Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 09:03 AM JST

PDB ID	:	8Z9R
EMDB ID	:	EMD-39868
Title	:	Cryo-EM structure of Thogoto virus polymerase in a replication elongation-reception conformation
Authors	:	Xue, L.; Chang, T.; Li, Z.; Zhao, H.; Li, M.; He, J.; Chen, X.; Xiong, X.
Deposited on	:	2024-04-23
Resolution	:	2.58 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:

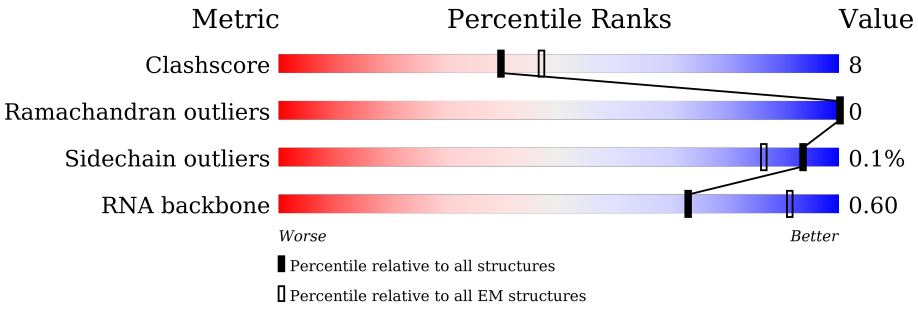
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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	622	82% 18%
1	H	622	58% 14% 28%
2	B	710	78% 17% 5%
2	I	710	9% 67% 21% 12%
3	C	827	6% 73% 17% 10%
3	J	827	14% 23% 6% 71%
4	D	18	6% 39% 11% 17% 33%

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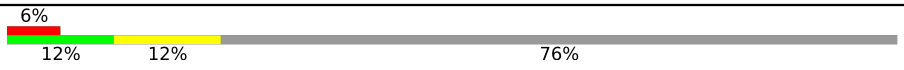
Mol	Chain	Length	Quality of chain
5	E	17	
5	F	17	
6	G	10	
6	K	10	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28075 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	621	Total	C	N	O	S	0	0
			5021	3172	874	947	28		
1	H	449	Total	C	N	O	S	0	0
			3616	2290	630	675	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	GLU	GLY	conflict	UNP P27194
H	471	GLU	GLY	conflict	UNP P27194

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	676	Total	C	N	O	S	0	0
			5422	3447	943	996	36		
2	I	628	Total	C	N	O	S	0	0
			5021	3202	860	926	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LEU	ARG	conflict	UNP O41353
B	230	TRP	CYS	conflict	UNP O41353
I	7	LEU	ARG	conflict	UNP O41353
I	230	TRP	CYS	conflict	UNP O41353

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	747	Total	C	N	O	S	3	0
			6005	3797	1050	1123	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	237	Total	C	N	O	S	0	0
			1926	1228	337	348	13		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	770	LEU	-	expression tag	UNP Q9YNA4
C	771	GLU	-	expression tag	UNP Q9YNA4
C	772	VAL	-	expression tag	UNP Q9YNA4
C	773	LEU	-	expression tag	UNP Q9YNA4
C	774	PHE	-	expression tag	UNP Q9YNA4
C	775	GLN	-	expression tag	UNP Q9YNA4
C	776	GLY	-	expression tag	UNP Q9YNA4
C	777	PRO	-	expression tag	UNP Q9YNA4
C	778	GLY	-	expression tag	UNP Q9YNA4
C	779	HIS	-	expression tag	UNP Q9YNA4
C	780	HIS	-	expression tag	UNP Q9YNA4
C	781	HIS	-	expression tag	UNP Q9YNA4
C	782	HIS	-	expression tag	UNP Q9YNA4
C	783	HIS	-	expression tag	UNP Q9YNA4
C	784	HIS	-	expression tag	UNP Q9YNA4
C	785	HIS	-	expression tag	UNP Q9YNA4
C	786	HIS	-	expression tag	UNP Q9YNA4
C	787	SER	-	expression tag	UNP Q9YNA4
C	788	ALA	-	expression tag	UNP Q9YNA4
C	789	ASP	-	expression tag	UNP Q9YNA4
C	790	TYR	-	expression tag	UNP Q9YNA4
C	791	LYS	-	expression tag	UNP Q9YNA4
C	792	ASP	-	expression tag	UNP Q9YNA4
C	793	ASP	-	expression tag	UNP Q9YNA4
C	794	ASP	-	expression tag	UNP Q9YNA4
C	795	ASP	-	expression tag	UNP Q9YNA4
C	796	LYS	-	expression tag	UNP Q9YNA4
C	797	GLY	-	expression tag	UNP Q9YNA4
C	798	GLY	-	expression tag	UNP Q9YNA4
C	799	TRP	-	expression tag	UNP Q9YNA4
C	800	SER	-	expression tag	UNP Q9YNA4
C	801	HIS	-	expression tag	UNP Q9YNA4
C	802	PRO	-	expression tag	UNP Q9YNA4
C	803	GLN	-	expression tag	UNP Q9YNA4
C	804	PHE	-	expression tag	UNP Q9YNA4
C	805	GLU	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	806	LYS	-	expression tag	UNP Q9YNA4
C	807	GLY	-	expression tag	UNP Q9YNA4
C	808	GLY	-	expression tag	UNP Q9YNA4
C	809	GLY	-	expression tag	UNP Q9YNA4
C	810	SER	-	expression tag	UNP Q9YNA4
C	811	GLY	-	expression tag	UNP Q9YNA4
C	812	GLY	-	expression tag	UNP Q9YNA4
C	813	GLY	-	expression tag	UNP Q9YNA4
C	814	GLY	-	expression tag	UNP Q9YNA4
C	815	SER	-	expression tag	UNP Q9YNA4
C	816	GLY	-	expression tag	UNP Q9YNA4
C	817	GLY	-	expression tag	UNP Q9YNA4
C	818	SER	-	expression tag	UNP Q9YNA4
C	819	ALA	-	expression tag	UNP Q9YNA4
C	820	TRP	-	expression tag	UNP Q9YNA4
C	821	SER	-	expression tag	UNP Q9YNA4
C	822	HIS	-	expression tag	UNP Q9YNA4
C	823	PRO	-	expression tag	UNP Q9YNA4
C	824	GLN	-	expression tag	UNP Q9YNA4
C	825	PHE	-	expression tag	UNP Q9YNA4
C	826	GLU	-	expression tag	UNP Q9YNA4
C	827	LYS	-	expression tag	UNP Q9YNA4
J	770	LEU	-	expression tag	UNP Q9YNA4
J	771	GLU	-	expression tag	UNP Q9YNA4
J	772	VAL	-	expression tag	UNP Q9YNA4
J	773	LEU	-	expression tag	UNP Q9YNA4
J	774	PHE	-	expression tag	UNP Q9YNA4
J	775	GLN	-	expression tag	UNP Q9YNA4
J	776	GLY	-	expression tag	UNP Q9YNA4
J	777	PRO	-	expression tag	UNP Q9YNA4
J	778	GLY	-	expression tag	UNP Q9YNA4
J	779	HIS	-	expression tag	UNP Q9YNA4
J	780	HIS	-	expression tag	UNP Q9YNA4
J	781	HIS	-	expression tag	UNP Q9YNA4
J	782	HIS	-	expression tag	UNP Q9YNA4
J	783	HIS	-	expression tag	UNP Q9YNA4
J	784	HIS	-	expression tag	UNP Q9YNA4
J	785	HIS	-	expression tag	UNP Q9YNA4
J	786	HIS	-	expression tag	UNP Q9YNA4
J	787	SER	-	expression tag	UNP Q9YNA4
J	788	ALA	-	expression tag	UNP Q9YNA4
J	789	ASP	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	790	TYR	-	expression tag	UNP Q9YNA4
J	791	LYS	-	expression tag	UNP Q9YNA4
J	792	ASP	-	expression tag	UNP Q9YNA4
J	793	ASP	-	expression tag	UNP Q9YNA4
J	794	ASP	-	expression tag	UNP Q9YNA4
J	795	ASP	-	expression tag	UNP Q9YNA4
J	796	LYS	-	expression tag	UNP Q9YNA4
J	797	GLY	-	expression tag	UNP Q9YNA4
J	798	GLY	-	expression tag	UNP Q9YNA4
J	799	TRP	-	expression tag	UNP Q9YNA4
J	800	SER	-	expression tag	UNP Q9YNA4
J	801	HIS	-	expression tag	UNP Q9YNA4
J	802	PRO	-	expression tag	UNP Q9YNA4
J	803	GLN	-	expression tag	UNP Q9YNA4
J	804	PHE	-	expression tag	UNP Q9YNA4
J	805	GLU	-	expression tag	UNP Q9YNA4
J	806	LYS	-	expression tag	UNP Q9YNA4
J	807	GLY	-	expression tag	UNP Q9YNA4
J	808	GLY	-	expression tag	UNP Q9YNA4
J	809	GLY	-	expression tag	UNP Q9YNA4
J	810	SER	-	expression tag	UNP Q9YNA4
J	811	GLY	-	expression tag	UNP Q9YNA4
J	812	GLY	-	expression tag	UNP Q9YNA4
J	813	GLY	-	expression tag	UNP Q9YNA4
J	814	GLY	-	expression tag	UNP Q9YNA4
J	815	SER	-	expression tag	UNP Q9YNA4
J	816	GLY	-	expression tag	UNP Q9YNA4
J	817	GLY	-	expression tag	UNP Q9YNA4
J	818	SER	-	expression tag	UNP Q9YNA4
J	819	ALA	-	expression tag	UNP Q9YNA4
J	820	TRP	-	expression tag	UNP Q9YNA4
J	821	SER	-	expression tag	UNP Q9YNA4
J	822	HIS	-	expression tag	UNP Q9YNA4
J	823	PRO	-	expression tag	UNP Q9YNA4
J	824	GLN	-	expression tag	UNP Q9YNA4
J	825	PHE	-	expression tag	UNP Q9YNA4
J	826	GLU	-	expression tag	UNP Q9YNA4
J	827	LYS	-	expression tag	UNP Q9YNA4

- Molecule 4 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*AP*GP*GP*CP*AP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	12	Total	C	N	O	P	0	0
			260	118	55	76	11		

- Molecule 5 is a RNA chain called RNA (5'-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	4	Total	C	N	O	P	0	0
			83	37	12	30	4		
5	F	13	Total	C	N	O	P	0	0
			269	120	38	98	13		

- Molecule 6 is a RNA chain called RNA (5'-D(*(ATP))-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3').

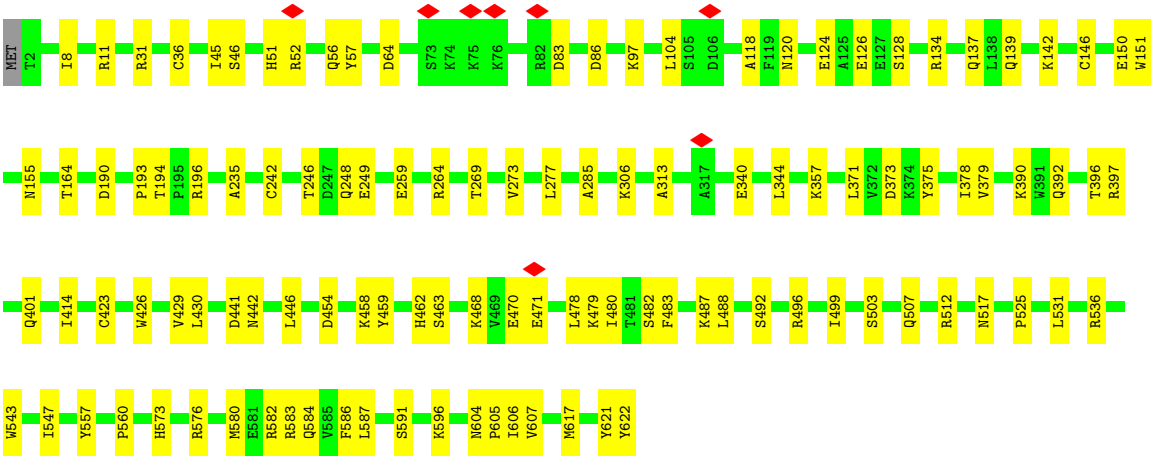
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	10	Total	C	N	O	P	0	0
			226	98	46	70	12		
6	K	10	Total	C	N	O	P	0	0
			226	98	46	70	12		

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.

