



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 06:15 AM UTC

PDB ID : 5M1S / pdb_00005m1s
EMDB ID : EMD-4141
Title : Cryo-EM structure of the E. coli replicative DNA polymerase-clamp-exonuclease-theta complex bound to DNA in the editing mode
Authors : Fernandez-Leiro, R.; Conrad, J.; Scheres, S.H.W.; Lamers, M.H.
Deposited on : 2016-10-10
Resolution : 6.70 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:

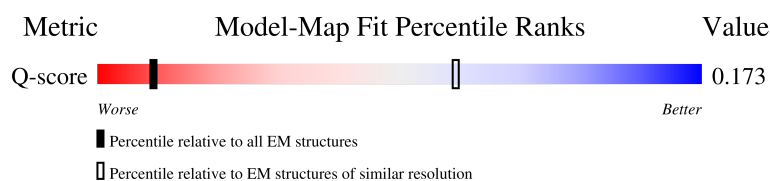
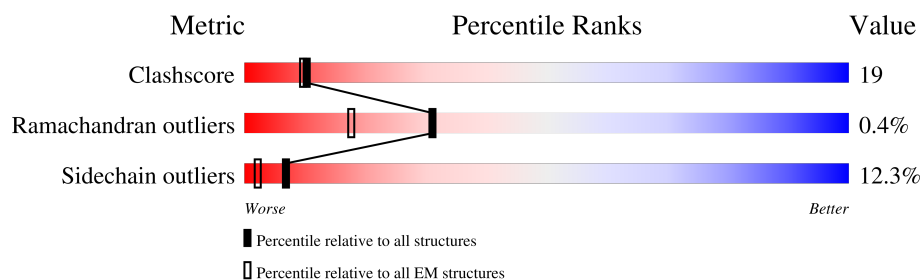
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.70 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	523 (6.20 - 7.20)

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	927	13% 65% 30% 5%
2	B	366	14% 68% 27% 5%
2	C	366	14% 57% 37% 6%
3	D	243	21% 52% 37% 5% 6%

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Mol	Chain	Length	Quality of chain
4	P	17	18%65%29%6%
5	T	22	18%55%45%
6	F	56	29%46%45%9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	927	Total	C	N	O	S	0	0
			7274	4630	1240	1363	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	921	LEU	ALA	engineered mutation	UNP P10443
A	923	LEU	MET	engineered mutation	UNP P10443

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		
2	C	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		

- Molecule 3 is a protein called DNA polymerase III subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	229	Total	C	N	O	S	0	0
			1800	1140	316	335	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	LEU	THR	engineered mutation	UNP P03007
D	185	LEU	MET	engineered mutation	UNP P03007
D	186	PRO	ALA	engineered mutation	UNP P03007
D	187	LEU	PHE	engineered mutation	UNP P03007

- Molecule 4 is a DNA chain called DNA Primer Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	17	Total	C	N	O	P	0	0
			354	168	69	100	17		

- Molecule 5 is a DNA chain called DNA Template Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	22	Total	C	N	O	P	0	0
			448	214	77	135	22		

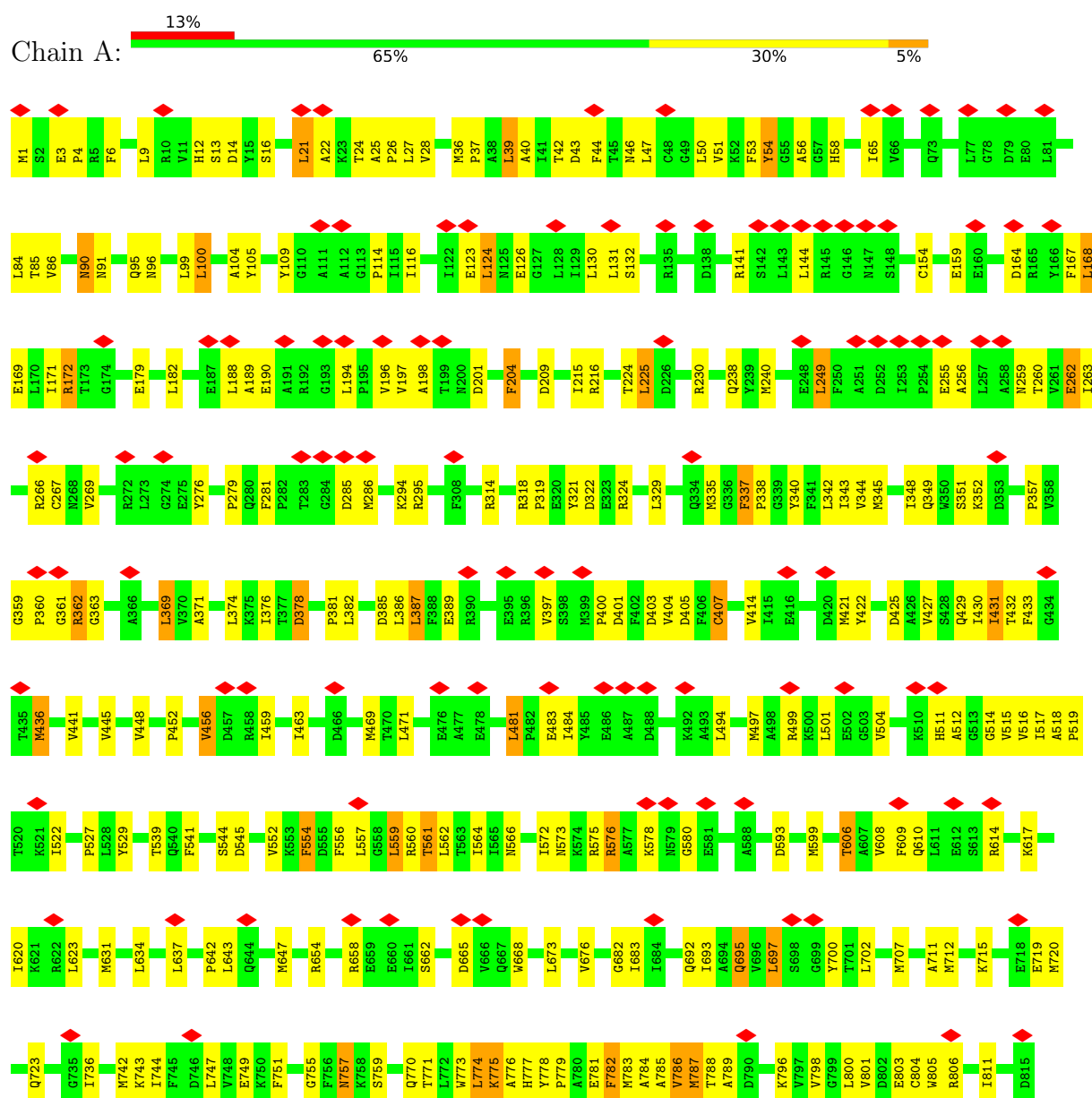
- Molecule 6 is a protein called DNA polymerase III subunit theta.

