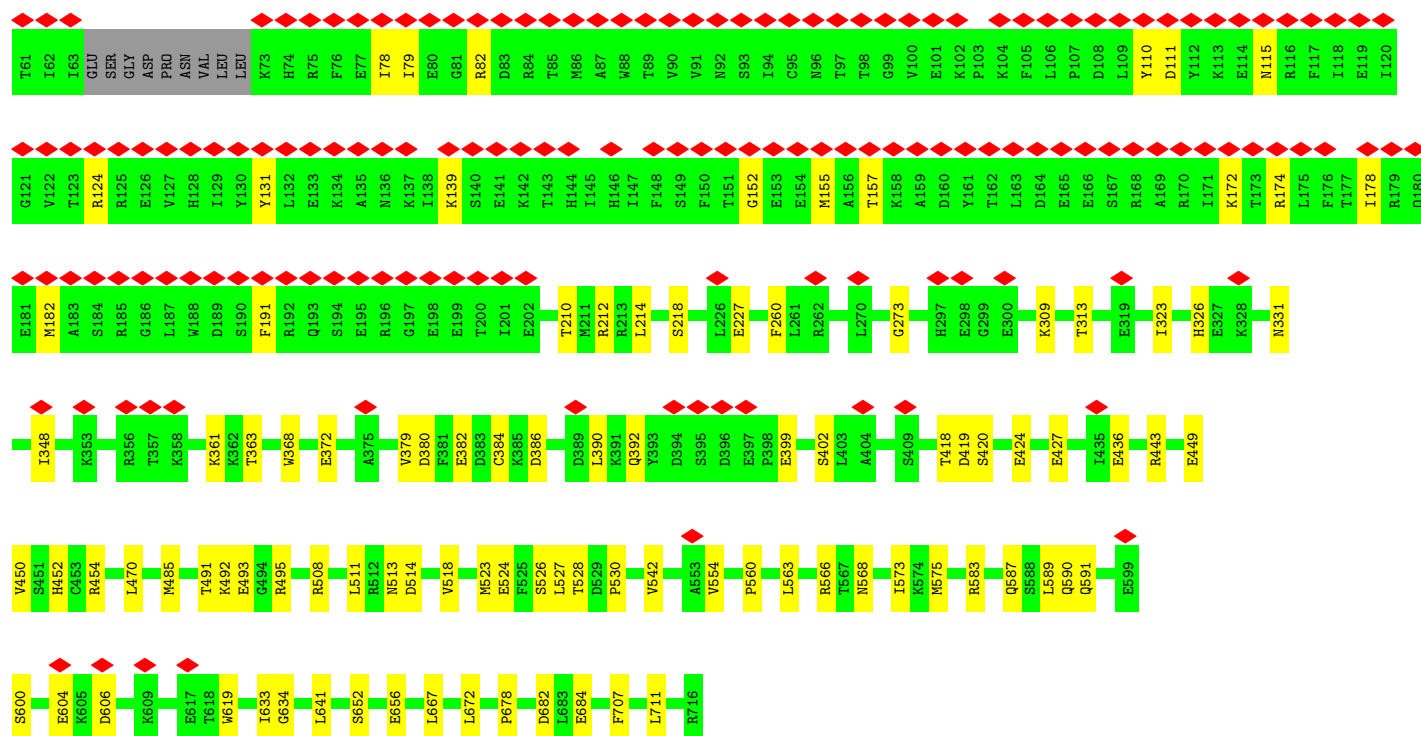
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

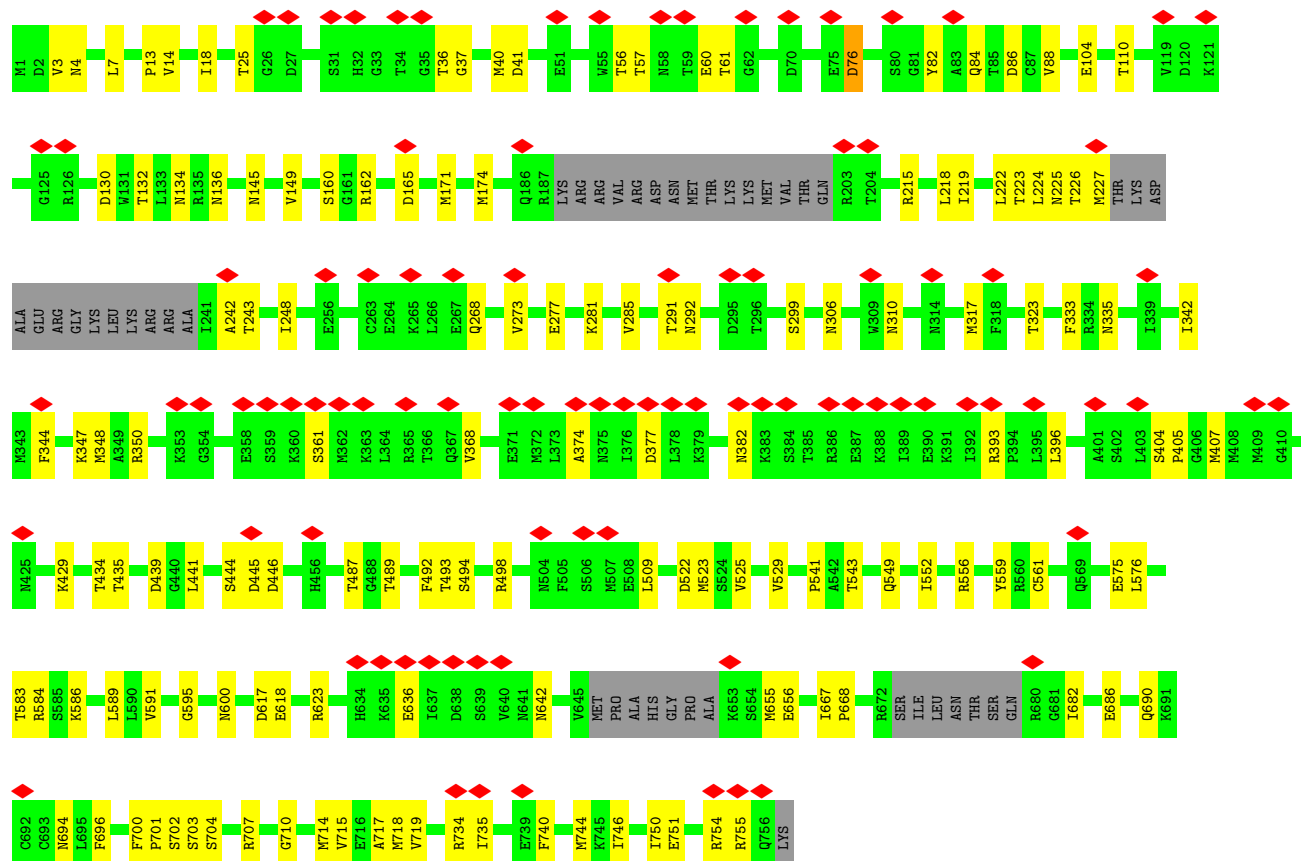
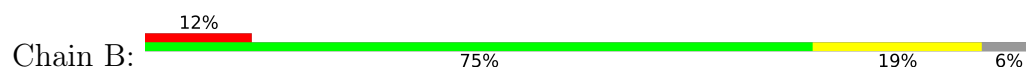


• Molecule 1: Polymerase acidic protein

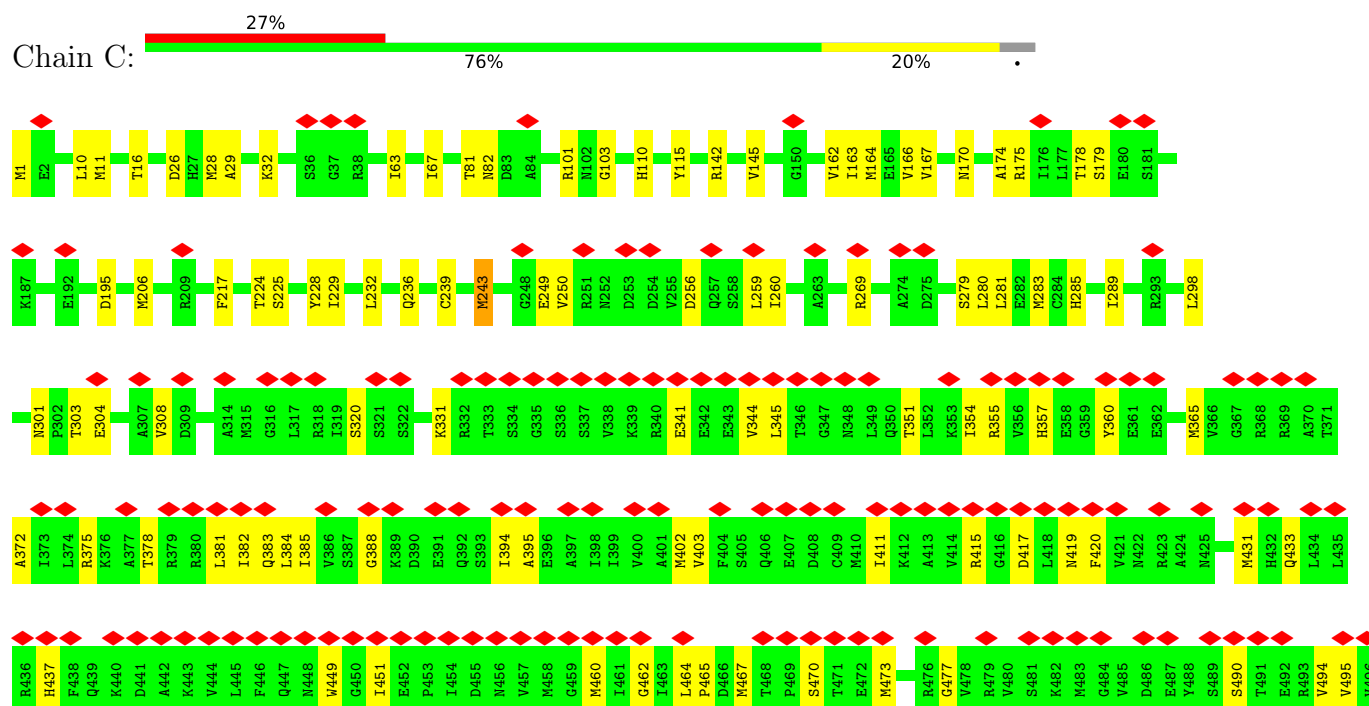




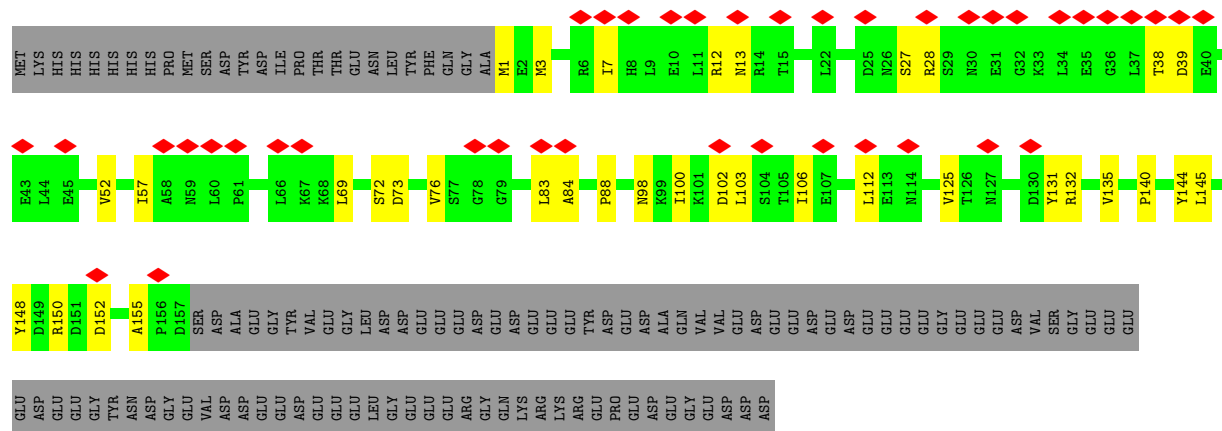
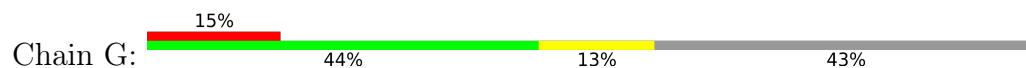
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



Chain E: 65% 16% 19%



- Molecule 4: Acidic leucine-rich nuclear phosphoprotein 32 family member A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.643	Depositor
Minimum map value	-0.903	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	352.8, 352.8, 352.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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

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	0.11	0/5870	0.30	0/7911
1	D	0.09	0/5861	0.23	0/7900
2	B	0.11	0/5813	0.29	0/7837
2	E	0.10	0/4970	0.25	0/6717
3	C	0.13	0/6121	0.30	0/8253
3	F	0.09	0/4963	0.28	0/6699
4	G	0.10	0/1268	0.23	0/1708
All	All	0.11	0/34866	0.27	0/47025

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	5748	5689	5689	110	0
1	D	5739	5678	5678	90	0
2	B	5703	5673	5673	119	0
2	E	4870	4830	4830	96	0
3	C	6023	6163	6163	132	0
3	F	4876	4945	4944	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1254	1274	1276	22	0
5	B	1	0	0	0	0
All	All	34214	34252	34253	616	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 9.