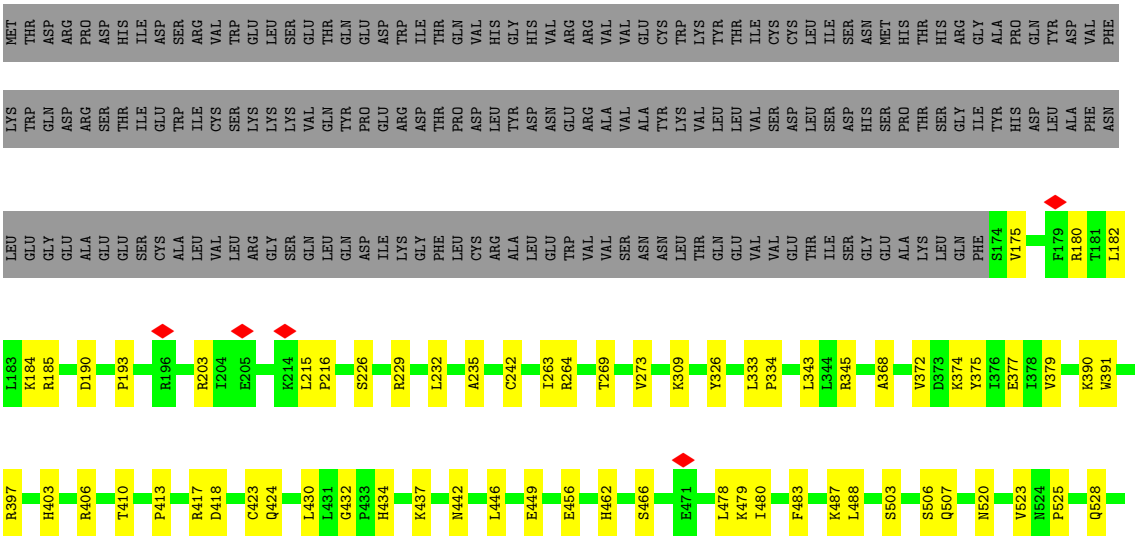
• Molecule 1: Polymerase acidic protein

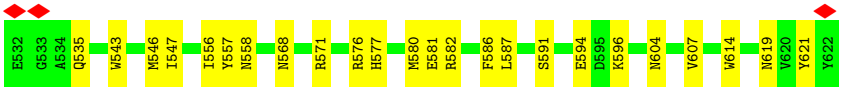
Chain A:



• Molecule 1: Polymerase acidic protein

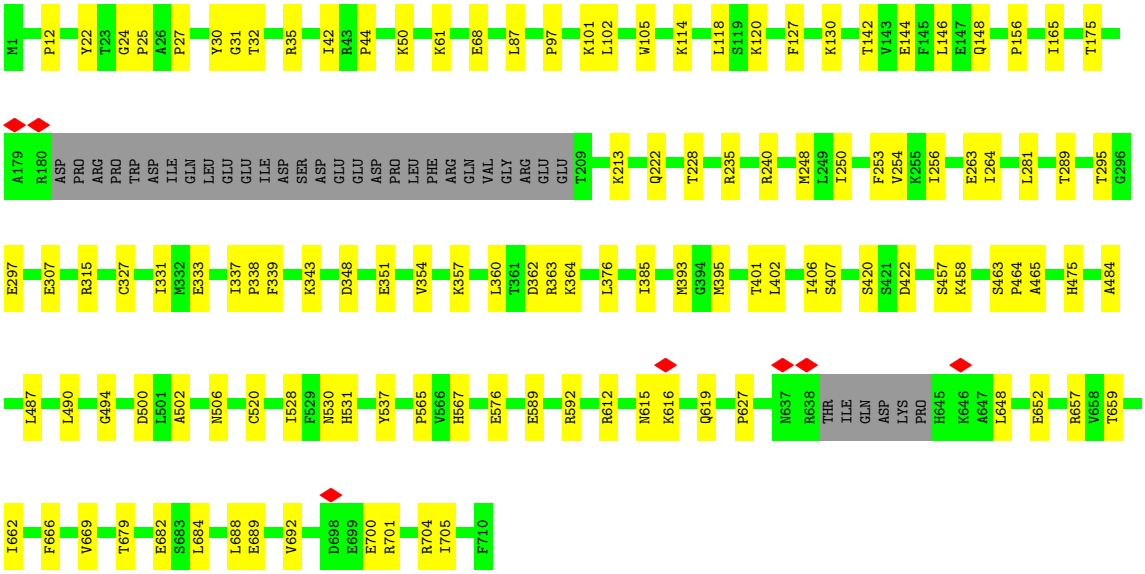
Chain H:





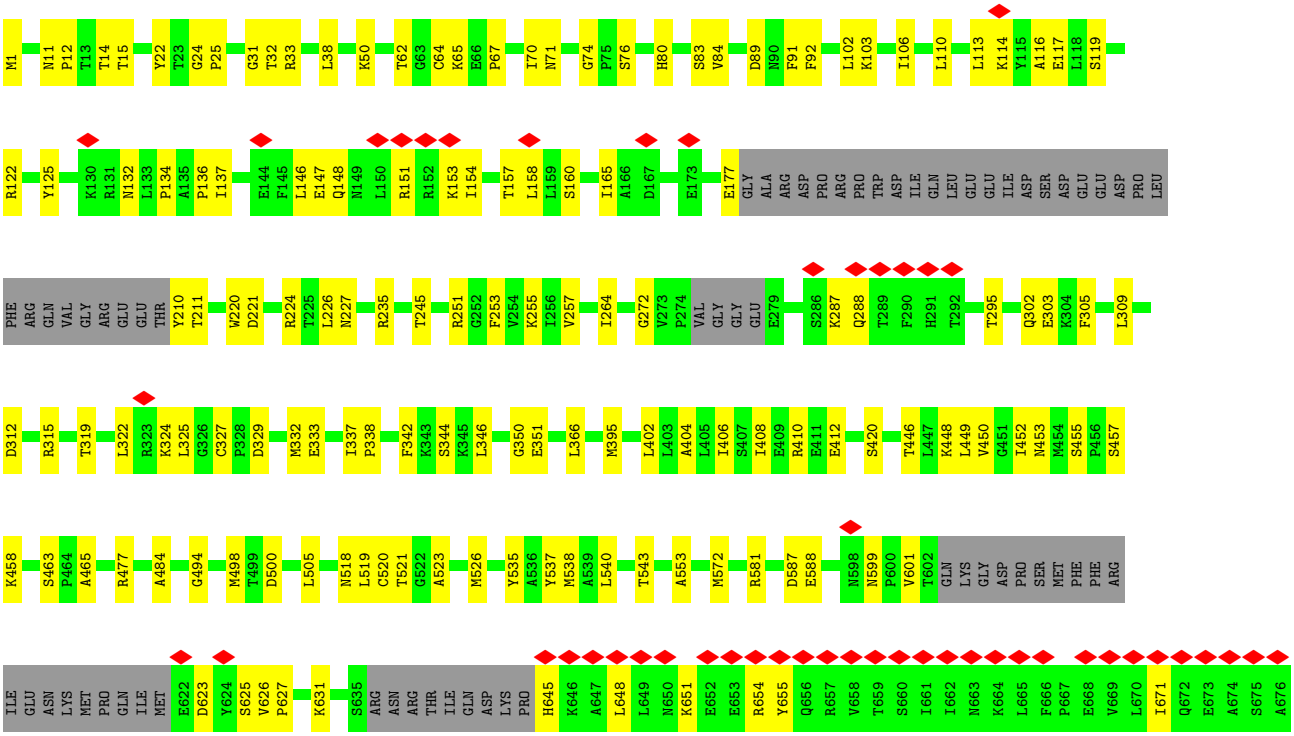
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

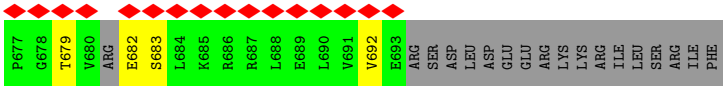
Chain B:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

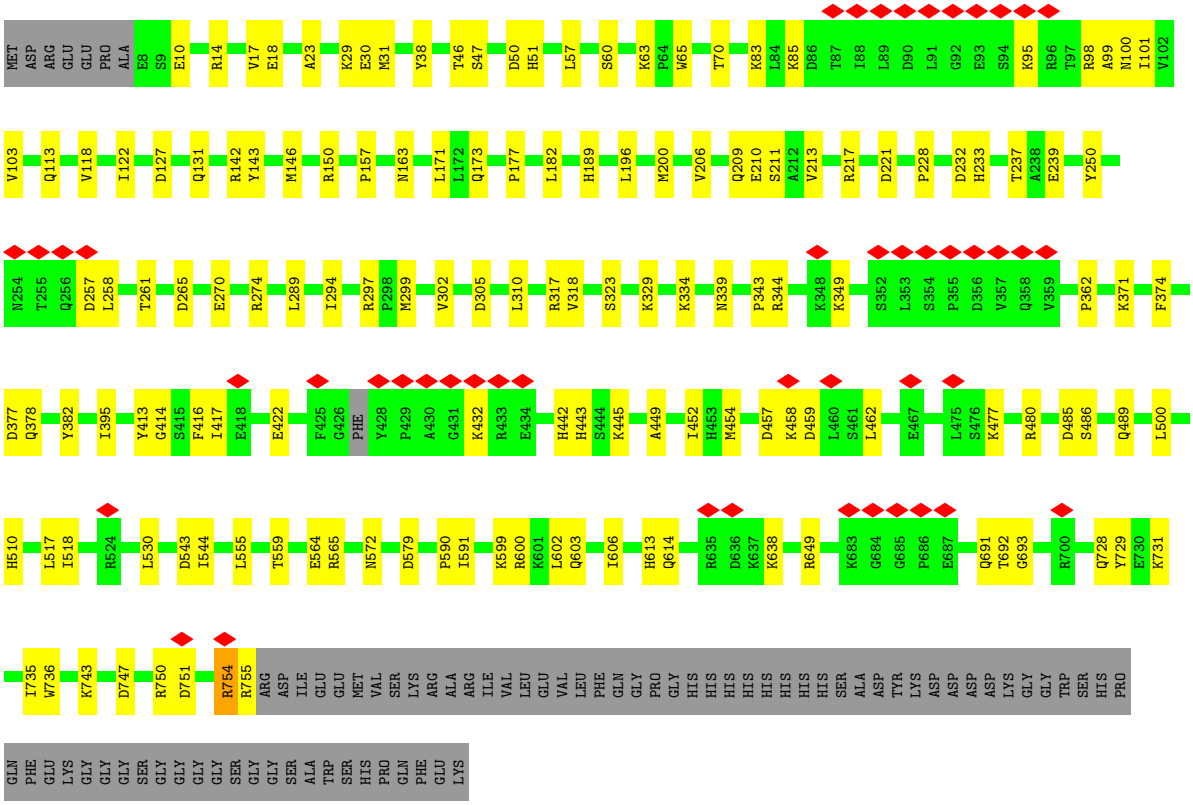
Chain I:





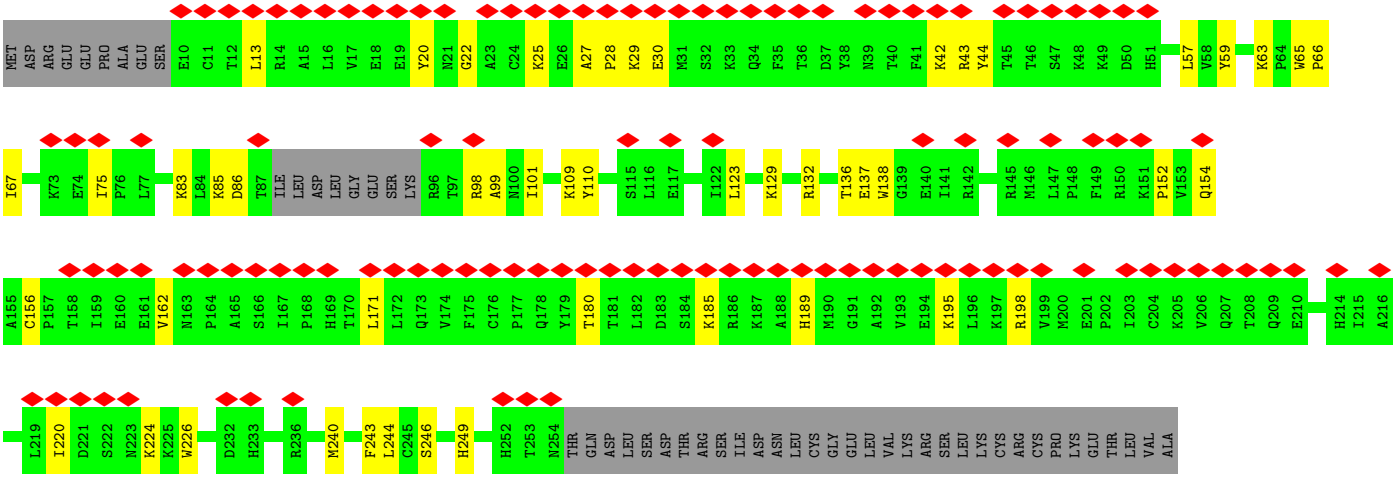
• Molecule 3: Polymerase basic protein 2

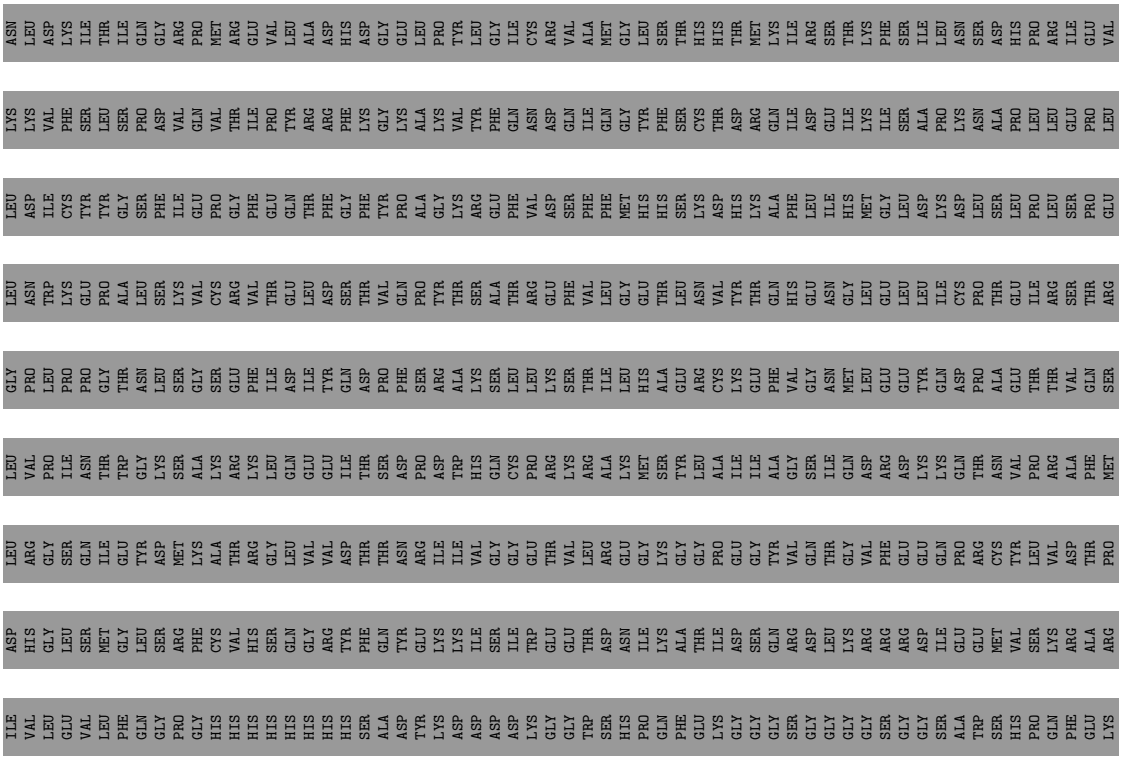
Chain C:



• Molecule 3: Polymerase basic protein 2

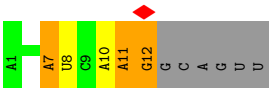
Chain J:





• Molecule 4: RNA (5’-R(*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*AP*GP*GP*CP*AP*GP*UP*U)-3’)

Chain D:

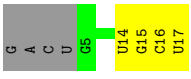


• Molecule 5: RNA (5’-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3’)

Chain E:

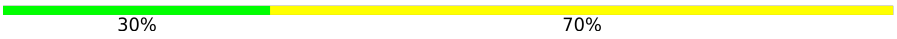
• Molecule 5: RNA (5’-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3’)

Chain F:



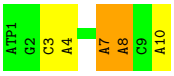
• Molecule 6: RNA (5’-D(*(ATP))-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3’)

Chain G:



• Molecule 6: RNA (5'-D(*(ATP))-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3')

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86841	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	4.117	Depositor
Minimum map value	-1.578	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.459	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97333336, 0.97333336, 0.97333336	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/5136	0.48	0/6967
1	H	0.25	0/3697	0.49	0/5011
2	B	0.25	0/5532	0.49	0/7468
2	I	0.25	0/5123	0.49	0/6923
3	C	0.25	0/6140	0.50	0/8302
3	J	0.24	0/1975	0.49	0/2676
4	D	0.18	0/293	0.70	0/456
5	E	0.22	0/91	0.75	0/139
5	F	0.21	0/297	0.73	0/459
6	G	0.28	0/219	0.70	0/339
6	K	0.21	0/219	0.69	0/339
All	All	0.25	0/28722	0.50	0/39079