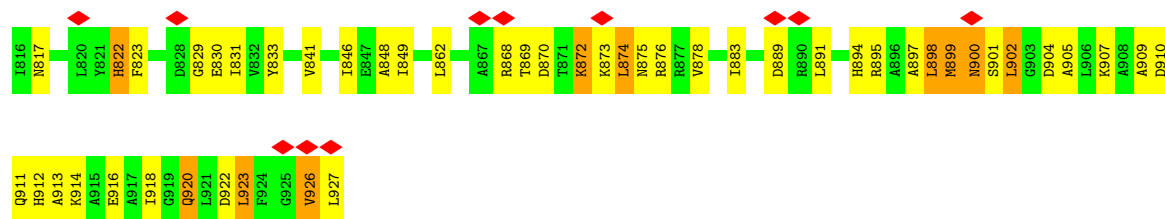
Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	56	Total	C	N	O	S	0	0
			456	285	86	83	2		

3 Residue-property plots

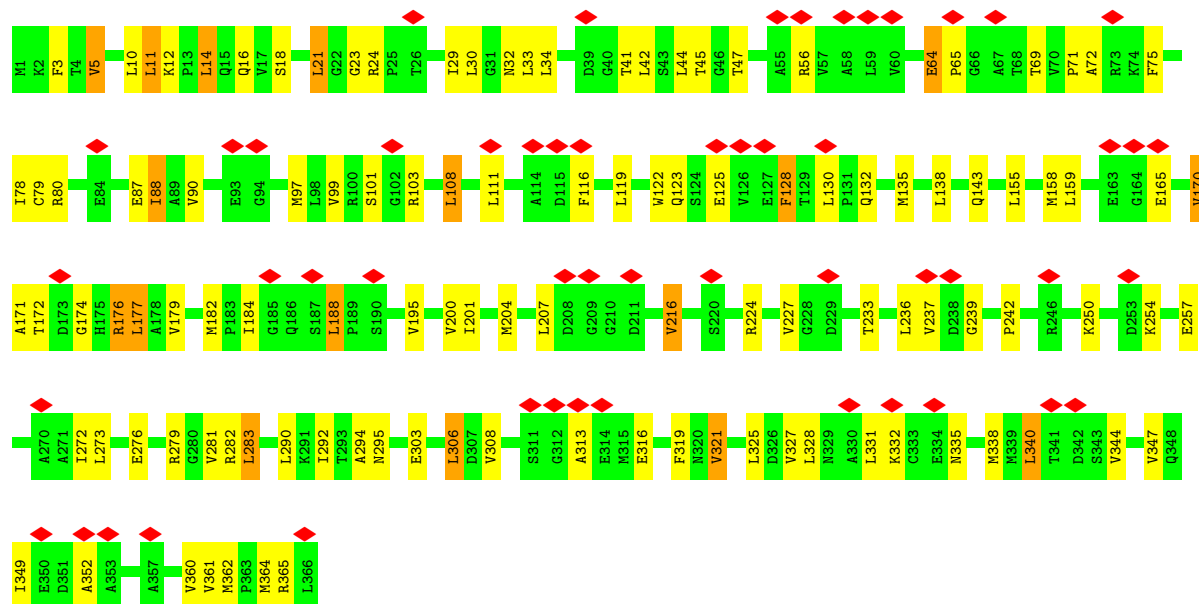
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA polymerase III subunit alpha