All (616) 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:D:450:VAL:HG21	1:D:641:LEU:CD2	1.77	1.12
1:D:450:VAL:CG2	1:D:641:LEU:HD23	1.83	1.09
1:A:609:LYS:HD3	1:D:386:ASP:OD2	1.52	1.08
1:D:450:VAL:HG21	1:D:641:LEU:HD22	1.36	1.06
3:C:225:SER:HB3	3:C:228:TYR:HD2	1.24	1.03
1:D:450:VAL:CG2	1:D:641:LEU:CD2	2.40	0.99
3:C:341:GLU:HG2	3:C:355:ARG:HD2	1.46	0.96
1:A:112:TYR:O	1:A:115:ASN:ND2	1.99	0.95
1:A:609:LYS:CD	1:D:386:ASP:OD2	2.17	0.92
3:C:525:GLU:OE1	3:C:670:LYS:NZ	2.06	0.89
3:C:341:GLU:HG2	3:C:355:ARG:CD	2.03	0.89
1:A:335:LEU:HD12	1:A:543:LEU:HD13	1.56	0.88
3:C:341:GLU:CG	3:C:355:ARG:HD2	2.05	0.85
2:E:413:ASN:OD1	2:E:444:SER:OG	1.95	0.85
1:D:392:GLN:NE2	2:E:382:ASN:OD1	2.10	0.85
3:C:225:SER:HB3	3:C:228:TYR:CD2	2.12	0.85
2:B:522:ASP:OD2	2:B:559:TYR:OH	1.95	0.84
3:C:530:THR:OG1	3:C:551:GLN:OE1	1.92	0.84
3:C:301:ASN:OD1	3:C:303:THR:OG1	1.96	0.84
3:C:10:LEU:O	3:C:16:THR:OG1	1.94	0.83
2:B:429:LYS:O	2:B:429:LYS:NZ	2.12	0.83
2:B:583:THR:OG1	2:B:617:ASP:OD2	1.97	0.82
4:G:132:ARG:NH1	4:G:152:ASP:OD1	2.14	0.81
1:A:118:ILE:HG22	1:A:144:HIS:HB3	1.62	0.81
1:A:426:ASP:O	2:B:549:GLN:NE2	2.14	0.79
1:D:530:PRO:HG3	1:D:542:VAL:HG11	1.65	0.79
2:B:636:GLU:HB3	3:C:32:LYS:NZ	1.98	0.79
3:C:525:GLU:OE1	3:C:544:SER:OG	2.00	0.78
2:B:575:GLU:OE1	3:C:101:ARG:NE	2.18	0.77
1:D:260:PHE:CE2	1:D:672:LEU:HD22	2.19	0.77
3:F:596:VAL:HG22	3:F:618:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:GLU:OE2	1:D:508:ARG:CZ	2.34	0.76
2:B:160:SER:OG	2:B:165:ASP:OD2	2.03	0.76
2:B:690:GLN:O	2:B:694:ASN:ND2	2.19	0.76
3:F:581:GLN:O	3:F:589:ARG:NH2	2.19	0.75
4:G:1:MET:SD	4:G:1:MET:N	2.60	0.75
2:E:60:GLU:O	2:E:215:ARG:NE	2.20	0.74
3:F:243:MET:SD	3:F:243:MET:N	2.61	0.74
1:A:506:LYS:NZ	1:A:507:GLY:O	2.21	0.74
2:B:636:GLU:HB3	3:C:32:LYS:HZ1	1.52	0.73
1:A:55:ASP:OD1	1:A:59:GLU:N	2.19	0.73
1:A:245:LYS:NZ	2:B:86:ASP:OD2	2.21	0.73
3:C:178:THR:O	3:C:178:THR:HG22	1.88	0.73
3:C:283:MET:SD	3:C:536:MET:HE2	2.29	0.73
1:D:273:GLY:O	1:D:402:SER:OG	2.06	0.73
3:F:449:TRP:O	3:F:476:ARG:NH1	2.21	0.73
3:F:333:THR:OG1	3:F:362:GLU:OE1	2.06	0.73
3:C:110:HIS:NE2	3:C:195:ASP:O	2.22	0.73
3:C:637:THR:OG1	3:C:646:ARG:NH1	2.23	0.72
1:A:75:ARG:NE	1:A:111:ASP:OD1	2.19	0.72
1:A:78:ILE:O	1:A:82:ARG:NH1	2.22	0.72
2:B:82:TYR:O	2:B:84:GLN:NE2	2.22	0.72
2:B:134:ASN:OD1	2:B:350:ARG:NH2	2.23	0.72
3:F:113:LYS:O	3:F:116:LYS:NZ	2.22	0.72
4:G:57:ILE:HD12	4:G:83:LEU:HD13	1.72	0.72
3:C:525:GLU:CD	3:C:670:LYS:HZ2	1.98	0.71
1:A:684:GLU:OE1	1:A:684:GLU:N	2.24	0.71
3:F:463:ILE:O	3:F:475:LEU:N	2.23	0.71
3:F:576:GLU:N	3:F:576:GLU:OE1	2.24	0.71
3:F:408:ASP:OD2	3:F:412:LYS:NZ	2.24	0.71
3:F:424:ALA:O	3:F:425:ASN:ND2	2.24	0.70
1:D:124:ARG:NH1	1:D:191:PHE:O	2.25	0.69
2:B:268:GLN:NE2	2:B:439:ASP:OD1	2.24	0.69
3:F:694:PHE:CE2	3:F:713:LEU:HD22	2.27	0.69
1:A:485:MET:HE1	1:A:524:GLU:HG2	1.73	0.69
1:D:139:LYS:NZ	1:D:157:THR:OG1	2.25	0.69
2:E:82:TYR:O	2:E:84:GLN:NE2	2.26	0.69
2:B:700:PHE:O	2:B:703:SER:OG	2.09	0.69
3:F:560:VAL:HG23	3:F:571:LEU:HD11	1.73	0.69
3:C:63:ILE:HD11	3:C:67:ILE:HD12	1.76	0.68
1:D:326:HIS:N	1:D:331:ASN:OD1	2.27	0.68
1:D:527:LEU:O	1:D:527:LEU:HG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:737:ARG:NH2	3:C:741:SER:O	2.26	0.68
1:A:45:CYS:SG	1:A:120:ILE:HD11	2.34	0.67
1:D:210:THR:HG23	2:E:60:GLU:OE2	1.94	0.67
3:F:384:LEU:HD23	3:F:478:VAL:HG12	1.76	0.67
3:C:709:SER:OG	3:C:712:GLU:OE2	2.12	0.67
3:C:243:MET:HB3	1:D:368:TRP:HH2	1.58	0.67
3:F:242:GLN:NE2	3:F:243:MET:O	2.28	0.67
3:C:304:GLU:OE2	3:C:320:SER:OG	2.04	0.66
2:B:130:ASP:OD1	2:B:132:THR:OG1	2.09	0.66
2:B:583:THR:HG21	2:B:589:LEU:HD11	1.77	0.66
3:F:713:LEU:HD11	3:F:724:VAL:HG21	1.77	0.66
1:D:418:THR:HG22	1:D:419:ASP:H	1.61	0.65
3:F:420:PHE:O	3:F:433:GLN:NE2	2.29	0.65
3:F:475:LEU:O	3:F:479:ARG:NH1	2.29	0.65
1:A:12:MET:HE2	3:C:754:ILE:CG2	2.26	0.65
1:D:573:ILE:HD11	2:E:29:PRO:O	1.97	0.65
3:C:528:THR:HG21	3:C:551:GLN:NE2	2.12	0.64
1:D:47:MET:HE2	1:D:47:MET:N	2.13	0.64
3:C:697:LEU:N	3:C:733:LEU:O	2.31	0.64
1:D:12:MET:SD	1:D:13:ILE:N	2.71	0.63
4:G:76:VAL:O	4:G:98:ASN:ND2	2.32	0.63
1:A:454:ARG:NH1	1:A:457:GLU:OE1	2.31	0.63
3:F:592:TYR:O	3:F:596:VAL:HG23	1.98	0.63
2:E:266:LEU:HD13	2:E:421:VAL:HG11	1.81	0.62
3:C:384:LEU:N	3:C:477:GLY:O	2.32	0.62
2:B:104:GLU:N	2:B:104:GLU:OE1	2.33	0.62
2:B:618:GLU:OE1	2:B:618:GLU:N	2.30	0.62
2:E:108:LEU:HD12	2:E:109:GLU:N	2.15	0.62
3:C:360:TYR:O	3:C:375:ARG:NH1	2.33	0.62
2:E:493:THR:O	2:E:494:SER:OG	2.16	0.62
2:B:656:GLU:N	2:B:656:GLU:OE2	2.31	0.62
2:E:425:ASN:C	2:E:425:ASN:HD22	2.06	0.62
2:B:710:GLY:N	3:C:26:ASP:OD1	2.30	0.62
1:A:280:SER:OG	1:A:282:PHE:O	2.17	0.62
3:F:267:VAL:O	3:F:271:THR:HG23	1.99	0.61
3:C:417:ASP:OD2	3:C:419:ASN:ND2	2.34	0.61
1:D:131:TYR:CB	1:D:155:MET:HE1	2.31	0.61
3:C:535:MET:SD	3:C:535:MET:N	2.71	0.61
4:G:69:LEU:CD2	4:G:83:LEU:HD11	2.30	0.61
2:B:529:VAL:HG22	2:B:655:MET:HE1	1.82	0.61
2:B:291:THR:OG1	3:C:460:MET:SD	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:623:ARG:NE	3:C:103:GLY:O	2.33	0.61
1:A:334:TYR:O	1:A:337:THR:OG1	2.19	0.61
3:C:497:SER:OG	3:C:505:ARG:O	2.18	0.61
2:E:46:THR:HG21	2:E:403:LEU:HD11	1.83	0.61
3:F:495:VAL:O	3:F:507:GLN:NE2	2.34	0.61
1:D:218:SER:O	1:D:218:SER:OG	2.19	0.60
2:B:88:VAL:HG21	2:B:317:MET:SD	2.41	0.60
3:C:281:LEU:O	3:C:285:HIS:ND1	2.35	0.60
3:F:713:LEU:HD21	3:F:724:VAL:CG2	2.31	0.60
2:E:316:ARG:NH1	2:E:345:SER:OG	2.35	0.60
1:A:389:ASP:OD2	2:B:361:SER:N	2.34	0.60
1:A:420:SER:OG	1:A:489:CYS:SG	2.47	0.60
3:F:713:LEU:HD21	3:F:724:VAL:HG21	1.84	0.60
2:B:489:THR:HG22	2:B:498:ARG:HA	1.84	0.59
3:C:541:GLY:O	3:C:545:VAL:HG23	2.02	0.59
1:D:485:MET:HE1	1:D:524:GLU:OE1	2.02	0.59
2:E:263:CYS:HA	2:E:266:LEU:HD12	1.82	0.59
1:A:285:MET:HE1	1:A:409:SER:OG	2.02	0.59
1:A:417:LEU:HD22	1:A:452:HIS:HB2	1.85	0.58
3:C:462:GLY:N	3:C:470:SER:O	2.35	0.58
3:C:557:TRP:CZ2	3:C:612:THR:HG23	2.38	0.58
2:E:213:ASN:OD1	2:E:215:ARG:N	2.36	0.58
1:D:382:GLU:OE1	1:D:382:GLU:N	2.36	0.58
1:A:12:MET:HG2	3:C:751:THR:HG23	1.84	0.58
2:B:76:ASP:OD1	2:B:76:ASP:N	2.35	0.58
3:C:528:THR:CG2	3:C:551:GLN:NE2	2.66	0.58
1:D:131:TYR:HB2	1:D:155:MET:HE1	1.84	0.58
1:A:309:LYS:O	1:A:313:THR:HG23	2.04	0.58
4:G:145:LEU:N	4:G:148:TYR:O	2.35	0.58
2:B:642:ASN:ND2	2:B:655:MET:O	2.37	0.58
3:C:525:GLU:CD	3:C:670:LYS:NZ	2.60	0.58
2:E:614:GLU:OE1	2:E:614:GLU:N	2.34	0.58
2:B:714:MET:HB3	2:B:718:MET:HE1	1.85	0.58
3:F:264:ARG:NH2	3:F:305:GLU:OE2	2.37	0.58
3:F:407:GLU:H	3:F:410:MET:HE2	1.69	0.57
3:F:108:THR:HG23	3:F:108:THR:O	2.05	0.57
1:D:380:ASP:N	1:D:380:ASP:OD1	2.38	0.57
3:F:279:SER:O	3:F:283:MET:HG3	2.04	0.57
1:A:709:SER:O	1:A:712:THR:OG1	2.20	0.57
3:F:506:ASP:HB3	3:F:512:LEU:HD11	1.85	0.57
3:C:331:LYS:NZ	3:C:490:SER:O	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:GLU:HG2	1:D:634:GLY:HA2	1.86	0.57
1:D:619:TRP:CH2	1:D:633:ILE:HD13	2.40	0.57
1:A:53:PHE:CD2	1:A:63:ILE:HD12	2.39	0.57
3:C:384:LEU:C	3:C:385:ILE:HD12	2.30	0.57
3:F:599:LEU:HD21	3:F:689:ALA:O	2.05	0.57
1:A:418:THR:OG1	1:A:452:HIS:O	2.11	0.56
3:F:268:ARG:NH2	3:F:271:THR:OG1	2.38	0.56
2:B:171:MET:HE3	2:B:171:MET:HA	1.87	0.56
2:B:444:SER:OG	2:B:445:ASP:N	2.38	0.56
3:C:528:THR:HG21	3:C:551:GLN:HE21	1.69	0.56
3:C:506:ASP:OD1	3:C:510:ASN:N	2.39	0.56
1:A:485:MET:CE	1:A:524:GLU:HG2	2.35	0.56
3:C:259:LEU:HD23	3:C:260:ILE:HD13	1.88	0.56
2:B:434:THR:HG22	2:B:435:THR:H	1.70	0.56
1:D:418:THR:N	1:D:452:HIS:O	2.35	0.56
4:G:72:SER:OG	4:G:73:ASP:OD1	2.23	0.56
2:E:46:THR:CG2	2:E:403:LEU:HD11	2.36	0.56
2:E:631:PHE:CE2	3:F:96:VAL:HG22	2.40	0.56
1:A:429:GLY:O	2:B:600:ASN:ND2	2.39	0.56
1:A:593:GLU:OE1	2:B:543:THR:OG1	2.24	0.56
2:E:557:TYR:O	2:E:560:ARG:NE	2.39	0.56
2:B:132:THR:HB	2:B:682:ILE:HD11	1.88	0.55
2:B:686:GLU:N	2:B:686:GLU:OE2	2.39	0.55
1:D:436:GLU:OE2	2:E:600:ASN:ND2	2.39	0.55
2:E:15:GLN:OE1	2:E:498:ARG:NH1	2.39	0.55
3:F:463:ILE:HD11	3:F:480:VAL:HG23	1.89	0.55
3:C:570:MET:HE3	3:C:570:MET:HA	1.88	0.55
3:C:81:THR:HG22	3:C:82:ASN:H	1.71	0.55
3:F:694:PHE:HE2	3:F:713:LEU:HD22	1.72	0.55
3:C:289:ILE:HD13	3:C:529:ILE:HG23	1.88	0.55
3:C:382:ILE:HG22	3:C:383:GLN:HG2	1.88	0.55
1:D:178:ILE:HG22	1:D:182:MET:SD	2.46	0.55
1:D:554:VAL:HG12	1:D:554:VAL:O	2.06	0.55
1:A:606:ASP:OD1	1:A:607:LEU:N	2.40	0.55
1:A:600:SER:O	1:A:604:GLU:N	2.40	0.55
2:E:86:ASP:OD1	2:E:87:CYS:N	2.39	0.55
3:F:463:ILE:HD12	3:F:478:VAL:O	2.07	0.55
3:C:402:MET:SD	3:C:403:VAL:HG13	2.47	0.54
2:B:492:PHE:CD1	2:B:493:THR:HG23	2.42	0.54
3:C:638:VAL:N	3:C:645:MET:O	2.40	0.54
1:D:260:PHE:HE2	1:D:672:LEU:HB2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:27:SER:OG	4:G:28:ARG:N	2.41	0.54
1:A:590:GLN:OE1	2:B:509:LEU:HD21	2.07	0.54
3:C:345:LEU:CD2	3:C:351:THR:OG1	2.54	0.54
2:E:593:ASP:OD2	3:F:100:ASN:ND2	2.39	0.54
3:C:534:SER:O	3:C:536:MET:N	2.40	0.54
1:A:126:GLU:OE1	1:A:127:VAL:N	2.39	0.54
1:D:372:GLU:OE2	1:D:508:ARG:NH2	2.40	0.54
2:E:413:ASN:O	2:E:416:SER:OG	2.21	0.54
4:G:140:PRO:O	4:G:150:ARG:NH2	2.40	0.54
3:C:341:GLU:HG3	3:C:355:ARG:HD2	1.89	0.54
3:F:418:LEU:HD21	3:F:437:HIS:HB2	1.88	0.54
3:F:473:MET:HA	3:F:473:MET:HE2	1.89	0.54
3:C:279:SER:OG	3:C:283:MET:HE2	2.08	0.54
1:A:601:SER:N	3:C:239:CYS:SG	2.80	0.53
3:C:676:MET:SD	3:C:676:MET:N	2.81	0.53
1:A:3:ASP:N	1:A:3:ASP:OD1	2.41	0.53
2:B:715:VAL:O	2:B:719:VAL:HG23	2.08	0.53
1:D:656:GLU:OE1	2:E:30:TYR:OH	2.26	0.53
3:F:614:GLN:NE2	3:F:649:VAL:O	2.40	0.53
3:C:378:THR:O	3:C:378:THR:HG23	2.08	0.53
1:D:424:GLU:O	2:E:553:LYS:NZ	2.30	0.53
1:D:583:ARG:NH1	2:E:510:PRO:O	2.41	0.53
3:F:596:VAL:HG13	3:F:618:LEU:HG	1.90	0.53
1:A:523:MET:HB2	1:A:563:LEU:HD21	1.90	0.53
1:A:422:TRP:O	1:A:456:THR:HG22	2.08	0.53
2:E:40:MET:HE1	2:E:351:LEU:HD13	1.91	0.53
3:F:496:VAL:HG21	3:F:504:VAL:HG12	1.90	0.53
1:A:317:TRP:HZ3	1:A:545:ILE:HD12	1.73	0.53
2:B:285:VAL:HG11	2:B:441:LEU:HD11	1.90	0.53
3:C:597:ARG:NH1	3:C:624:ALA:O	2.41	0.53
1:D:56:GLU:N	1:D:56:GLU:OE1	2.42	0.53
1:D:152:GLY:O	1:D:172:LYS:NZ	2.23	0.53
3:F:554:ILE:HD11	3:F:674:ALA:O	2.08	0.53
3:F:629:SER:O	3:F:692:ARG:NH1	2.42	0.53
2:B:714:MET:O	2:B:718:MET:SD	2.67	0.53
3:F:78:TRP:HB3	3:F:91:VAL:HG12	1.91	0.53
1:A:129:ILE:O	1:A:133:GLU:HG2	2.09	0.52
1:D:684:GLU:N	1:D:684:GLU:OE2	2.41	0.52
1:A:391:LYS:HD3	1:A:392:GLN:N	2.25	0.52
3:C:530:THR:OG1	3:C:551:GLN:CD	2.49	0.52
3:C:697:LEU:HD11	3:C:735:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:ASN:OD1	2:E:60:GLU:N	2.41	0.52
1:A:233:VAL:HG11	2:B:323:THR:HG22	1.91	0.52
2:B:715:VAL:HG21	3:C:11:MET:HE3	1.92	0.52
1:D:78:ILE:O	1:D:82:ARG:NH1	2.42	0.52
3:F:231:VAL:HG12	3:F:231:VAL:O	2.09	0.52
3:C:656:PHE:CZ	3:C:665:LEU:HD11	2.45	0.52
2:E:273:VAL:HG23	2:E:278:LYS:HG3	1.90	0.52
4:G:84:ALA:HA	4:G:112:LEU:HD21	1.91	0.52
1:A:118:ILE:HG22	1:A:144:HIS:CB	2.38	0.52
1:D:178:ILE:O	1:D:182:MET:SD	2.67	0.52
2:E:432:THR:OG1	2:E:434:THR:OG1	2.21	0.52
1:A:86:MET:O	1:A:90:VAL:HG13	2.10	0.52
1:D:443:ARG:NH1	2:E:549:GLN:OE1	2.43	0.52
2:E:419:LEU:O	2:E:422:SER:OG	2.24	0.52
2:E:445:ASP:OD1	2:E:446:ASP:N	2.43	0.52
2:E:457:GLU:N	2:E:457:GLU:OE1	2.42	0.52
3:F:599:LEU:HD23	3:F:618:LEU:CD2	2.39	0.52
1:A:211:MET:HE2	2:B:174:MET:SD	2.51	0.51
3:C:178:THR:O	3:C:178:THR:CG2	2.58	0.51
3:C:528:THR:HG22	3:C:551:GLN:HE22	1.75	0.51
1:D:493:GLU:OE2	1:D:495:ARG:NH2	2.39	0.51
1:A:322:ILE:HD13	1:A:335:LEU:HD13	1.92	0.51
3:F:583:LEU:O	3:F:639:ASN:ND2	2.43	0.51
2:B:740:PHE:CE1	2:B:744:MET:HE3	2.45	0.51
2:E:521:ALA:O	2:E:525:VAL:HG12	2.11	0.51
3:F:398:ILE:O	3:F:402:MET:HG3	2.11	0.51
2:B:36:THR:HG22	2:B:40:MET:SD	2.51	0.51
1:A:55:ASP:OD1	1:A:58:GLY:N	2.44	0.51
2:E:572:ARG:NH1	3:F:97:THR:OG1	2.43	0.51
2:E:158:ASN:N	2:E:169:ASP:OD2	2.44	0.51
3:F:231:VAL:O	3:F:231:VAL:CG1	2.58	0.51
2:B:145:ASN:HB3	2:B:682:ILE:HD12	1.92	0.51
2:E:438:TRP:CB	2:E:451:VAL:HG22	2.41	0.51
1:A:374:MET:O	1:A:374:MET:HG2	2.11	0.50
2:B:248:ILE:HD12	2:B:347:LYS:HE3	1.92	0.50
2:B:292:ASN:OD1	2:B:292:ASN:O	2.29	0.50
2:E:213:ASN:OD1	2:E:213:ASN:C	2.53	0.50
3:F:701:ASN:O	3:F:723:ASN:ND2	2.45	0.50
4:G:88:PRO:HA	4:G:112:LEU:HD22	1.93	0.50
1:D:652:SER:N	2:E:24:TYR:OH	2.44	0.50
1:A:342:LEU:O	1:A:346:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:ASP:OD1	2:B:377:ASP:N	2.45	0.50
2:B:60:GLU:O	2:B:215:ARG:NE	2.44	0.50
2:B:219:ILE:O	2:B:223:THR:OG1	2.29	0.50
2:E:110:THR:HG21	2:E:258:LEU:HD12	1.94	0.50
2:B:374:ALA:O	2:B:393:ARG:NE	2.45	0.50
3:C:415:ARG:O	3:C:437:HIS:NE2	2.45	0.50
1:D:111:ASP:O	1:D:115:ASN:N	2.44	0.50
2:E:227:MET:SD	2:E:227:MET:N	2.84	0.50
2:E:582:GLN:NE2	3:F:101:ARG:O	2.43	0.50
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.11	0.50
1:D:606:ASP:OD1	1:D:606:ASP:N	2.45	0.50
2:E:40:MET:CE	2:E:351:LEU:HD22	2.42	0.50
3:F:553:ILE:HD11	3:F:577:PHE:CE1	2.47	0.50
2:E:255:VAL:CG2	2:E:415:LEU:HD11	2.41	0.49
3:F:298:LEU:HD21	3:F:312:LYS:HG2	1.93	0.49
1:A:647:ASN:OD1	1:A:699:TRP:NE1	2.37	0.49
2:B:306:ASN:ND2	2:B:444:SER:O	2.45	0.49
1:D:491:THR:HG22	1:D:492:LYS:H	1.77	0.49
1:D:511:LEU:HD11	1:D:518:VAL:CG2	2.42	0.49
1:A:215:ALA:HA	2:B:342:ILE:HD12	1.94	0.49
3:F:571:LEU:HD12	3:F:574:LYS:HD2	1.94	0.49
2:E:25:THR:HG22	2:E:25:THR:O	2.11	0.49
2:E:474:GLY:O	2:E:476:ASN:ND2	2.46	0.49
3:F:659:ASN:O	3:F:663:LYS:N	2.45	0.49
3:C:570:MET:HE3	3:C:570:MET:CA	2.43	0.49
2:E:526:GLY:HA3	2:E:551:PHE:CE2	2.48	0.49