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

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	5021	0	4960	79	0
1	H	3616	0	3614	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5422	0	5493	91	0
2	I	5021	0	5075	107	0
3	C	6005	0	6008	98	0
3	J	1926	0	1938	38	0
4	D	260	0	133	8	0
5	E	83	0	43	4	0
5	F	269	0	137	3	0
6	G	226	0	111	8	0
6	K	226	0	111	5	0
All	All	28075	0	27623	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (426) 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)
2:I:253:PHE:HB3	2:I:338:PRO:HG3	1.48	0.93
1:A:396:THR:HG21	5:E:16:C:H41	1.38	0.88
2:B:253:PHE:HB3	2:B:338:PRO:HG3	1.63	0.79
2:I:89:ASP:OD1	2:I:324:LYS:NZ	2.22	0.72
3:C:150:ARG:O	3:C:489:GLN:NE2	2.23	0.70
3:C:329:LYS:HG2	3:C:334:LYS:HG2	1.74	0.69
3:C:29:LYS:HG3	3:C:30:GLU:H	1.56	0.69
1:A:517:ASN:O	3:C:142:ARG:NH2	2.26	0.69
1:H:235:ALA:HB1	1:H:343:LEU:HD22	1.75	0.68
2:B:701:ARG:NH1	3:C:10:GLU:OE1	2.26	0.68
3:C:692:THR:O	3:C:728:GLN:NE2	2.26	0.68
2:I:599:ASN:ND2	2:I:601:VAL:O	2.27	0.68
2:I:22:TYR:OH	2:I:484:ALA:O	2.12	0.68
3:C:377:ASP:OD1	3:C:378:GLN:N	2.26	0.67
1:A:397:ARG:O	1:A:401:GLN:NE2	2.26	0.67
3:C:157:PRO:HD3	3:C:237:THR:HG21	1.76	0.67
2:I:500:ASP:OD2	2:I:537:TYR:OH	2.13	0.67
1:A:392:GLN:NE2	1:A:492:SER:O	2.27	0.67
3:C:237:THR:HG22	3:C:239:GLU:H	1.59	0.67
1:A:259:GLU:HB2	1:A:468:LYS:HB3	1.78	0.66
2:B:679:THR:HG22	2:B:682:GLU:HG2	1.75	0.66
2:B:627:PRO:HB3	3:C:122:ILE:HD13	1.77	0.66
1:A:517:ASN:ND2	3:C:143:TYR:O	2.27	0.66
2:I:679:THR:HA	2:I:683:SER:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:GLY:O	2:I:235:ARG:NH2	2.30	0.65
3:C:317:ARG:NH1	3:C:323:SER:O	2.30	0.64
1:H:397:ARG:NH1	1:H:413:PRO:O	2.31	0.64
2:I:505:LEU:HD12	2:I:572:MET:HB2	1.79	0.64
1:H:216:PRO:HB3	1:H:594:GLU:HB3	1.81	0.63
3:C:362:PRO:O	3:C:432:LYS:NZ	2.29	0.63
1:H:273:VAL:HG23	1:H:478:LEU:HD13	1.79	0.63
1:A:31:ARG:HD2	1:A:164:THR:HG23	1.81	0.63
1:H:417:ARG:NH1	1:H:423:CYS:SG	2.72	0.63
2:B:362:ASP:OD2	2:B:364:LYS:NZ	2.31	0.62
1:A:146:CYS:SG	3:C:693:GLY:N	2.70	0.62
2:B:502:ALA:O	2:B:506:ASN:ND2	2.31	0.62
1:H:528:GLN:OE1	1:H:535:GLN:NE2	2.31	0.62
2:B:648:LEU:O	2:B:652:GLU:HG2	1.99	0.62
1:H:430:LEU:HD12	1:H:446:LEU:HD23	1.81	0.62
1:A:430:LEU:HD12	1:A:446:LEU:HD23	1.81	0.62
1:A:496:ARG:HG2	2:B:490:LEU:HD23	1.81	0.62
2:B:35:ARG:NH1	4:D:7:A:OP1	2.30	0.62
1:H:520:ASN:HB3	1:H:523:VAL:HG23	1.82	0.61
3:C:99:ALA:HB1	3:C:103:VAL:HG21	1.83	0.61
2:I:581:ARG:HH11	3:J:123:LEU:HD13	1.65	0.61
3:C:189:HIS:HD2	3:C:297:ARG:HH11	1.48	0.61
1:H:368:ALA:HB2	2:I:519:LEU:HD12	1.84	0.60
6:G:7:A:H2'	6:G:8:A:H8	1.65	0.60
1:A:194:THR:HB	1:A:196:ARG:HH22	1.67	0.60
6:G:7:A:H2'	6:G:8:A:C8	2.38	0.59
2:I:553:ALA:O	3:J:109:LYS:NZ	2.34	0.59
2:B:393:MET:HE3	2:B:395:MET:HB2	1.83	0.59
3:C:572:ASN:ND2	3:C:579:ASP:OD1	2.34	0.59
1:H:390:LYS:NZ	1:H:449:GLU:OE2	2.31	0.59
2:B:662:ILE:HG12	2:B:684:LEU:HD11	1.85	0.59
2:I:74:GLY:O	2:I:448:LYS:NZ	2.35	0.59
3:J:246:SER:HG	3:J:249:HIS:CE1	2.21	0.58
2:B:484:ALA:HA	2:B:487:LEU:HG	1.85	0.58
2:I:31:GLY:HA2	6:K:8:A:H5'	1.86	0.58
1:A:242:CYS:HB2	1:A:423:CYS:HB2	1.84	0.58
3:C:14:ARG:O	3:C:18:GLU:HG2	2.03	0.58
3:J:195:LYS:HA	3:J:198:ARG:HH21	1.68	0.58
2:I:12:PRO:HA	2:I:15:THR:HG22	1.84	0.58
3:J:59:TYR:O	3:J:63:LYS:N	2.37	0.58
2:B:289:THR:HG21	3:C:371:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:148:GLN:HA	2:I:151:ARG:HH21	1.69	0.57
3:J:154:GLN:NE2	3:J:156:CYS:O	2.37	0.57
1:H:345:ARG:NH1	1:H:546:MET:SD	2.77	0.57
1:A:264:ARG:NH2	1:A:459:TYR:O	2.37	0.57
2:I:114:LYS:HG3	2:I:116:ALA:H	1.69	0.57
1:A:248:GLN:NE2	1:A:285:ALA:O	2.32	0.57
2:B:657:ARG:HD3	3:C:23:ALA:HA	1.86	0.57
2:I:671:ILE:HD12	3:J:171:LEU:HB3	1.87	0.57
1:A:269:THR:O	1:A:463:SER:OG	2.23	0.57
2:B:333:GLU:O	2:B:337:ILE:HG12	2.04	0.57
2:I:210:TYR:CD2	2:I:211:THR:HG23	2.39	0.57
2:I:102:LEU:HD22	2:I:264:ILE:HD12	1.86	0.57
1:H:232:LEU:HB2	1:H:391:TRP:CE2	2.40	0.56
2:I:210:TYR:HD2	2:I:211:THR:HG23	1.70	0.56
2:I:627:PRO:HA	2:I:631:LYS:HG3	1.88	0.56
2:B:42:ILE:HB	2:B:376:LEU:HD11	1.88	0.56
2:I:648:LEU:HA	2:I:651:LYS:HZ2	1.71	0.56
3:C:171:LEU:HD23	3:C:213:VAL:HG13	1.87	0.56
2:I:80:HIS:ND1	2:I:83:SER:OG	2.37	0.55
2:I:410:ARG:NH1	2:I:446:THR:OG1	2.38	0.55
2:B:619:GLN:OE1	3:C:209:GLN:NE2	2.39	0.55
1:H:345:ARG:HD3	1:H:546:MET:HG2	1.88	0.55
1:H:434:HIS:ND1	1:H:434:HIS:O	2.39	0.55
2:I:65:LYS:HD3	2:I:70:ILE:HG12	1.87	0.55
1:A:46:SER:HB3	1:A:57:TYR:HB2	1.87	0.55
2:B:50:LYS:NZ	2:B:68:GLU:O	2.39	0.55
2:B:531:HIS:ND1	5:E:16:C:O2	2.39	0.55
2:B:87:LEU:HD13	2:B:407:SER:HA	1.88	0.55
2:B:295:THR:O	2:B:465:ALA:N	2.38	0.55
2:I:76:SER:O	2:I:453:ASN:ND2	2.34	0.55
2:I:106:ILE:HG13	2:I:110:LEU:HD22	1.90	0.54
2:I:134:PRO:HD2	2:I:137:ILE:HD12	1.89	0.54
2:B:30:TYR:HB3	4:D:8:U:H1'	1.90	0.54
2:B:102:LEU:HD22	2:B:264:ILE:HD11	1.90	0.54
2:B:679:THR:OG1	3:C:31:MET:O	2.23	0.54
3:C:50:ASP:OD1	3:C:51:HIS:N	2.40	0.53
1:A:306:LYS:NZ	4:D:10:A:OP2	2.27	0.53
2:B:567:HIS:HE1	2:B:576:GLU:HB2	1.74	0.53
1:A:560:PRO:HD3	2:B:27:PRO:HB3	1.89	0.53
1:H:543:TRP:CE2	1:H:547:ILE:HD11	2.43	0.53
2:I:322:LEU:HB3	2:I:327:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:ARG:NH1	3:C:413:TYR:O	2.36	0.53
3:C:349:LYS:HG2	3:C:422:GLU:HA	1.91	0.53
1:H:403:HIS:HB3	3:J:59:TYR:CD2	2.44	0.53
2:I:119:SER:OG	3:J:43:ARG:NH1	2.42	0.53
3:J:66:PRO:HG2	3:J:101:ILE:HB	1.91	0.53
6:G:4:A:H2'	6:G:5:A:H8	1.74	0.53
1:H:581:GLU:OE2	2:I:477:ARG:NE	2.41	0.53
1:A:151:TRP:O	1:A:155:ASN:ND2	2.32	0.52
1:H:614:TRP:HB2	2:I:1:MET:HG2	1.92	0.52
2:B:401:THR:OG1	2:B:420:SER:O	2.17	0.52
3:C:265:ASP:OD2	3:C:310:LEU:HB3	2.09	0.52
2:I:682:GLU:OE1	3:J:20:TYR:OH	2.27	0.52
1:A:430:LEU:HB2	1:A:446:LEU:HB3	1.91	0.52
1:A:576:ARG:HD3	1:A:617:MET:HE1	1.90	0.52
2:I:303:GLU:HB3	2:I:455:SER:HB2	1.90	0.52
1:H:580:MET:HG2	1:H:621:TYR:CE2	2.44	0.52
2:I:113:LEU:HB2	2:I:158:LEU:HD22	1.92	0.52
1:H:193:PRO:HD2	2:I:319:THR:HG21	1.91	0.52
2:I:535:TYR:HB2	2:I:540:LEU:HD12	1.92	0.52
2:I:518:ASN:H	2:I:521:THR:HG1	1.53	0.52
1:A:51:HIS:CD2	1:A:52:ARG:HG3	2.45	0.51
2:B:24:GLY:O	2:B:235:ARG:NH2	2.39	0.51
3:C:10:GLU:OE2	3:C:14:ARG:NH2	2.43	0.51
1:A:587:LEU:HB3	1:A:591:SER:HB3	1.92	0.51
2:B:120:LYS:NZ	6:G:3:C:OP2	2.39	0.51
2:I:626:VAL:HG11	3:J:123:LEU:HA	1.93	0.51
3:C:257:ASP:OD1	3:C:258:LEU:N	2.43	0.51
2:I:402:LEU:O	2:I:406:ILE:HG23	2.10	0.51
3:J:28:PRO:O	3:J:29:LYS:HG2	2.10	0.51
2:B:376:LEU:HB3	2:B:385:ILE:HD11	1.92	0.51
3:C:590:PRO:HA	3:C:649:ARG:HE	1.76	0.51
2:I:404:ALA:O	2:I:408:ILE:HG12	2.11	0.51
2:B:228:THR:OG1	2:B:348:ASP:O	2.17	0.51
3:C:270:GLU:OE1	3:C:274:ARG:NH1	2.41	0.51
2:B:105:TRP:HH2	2:B:256:ILE:HG23	1.76	0.51
3:C:485:ASP:OD1	3:C:486:SER:N	2.43	0.51
3:C:530:LEU:HD11	3:C:544:ILE:HG22	1.93	0.51
2:I:50:LYS:HE3	2:I:71:ASN:HA	1.93	0.51
3:J:75:ILE:O	3:J:85:LYS:NZ	2.39	0.51
2:I:295:THR:O	2:I:465:ALA:N	2.44	0.51
3:J:180:THR:HG21	3:J:185:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ARG:O	2:B:705:ILE:HG13	2.11	0.50
2:I:84:VAL:HG22	2:I:450:VAL:HG12	1.93	0.50
2:I:148:GLN:OE1	2:I:177:GLU:N	2.44	0.50
1:A:45:ILE:O	1:A:137:GLN:NE2	2.45	0.50
1:A:104:LEU:HG	1:A:120:ASN:HB3	1.94	0.50
1:A:126:GLU:OE2	1:A:128:SER:OG	2.28	0.50
2:B:688:LEU:HD21	3:C:17:VAL:HG22	1.94	0.50
3:C:459:ASP:HB3	3:C:462:LEU:HD13	1.93	0.50
2:I:92:PHE:CD2	2:I:324:LYS:HE2	2.47	0.50
3:C:339:ASN:HD21	3:C:371:LYS:HE2	1.77	0.49
3:J:152:PRO:HB2	3:J:224:LYS:HD3	1.94	0.49
2:I:410:ARG:NH2	2:I:412:GLU:OE2	2.45	0.49
3:C:127:ASP:O	3:C:131:GLN:HG2	2.12	0.49
3:C:261:THR:HG22	3:C:310:LEU:HD12	1.94	0.49
1:A:142:LYS:HD3	3:C:692:THR:HG23	1.92	0.49
1:A:193:PRO:HD3	2:B:315:ARG:HH21	1.78	0.49
3:C:118:VAL:HG13	3:C:206:VAL:HG11	1.94	0.49
3:C:599:LYS:O	3:C:603:GLN:HG2	2.12	0.49
2:B:327:CYS:HB3	2:B:331:ILE:HG21	1.94	0.49
2:I:119:SER:HB2	2:I:136:PRO:HG3	1.94	0.49
3:J:67:ILE:O	3:J:99:ALA:N	2.37	0.49
2:I:312:ASP:OD1	2:I:315:ARG:NH1	2.45	0.49
2:B:354:VAL:HG21	4:D:7:A:H3'	1.94	0.49
6:G:4:A:H2'	6:G:5:A:C8	2.47	0.49
2:I:692:VAL:HG22	3:J:13:LEU:HD21	1.94	0.49
1:H:586:PHE:CE2	2:I:463:SER:HB2	2.48	0.48
2:I:32:THR:HG22	2:I:351:GLU:HB2	1.94	0.48
2:B:494:GLY:HA2	3:C:57:LEU:HD13	1.94	0.48
2:I:302:GLN:OE1	2:I:452:ILE:HG22	2.13	0.48
3:C:299:MET:HA	3:C:302:VAL:HG12	1.94	0.48
3:C:613:HIS:ND1	3:C:614:GLN:OE1	2.45	0.48
1:A:83:ASP:OD1	1:A:83:ASP:N	2.44	0.48
1:A:139:GLN:NE2	3:C:731:LYS:O	2.46	0.48
2:B:175:THR:HG22	2:B:213:LYS:HD3	1.94	0.48
3:C:83:LYS:NZ	3:C:85:LYS:O	2.47	0.48
3:C:747:ASP:OD1	3:C:750:ARG:NH2	2.47	0.48
1:A:340:GLU:OE1	1:A:458:LYS:NZ	2.33	0.47
1:A:487:LYS:HG2	2:B:25:PRO:HB3	1.96	0.47
2:B:589:GLU:HG3	3:C:113:GLN:HE22	1.78	0.47
3:C:232:ASP:O	3:C:233:HIS:ND1	2.47	0.47
2:I:122:ARG:H	2:I:251:ARG:HH12	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:494:GLY:HA2	3:J:57:LEU:HD22	1.95	0.47
3:J:240:MET:HB2	3:J:243:PHE:CE1	2.48	0.47
3:C:60:SER:HA	3:C:63:LYS:HE2	1.95	0.47
1:H:242:CYS:HB2	1:H:423:CYS:HB2	1.96	0.47
2:I:220:TRP:O	2:I:224:ARG:HG3	2.14	0.47
3:J:65:TRP:HB3	3:J:98:ARG:HB3	1.95	0.47
3:J:137:GLU:N	3:J:137:GLU:OE1	2.48	0.47
1:A:273:VAL:HG23	1:A:478:LEU:HD21	1.96	0.47
2:B:105:TRP:HB2	2:B:263:GLU:HG2	1.97	0.47
2:I:287:LYS:NZ	2:I:288:GLN:O	2.40	0.47
1:A:531:LEU:HD23	1:A:536:ARG:HG2	1.95	0.47
1:A:584:GLN:HB2	2:B:463:SER:OG	2.15	0.47
2:B:688:LEU:O	2:B:692:VAL:HG23	2.15	0.47
3:C:457:ASP:O	3:C:477:LYS:N	2.42	0.47
1:H:523:VAL:HG12	1:H:525:PRO:HD3	1.96	0.47
2:I:455:SER:HB3	2:I:458:LYS:HB2	1.95	0.47
1:A:462:HIS:NE2	1:A:479:LYS:HD2	2.30	0.47
3:C:217:ARG:O	3:C:221:ASP:HB2	2.14	0.47
1:H:375:TYR:O	1:H:379:VAL:HG22	2.15	0.47
2:B:146:LEU:HD21	2:B:165:ILE:HD13	1.95	0.47
3:C:196:LEU:O	3:C:200:MET:HG2	2.15	0.47
1:H:483:PHE:CE2	1:H:487:LYS:HB3	2.49	0.47
1:H:587:LEU:HB3	1:H:591:SER:HB3	1.97	0.47
2:I:103:LYS:HA	2:I:106:ILE:HG22	1.96	0.47
1:A:86:ASP:OD1	1:A:97:LYS:NZ	2.47	0.46
4:D:7:A:O2'	4:D:8:U:OP2	2.31	0.46
1:H:604:ASN:HB3	1:H:607:VAL:HB	1.96	0.46
1:A:235:ALA:HB2	1:A:344:LEU:HG	1.97	0.46
1:A:573:HIS:NE2	2:B:12:PRO:HB3	2.30	0.46
2:I:220:TRP:CE2	2:I:224:ARG:HD3	2.50	0.46
2:B:142:THR:O	2:B:146:LEU:HG	2.16	0.46
1:H:582:ARG:HH22	1:H:621:TYR:HB3	1.79	0.46
3:J:240:MET:HG3	3:J:244:LEU:HD11	1.98	0.46
2:B:689:GLU:O	2:B:692:VAL:N	2.48	0.46
3:C:414:GLY:HA3	3:C:416:PHE:CZ	2.51	0.46