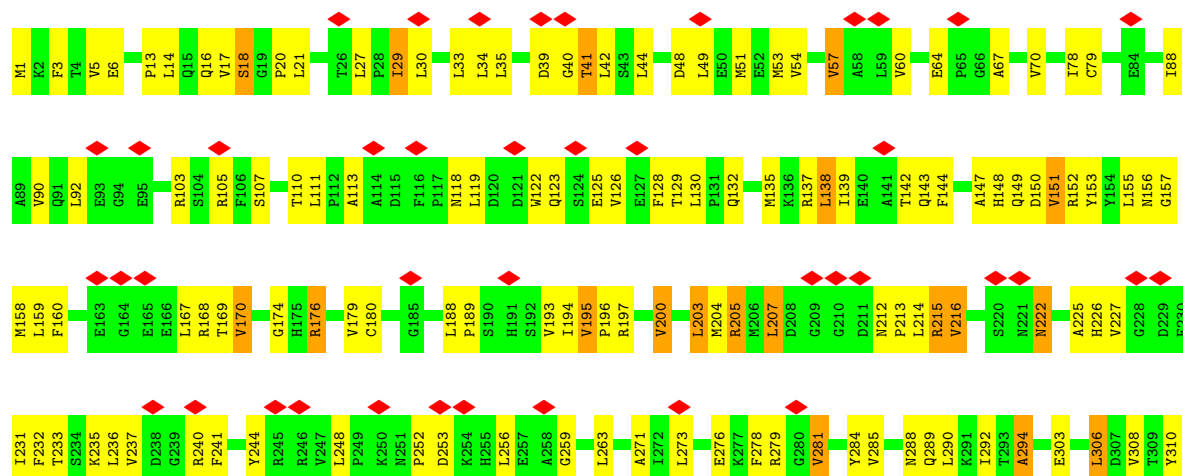




• Molecule 2: DNA polymerase III subunit beta

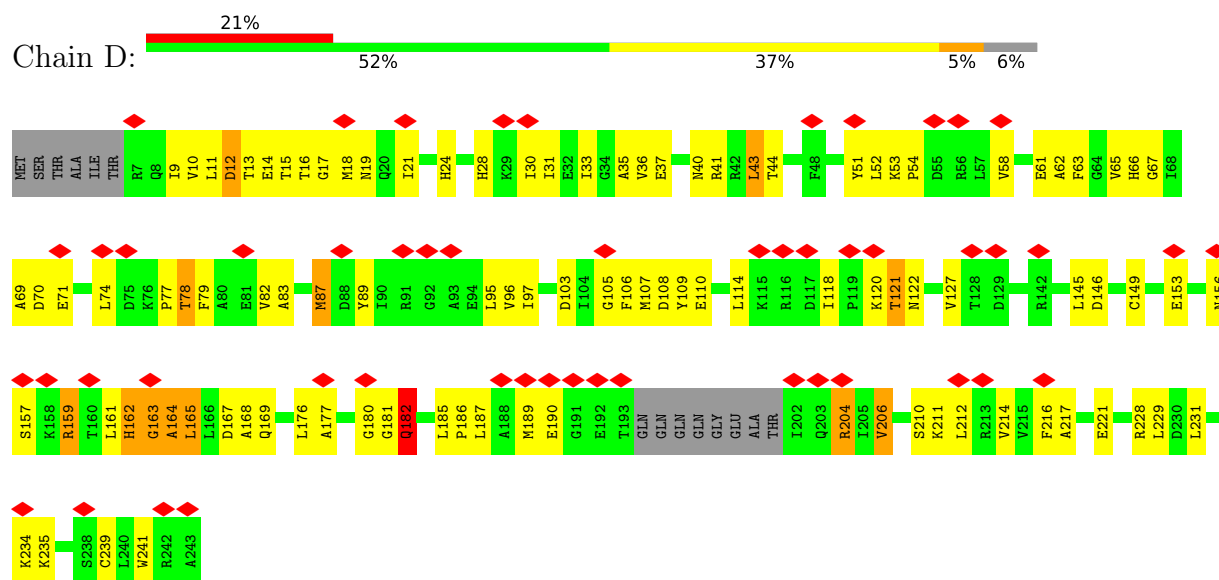


• Molecule 2: DNA polymerase III subunit beta

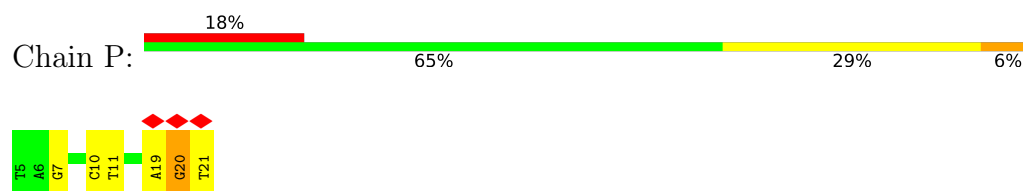




• Molecule 3: DNA polymerase III subunit epsilon



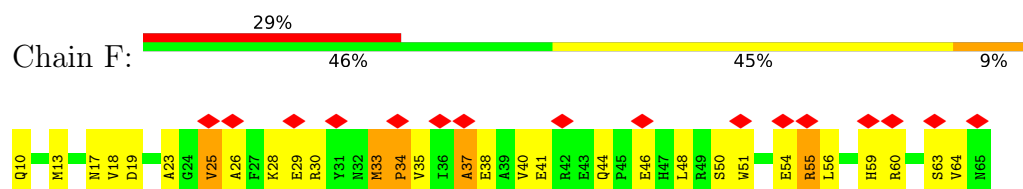
• Molecule 4: DNA Primer Strand



• Molecule 5: DNA Template Strand



• Molecule 6: DNA polymerase III subunit theta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15616	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	79545	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.343	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	246.4, 246.4, 246.4	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.76, 1.76, 1.76	Depositor

5 Model quality

5.1 Standard geometry

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	0.77	2/7427 (0.0%)	1.06	9/10040 (0.1%)
2	B	0.71	0/2893	0.98	4/3915 (0.1%)
2	C	0.77	0/2893	1.00	4/3915 (0.1%)
3	D	0.91	1/1830 (0.1%)	1.09	3/2469 (0.1%)
4	P	0.37	0/398	0.92	1/613 (0.2%)
5	T	0.43	0/500	0.95	0/769
6	F	1.45	3/464 (0.6%)	1.36	3/626 (0.5%)
All	All	0.79	6/16405 (0.0%)	1.04	24/22347 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	C	0	1
3	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	33	MET	CA-C	7.05	1.59	1.52
6	F	37	ALA	N-CA	6.17	1.53	1.46
6	F	41	GLU	N-CA	6.13	1.54	1.46
1	A	775	LYS	C-O	-5.50	1.17	1.24
1	A	775	LYS	CA-C	-5.29	1.46	1.52
3	D	182	GLN	N-CA	5.09	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	164	ALA	N-CA-C	8.65	123.97	113.41
2	B	72	ALA	N-CA-C	7.98	119.88	111.03
1	A	387	LEU	N-CA-C	7.53	120.69	108.41
2	C	143	GLN	N-CA-C	7.45	120.34	111.33
6	F	37	ALA	N-CA-C	7.40	119.35	111.28
1	A	560	ARG	N-CA-C	-6.78	104.11	112.38
2	B	306	LEU	N-CA-C	6.71	118.96	108.96
1	A	276	TYR	N-CA-C	6.54	119.96	110.28
3	D	206	VAL	N-CA-C	6.46	118.04	111.00
1	A	561	THR	N-CA-C	6.42	119.97	111.75
2	B	239	GLY	N-CA-C	6.41	122.04	111.59
6	F	34	PRO	N-CA-C	6.34	120.80	111.03
6	F	46	GLU	N-CA-C	6.33	118.26	111.36
1	A	204	PHE	N-CA-C	6.25	117.73	108.60
2	C	253	ASP	N-CA-C	6.16	118.07	111.36
2	C	306	LEU	N-CA-C	5.83	116.26	108.38
2	C	18	SER	N-CA-C	5.58	118.29	111.82
1	A	874	LEU	N-CA-C	5.55	118.42	107.98
3	D	204	ARG	N-CA-C	5.47	118.49	109.85
1	A	4	PRO	N-CA-C	5.29	119.51	110.95
1	A	841	VAL	N-CA-C	5.21	116.31	109.58
2	B	128	PHE	N-CA-C	5.11	116.60	108.79
4	P	20	DG	C4'-C3'-O3'	5.03	117.54	110.00
1	A	786	VAL	CB-CA-C	-5.02	105.45	111.88