2:B:494:SER:O	2:B:494:SER:OG	2.29	0.49
3:C:163:ILE:O	3:C:167:VAL:HG12	2.13	0.49
3:F:384:LEU:HD22	3:F:401:ALA:CB	2.43	0.49
2:B:734:ARG:O	2:B:735:ILE:HD13	2.13	0.49
2:B:556:ARG:NH2	2:B:595:GLY:O	2.46	0.49
3:C:259:LEU:HD21	3:C:308:VAL:HG21	1.95	0.49
3:C:656:PHE:CE1	3:C:665:LEU:HD11	2.48	0.49
1:D:511:LEU:HD11	1:D:518:VAL:HG22	1.94	0.49
2:B:306:ASN:ND2	2:B:445:ASP:O	2.46	0.48
1:D:427:GLU:OE1	1:D:427:GLU:N	2.41	0.48
2:E:95:LEU:HD23	2:E:95:LEU:C	2.37	0.48
3:F:78:TRP:CB	3:F:91:VAL:HG12	2.43	0.48
4:G:12:ARG:O	4:G:13:ASN:OD1	2.31	0.48
2:B:446:ASP:OD1	2:B:446:ASP:N	2.45	0.48
2:E:619:ASP:OD1	2:E:619:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD13	1:A:543:LEU:HD22	1.95	0.48
3:C:115:TYR:HA	3:C:206:MET:HE2	1.96	0.48
3:C:537:TRP:HE1	3:C:548:ASN:CG	2.21	0.48
2:E:436:TYR:CD1	2:E:436:TYR:C	2.92	0.48
2:B:222:LEU:O	2:B:348:MET:N	2.39	0.48
1:D:210:THR:HG21	2:E:218:LEU:HD13	1.94	0.48
2:E:396:LEU:C	2:E:397:ILE:HD13	2.38	0.48
3:F:280:LEU:HD23	3:F:280:LEU:C	2.38	0.48
2:B:218:LEU:HD23	2:B:222:LEU:HD13	1.96	0.48
1:D:587:GLN:O	1:D:591:GLN:HG3	2.14	0.48
2:E:113:ILE:O	2:E:117:THR:HG23	2.12	0.48
1:A:94:ILE:HG21	1:A:117:PHE:HE1	1.78	0.48
1:A:609:LYS:NZ	1:D:386:ASP:OD2	2.47	0.48
3:C:666:THR:OG1	3:C:670:LYS:O	2.16	0.48
1:D:450:VAL:HG23	1:D:641:LEU:HD23	1.86	0.48
3:F:554:ILE:HD11	3:F:675:LEU:HA	1.96	0.48
3:F:352:LEU:HD22	3:F:430:PRO:HB3	1.95	0.48
3:C:355:ARG:HH22	3:C:511:VAL:HG23	1.78	0.47
3:F:348:ASN:ND2	3:F:417:ASP:OD1	2.47	0.47
1:A:370:LEU:HD13	1:A:507:GLY:HA2	1.96	0.47
1:A:404:ALA:HB3	1:A:406:TRP:CD1	2.49	0.47
1:A:563:LEU:HD23	1:A:563:LEU:O	2.13	0.47
2:B:310:ASN:O	2:B:407:MET:N	2.44	0.47
3:F:499:ASP:OD1	3:F:503:ARG:N	2.47	0.47
2:E:56:THR:HG22	2:E:57:THR:N	2.29	0.47
3:F:538:GLU:O	3:F:538:GLU:HG2	2.14	0.47
4:G:76:VAL:N	4:G:98:ASN:OD1	2.44	0.47
3:C:269:ARG:HB2	3:C:536:MET:HE1	1.96	0.47
2:E:258:LEU:HD22	2:E:337:LEU:HD13	1.95	0.47
1:A:292:ILE:HG22	1:A:313:THR:HG21	1.97	0.47
1:D:524:GLU:O	1:D:563:LEU:HD12	2.15	0.47
2:B:525:VAL:O	2:B:529:VAL:HG23	2.15	0.47
2:B:529:VAL:CG2	2:B:655:MET:HE1	2.44	0.47
3:C:1:MET:HE2	3:C:1:MET:N	2.30	0.47
3:C:619:LEU:O	3:C:619:LEU:HD12	2.15	0.47
1:D:260:PHE:CE2	1:D:672:LEU:HB2	2.50	0.47
1:D:450:VAL:HG22	1:D:641:LEU:CD2	2.41	0.47
4:G:69:LEU:HD21	4:G:83:LEU:HD11	1.96	0.47
3:C:344:VAL:HG11	3:C:411:ILE:HD12	1.97	0.47
2:E:171:MET:HE1	2:E:339:ILE:HD11	1.96	0.47
3:F:652:ASN:ND2	3:F:657:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HD13	1:A:585:LEU:CD1	2.45	0.47
1:A:670:GLN:OE1	2:B:14:VAL:HG23	2.15	0.47
3:C:395:ALA:HA	3:C:467:MET:HE3	1.96	0.47
2:E:295:ASP:OD1	2:E:295:ASP:N	2.48	0.47
3:F:496:VAL:HG21	3:F:504:VAL:CG1	2.45	0.47
3:F:475:LEU:HD23	3:F:478:VAL:HG21	1.97	0.46
3:F:617:LYS:NZ	3:F:651:GLY:O	2.42	0.46
1:A:225:SER:OG	1:A:228:ASN:OD1	2.30	0.46
2:B:583:THR:O	2:B:586:LYS:NZ	2.49	0.46
4:G:38:THR:OG1	4:G:39:ASP:N	2.48	0.46
1:A:2:GLU:OE1	1:A:32:THR:OG1	2.28	0.46
1:A:12:MET:HE2	3:C:754:ILE:HG23	1.97	0.46
2:E:147:ILE:HG13	2:E:148:GLU:N	2.29	0.46
1:A:611:PHE:O	1:A:633:ILE:HG21	2.15	0.46
2:B:636:GLU:CB	3:C:32:LYS:NZ	2.76	0.46
4:G:100:ILE:HG23	4:G:125:VAL:HG23	1.97	0.46
2:B:136:ASN:ND2	2:B:227:MET:SD	2.88	0.46
1:D:493:GLU:OE2	1:D:495:ARG:NH1	2.49	0.46
2:E:131:TRP:CH2	2:E:149:VAL:HG11	2.50	0.46
1:A:707:PHE:CD1	1:A:707:PHE:C	2.93	0.46
2:E:603:ASN:HB2	3:F:125:LEU:HD21	1.98	0.46
1:A:151:THR:O	1:A:151:THR:HG22	2.16	0.46
3:F:306:GLN:HG2	3:F:518:VAL:HG22	1.97	0.46
2:B:299:SER:OG	2:B:487:THR:HG21	2.16	0.46
4:G:102:ASP:HA	4:G:125:VAL:HG22	1.97	0.46
3:C:259:LEU:HD11	3:C:298:LEU:HD23	1.98	0.45
1:D:418:THR:HG22	1:D:419:ASP:N	2.30	0.45
2:B:61:THR:HG22	2:B:218:LEU:HD22	1.98	0.45
2:B:132:THR:CB	2:B:682:ILE:HD11	2.47	0.45
1:D:566:ARG:NE	1:D:568:ASN:OD1	2.48	0.45
3:C:581:GLN:O	3:C:589:ARG:NH2	2.49	0.45
1:D:450:VAL:HG22	1:D:450:VAL:O	2.16	0.45
1:D:523:MET:HB3	1:D:563:LEU:HD11	1.97	0.45
2:E:438:TRP:CD1	2:E:449:LEU:HD11	2.51	0.45
3:F:494:VAL:HG12	3:F:495:VAL:N	2.32	0.45
3:F:596:VAL:HG21	3:F:621:PHE:HB2	1.99	0.45
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.49	0.45
2:E:248:ILE:HD11	2:E:344:PHE:CD1	2.52	0.45
3:F:318:ARG:HE	3:F:495:VAL:HA	1.81	0.45
1:A:541:CYS:SG	1:A:543:LEU:HD21	2.57	0.45
1:A:670:GLN:OE1	2:B:14:VAL:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:THR:HG22	2:B:333:PHE:HE1	1.82	0.45
3:C:170:ASN:OD1	3:C:170:ASN:N	2.46	0.45
1:D:399:GLU:H	1:D:399:GLU:CD	2.24	0.45
1:D:667:LEU:HD21	2:E:18:ILE:HD11	1.98	0.45
2:B:61:THR:CG2	2:B:218:LEU:HD22	2.47	0.45
3:C:420:PHE:O	3:C:433:GLN:NE2	2.44	0.45
2:E:124:GLN:CD	2:E:124:GLN:C	2.85	0.45
3:F:64:MET:HE1	3:F:69:GLU:OE1	2.16	0.45
3:F:298:LEU:C	3:F:298:LEU:HD23	2.42	0.45
3:F:336:SER:N	3:F:360:TYR:O	2.49	0.45
1:A:12:MET:HE2	3:C:754:ILE:HG21	1.99	0.45
3:C:563:GLN:O	3:C:567:ASP:N	2.45	0.45
3:F:520:GLU:OE1	3:F:520:GLU:N	2.49	0.45
1:A:288:LEU:HD22	1:A:527:LEU:CD2	2.46	0.45
2:B:273:VAL:HG11	2:B:281:LYS:CE	2.47	0.45
3:F:525:GLU:OE1	3:F:529:ILE:N	2.50	0.45
3:F:686:VAL:HG22	3:F:697:LEU:HD12	1.99	0.45
4:G:131:TYR:CE1	4:G:135:VAL:HG21	2.52	0.45
1:A:322:ILE:CD1	1:A:335:LEU:HD13	2.46	0.45
3:C:162:VAL:O	3:C:166:VAL:HG23	2.17	0.45
3:C:451:ILE:HG22	3:C:473:MET:HE2	1.98	0.45
3:C:537:TRP:NE1	3:C:548:ASN:OD1	2.49	0.45
1:A:91:VAL:HG23	1:A:117:PHE:CE2	2.53	0.44
1:A:261:LEU:N	1:A:261:LEU:HD23	2.32	0.44
2:B:37:GLY:HA2	2:B:40:MET:HE2	2.00	0.44
2:B:523:MET:HE1	2:B:591:VAL:CG2	2.47	0.44
3:C:497:SER:O	3:C:505:ARG:N	2.40	0.44
1:A:331:ASN:N	1:A:332:PRO:HD2	2.33	0.44
3:C:279:SER:O	3:C:283:MET:HG3	2.17	0.44
2:E:438:TRP:HB2	2:E:451:VAL:HG22	2.00	0.44
2:B:37:GLY:O	2:B:41:ASP:OD2	2.34	0.44
2:B:696:PHE:CD2	3:C:28:MET:HE2	2.52	0.44
2:E:143:LEU:O	2:E:147:ILE:HG23	2.18	0.44
3:F:556:ASN:OD1	3:F:556:ASN:N	2.49	0.44
1:A:106:LEU:HD12	1:A:107:PRO:N	2.31	0.44
3:C:431:MET:SD	3:C:431:MET:N	2.88	0.44
1:D:526:SER:OG	1:D:528:THR:HG22	2.18	0.44
2:E:177:GLU:O	2:E:214:LYS:N	2.50	0.44
3:F:64:MET:HE3	3:F:64:MET:O	2.17	0.44
3:F:407:GLU:N	3:F:410:MET:HE2	2.32	0.44
1:D:589:LEU:O	1:D:590:GLN:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:GLU:OE1	2:E:104:GLU:N	2.43	0.44
3:C:528:THR:CG2	3:C:551:GLN:HE22	2.28	0.44
2:E:565:ASP:OD1	2:E:566:THR:N	2.51	0.44
3:F:334:SER:O	3:F:362:GLU:N	2.49	0.44
1:A:128:HIS:O	1:A:132:LEU:HG	2.17	0.44
1:D:420:SER:O	1:D:452:HIS:ND1	2.45	0.44
1:A:1:MET:HA	1:A:187:LEU:HD13	2.00	0.44
2:B:277:GLU:OE1	2:B:277:GLU:N	2.46	0.44
1:D:530:PRO:CG	1:D:542:VAL:HG11	2.39	0.44
4:G:3:MET:O	4:G:7:ILE:HG13	2.18	0.44
3:C:743:ILE:O	3:C:743:ILE:HG22	2.18	0.44
2:E:422:SER:O	2:E:426:LEU:HD13	2.18	0.44
3:F:268:ARG:O	3:F:271:THR:OG1	2.26	0.44
1:A:12:MET:HE3	1:A:12:MET:O	2.17	0.43
1:A:106:LEU:HD12	1:A:107:PRO:HD2	1.99	0.43
3:C:388:GLY:N	3:C:394:ILE:HD11	2.33	0.43
1:A:360:MET:SD	1:A:505:ILE:HD11	2.58	0.43
2:B:382:ASN:N	2:B:382:ASN:OD1	2.48	0.43
2:B:754:ARG:HG3	2:B:755:ARG:HD2	1.98	0.43
1:D:491:THR:HG22	1:D:492:LYS:N	2.33	0.43
1:A:447:THR:O	1:A:451:SER:N	2.51	0.43
2:E:492:PHE:O	2:E:493:THR:OG1	2.31	0.43
2:B:523:MET:HE1	2:B:591:VAL:HG21	2.01	0.43
2:B:583:THR:OG1	2:B:584:ARG:N	2.52	0.43
2:B:701:PRO:O	2:B:704:SER:OG	2.35	0.43
2:E:40:MET:HE3	2:E:351:LEU:HD22	1.99	0.43
3:F:133:VAL:HG12	3:F:242:GLN:CG	2.49	0.43
4:G:144:TYR:CD1	4:G:155:ALA:HB2	2.54	0.43
1:A:612:PHE:CZ	1:A:633:ILE:HD11	2.53	0.43
1:A:621:ILE:HD13	1:A:636:VAL:HG22	1.99	0.43
3:C:174:ALA:HB2	3:C:726:ILE:HD12	2.00	0.43
2:E:428:GLN:O	2:E:432:THR:HG22	2.18	0.43
1:A:439:ALA:HB2	2:B:541:PRO:HB2	2.00	0.43
2:B:702:SER:HB2	3:C:164:MET:HE1	2.01	0.43
2:B:751:GLU:O	2:B:755:ARG:HG2	2.19	0.43
3:C:145:VAL:HG21	3:C:229:ILE:HD12	2.00	0.43
3:C:256:ASP:OD1	3:C:301:ASN:ND2	2.52	0.43
3:C:494:VAL:HG22	3:C:495:VAL:N	2.34	0.43
2:E:316:ARG:NH2	2:E:404:SER:OG	2.49	0.43
3:F:538:GLU:OE1	3:F:538:GLU:N	2.42	0.43
4:G:103:LEU:HA	4:G:106:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:NH2	2:B:335:ASN:OD1	2.52	0.43
1:A:665:LEU:O	1:A:669:VAL:HG22	2.18	0.43
1:D:470:LEU:HD12	1:D:575:MET:HB3	2.01	0.43
3:F:611:ASP:O	3:F:615:ILE:HG13	2.18	0.43
1:A:203:GLU:OE2	2:B:162:ARG:NH2	2.46	0.43
3:C:249:GLU:OE1	3:C:250:VAL:N	2.52	0.43
3:C:570:MET:HE3	3:C:570:MET:O	2.19	0.43
2:B:224:LEU:HG	2:B:347:LYS:HE2	2.00	0.43
2:E:219:ILE:HD11	2:E:348:MET:HE2	2.01	0.43
1:A:237:GLU:N	1:A:237:GLU:OE1	2.50	0.43
2:B:149:VAL:HG23	2:B:682:ILE:HD13	2.01	0.43
2:B:404:SER:HB3	2:B:405:PRO:HD3	2.01	0.43
2:E:438:TRP:HB3	2:E:451:VAL:HG22	2.00	0.43
1:A:391:LYS:HD3	1:A:392:GLN:O	2.19	0.42
2:B:14:VAL:HG12	2:B:18:ILE:CD1	2.49	0.42
2:B:347:LYS:HG3	2:B:348:MET:N	2.34	0.42
1:D:600:SER:O	1:D:604:GLU:N	2.47	0.42
3:F:98:TRP:CD1	3:F:102:ASN:HD21	2.37	0.42
3:F:280:LEU:HD23	3:F:280:LEU:O	2.19	0.42
2:B:561:CYS:HA	2:B:576:LEU:HD11	2.01	0.42
2:B:707:ARG:CZ	3:C:29:ALA:HB3	2.49	0.42
3:C:232:LEU:HD11	3:C:236:GLN:OE1	2.19	0.42
1:D:590:GLN:HG3	2:E:543:THR:HG21	2.01	0.42
1:A:164:ASP:OD1	1:A:165:GLU:N	2.51	0.42
1:D:214:LEU:HD22	2:E:346:ASN:OD1	2.19	0.42
1:A:51:PHE:N	1:A:51:PHE:CD1	2.86	0.42
1:A:563:LEU:HD23	1:A:565:VAL:HG23	2.00	0.42
2:B:291:THR:HG21	3:C:385:ILE:CG1	2.49	0.42
2:B:667:ILE:HG13	2:B:668:PRO:HD2	2.02	0.42
3:C:381:LEU:HD23	3:C:449:TRP:CZ2	2.54	0.42
3:C:678:ASP:HB3	3:C:679:PRO:HD3	2.01	0.42
1:D:260:PHE:HD2	1:D:678:PRO:HG2	1.84	0.42
3:F:659:ASN:OD1	3:F:662:THR:N	2.45	0.42
1:D:707:PHE:HE1	1:D:711:LEU:HD11	1.84	0.42
2:E:268:GLN:HB2	2:E:421:VAL:HG23	2.02	0.42
1:A:580:GLU:O	1:A:580:GLU:CG	2.68	0.42
2:B:149:VAL:CG2	2:B:682:ILE:HD13	2.49	0.42
2:E:255:VAL:HG22	2:E:415:LEU:HD11	2.01	0.42
4:G:3:MET:HE2	4:G:52:VAL:HG21	2.02	0.42
1:A:261:LEU:O	1:A:261:LEU:HG	2.19	0.42
2:B:25:THR:O	2:B:25:THR:OG1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:PHE:CE1	1:D:711:LEU:HD11	2.54	0.42
2:E:624:LEU:O	2:E:663:THR:OG1	2.25	0.42
3:F:262:ALA:O	3:F:266:ILE:HG12	2.20	0.42
3:F:403:VAL:HG12	3:F:438:PHE:CD2	2.54	0.42
1:A:106:LEU:HD12	1:A:107:PRO:CD	2.50	0.42
1:A:392:GLN:NE2	2:B:382:ASN:OD1	2.53	0.42
3:C:256:ASP:O	3:C:260:ILE:HG12	2.19	0.42
3:C:280:LEU:HD12	3:C:280:LEU:C	2.45	0.42
1:A:621:ILE:O	1:A:621:ILE:HG23	2.18	0.42
2:B:171:MET:HE3	2:B:171:MET:CA	2.49	0.42
3:C:579:PRO:HD2	3:C:580:PHE:H	1.85	0.42
1:D:527:LEU:HD12	1:D:560:PRO:O	2.20	0.42
2:E:101:GLY:O	2:E:105:ASN:OD1	2.37	0.42
3:C:175:ARG:O	3:C:179:SER:OG	2.30	0.41
3:C:341:GLU:CG	3:C:355:ARG:CD	2.80	0.41
1:D:379:VAL:HG12	2:E:364:LEU:HD22	2.02	0.41
2:E:42:THR:HG21	2:E:408:MET:HE1	2.02	0.41
3:F:570:MET:N	3:F:570:MET:SD	2.93	0.41
1:A:599:GLU:HB3	1:A:607:LEU:HD13	2.01	0.41
2:B:243:THR:HG23	2:B:243:THR:O	2.18	0.41
3:F:496:VAL:HG22	3:F:497:SER:N	2.35	0.41
1:A:211:MET:HE3	2:B:171:MET:SD	2.60	0.41
2:B:291:THR:HG21	3:C:385:ILE:HD11	2.02	0.41
3:C:725:LEU:HD23	3:C:725:LEU:O	2.20	0.41
1:D:384:CYS:O	1:D:390:LEU:HD22	2.20	0.41
2:E:258:LEU:HD12	2:E:258:LEU:HA	1.92	0.41
3:F:71:ASN:N	3:F:75:GLN:O	2.52	0.41
1:A:347:ASP:O	1:A:351:GLU:HG2	2.20	0.41
3:C:530:THR:HG1	3:C:551:GLN:CD	2.05	0.41
2:E:131:TRP:HH2	2:E:149:VAL:HG11	1.85	0.41
3:F:110:HIS:O	3:F:114:VAL:HG12	2.20	0.41
3:F:269:ARG:NH2	3:F:535:MET:SD	2.93	0.41
3:F:453:PRO:HA	3:F:473:MET:HE1	2.02	0.41
1:A:584:CYS:O	1:A:585:LEU:C	2.64	0.41
2:B:4:ASN:ND2	2:B:7:LEU:HD13	2.35	0.41
2:B:714:MET:O	2:B:717:ALA:N	2.53	0.41
3:C:365:MET:HE2	3:C:372:ALA:HB3	2.02	0.41
3:C:512:LEU:O	3:C:513:LEU:HD12	2.21	0.41
2:E:438:TRP:CD1	2:E:438:TRP:C	2.99	0.41
3:F:328:PHE:CE2	3:F:400:VAL:HG21	2.56	0.41
3:F:486:ASP:O	3:F:487:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:616:ILE:HD13	3:F:675:LEU:HD13	2.02	0.41
1:A:111:ASP:OD2	1:A:114:GLU:N	2.43	0.41
2:B:368:VAL:O	2:B:368:VAL:HG13	2.21	0.41
1:D:323:ILE:HD13	1:D:323:ILE:N	2.35	0.41
3:F:481:SER:OG	3:F:482:LYS:N	2.54	0.41
1:A:251:LYS:O	1:A:254:ASN:ND2	2.41	0.41
1:A:462:GLY:O	1:A:466:ASN:ND2	2.54	0.41
1:A:543:LEU:O	1:A:545:ILE:HG23	2.20	0.41
2:B:56:THR:HG22	2:B:57:THR:N	2.35	0.41
2:E:322:ILE:HG23	2:E:337:LEU:CD2	2.51	0.41
1:A:639:THR:HG23	2:B:3:VAL:HG11	2.01	0.41
2:B:344:PHE:CE1	2:B:347:LYS:NZ	2.88	0.41
2:B:374:ALA:HB2	2:B:396:LEU:HD23	2.02	0.41
3:C:224:THR:O	3:C:224:THR:HG22	2.20	0.41
1:D:79:ILE:HD11	1:D:110:TYR:HB2	2.03	0.41
1:D:174:ARG:NH2	1:D:178:ILE:HD11	2.36	0.41
1:D:212:ARG:NH1	1:D:227:GLU:OE2	2.42	0.41
1:A:562:PHE:N	1:A:562:PHE:CD1	2.89	0.41
1:A:670:GLN:OE1	2:B:13:PRO:HA	2.21	0.41
2:B:746:ILE:O	2:B:750:ILE:HG12	2.21	0.41
3:C:81:THR:HG22	3:C:82:ASN:N	2.35	0.41
3:C:528:THR:OG1	3:C:671:ASP:O	2.35	0.41
2:E:134:ASN:OD1	2:E:350:ARG:NH1	2.48	0.41
2:E:255:VAL:CG2	2:E:322:ILE:HD11	2.51	0.41
2:E:397:ILE:O	2:E:400:THR:OG1	2.33	0.41
3:F:281:LEU:O	3:F:285:HIS:ND1	2.54	0.41
3:C:1:MET:HE2	3:C:1:MET:H1	1.84	0.41
3:C:142:ARG:HB3	3:C:217:PHE:CZ	2.56	0.41
3:C:499:ASP:OD1	3:C:503:ARG:N	2.49	0.41
1:D:513:ASN:OD1	1:D:514:ASP:N	2.54	0.41
2:E:104:GLU:O	2:E:108:LEU:HG	2.21	0.41
2:E:318:PHE:O	2:E:322:ILE:HG13	2.21	0.41
3:F:624:ALA:O	3:F:626:PRO:HD3	2.21	0.41
3:F:690:VAL:HB	3:F:696:ILE:HD13	2.02	0.41
1:A:289:LYS:HB2	1:A:499:ASN:HB3	2.03	0.40
1:D:309:LYS:O	1:D:313:THR:HG23	2.21	0.40
1:D:450:VAL:HG22	1:D:641:LEU:HD23	1.89	0.40
3:C:355:ARG:NH2	3:C:511:VAL:HG23	2.35	0.40
2:E:273:VAL:HG23	2:E:278:LYS:CG	2.51	0.40
3:F:478:VAL:O	3:F:478:VAL:HG23	2.21	0.40
2:B:226:THR:HG22	2:B:242:ALA:HB2	2.03	0.40