1:A:605:PRO:HG2	1:A:606:ILE:HD12	1.98	0.46
3:C:100:ASN:OD1	3:C:101:ILE:N	2.48	0.46
6:G:1:ATP:H2'	6:G:2:G:C8	2.51	0.46
1:A:414:ILE:HD11	1:A:429:VAL:HG23	1.98	0.46
1:H:462:HIS:NE2	1:H:479:LYS:HD2	2.30	0.46
2:I:655:TYR:HE1	3:J:30:GLU:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HB3	2:B:520:CYS:HB2	1.98	0.46
3:C:70:THR:HG22	3:C:95:LYS:HD3	1.96	0.46
3:C:189:HIS:CD2	3:C:297:ARG:HH11	2.32	0.46
3:C:374:PHE:HZ	3:C:395:ILE:HG12	1.81	0.46
5:F:14:U:H2'	5:F:15:G:C8	2.51	0.46
1:H:374:LYS:HA	1:H:377:GLU:HG2	1.96	0.46
2:I:221:ASP:OD1	2:I:224:ARG:NH2	2.46	0.46
2:B:531:HIS:HE1	5:E:16:C:H1'	1.81	0.46
2:B:592:ARG:NE	3:C:113:GLN:OE1	2.47	0.46
1:H:483:PHE:HD2	1:H:488:LEU:HG	1.81	0.46
2:I:146:LEU:HD21	2:I:165:ILE:HD13	1.98	0.46
1:H:577:HIS:ND1	2:I:12:PRO:HD2	2.32	0.45
1:A:390:LYS:HD3	1:A:426:TRP:CE3	2.51	0.45
2:B:351:GLU:HG3	2:B:363:ARG:NH1	2.31	0.45
3:C:343:PRO:HG3	3:C:510:HIS:HB3	1.98	0.45
3:C:543:ASP:OD1	3:C:543:ASP:N	2.46	0.45
1:H:175:VAL:HG11	1:H:180:ARG:HH11	1.81	0.45
2:I:253:PHE:O	2:I:257:VAL:HG22	2.15	0.45
6:K:3:C:H2'	6:K:4:A:O4'	2.17	0.45
1:A:56:GLN:HE22	1:A:134:ARG:HH22	1.64	0.45
1:H:558:ASN:ND2	2:I:25:PRO:O	2.48	0.45
3:J:22:GLY:HA2	3:J:25:LYS:HE3	1.97	0.45
1:A:375:TYR:O	1:A:379:VAL:HG22	2.16	0.45
2:B:289:THR:HG23	3:C:382:TYR:CE2	2.51	0.45
3:C:449:ALA:HA	3:C:452:ILE:HG12	1.98	0.45
1:H:184:LYS:HE3	1:H:190:ASP:HA	1.98	0.45
1:A:503:SER:O	1:A:507:GLN:HG3	2.16	0.45
1:A:583:ARG:HG2	2:B:464:PRO:HG2	1.99	0.45
1:H:269:THR:HG23	1:H:480:ILE:HG13	1.98	0.45
1:H:442:ASN:ND2	6:K:3:C:O2	2.50	0.45
2:B:118:LEU:HD13	2:B:248:MET:HE3	1.98	0.45
3:C:146:MET:HE1	3:C:250:TYR:HD1	1.81	0.45
3:C:602:LEU:O	3:C:606:ILE:HG12	2.15	0.45
2:B:402:LEU:O	2:B:406:ILE:HG23	2.16	0.45
1:A:120:ASN:ND2	1:A:124:GLU:HB2	2.33	0.44
2:B:666:PHE:O	2:B:669:VAL:HG22	2.17	0.44
2:I:325:LEU:HD11	2:I:327:CYS:HB3	1.98	0.44
3:J:42:LYS:HB3	3:J:42:LYS:HE2	1.80	0.44
1:H:418:ASP:HB3	1:H:424:GLN:NE2	2.32	0.44
1:A:604:ASN:HB3	1:A:607:VAL:HB	2.00	0.44
3:C:182:LEU:HD13	3:C:729:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:VAL:HG12	3:C:500:LEU:HB2	2.00	0.44
2:I:125:TYR:HB2	2:I:227:ASN:HD22	1.81	0.44
1:H:596:LYS:HE3	2:I:458:LYS:HG3	1.99	0.44
2:I:272:GLY:HA3	2:I:420:SER:HB3	2.00	0.44
2:I:645:HIS:O	2:I:645:HIS:ND1	2.50	0.44
3:J:129:LYS:HG2	3:J:132:ARG:HH22	1.82	0.44
2:B:494:GLY:HA2	3:C:57:LEU:HD22	1.99	0.44
3:C:29:LYS:HG3	3:C:30:GLU:N	2.27	0.44
3:C:564:GLU:HG2	3:C:565:ARG:N	2.31	0.44
1:A:499:ILE:HD11	2:B:528:ILE:HD12	1.99	0.44
3:C:417:ILE:HD12	3:C:443:HIS:CD2	2.53	0.44
1:A:441:ASP:N	1:A:441:ASP:OD1	2.51	0.44
3:J:65:TRP:HH2	3:J:83:LYS:HG3	1.83	0.44
2:B:500:ASP:OD2	2:B:537:TYR:OH	2.30	0.44
3:C:289:LEU:O	3:C:299:MET:HB3	2.18	0.44
3:C:691:GLN:HA	3:C:729:TYR:CD2	2.53	0.44
3:C:754:ARG:NH1	3:C:755:ARG:HB2	2.33	0.44
1:H:586:PHE:HE2	2:I:463:SER:HB2	1.83	0.44
2:I:125:TYR:HB2	2:I:227:ASN:ND2	2.32	0.44
2:I:157:THR:HG23	2:I:160:SER:H	1.83	0.44
3:J:129:LYS:HG2	3:J:132:ARG:NH2	2.33	0.44
1:A:277:LEU:HA	1:A:430:LEU:HD11	1.99	0.44
2:B:144:GLU:O	2:B:148:GLN:HG2	2.17	0.44
2:B:254:VAL:HG11	2:B:395:MET:HG3	1.99	0.44
2:B:422:ASP:OD1	2:B:422:ASP:N	2.50	0.44
1:H:556:ILE:HG13	1:H:557:TYR:HD1	1.82	0.44
2:I:312:ASP:HA	2:I:315:ARG:HD3	2.00	0.44
3:J:162:VAL:HA	3:J:189:HIS:CD2	2.52	0.44
3:C:46:THR:HG22	3:C:47:SER:N	2.32	0.43
2:I:333:GLU:O	2:I:337:ILE:HG13	2.18	0.43
1:A:596:LYS:HD3	2:B:458:LYS:HE3	2.00	0.43
4:D:11:A:HO2'	4:D:12:G:H8	1.64	0.43
2:I:62:THR:HG22	2:I:64:CYS:H	1.83	0.43
2:I:523:ALA:HA	2:I:526:MET:HG2	1.98	0.43
1:H:406:ARG:NH1	1:H:410:THR:OG1	2.51	0.43
2:I:587:ASP:OD1	2:I:588:GLU:N	2.52	0.43
1:A:104:LEU:HD22	1:A:126:GLU:HB3	2.00	0.43
1:A:190:ASP:O	2:B:315:ARG:NH2	2.52	0.43
1:A:557:TYR:CG	1:A:606:ILE:HD13	2.54	0.43
2:B:357:LYS:HE3	2:B:357:LYS:HB2	1.79	0.43
3:C:751:ASP:HA	3:C:754:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:15:G:H2'	5:F:16:C:C6	2.53	0.43
1:H:503:SER:O	1:H:507:GLN:HG3	2.18	0.43
2:I:245:THR:OG1	2:I:251:ARG:NH2	2.51	0.43
1:A:11:ARG:HH12	3:C:743:LYS:HB2	1.83	0.43
1:A:560:PRO:HB3	2:B:240:ARG:HH12	1.83	0.43
2:B:127:PHE:HB2	2:B:222:GLN:HB3	2.01	0.43
2:B:281:LEU:HB3	3:C:150:ARG:NH1	2.34	0.43
2:B:297:GLU:OE2	2:B:475:HIS:NE2	2.49	0.43
3:C:751:ASP:O	3:C:754:ARG:NE	2.51	0.43
2:I:33:ARG:CZ	2:I:350:GLY:HA2	2.49	0.43
2:I:226:LEU:HD21	2:I:395:MET:HE1	2.01	0.43
3:C:454:MET:HA	3:C:480:ARG:HH21	1.84	0.43
1:H:326:TYR:CZ	6:K:7:A:H8	2.37	0.43
2:I:132:ASN:HD21	2:I:227:ASN:ND2	2.16	0.43
2:I:623:ASP:OD1	2:I:625:SER:OG	2.27	0.43
1:A:375:TYR:HA	1:A:378:ILE:HG12	2.01	0.43
2:B:250:ILE:HD11	2:B:338:PRO:HA	2.01	0.43
2:B:612:ARG:HD3	2:B:612:ARG:HA	1.93	0.43
3:C:163:ASN:N	3:C:305:ASP:OD1	2.46	0.43
1:H:345:ARG:HD3	1:H:546:MET:CG	2.49	0.43
1:H:372:VAL:HG21	2:I:523:ALA:HB3	2.01	0.43
2:I:147:GLU:OE2	2:I:154:ILE:HG12	2.19	0.43
2:I:226:LEU:HD11	2:I:342:PHE:CE1	2.54	0.43
1:H:309:LYS:HE2	6:K:10:A:N1	2.34	0.43
1:H:434:HIS:O	1:H:434:HIS:CG	2.72	0.43
2:I:538:MET:HB3	2:I:543:THR:HG21	2.00	0.43
3:J:109:LYS:HG2	3:J:110:TYR:CD1	2.54	0.43
1:H:215:LEU:HD13	1:H:576:ARG:HH21	1.83	0.43
2:I:38:LEU:HD21	2:I:366:LEU:HD22	2.00	0.43
1:A:512:ARG:NH2	1:A:525:PRO:HB3	2.34	0.42
2:B:659:THR:HG23	3:C:38:TYR:HE1	1.83	0.42
2:I:91:PHE:CG	2:I:406:ILE:HG22	2.54	0.42
2:B:700:GLU:OE1	2:B:704:ARG:NH2	2.47	0.42
3:C:173:GLN:O	3:C:177:PRO:HG3	2.19	0.42
1:A:8:ILE:HD12	1:A:36:CYS:HB3	2.00	0.42
1:A:483:PHE:HD2	1:A:488:LEU:HG	1.85	0.42
1:A:586:PHE:HE2	2:B:463:SER:HB3	1.84	0.42
3:C:735:ILE:HG13	3:C:736:TRP:CD1	2.54	0.42
2:I:648:LEU:HG	2:I:651:LYS:HZ2	1.85	0.42
2:B:531:HIS:CE1	5:E:16:C:H1'	2.54	0.42
2:I:305:PHE:O	2:I:309:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASN:HB3	3:C:142:ARG:NH2	2.34	0.42
3:C:65:TRP:HB3	3:C:98:ARG:HB3	2.02	0.42
1:H:215:LEU:HB2	1:H:619:ASN:HB2	2.01	0.42
1:H:596:LYS:HE2	2:I:457:SER:HB2	2.00	0.42
2:B:31:GLY:HA3	4:D:7:A:O3'	2.19	0.42
1:H:437:LYS:HA	1:H:437:LYS:HD3	1.78	0.42
1:A:357:LYS:NZ	1:A:373:ASP:OD1	2.47	0.42
1:A:264:ARG:NH1	1:A:454:ASP:OD1	2.52	0.42
3:C:457:ASP:OD1	3:C:458:LYS:N	2.52	0.42
2:I:224:ARG:HD2	2:I:344:SER:O	2.20	0.42
3:J:86:ASP:OD2	3:J:98:ARG:NH2	2.49	0.42
2:I:11:ASN:OD1	2:I:14:THR:HG23	2.19	0.42
2:B:315:ARG:HG3	2:B:339:PHE:HB2	2.02	0.42
3:C:150:ARG:HE	3:C:228:PRO:HB3	1.85	0.42
1:H:232:LEU:HD12	1:H:390:LYS:HE2	2.02	0.42
1:H:577:HIS:HD1	2:I:12:PRO:HD2	1.85	0.42
1:H:264:ARG:HD2	1:H:456:GLU:OE1	2.20	0.41
1:H:333:LEU:HD12	1:H:334:PRO:HD2	2.02	0.41
1:H:581:GLU:O	1:H:581:GLU:HG2	2.20	0.41
2:I:654:ARG:HD2	3:J:27:ALA:HA	2.02	0.41
2:B:61:LYS:O	2:B:343:LYS:NZ	2.47	0.41
2:I:329:ASP:O	2:I:332:MET:HB2	2.20	0.41
2:B:44:PRO:HG3	2:B:307:GLU:HB2	2.01	0.41
2:B:97:PRO:O	2:B:101:LYS:HG2	2.20	0.41
2:B:530:ASN:ND2	2:B:565:PRO:HG3	2.35	0.41
6:G:3:C:H2'	6:G:4:A:H8	1.84	0.41
2:I:117:GLU:HG3	2:I:255:LYS:HE3	2.01	0.41
1:A:120:ASN:HD21	1:A:124:GLU:HB2	1.86	0.41
1:A:246:THR:HG22	1:A:249:GLU:HG3	2.02	0.41
3:C:46:THR:HG22	3:C:47:SER:H	1.86	0.41
1:H:182:LEU:O	1:H:185:ARG:HG2	2.20	0.41
1:H:568:ASN:OD1	1:H:571:ARG:NH2	2.53	0.41
2:I:147:GLU:OE2	2:I:153:LYS:HD2	2.21	0.41
3:J:152:PRO:HD3	3:J:226:TRP:CZ3	2.55	0.41
3:J:162:VAL:HG21	3:J:220:ILE:HB	2.03	0.41
3:C:600:ARG:O	3:C:603:GLN:N	2.53	0.41
1:A:269:THR:HG23	1:A:480:ILE:HG13	2.03	0.41
3:C:442:HIS:HA	3:C:445:LYS:NZ	2.35	0.41
1:A:313:ALA:HB1	2:B:360:LEU:HD23	2.02	0.41
2:B:22:TYR:HD2	2:B:484:ALA:O	2.04	0.41
1:A:582:ARG:NH1	1:A:622:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LYS:HE2	2:B:457:SER:HB2	2.02	0.41
2:B:701:ARG:HA	2:B:704:ARG:HG2	2.02	0.41
3:C:210:GLU:HG2	3:C:211:SER:N	2.35	0.41
1:H:432:GLY:O	1:H:434:HIS:HD2	2.03	0.41
3:J:83:LYS:HE2	3:J:85:LYS:O	2.20	0.41
1:A:150:GLU:HB2	3:C:691:GLN:HE22	1.86	0.41
1:A:543:TRP:CE2	1:A:547:ILE:HD11	2.56	0.41
2:B:32:THR:HG23	4:D:8:U:OP1	2.20	0.41
3:C:517:LEU:HG	3:C:518:ILE:HG13	2.02	0.41
3:C:555:LEU:O	3:C:559:THR:HG23	2.21	0.41
2:I:67:PRO:HD3	2:I:80:HIS:CD2	2.55	0.41
2:B:114:LYS:HD2	2:B:156:PRO:HB2	2.03	0.41
1:H:506:SER:HB2	2:I:520:CYS:HB3	2.03	0.41
1:A:64:ASP:N	1:A:64:ASP:OD1	2.55	0.40
2:B:615:ASN:OD1	2:B:616:LYS:N	2.53	0.40
6:G:1:ATP:H2'	6:G:2:G:H8	1.85	0.40
2:I:226:LEU:HD11	2:I:342:PHE:HE1	1.86	0.40
3:J:136:THR:HG22	3:J:138:TRP:H	1.86	0.40
1:A:118:ALA:HB3	1:A:126:GLU:HG2	2.02	0.40
2:B:130:LYS:HE3	2:B:222:GLN:NE2	2.36	0.40
2:B:530:ASN:HD21	2:B:565:PRO:HG3	1.85	0.40
3:C:210:GLU:HG3	5:F:17:U:H2'	2.04	0.40
1:H:263:ILE:HD11	1:H:466:SER:HB2	2.03	0.40
1:A:470:GLU:O	1:A:471:GLU:HG3	2.21	0.40
1:A:580:MET:HG2	1:A:621:TYR:CE1	2.56	0.40
3:C:294:ILE:HD12	3:C:302:VAL:HG11	2.04	0.40
3:C:591:ILE:HD12	3:C:591:ILE:H	1.86	0.40
2:I:137:ILE:HG12	3:J:44:TYR:CZ	2.57	0.40
2:I:224:ARG:NH2	2:I:346:LEU:HD11	2.35	0.40
1:A:442:ASN:HB3	1:A:482:SER:HB2	2.03	0.40
1:H:226:SER:HB2	1:H:229:ARG:NH2	2.36	0.40
2:I:83:SER:HB3	2:I:449:LEU:HD13	2.03	0.40
2:I:498:MET:N	2:I:498:MET:SD	2.94	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	619/622 (100%)	596 (96%)	23 (4%)	0	100	100
1	H	447/622 (72%)	428 (96%)	19 (4%)	0	100	100
2	B	670/710 (94%)	645 (96%)	25 (4%)	0	100	100
2	I	616/710 (87%)	590 (96%)	26 (4%)	0	100	100
3	C	744/827 (90%)	705 (95%)	39 (5%)	0	100	100
3	J	233/827 (28%)	225 (97%)	8 (3%)	0	100	100
All	All	3329/4318 (77%)	3189 (96%)	140 (4%)	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	560/561 (100%)	560 (100%)	0	100	100
1	H	403/561 (72%)	402 (100%)	1 (0%)	93	98
2	B	600/633 (95%)	600 (100%)	0	100	100
2	I	557/633 (88%)	557 (100%)	0	100	100
3	C	674/736 (92%)	672 (100%)	2 (0%)	92	97
3	J	216/736 (29%)	216 (100%)	0	100	100
All	All	3010/3860 (78%)	3007 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	638	LYS
3	C	754	ARG
1	H	203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	GLN
2	B	476	HIS
2	B	672	GLN
1	H	434	HIS
1	H	528	GLN
1	H	535	GLN
2	I	132	ASN
2	I	227	ASN
2	I	476	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	11/18 (61%)	3 (27%)	0
5	E	3/17 (17%)	1 (33%)	0
5	F	12/17 (70%)	0	0
6	G	8/10 (80%)	0	0
6	K	8/10 (80%)	2 (25%)	0
All	All	42/72 (58%)	6 (14%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	7	A
4	D	11	A
4	D	12	G
5	E	17	U
6	K	7	A
6	K	8	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