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	556	PHE	Peptide
2	B	71	PRO	Peptide
2	C	294	ALA	Peptide
3	D	163	GLY	Peptide

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	7274	0	7219	304	0
2	B	2844	0	2861	80	0
2	C	2844	0	2861	105	0
3	D	1800	0	1802	114	0
4	P	354	0	192	9	0
5	T	448	0	250	9	0
6	F	456	0	450	20	0
All	All	16020	0	15635	604	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 19.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:HIS:O	1:A:898:LEU:CD2	1.73	1.37
1:A:899:MET:O	1:A:902:LEU:HG	1.17	1.29
1:A:894:HIS:O	1:A:898:LEU:HD23	1.36	1.14
2:B:18:SER:C	2:B:21:LEU:HD13	1.74	1.12
1:A:899:MET:HA	1:A:902:LEU:HD11	1.23	1.11
1:A:782:PHE:CE2	1:A:786:VAL:CG2	2.32	1.11
1:A:431:ILE:HG21	1:A:433:PHE:CZ	1.85	1.10
1:A:782:PHE:CE2	1:A:786:VAL:HG22	1.85	1.10
1:A:559:LEU:HD11	1:A:561:THR:HB	1.25	1.09
1:A:894:HIS:O	1:A:898:LEU:HD21	1.52	1.07
1:A:913:ALA:HA	1:A:916:GLU:OE1	1.55	1.06
1:A:912:HIS:CD2	1:A:916:GLU:OE2	2.09	1.06
1:A:559:LEU:HD11	1:A:561:THR:CB	1.86	1.04
1:A:431:ILE:HD13	1:A:433:PHE:CE1	1.93	1.03
1:A:776:ALA:CA	1:A:779:PRO:HG3	1.75	1.03
1:A:899:MET:C	1:A:902:LEU:HG	1.82	1.03
1:A:782:PHE:CZ	1:A:786:VAL:CG2	2.42	1.02
3:D:145:LEU:HD12	3:D:146:ASP:N	1.74	1.02
1:A:776:ALA:HA	1:A:779:PRO:HG3	1.37	1.01
1:A:899:MET:O	1:A:902:LEU:CG	2.10	1.00
1:A:901:SER:HA	1:A:904:ASP:OD1	1.59	0.99
1:A:776:ALA:C	1:A:779:PRO:HD3	1.89	0.98
1:A:559:LEU:CD1	1:A:561:THR:HB	1.92	0.98
3:D:163:GLY:O	3:D:167:ASP:CG	2.08	0.96
2:C:281:VAL:HG23	2:C:294:ALA:HB2	1.45	0.95
1:A:899:MET:HA	1:A:902:LEU:CD1	1.94	0.95
1:A:431:ILE:HG21	1:A:433:PHE:CE2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:PHE:CZ	1:A:786:VAL:HG22	2.02	0.93
1:A:912:HIS:O	1:A:916:GLU:CD	2.12	0.93
2:B:18:SER:O	2:B:21:LEU:HD13	1.66	0.93
1:A:431:ILE:CD1	1:A:433:PHE:CE1	2.52	0.92
1:A:182:LEU:HD22	3:D:206:VAL:HG21	1.50	0.92
5:T:12:DT:H2"	5:T:13:DC:C5	2.06	0.89
1:A:901:SER:HA	1:A:904:ASP:CG	1.94	0.89
1:A:782:PHE:CE2	1:A:786:VAL:HG23	2.07	0.89
1:A:712:MET:HE2	1:A:720:MET:HE1	1.55	0.89
1:A:776:ALA:CA	1:A:779:PRO:CG	2.50	0.88
1:A:776:ALA:C	1:A:779:PRO:CD	2.46	0.88
3:D:41:ARG:HB3	3:D:176:LEU:HD21	1.56	0.88
2:C:351:ASP:HB3	2:C:354:SER:HB3	1.56	0.88
1:A:559:LEU:CD1	1:A:562:LEU:N	2.36	0.88
1:A:559:LEU:HD12	1:A:562:LEU:HD22	1.54	0.87
1:A:899:MET:CA	1:A:902:LEU:HD11	2.03	0.87
1:A:776:ALA:HA	1:A:779:PRO:CG	2.05	0.87
2:C:14:LEU:O	2:C:18:SER:OG	1.93	0.85
2:B:279:ARG:HB3	2:B:321:VAL:HG12	1.59	0.84
5:T:12:DT:H2"	5:T:13:DC:C6	2.13	0.82
1:A:913:ALA:CA	1:A:916:GLU:OE1	2.25	0.82
3:D:177:ALA:O	3:D:181:GLY:N	2.12	0.82
1:A:362:ARG:NE	1:A:378:ASP:OD1	2.13	0.82
2:C:157:GLY:HA3	2:C:195:VAL:O	1.79	0.82
1:A:559:LEU:CD1	1:A:561:THR:CA	2.58	0.81
3:D:71:GLU:OE2	6:F:59:HIS:O	1.97	0.81
1:A:431:ILE:HG12	1:A:433:PHE:CD1	2.17	0.80
3:D:63:PHE:O	3:D:67:GLY:N	2.14	0.80
2:B:176:ARG:HB3	2:B:361:VAL:HG12	1.61	0.80
3:D:62:ALA:O	3:D:66:HIS:CE1	2.34	0.80
1:A:559:LEU:HD11	1:A:561:THR:CA	2.11	0.80
1:A:899:MET:CA	1:A:902:LEU:HD21	2.11	0.79
1:A:775:LYS:HA	1:A:779:PRO:HA	1.65	0.79
1:A:559:LEU:HD13	1:A:562:LEU:H	1.47	0.79
1:A:559:LEU:HD12	1:A:562:LEU:CD2	2.14	0.77