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:VAL:HG21	3:C:354:ILE:HD11	2.03	0.40
3:C:520:GLU:N	3:C:520:GLU:OE1	2.54	0.40
3:C:536:MET:HE3	3:C:536:MET:HB3	1.95	0.40
3:C:606:VAL:HG12	3:C:607:LEU:N	2.36	0.40
1:D:55:ASP:OD1	1:D:59:GLU:N	2.54	0.40
2:E:107:CYS:O	2:E:111:MET:HG3	2.21	0.40
2:B:549:GLN:O	2:B:552:ILE:HG22	2.21	0.40
3:C:464:LEU:HB3	3:C:465:PRO:HD3	2.03	0.40
1:D:361:LYS:O	1:D:363:THR:HG23	2.21	0.40
3:F:640:VAL:O	3:F:640:VAL:HG23	2.21	0.40
3:F:694:PHE:C	3:F:695:LEU:HD12	2.46	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	704/716 (98%)	682 (97%)	22 (3%)	0	100	100
1	D	703/716 (98%)	673 (96%)	30 (4%)	0	100	100
2	B	704/757 (93%)	672 (96%)	32 (4%)	0	100	100
2	E	605/757 (80%)	579 (96%)	26 (4%)	0	100	100
3	C	757/788 (96%)	725 (96%)	31 (4%)	1 (0%)	48	76
3	F	611/788 (78%)	579 (95%)	30 (5%)	2 (0%)	36	66
4	G	155/275 (56%)	148 (96%)	7 (4%)	0	100	100
All	All	4239/4797 (88%)	4058 (96%)	178 (4%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	251	ARG
3	F	487	GLU
3	C	678	ASP