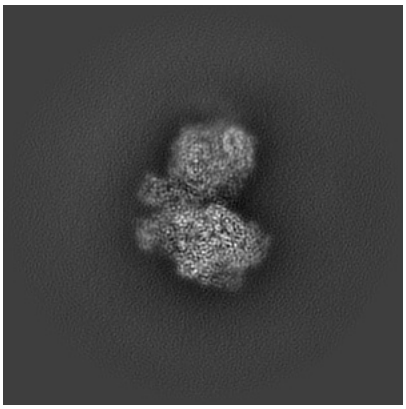
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39868. These allow visual inspection of the internal detail of the map and identification of artifacts.

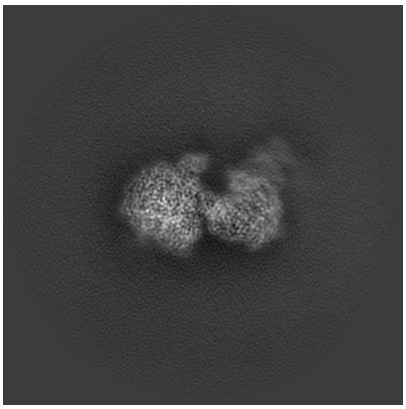
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

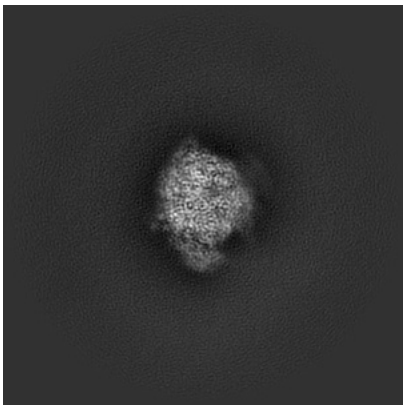
6.1.1 Primary map



X

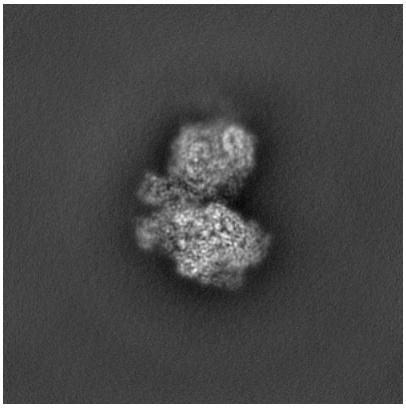


Y

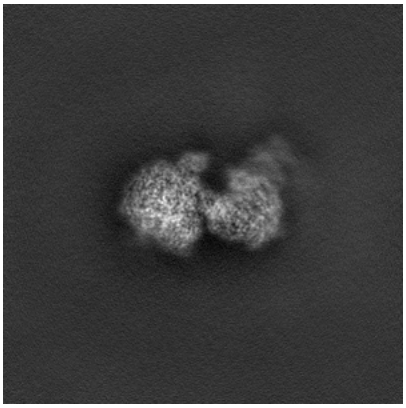


Z

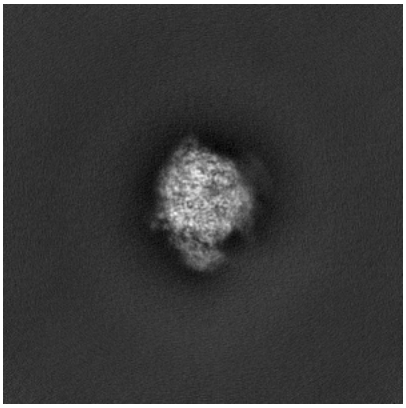
6.1.2 Raw map



X



Y

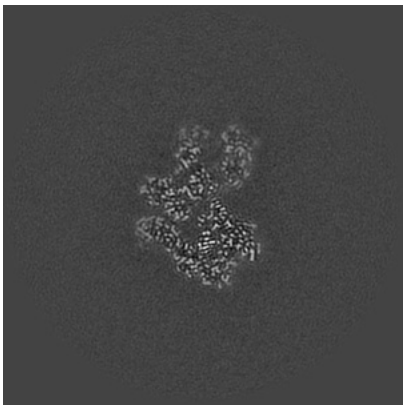


Z

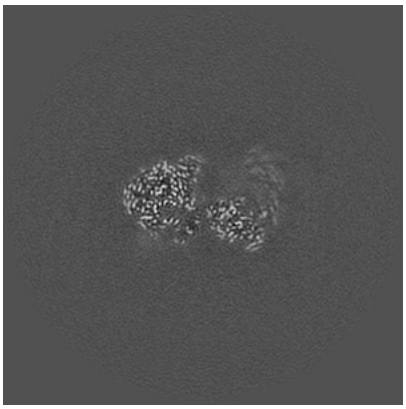
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

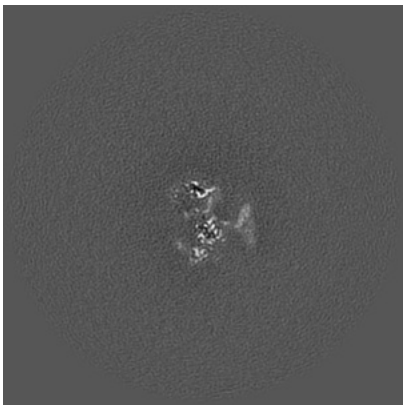
6.2.1 Primary map



X Index: 192

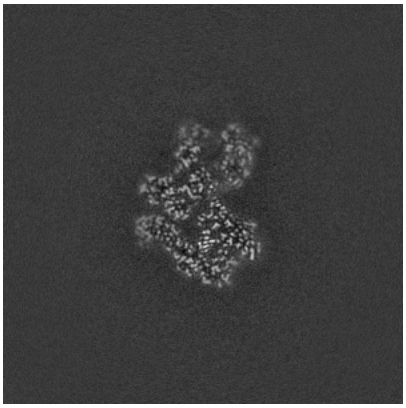


Y Index: 192

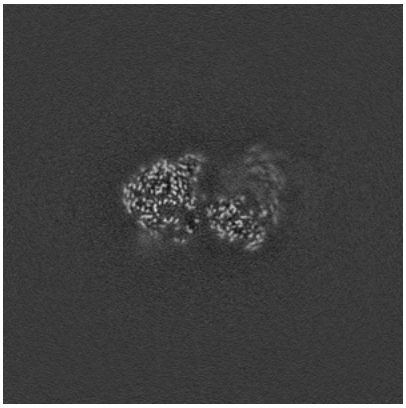


Z Index: 192

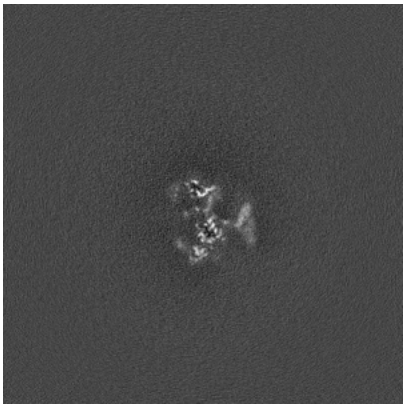
6.2.2 Raw map



X Index: 192



Y Index: 192

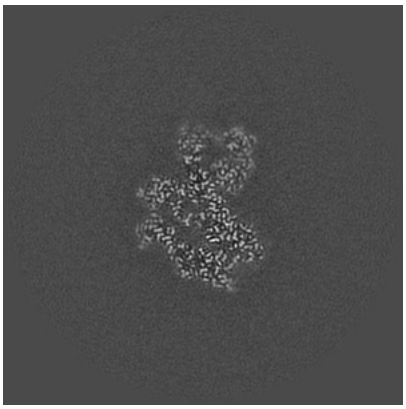


Z Index: 192

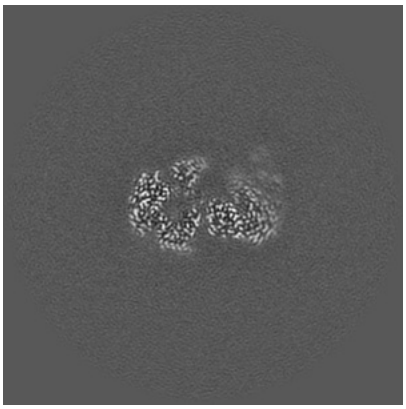
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

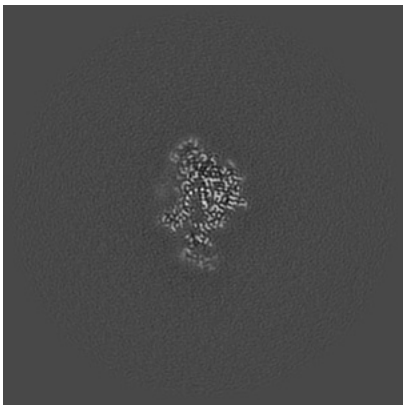
6.3.1 Primary map



X Index: 188

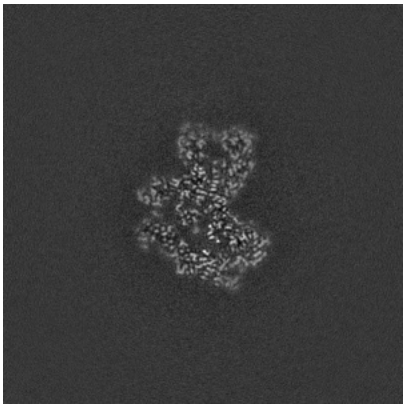


Y Index: 181

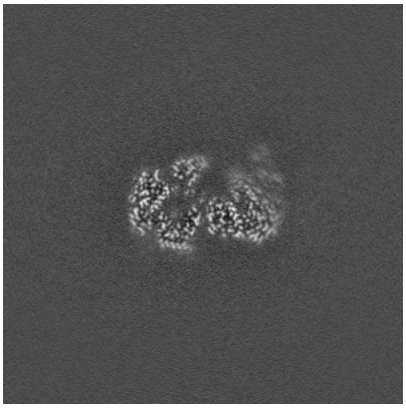


Z Index: 155

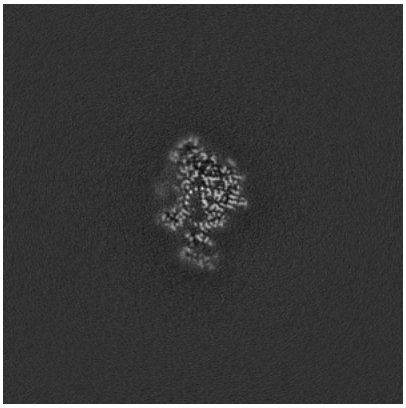
6.3.2 Raw map



X Index: 185



Y Index: 181

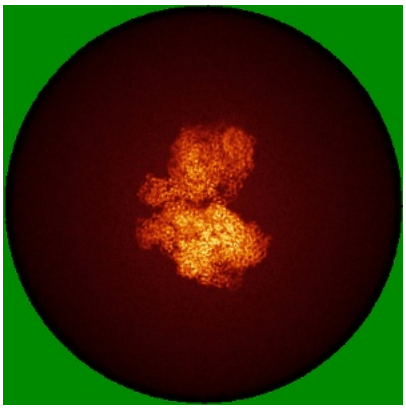


Z Index: 155

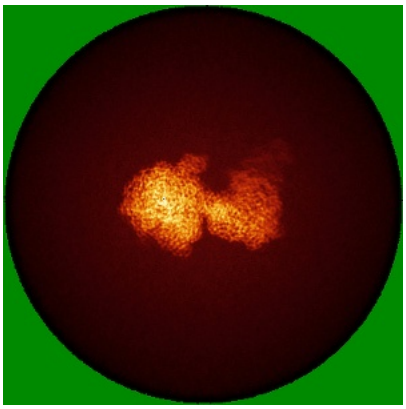
The images above show the largest variance slices of the map in three orthogonal directions.

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

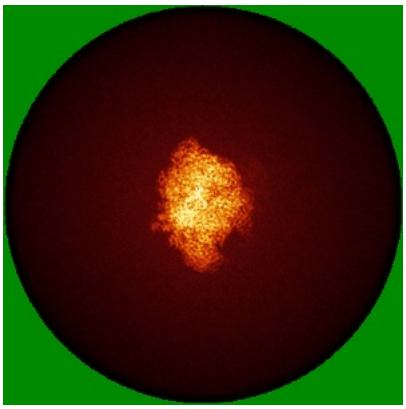
6.4.1 Primary map



X

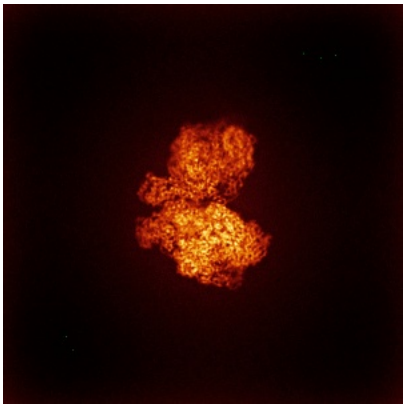


Y

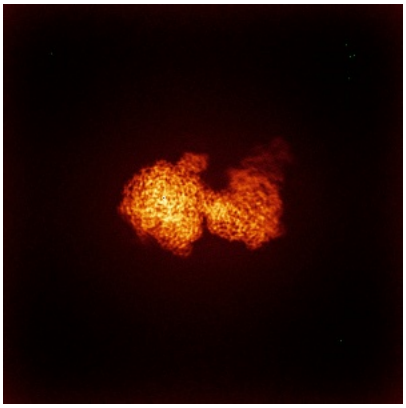


Z

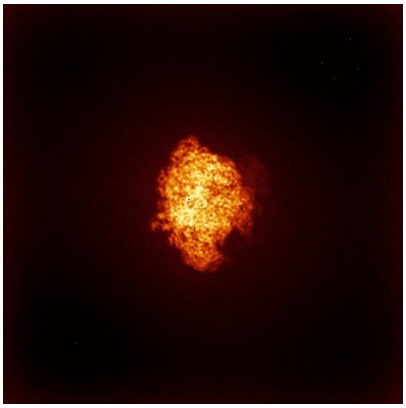
6.4.2 Raw map



X



Y

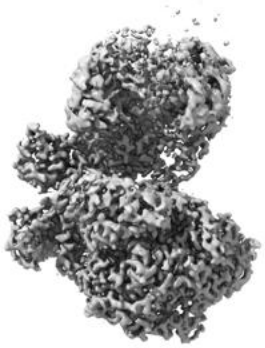


Z

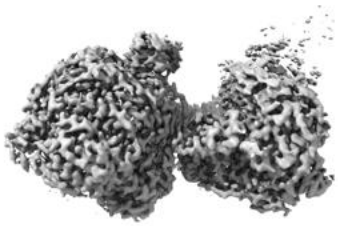
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

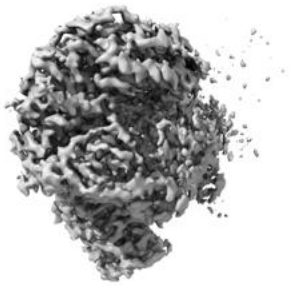
6.5.1 Primary map



X



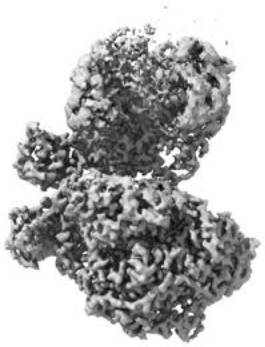
Y



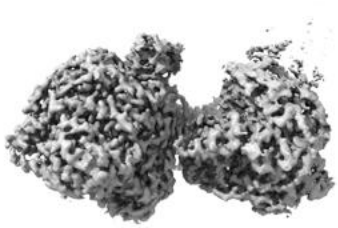
Z

The images above show the 3D surface view of the map at the recommended contour level 0.459. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

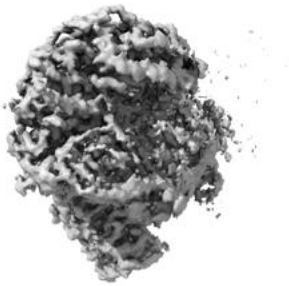
6.5.2 Raw map



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.