3:D:176:LEU:O	3:D:180:GLY:N	2.17	0.77
1:A:16:SER:HA	1:A:46:ASN:HD21	1.50	0.77
1:A:901:SER:CA	1:A:904:ASP:OD1	2.33	0.77
1:A:559:LEU:CD1	1:A:562:LEU:H	1.99	0.76
1:A:901:SER:CA	1:A:904:ASP:CG	2.57	0.76
1:A:431:ILE:CG2	1:A:433:PHE:CE2	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:14:GLU:OE2	3:D:163:GLY:HA3	1.85	0.75
1:A:559:LEU:CD1	1:A:561:THR:CB	2.60	0.75
1:A:608:VAL:HG13	1:A:771:THR:OG1	1.86	0.74
2:B:18:SER:HA	2:B:21:LEU:CD1	2.17	0.74
1:A:894:HIS:C	1:A:898:LEU:CD2	2.61	0.74
2:B:18:SER:HA	2:B:21:LEU:HD11	1.68	0.73
1:A:899:MET:HA	1:A:902:LEU:HD21	1.68	0.73
3:D:163:GLY:O	3:D:167:ASP:CB	2.36	0.73
1:A:899:MET:C	1:A:902:LEU:CG	2.59	0.73
1:A:159:GLU:HG2	1:A:194:LEU:HD21	1.69	0.73
4:P:20:DG:H2"	4:P:21:DT:OP2	1.87	0.72
1:A:559:LEU:HD21	1:A:561:THR:CB	2.19	0.72
2:C:355:GLN:HE21	2:C:355:GLN:HA	1.54	0.72
1:A:559:LEU:CG	1:A:561:THR:HB	2.19	0.72
3:D:30:ILE:HD11	3:D:106:PHE:HB3	1.71	0.71
1:A:198:ALA:HB2	1:A:256:ALA:HB1	1.72	0.71
3:D:107:MET:HE2	3:D:121:THR:HG21	1.72	0.71
2:C:351:ASP:HB3	2:C:354:SER:CB	2.19	0.71
2:C:271:ALA:HB1	2:C:321:VAL:HG11	1.73	0.71
1:A:21:LEU:HD13	1:A:204:PHE:HB3	1.71	0.71
2:B:254:LYS:HE3	2:B:313:ALA:HB3	1.73	0.71
1:A:564:ILE:HG23	1:A:785:ALA:HB1	1.73	0.70
2:B:283:LEU:HG	2:B:290:LEU:HD11	1.73	0.70
1:A:899:MET:HA	1:A:902:LEU:CG	2.21	0.70
1:A:559:LEU:HD13	1:A:562:LEU:N	2.03	0.70
1:A:559:LEU:CD1	1:A:561:THR:C	2.64	0.69
3:D:79:PHE:CZ	3:D:110:GLU:HB3	2.27	0.69
2:B:47:THR:HG22	2:B:116:PHE:CZ	2.27	0.69
1:A:559:LEU:HD21	1:A:561:THR:HB	1.75	0.69
2:C:130:LEU:HD11	2:C:135:MET:HE2	1.75	0.69
1:A:559:LEU:HD21	1:A:561:THR:OG1	1.92	0.68
1:A:559:LEU:HD11	1:A:561:THR:C	2.19	0.68
1:A:784:ALA:HB1	1:A:823:PHE:HB3	1.75	0.68
1:A:559:LEU:HD13	1:A:561:THR:N	2.09	0.68
1:A:907:LYS:NZ	2:C:149:GLN:O	2.22	0.68
1:A:711:ALA:HB1	1:A:719:GLU:HB3	1.77	0.67
2:B:30:LEU:HG	2:B:47:THR:HG23	1.77	0.67
1:A:559:LEU:HD13	1:A:561:THR:CA	2.25	0.67
1:A:778:TYR:N	1:A:779:PRO:HD3	2.09	0.67
3:D:36:VAL:HG12	3:D:168:ALA:HB1	1.76	0.66
1:A:778:TYR:N	1:A:779:PRO:CD	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ILE:O	2:C:303:GLU:HA	1.95	0.66
3:D:53:LYS:CE	3:D:78:THR:HG22	2.26	0.66
1:A:13:SER:N	1:A:43:ASP:OD1	2.27	0.66
1:A:776:ALA:O	1:A:779:PRO:CD	2.42	0.66
1:A:894:HIS:C	1:A:898:LEU:HD21	2.20	0.66
2:C:157:GLY:CA	2:C:195:VAL:O	2.43	0.66
1:A:559:LEU:CD2	1:A:561:THR:HB	2.26	0.66
6:F:29:GLU:OE2	6:F:60:ARG:HB2	1.96	0.66
2:C:27:LEU:HD22	2:C:29:ILE:HG12	1.78	0.66
2:C:212:ASN:CG	2:C:213:PRO:HD2	2.21	0.66
3:D:58:VAL:HG23	3:D:70:ASP:OD1	1.95	0.65
2:C:197:ARG:NH1	4:P:7:DG:OP1	2.28	0.65
1:A:359:GLY:O	1:A:362:ARG:NH1	2.28	0.65
2:C:17:VAL:HG22	2:C:53:MET:HG3	1.79	0.65
6:F:28:LYS:HE3	6:F:37:ALA:HB2	1.78	0.65
3:D:17:GLY:HA2	3:D:62:ALA:HB2	1.78	0.65
2:C:147:ALA:HB3	2:C:156:ASN:HD21	1.62	0.65
1:A:898:LEU:H	1:A:898:LEU:HD22	1.61	0.65
2:C:263:LEU:HD12	2:C:306:LEU:HD11	1.78	0.65
6:F:26:ALA:HB2	6:F:59:HIS:HB3	1.77	0.65
2:C:29:ILE:HG23	2:C:111:LEU:HD23	1.79	0.65
3:D:61:GLU:O	3:D:65:VAL:HG23	1.97	0.65
2:B:273:LEU:HD13	2:C:78:ILE:HD11	1.77	0.64
1:A:899:MET:HA	1:A:902:LEU:CD2	2.27	0.64
1:A:431:ILE:HD13	1:A:433:PHE:HE1	1.59	0.64