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	638/645 (99%)	637 (100%)	1 (0%)	87	87
1	D	637/645 (99%)	634 (100%)	3 (0%)	81	82
2	B	630/667 (94%)	629 (100%)	1 (0%)	87	87
2	E	537/667 (80%)	535 (100%)	2 (0%)	84	84
3	C	667/686 (97%)	664 (100%)	3 (0%)	84	84
3	F	538/686 (78%)	538 (100%)	0	100	100
4	G	146/251 (58%)	146 (100%)	0	100	100
All	All	3793/4247 (89%)	3783 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	MET
2	B	76	ASP
3	C	243	MET
3	C	357	HIS
3	C	681	GLU
1	D	348	ILE
1	D	454	ARG
1	D	682	ASP
2	E	32	HIS
2	E	345	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	392	GLN
1	A	408	GLN
1	A	466	ASN
1	A	513	ASN
2	B	77	ASN
2	B	84	GLN
2	B	268	GLN
2	B	276	ASN
2	B	306	ASN
2	B	312	ASN
2	B	456	HIS
2	B	549	GLN
2	B	621	GLN
3	C	100	ASN
3	C	127	HIS
3	C	138	GLN
3	C	288	GLN
3	C	348	ASN
3	C	540	ASN
3	C	581	GLN
3	C	614	GLN
3	C	701	ASN
1	D	41	HIS
1	D	278	GLN
2	E	67	ASN
2	E	77	ASN
2	E	310	ASN
2	E	313	GLN
2	E	476	ASN
3	F	102	ASN
3	F	652	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