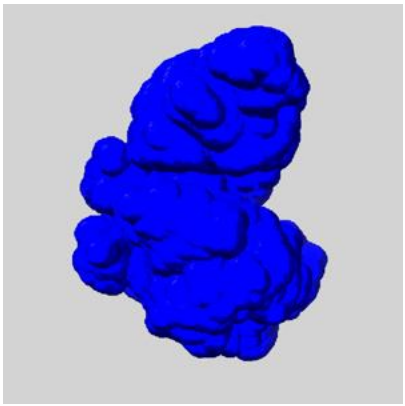
6.6 Mask visualisation (i)

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

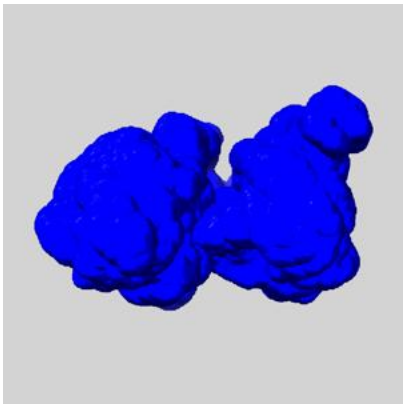
A mask typically either:

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

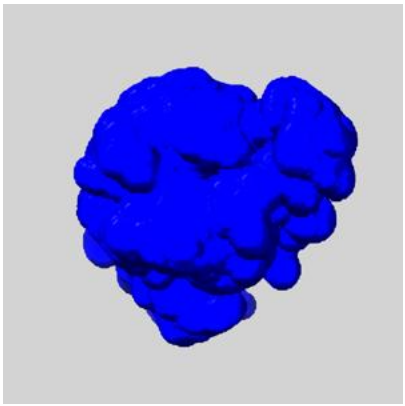
6.6.1 emd_39868_msk_1.map (i)



X



Y

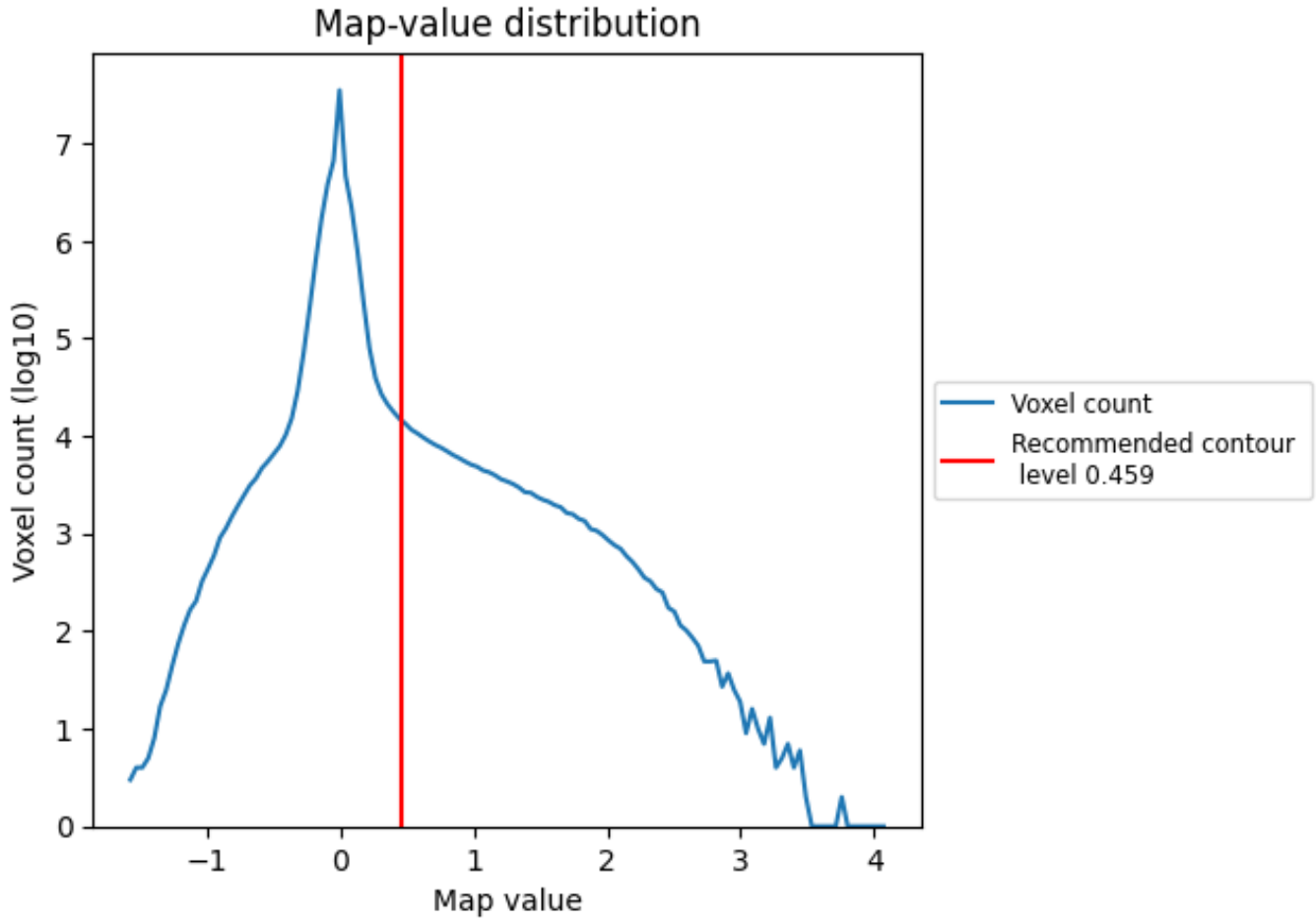


Z

7 Map analysis

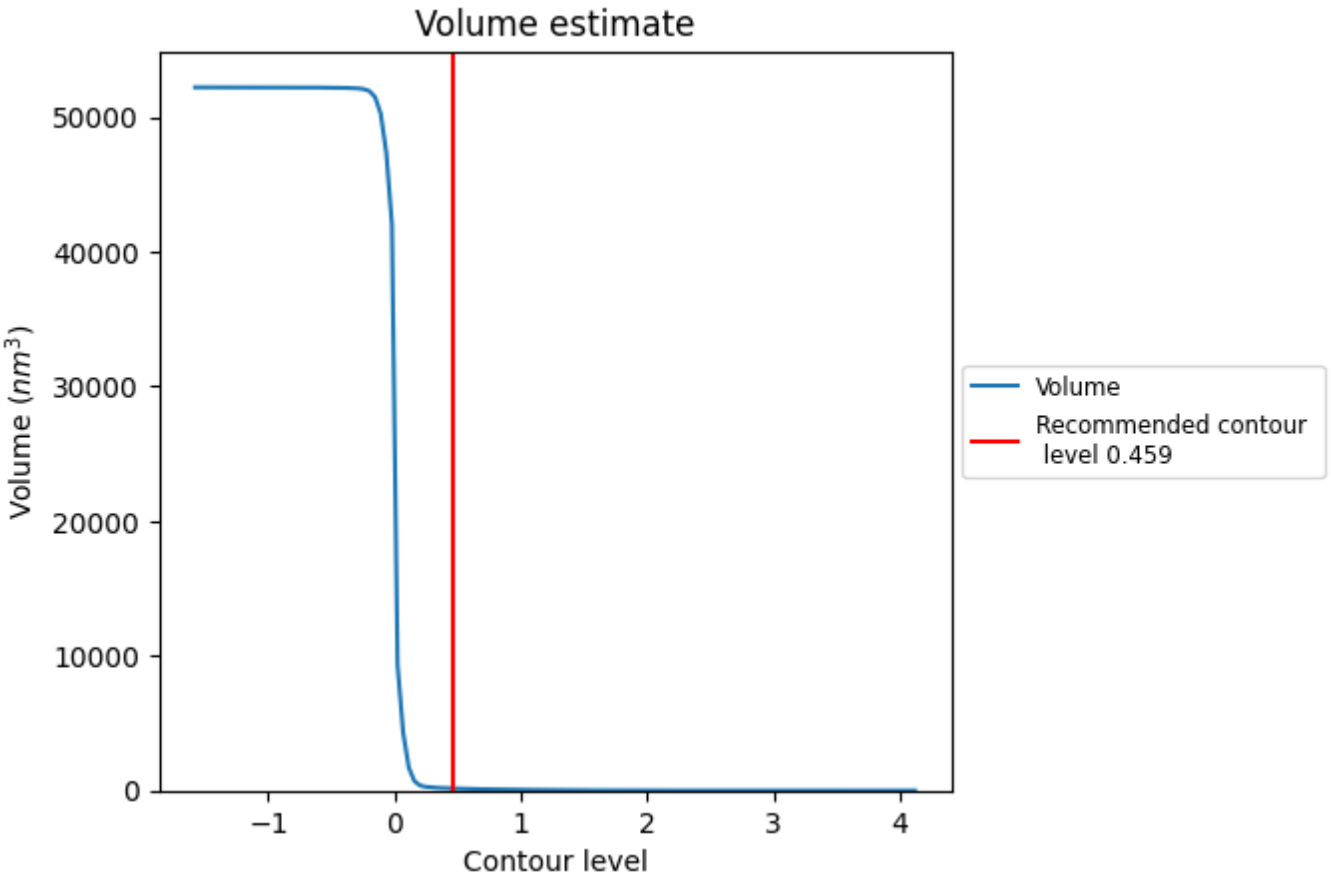
This section contains the results of statistical analysis of the map.

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.

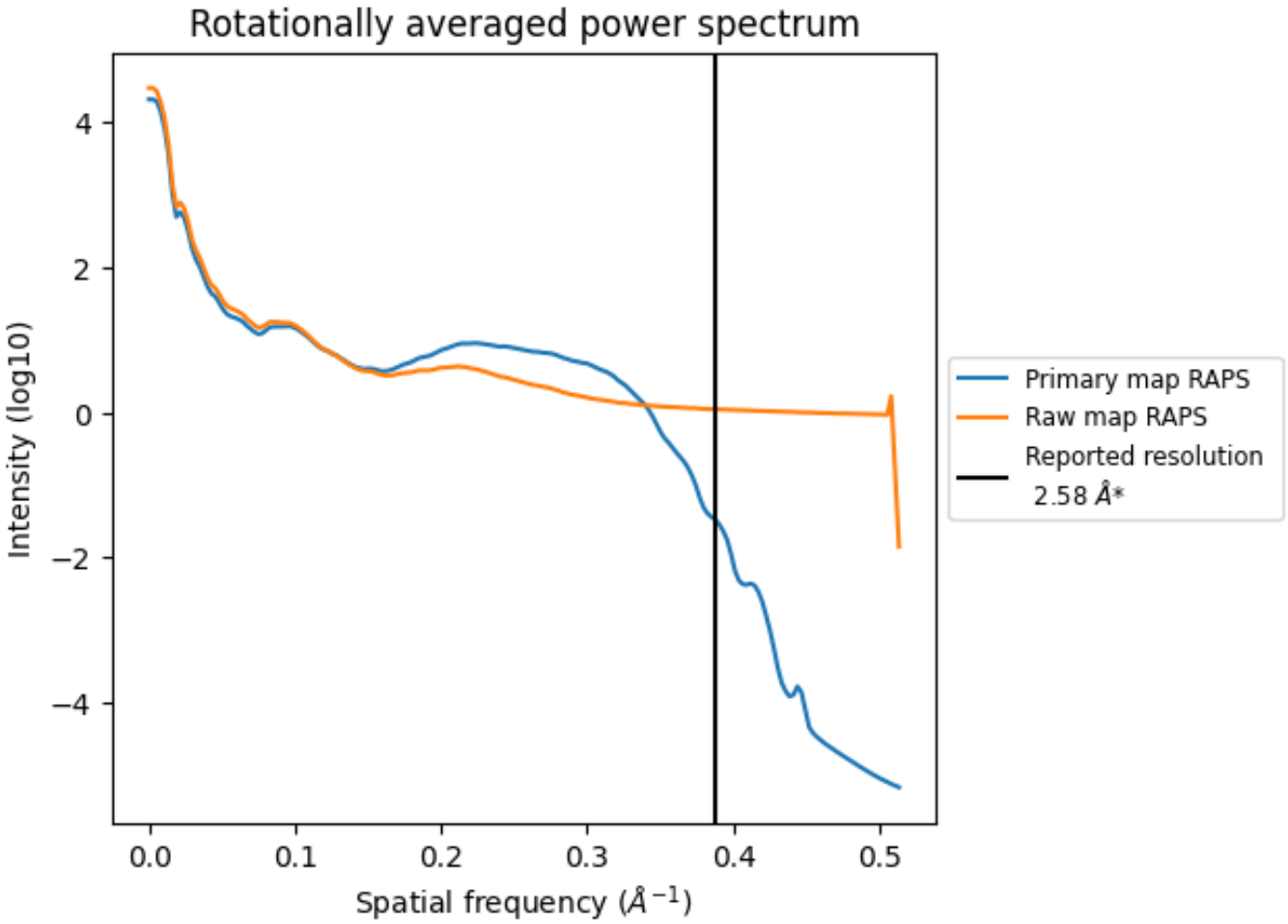
7.2 Volume estimate



The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 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)