1:A:431:ILE:HG12	1:A:433:PHE:CG	2.33	0.63
2:B:18:SER:CA	2:B:21:LEU:HD13	2.28	0.63
1:A:782:PHE:O	1:A:785:ALA:N	2.31	0.63
3:D:18:MET:HE1	4:P:20:DG:N2	2.13	0.63
1:A:100:LEU:HG	1:A:124:LEU:HD23	1.81	0.63
3:D:54:PRO:CG	3:D:74:LEU:HD23	2.28	0.63
1:A:673:LEU:HD22	1:A:693:ILE:HG23	1.81	0.63
3:D:33:ILE:HD11	3:D:52:LEU:HG	1.80	0.63
1:A:132:SER:HB3	1:A:168:LEU:HD23	1.79	0.62
3:D:79:PHE:CE2	3:D:110:GLU:HB3	2.35	0.62
2:C:158:MET:HE2	2:C:160:PHE:CZ	2.33	0.62
2:B:18:SER:C	2:B:21:LEU:CD1	2.64	0.62
1:A:781:GLU:N	1:A:781:GLU:OE1	2.30	0.62
2:C:150:ASP:CG	2:C:155:LEU:HD12	2.25	0.62
2:C:347:VAL:O	2:C:360:VAL:HA	2.00	0.62
3:D:95:LEU:HD13	3:D:107:MET:HE1	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:9:DC:H2'	5:T:10:DC:C6	2.35	0.61
1:A:164:ASP:O	1:A:266:ARG:NH2	2.34	0.61
2:B:78:ILE:HD11	2:C:273:LEU:CD1	2.31	0.61
2:B:177:LEU:HD21	2:B:179:VAL:HG23	1.83	0.61
1:A:912:HIS:O	1:A:916:GLU:OE1	2.19	0.61
2:B:128:PHE:CE2	2:B:216:VAL:HG13	2.36	0.61
1:A:606:THR:HG21	1:A:803:GLU:OE2	2.00	0.61
2:C:159:LEU:HD23	2:C:170:VAL:HG13	1.81	0.60
2:B:159:LEU:HD23	2:B:170:VAL:HG13	1.81	0.60
2:B:335:ASN:HB2	2:B:352:ALA:HB3	1.83	0.60
2:C:33:LEU:HD12	2:C:70:VAL:HG23	1.83	0.60
1:A:431:ILE:CD1	1:A:433:PHE:CD1	2.85	0.60
1:A:321:TYR:CD2	1:A:382:LEU:HD12	2.37	0.59
3:D:12:ASP:O	3:D:164:ALA:HB2	2.02	0.59
3:D:53:LYS:HE3	3:D:78:THR:HG22	1.84	0.59
1:A:85:THR:HB	1:A:131:LEU:HD12	1.84	0.59
1:A:432:THR:OG1	1:A:511:HIS:O	2.20	0.59
1:A:54:TYR:OH	1:A:269:VAL:O	2.18	0.59
2:C:39:ASP:CG	2:C:40:GLY:H	2.10	0.59
1:A:28:VAL:HG11	1:A:56:ALA:HB1	1.85	0.59
1:A:777:HIS:N	1:A:779:PRO:HD3	2.18	0.59
1:A:431:ILE:CG1	1:A:433:PHE:CE1	2.85	0.59
1:A:463:ILE:CG2	1:A:469:MET:HG2	2.33	0.58
1:A:899:MET:HG2	1:A:902:LEU:HD11	1.86	0.58
3:D:145:LEU:HD12	3:D:145:LEU:C	2.29	0.58
1:A:58:HIS:CE1	3:D:235:LYS:HB3	2.38	0.58
1:A:803:GLU:O	1:A:806:ARG:HG2	2.03	0.58
1:A:899:MET:CA	1:A:902:LEU:CG	2.81	0.58
3:D:145:LEU:HD11	3:D:162:HIS:CE1	2.39	0.58
1:A:564:ILE:HD11	1:A:789:ALA:HB2	1.85	0.58
6:F:29:GLU:HB3	6:F:64:VAL:HG22	1.84	0.58
1:A:899:MET:CA	1:A:902:LEU:CD2	2.82	0.57
1:A:6:PHE:CE1	1:A:260:THR:HG21	2.40	0.57
1:A:335:MET:HE1	1:A:397:VAL:HA	1.86	0.57
1:A:337:PHE:CZ	1:A:400:PRO:HB3	2.39	0.57
1:A:429:GLN:O	1:A:539:THR:HG23	2.04	0.57
1:A:901:SER:CB	1:A:904:ASP:OD1	2.52	0.57
2:B:18:SER:CA	2:B:21:LEU:CD1	2.82	0.57
1:A:9:LEU:HD11	1:A:260:THR:HA	1.85	0.57
1:A:862:LEU:HD11	1:A:905:ALA:CB	2.35	0.57
1:A:14:ASP:OD2	1:A:22:ALA:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:PRO:O	2:C:17:VAL:HG23	2.03	0.57
2:B:338:MET:HE3	2:B:349:ILE:HG12	1.85	0.57
1:A:431:ILE:CG1	1:A:433:PHE:CD1	2.87	0.57
1:A:869:THR:HG23	1:A:874:LEU:HD11	1.87	0.57
6:F:25:VAL:HG11	6:F:56:LEU:CD1	2.35	0.57
1:A:14:ASP:O	1:A:216:ARG:NH2	2.38	0.57
2:B:90:VAL:HG13	2:B:99:VAL:HG22	1.87	0.57
6:F:44:GLN:HB3	6:F:48:LEU:HD11	1.86	0.57
1:A:898:LEU:HD22	1:A:898:LEU:N	2.19	0.57
1:A:899:MET:CG	1:A:902:LEU:HD11	2.35	0.57
1:A:848:ALA:HB2	1:A:873:LYS:HG2	1.87	0.56
1:A:784:ALA:O	1:A:788:THR:HG23	2.05	0.56
2:B:155:LEU:HD22	2:B:172:THR:CG2	2.36	0.56
3:D:83:ALA:HB1	3:D:114:LEU:HD11	1.87	0.56