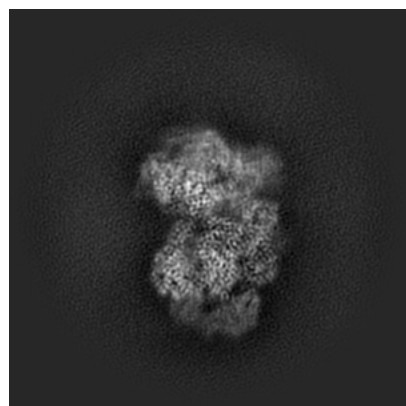
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19368. These allow visual inspection of the internal detail of the map and identification of artifacts.

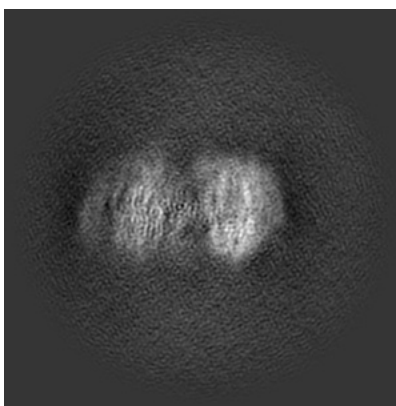
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

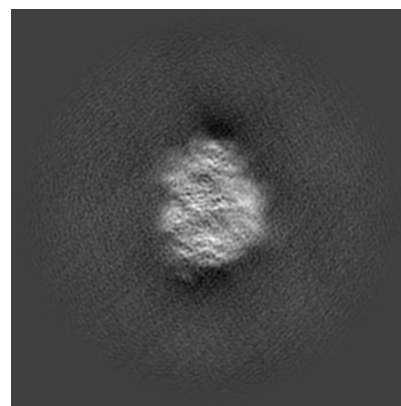
6.1.1 Primary map



X

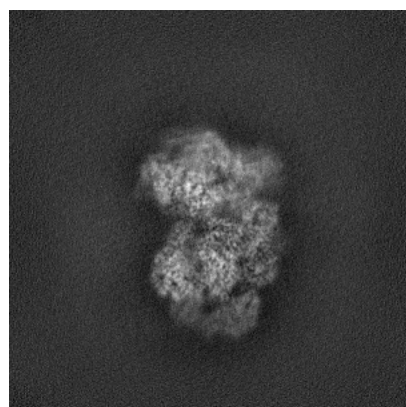


Y

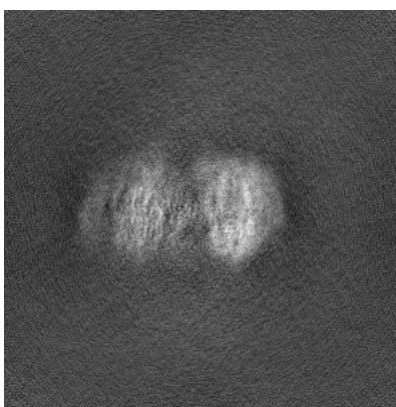


Z

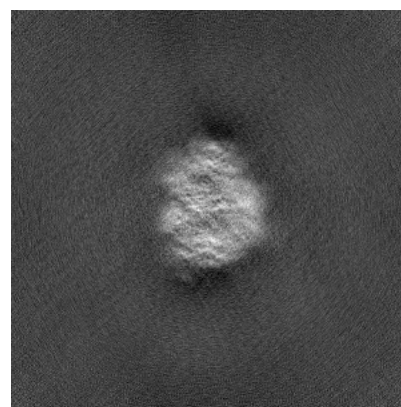
6.1.2 Raw map



X



Y

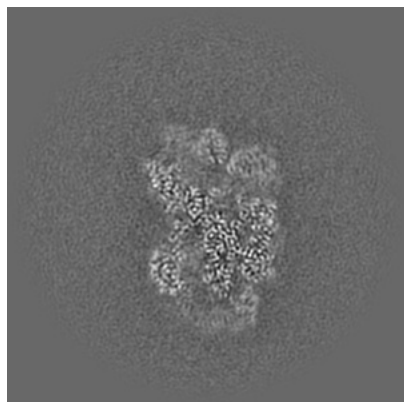


Z

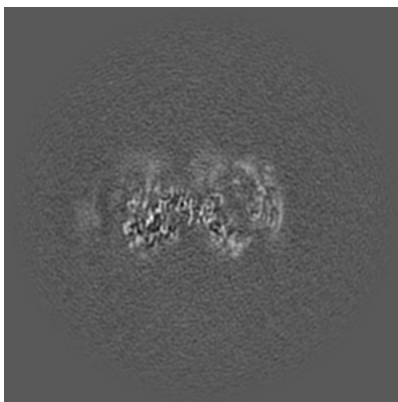
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

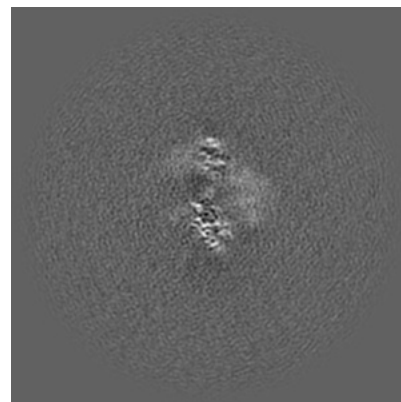
6.2.1 Primary map



X Index: 210

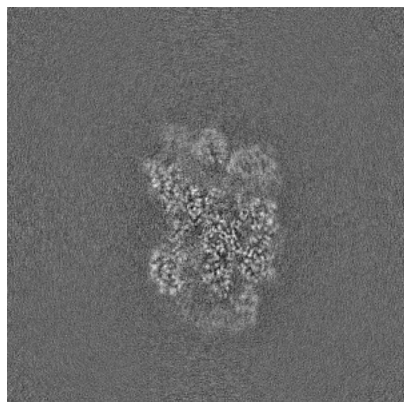


Y Index: 210

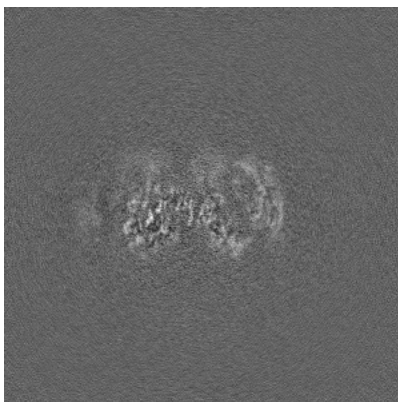


Z Index: 210

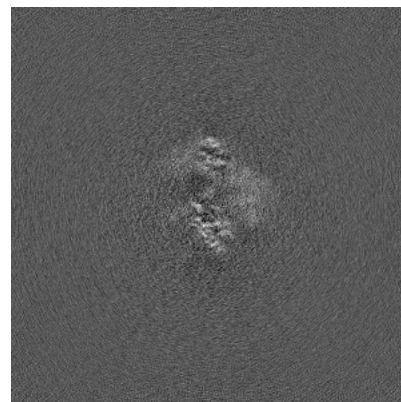
6.2.2 Raw map



X Index: 210



Y Index: 210

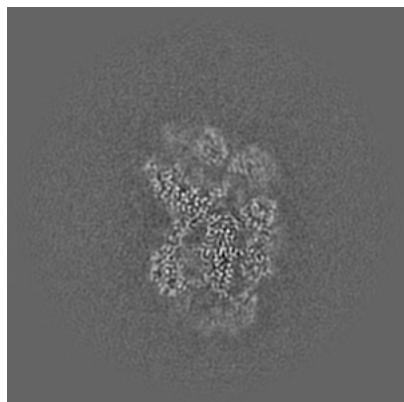


Z Index: 210

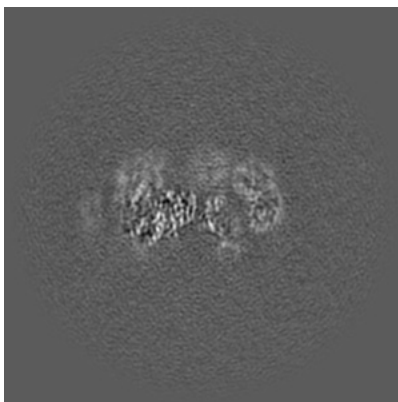
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

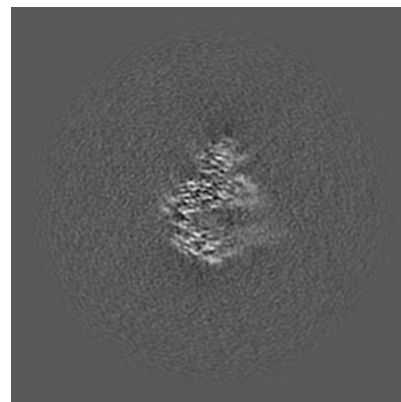
6.3.1 Primary map



X Index: 207

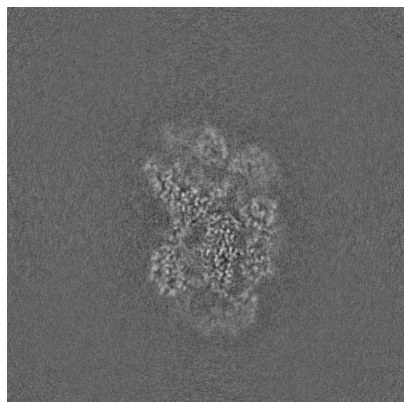


Y Index: 214

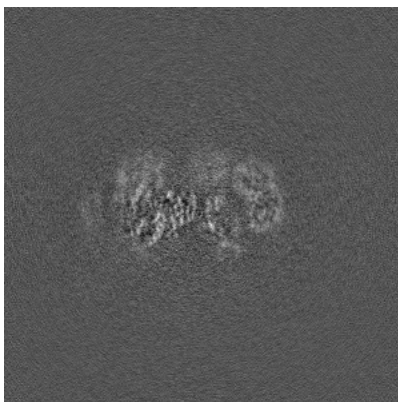


Z Index: 148

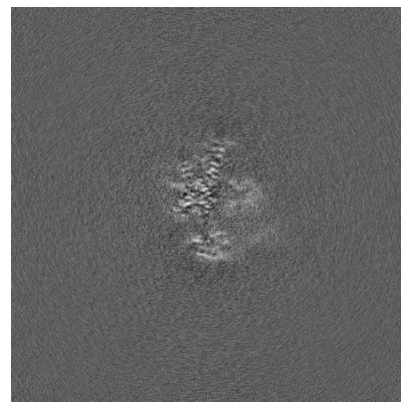
6.3.2 Raw map



X Index: 207



Y Index: 214

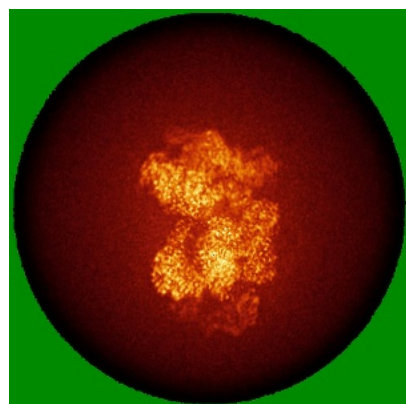


Z Index: 161

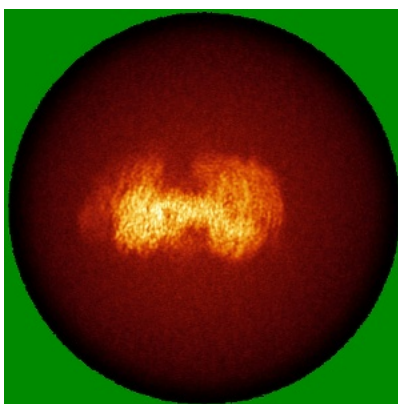
The images above show the largest variance slices of the map in three orthogonal directions.