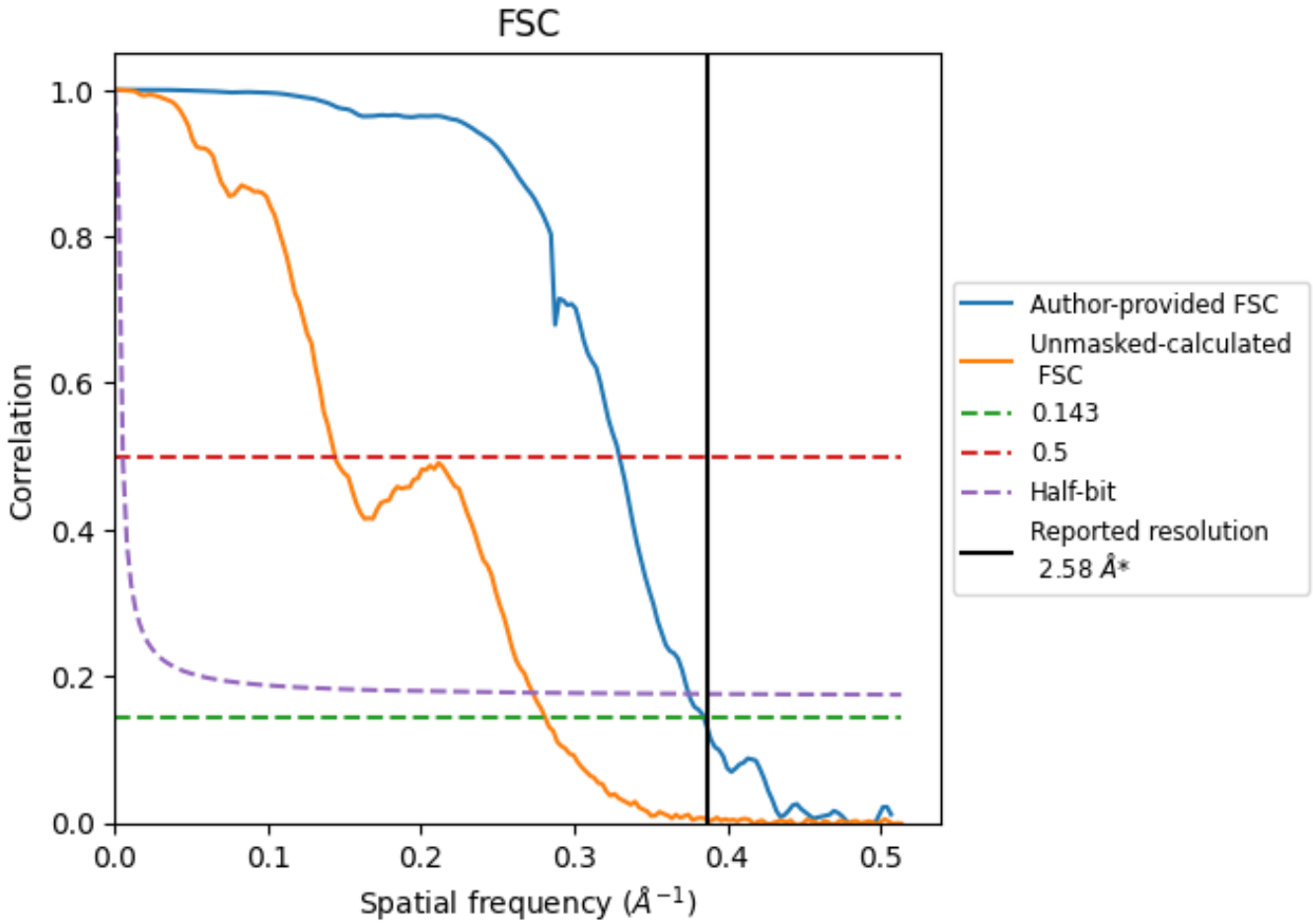


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

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 0.388 $Å^{-1}$

8.2 Resolution estimates (i)

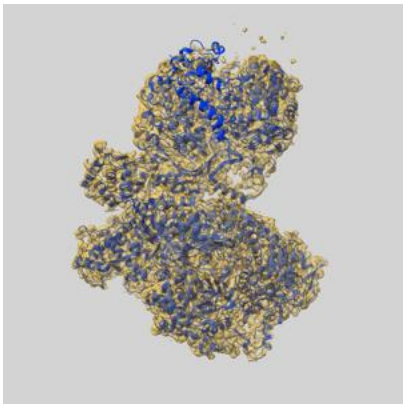
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.60	3.04	2.67
Unmasked-calculated*	3.56	6.95	3.66

*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 3.56 differs from the reported value 2.58 by more than 10 %

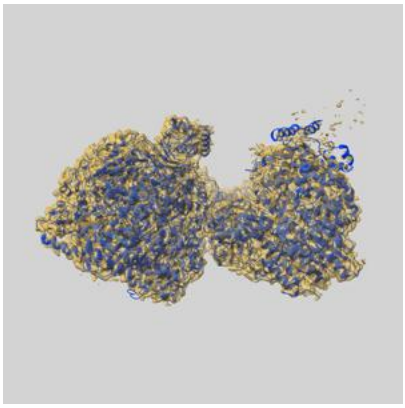
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39868 and PDB model 8Z9R. Per-residue inclusion information can be found in section 3 on page 9.

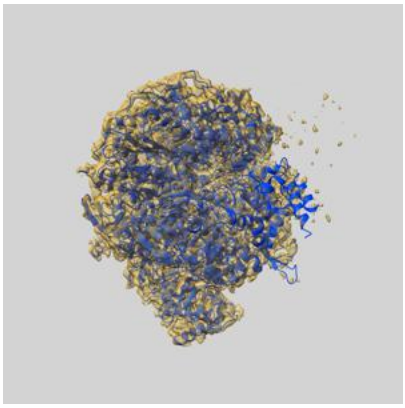
9.1 Map-model overlay



X



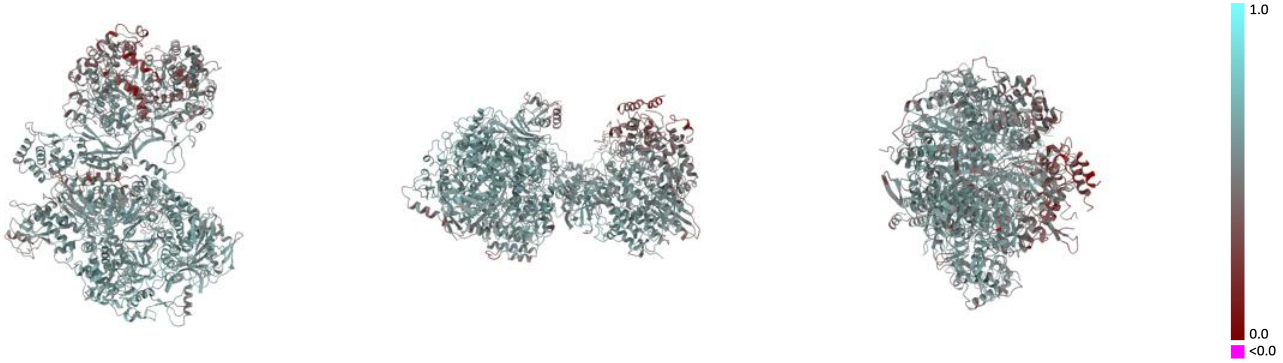
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.459 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.

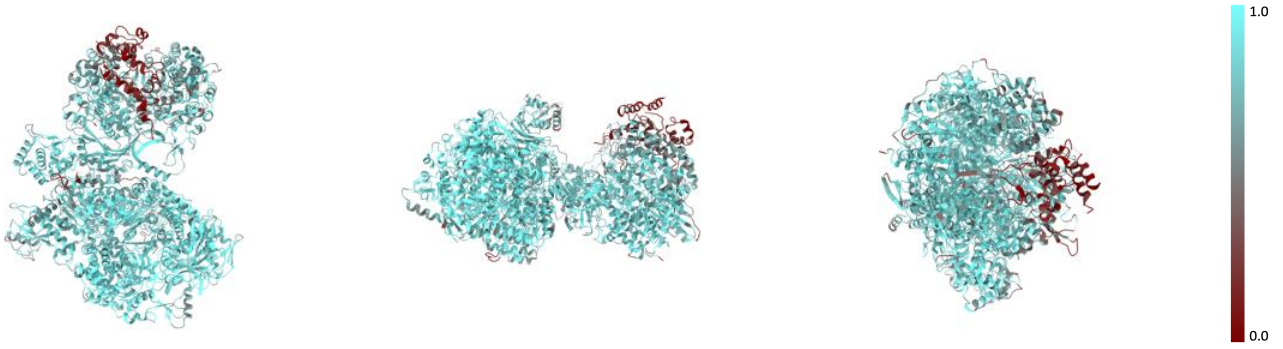
9.2 Q-score mapped to coordinate model (i)



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.

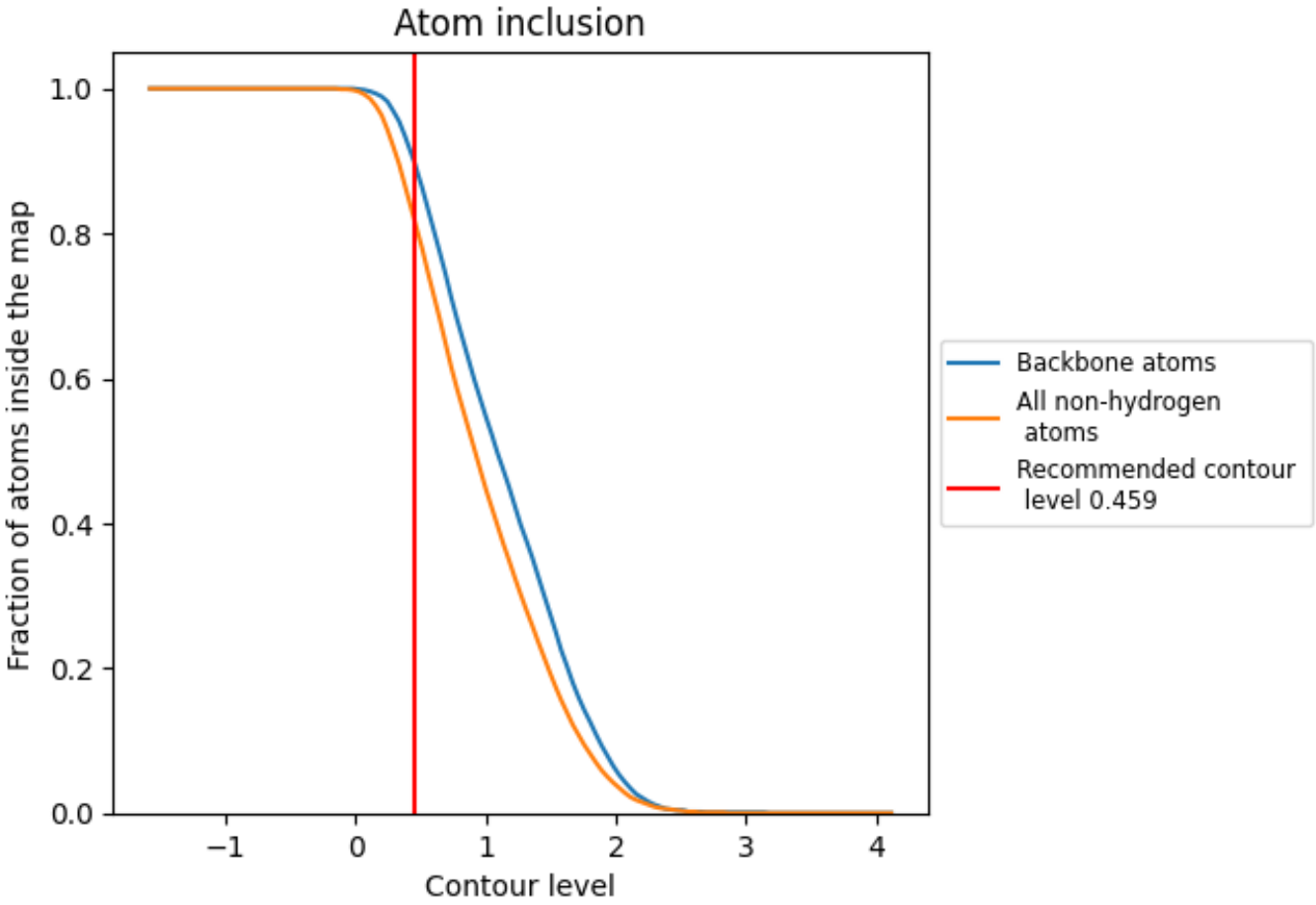
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.459).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.459) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5480
A	0.8790	0.5740
B	0.9150	0.5950
C	0.8250	0.5540
D	0.8460	0.5290
E	0.5780	0.5490
F	0.9630	0.6090
G	0.9960	0.6230
H	0.8570	0.5660
I	0.7330	0.4990
J	0.4230	0.4010
K	0.9250	0.5690