6:F:54:GLU:OE2	6:F:55:ARG:NH1	2.33	0.56
3:D:163:GLY:O	3:D:167:ASP:HB2	2.06	0.56
1:A:676:VAL:HG11	1:A:693:ILE:HG13	1.87	0.56
3:D:107:MET:CE	3:D:121:THR:HG21	2.34	0.56
3:D:145:LEU:HD12	3:D:146:ASP:CA	2.35	0.56
1:A:25:ALA:HB3	1:A:26:PRO:HD3	1.88	0.56
1:A:431:ILE:HG12	1:A:433:PHE:CE1	2.40	0.56
1:A:104:ALA:HB2	1:A:116:ILE:CG2	2.36	0.56
1:A:172:ARG:NH1	1:A:249:LEU:O	2.36	0.56
2:B:5:VAL:HG23	2:B:88:ILE:CG1	2.36	0.56
1:A:516:VAL:HG23	1:A:552:VAL:O	2.05	0.55
1:A:21:LEU:HD22	1:A:204:PHE:HA	1.88	0.55
3:D:108:ASP:HB3	3:D:120:LYS:HG2	1.89	0.55
2:C:158:MET:HE3	2:C:169:THR:HB	1.88	0.55
2:B:33:LEU:HD12	2:B:75:PHE:HD2	1.71	0.55
2:B:283:LEU:HG	2:B:290:LEU:HD21	1.88	0.55
2:C:35:LEU:HD13	2:C:70:VAL:HG22	1.87	0.55
2:B:11:LEU:HD11	2:B:80:ARG:HA	1.89	0.55
2:B:23:GLY:O	2:B:24:ARG:C	2.49	0.55
3:D:217:ALA:HA	3:D:221:GLU:OE1	2.06	0.55
1:A:623:LEU:HD23	1:A:634:LEU:HD21	1.88	0.55
1:A:776:ALA:C	1:A:779:PRO:CG	2.79	0.55
2:B:170:VAL:CG2	2:B:179:VAL:HG22	2.37	0.55
2:C:128:PHE:CE2	2:C:216:VAL:HG13	2.42	0.55
1:A:782:PHE:CZ	1:A:786:VAL:HG21	2.37	0.55
2:B:14:LEU:CD2	2:B:79:CYS:HB2	2.37	0.55
3:D:35:ALA:HB1	3:D:89:TYR:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG21	1:A:263:ILE:HD12	1.89	0.55
2:C:159:LEU:HD23	2:C:170:VAL:CG1	2.37	0.54
3:D:53:LYS:HE2	3:D:78:THR:HG22	1.88	0.54
1:A:631:MET:HA	1:A:634:LEU:HD12	1.89	0.54
3:D:145:LEU:HD11	3:D:162:HIS:NE2	2.22	0.54
1:A:9:LEU:HA	1:A:40:ALA:HB3	1.89	0.54
1:A:559:LEU:CD2	1:A:561:THR:CB	2.83	0.54
2:B:41:THR:HG21	2:B:56:ARG:HG3	1.89	0.54
2:B:170:VAL:HB	2:B:179:VAL:HG22	1.88	0.54
2:C:39:ASP:OD1	2:C:40:GLY:N	2.41	0.54
3:D:63:PHE:O	3:D:67:GLY:CA	2.55	0.54
1:A:642:PRO:HA	1:A:647:MET:HE3	1.90	0.54
1:A:889:ASP:OD1	1:A:895:ARG:NH2	2.41	0.54
1:A:894:HIS:CD2	1:A:897:ALA:HB3	2.43	0.54
1:A:923:LEU:HD23	1:A:923:LEU:N	2.22	0.54
3:D:41:ARG:HB3	3:D:176:LEU:CD2	2.35	0.54
1:A:363:GLY:HA3	1:A:403:ASP:CG	2.33	0.54
1:A:742:MET:HE3	1:A:742:MET:HA	1.90	0.54
2:B:172:THR:HB	2:B:177:LEU:HD12	1.89	0.54
3:D:165:LEU:HD12	3:D:165:LEU:O	2.07	0.54
1:A:36:MET:HE1	1:A:240:MET:HE2	1.90	0.54
1:A:431:ILE:CG2	1:A:433:PHE:CZ	2.75	0.54
2:B:159:LEU:HD23	2:B:170:VAL:CG1	2.38	0.54
2:C:39:ASP:CG	2:C:40:GLY:N	2.65	0.54
3:D:54:PRO:HG3	3:D:74:LEU:HD23	1.89	0.53
1:A:573:ASN:O	1:A:576:ARG:HB3	2.07	0.53
1:A:894:HIS:N	1:A:898:LEU:HD21	2.23	0.53
2:C:139:ILE:HD11	2:C:203:LEU:HD13	1.89	0.53
1:A:518:ALA:HB1	1:A:519:PRO:HD2	1.90	0.53
1:A:617:LYS:HA	1:A:620:ILE:HD12	1.91	0.53
1:A:927:LEU:HD12	1:A:927:LEU:N	2.23	0.53
2:C:6:GLU:OE2	2:C:60:VAL:HG12	2.09	0.53
1:A:515:VAL:HG13	1:A:554:PHE:CD1	2.44	0.53
1:A:131:LEU:HD13	1:A:169:GLU:HB2	1.90	0.53
1:A:159:GLU:OE2	1:A:194:LEU:HD11	2.09	0.53
3:D:163:GLY:O	3:D:167:ASP:OD2	2.24	0.53
1:A:104:ALA:HB2	1:A:116:ILE:HG22	1.91	0.53
1:A:846:ILE:HA	1:A:849:ILE:HD12	1.91	0.53
2:B:10:LEU:O	2:B:14:LEU:HB2	2.09	0.53
1:A:361:GLY:N	1:A:405:ASP:OD1	2.41	0.53
1:A:572:ILE:O	1:A:575:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:VAL:HG13	1:A:692:GLN:NE2	2.23	0.53
1:A:920:GLN:HE21	1:A:920:GLN:CA	2.21	0.53
2:C:138:LEU:HD12	2:C:180:CYS:SG	2.49	0.53
2:B:155:LEU:HD22	2:B:172:THR:HG23	1.91	0.53