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

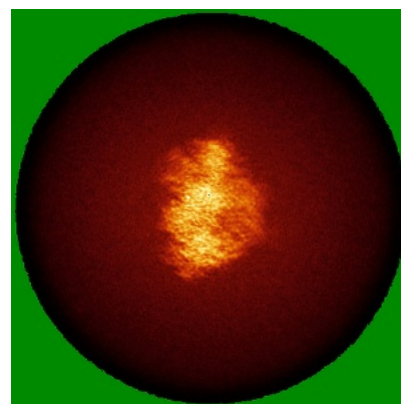
6.4.1 Primary map



X

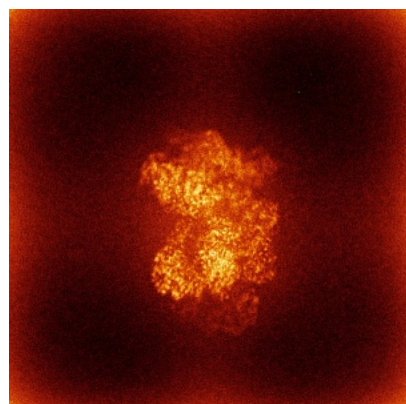


Y

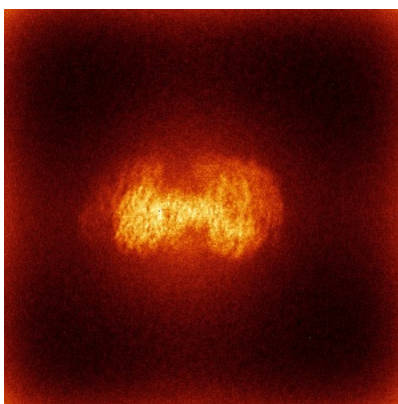


Z

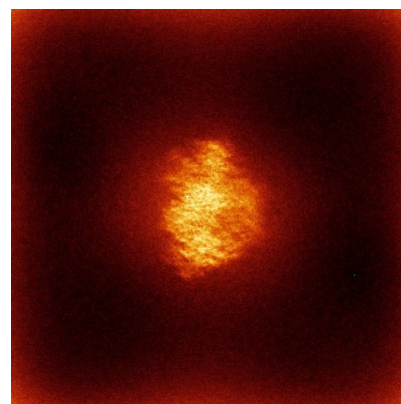
6.4.2 Raw map



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



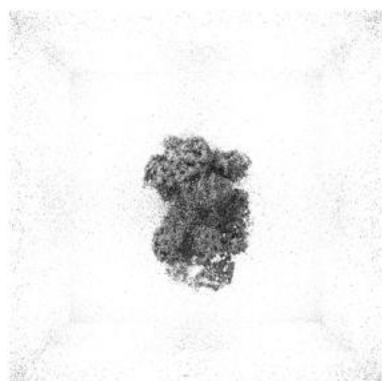
Y



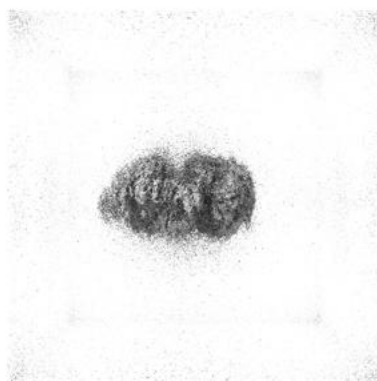
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

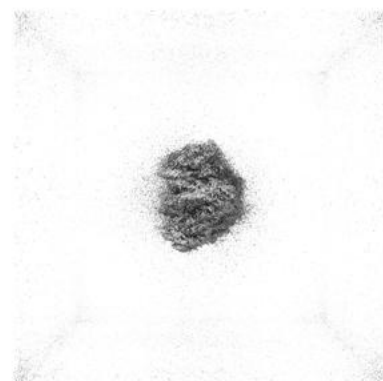
6.5.2 Raw map



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.

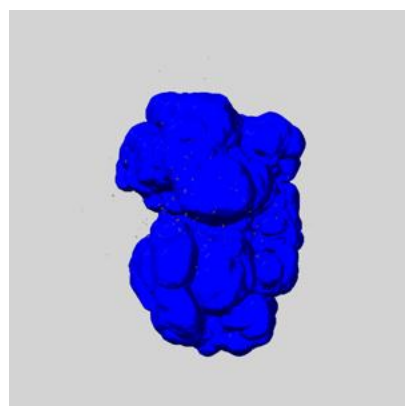
6.6 Mask visualisation [i](#)

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

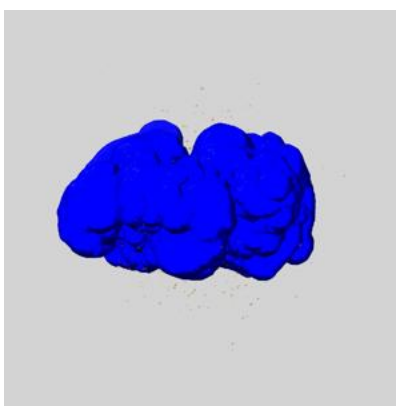
A mask typically either:

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

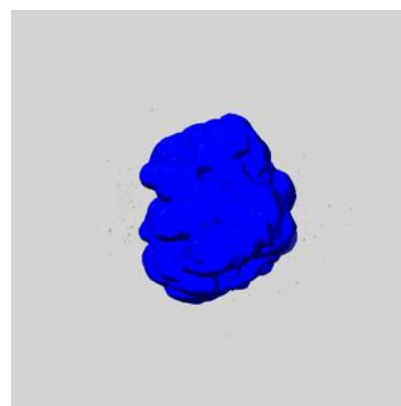
6.6.1 emd_19368_msk_1.map [i](#)



X



Y

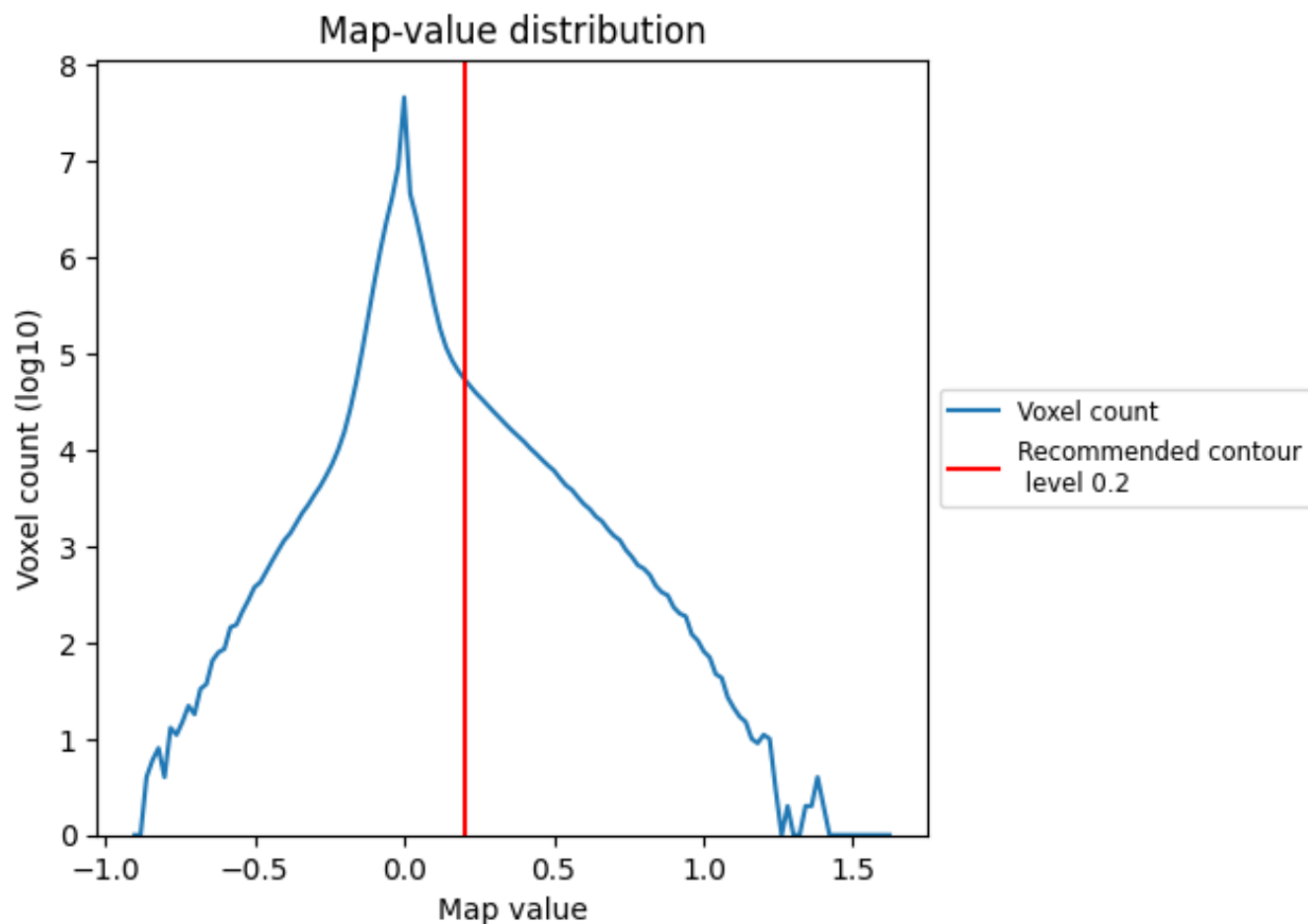


Z

7 Map analysis [i](#)

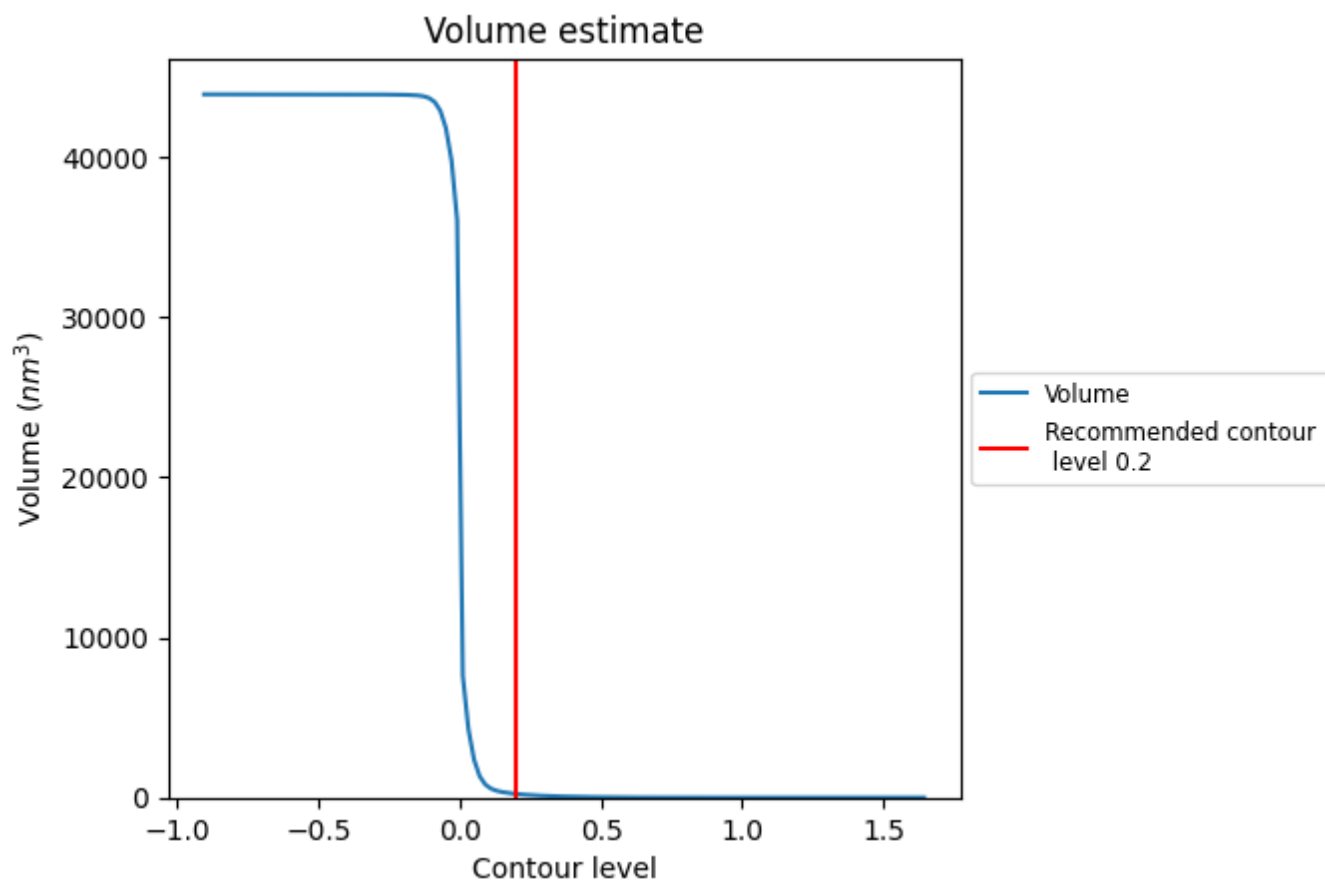
This section contains the results of statistical analysis of the map.

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.

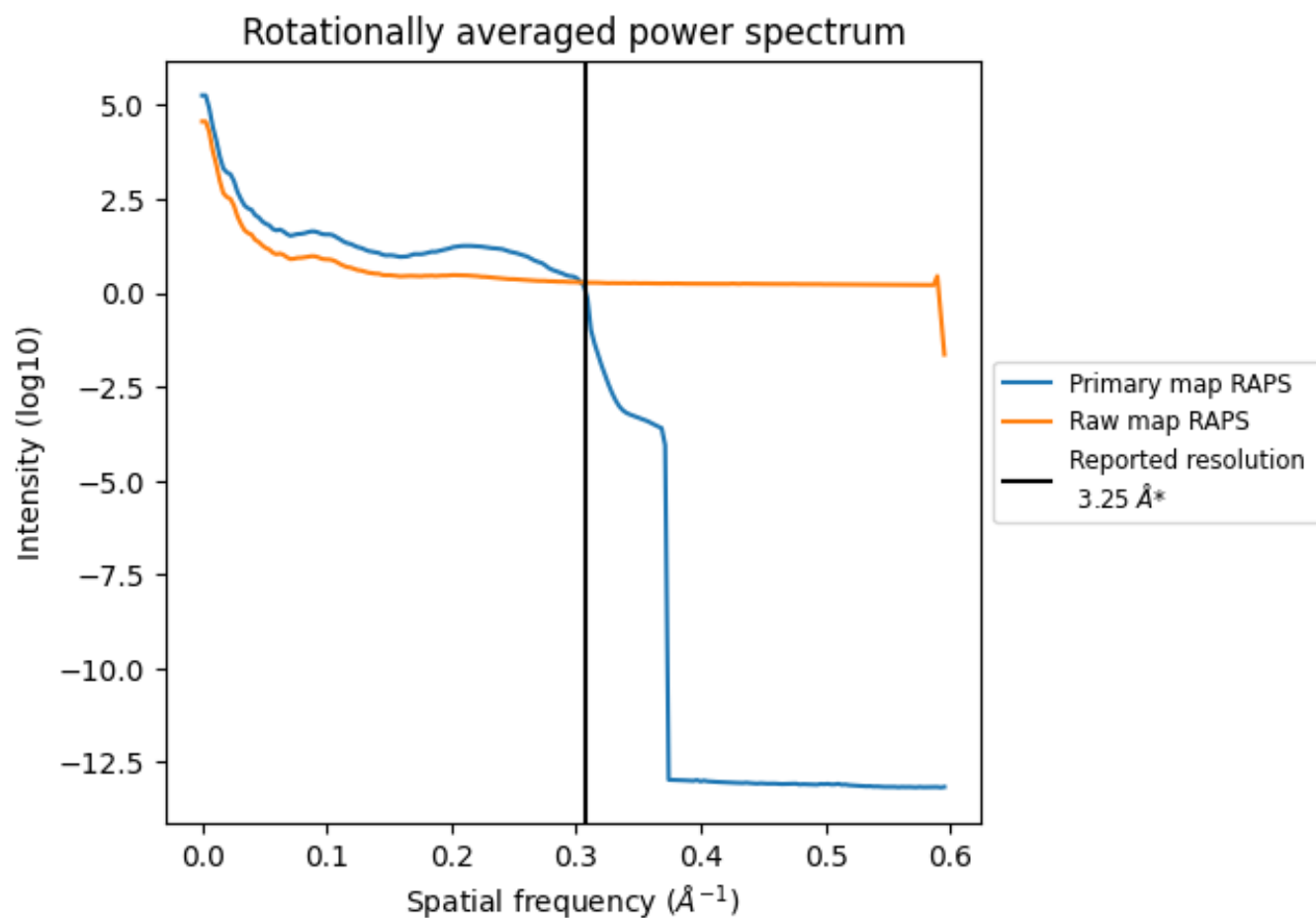
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm³; this corresponds to an approximate mass of 207 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 ⓘ

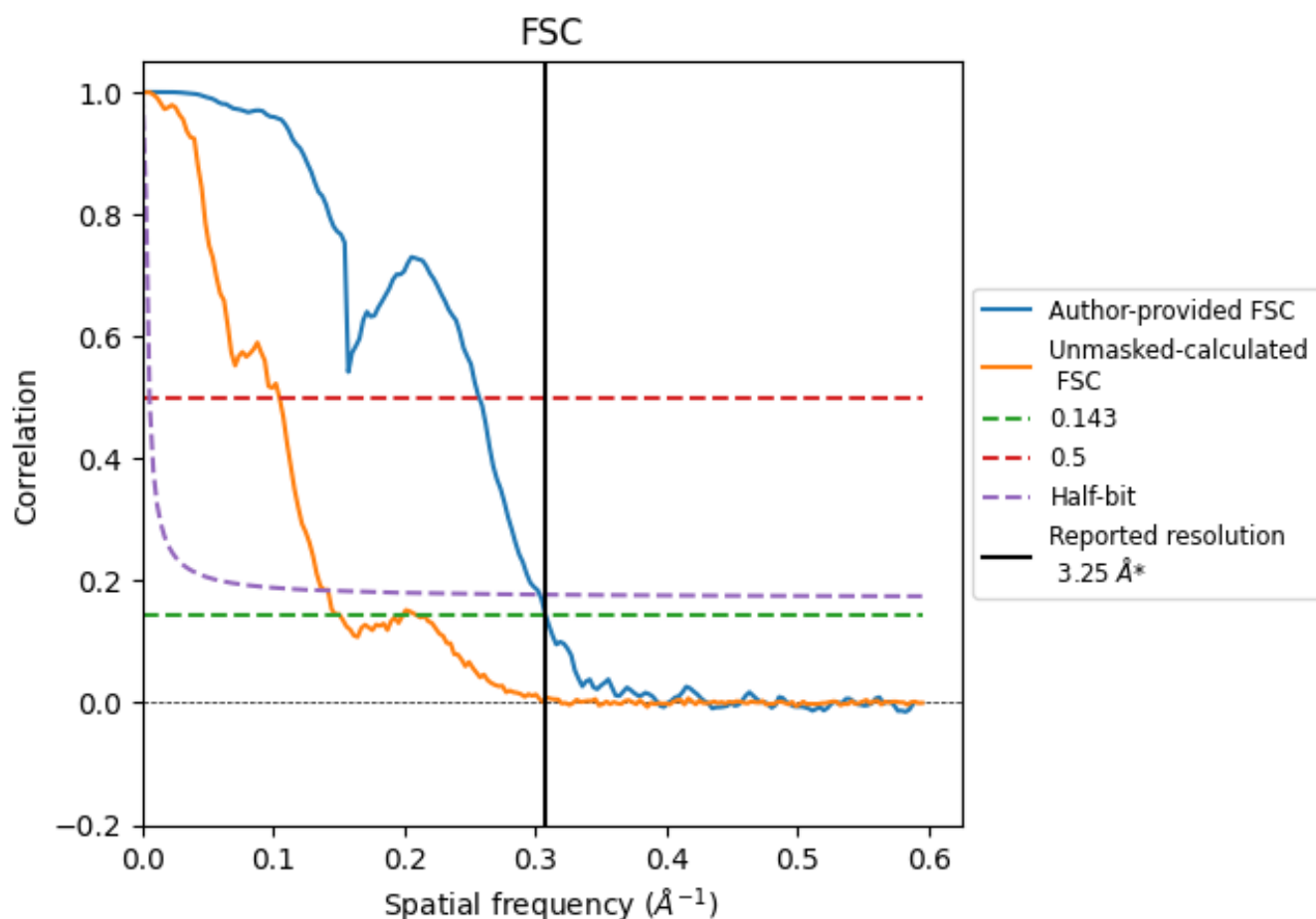


*Reported resolution corresponds to spatial frequency of 0.308 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.308 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.25	3.89	3.30
Unmasked-calculated*	6.63	9.56	7.05

*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 6.63 differs from the reported value 3.25 by more than 10 %

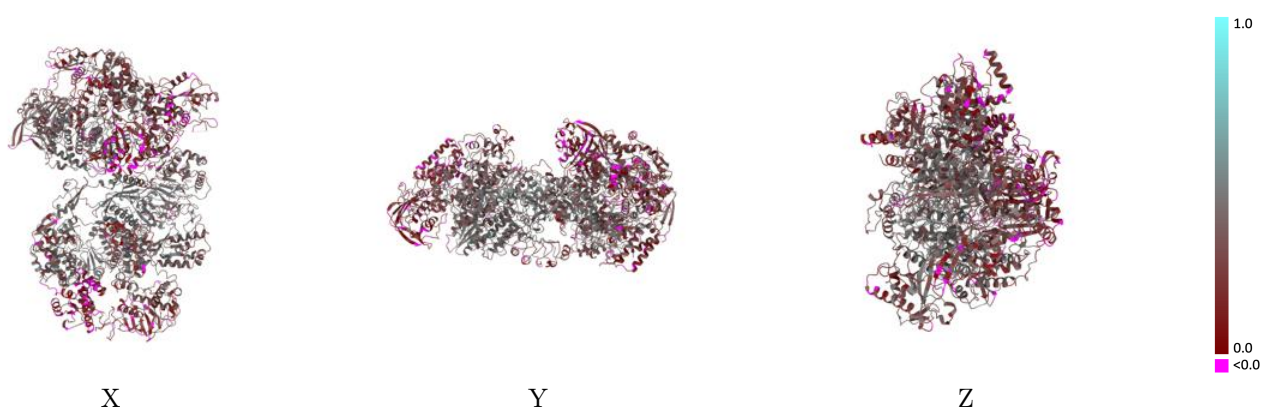
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19368 and PDB model 8RMR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

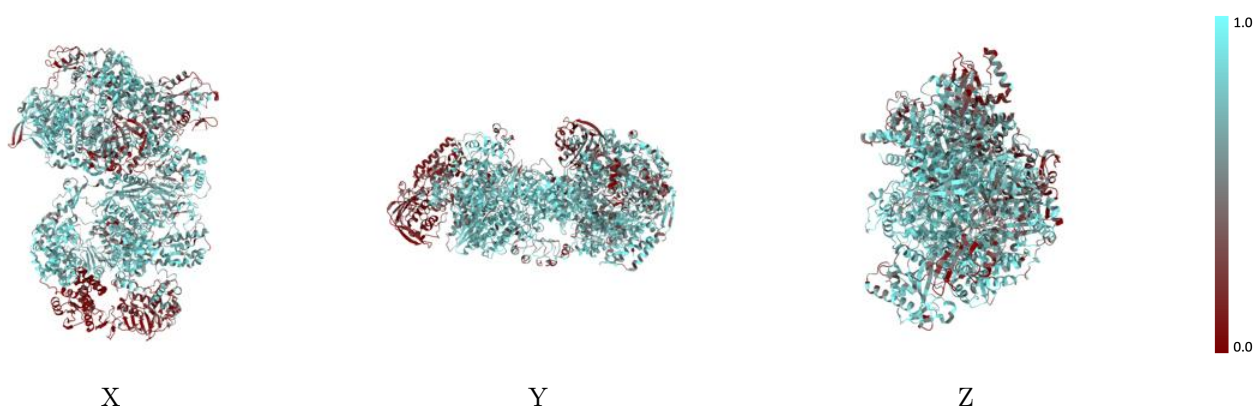
This section was not generated.

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



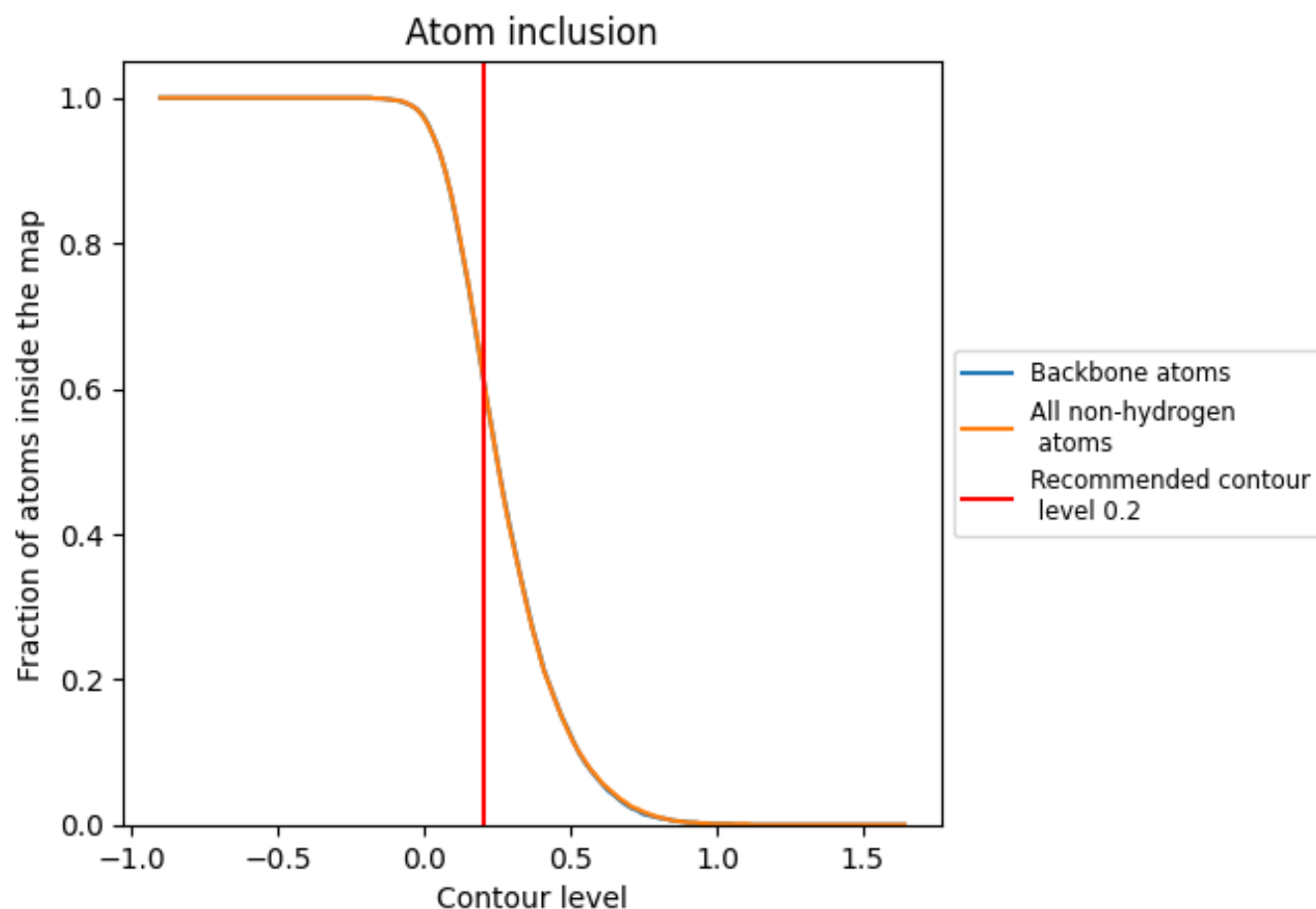
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 62% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.3260
A	0.6400	0.3040
B	0.6910	0.3300
C	0.6010	0.2920
D	0.5860	0.3470
E	0.7890	0.4030
F	0.4600	0.2860
G	0.5810	0.3320

1.0

0.0

<0.0