2:B:130:LEU:HD11	2:B:135:MET:HE2	1.90	0.52
2:C:132:GLN:NE2	2:C:227:VAL:HG11	2.24	0.52
2:B:32:ASN:CB	2:B:69:THR:HG22	2.39	0.52
2:B:128:PHE:CE1	2:B:216:VAL:HG22	2.45	0.52
6:F:23:ALA:HB2	6:F:59:HIS:CE1	2.44	0.52
1:A:281:PHE:CE2	1:A:422:TYR:CE2	2.97	0.52
2:B:158:MET:HG3	2:B:171:ALA:HB2	1.90	0.52
1:A:776:ALA:O	1:A:779:PRO:HD2	2.07	0.52
6:F:18:VAL:CG1	6:F:48:LEU:HD13	2.40	0.52
3:D:33:ILE:N	3:D:33:ILE:HD12	2.25	0.52
1:A:798:VAL:O	1:A:801:VAL:HG22	2.09	0.52
2:C:271:ALA:HB2	2:C:321:VAL:HG21	1.92	0.52
1:A:425:ASP:O	1:A:522:ILE:HG22	2.10	0.52
1:A:695:GLN:HA	1:A:700:TYR:HB2	1.91	0.52
1:A:920:GLN:HE21	1:A:920:GLN:HA	1.73	0.52
2:C:147:ALA:HB3	2:C:156:ASN:ND2	2.25	0.52
2:C:256:LEU:O	2:C:338:MET:N	2.43	0.52
5:T:12:DT:C2'	5:T:13:DC:C5	2.88	0.52
1:A:564:ILE:HD11	1:A:789:ALA:CB	2.41	0.51
1:A:673:LEU:HD21	1:A:697:LEU:HD23	1.92	0.51
2:B:242:PRO:CG	3:D:187:LEU:HD22	2.40	0.51
3:D:62:ALA:C	3:D:66:HIS:CE1	2.88	0.51
3:D:176:LEU:O	3:D:180:GLY:CA	2.57	0.51
1:A:343:ILE:HG23	1:A:422:TYR:OH	2.11	0.51
2:B:242:PRO:HG3	3:D:187:LEU:HD22	1.91	0.51
2:C:17:VAL:HG22	2:C:53:MET:CG	2.39	0.51
2:B:34:LEU:O	2:B:44:LEU:HA	2.11	0.51
3:D:62:ALA:O	3:D:66:HIS:ND1	2.42	0.51
2:C:48:ASP:HB3	2:C:51:MET:HE3	1.91	0.51
3:D:63:PHE:O	3:D:67:GLY:HA2	2.10	0.51
3:D:161:LEU:HD11	3:D:165:LEU:HD23	1.92	0.51
6:F:18:VAL:HG11	6:F:48:LEU:HB2	1.92	0.51
1:A:182:LEU:CD2	3:D:206:VAL:HG21	2.33	0.51
2:B:364:MET:SD	3:D:182:GLN:NE2	2.84	0.51
3:D:163:GLY:CA	3:D:167:ASP:OD2	2.59	0.51
1:A:381:PRO:HA	1:A:386:LEU:HD12	1.93	0.51
1:A:262:GLU:HG3	3:D:216:PHE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:GLN:HB2	2:C:53:MET:HE2	1.93	0.51
1:A:86:VAL:HG13	1:A:130:LEU:CD2	2.41	0.50
1:A:463:ILE:CD1	1:A:481:LEU:HD21	2.41	0.50
2:C:176:ARG:HB3	2:C:323:TYR:CD2	2.46	0.50
3:D:58:VAL:HG23	3:D:70:ASP:CG	2.36	0.50
3:D:108:ASP:HB3	3:D:120:LYS:CG	2.41	0.50
1:A:429:GLN:HB3	1:A:512:ALA:CB	2.41	0.50
3:D:11:LEU:O	3:D:97:ILE:HG23	2.11	0.50
2:B:78:ILE:HD11	2:C:273:LEU:HD13	1.93	0.50
2:C:129:THR:HG22	2:C:215:ARG:HB2	1.93	0.50
2:C:176:ARG:HA	2:C:361:VAL:HG12	1.94	0.50
6:F:19:ASP:HA	6:F:55:ARG:HG2	1.93	0.50
1:A:902:LEU:HD23	1:A:902:LEU:N	2.26	0.50
3:D:52:LEU:HD21	3:D:82:VAL:CG2	2.41	0.50
3:D:58:VAL:HG21	3:D:69:ALA:HA	1.94	0.50
1:A:225:LEU:O	1:A:230:ARG:NH1	2.45	0.50
3:D:53:LYS:HB2	3:D:78:THR:HA	1.94	0.50
1:A:804:CYS:HB3	1:A:811:ILE:HD11	1.93	0.50
1:A:559:LEU:HD13	1:A:559:LEU:C	2.37	0.50
1:A:801:VAL:O	1:A:805:TRP:HD1	1.94	0.50
2:C:158:MET:HE3	2:C:169:THR:CB	2.42	0.50
6:F:25:VAL:CG2	6:F:40:VAL:HG11	2.42	0.50
3:D:107:MET:HE2	3:D:121:THR:CG2	2.41	0.50
1:A:782:PHE:HE2	1:A:786:VAL:HG22	1.63	0.50
2:B:32:ASN:HB2	2:B:69:THR:HG22	1.94	0.50
1:A:37:PRO:HB2	3:D:241:TRP:HB2	1.92	0.49
3:D:229:LEU:HD22	3:D:239:CYS:SG	2.51	0.49
1:A:452:PRO:O	1:A:456:VAL:HG13	2.11	0.49
2:C:16:GLN:CB	2:C:53:MET:HE2	2.42	0.49
2:C:150:ASP:N	2:C:156:ASN:OD1	2.40	0.49
1:A:16:SER:HB3	1:A:44:PHE:HB3	1.95	0.49
1:A:337:PHE:N	1:A:338:PRO:CD	2.75	0.49
1:A:24:THR:HA	1:A:27:LEU:HD12	1.94	0.49
2:C:321:VAL:HG22	2:C:325:LEU:HD22	1.95	0.49
3:D:71:GLU:OE2	6:F:63:SER:N	2.45	0.49
1:A:96:ASN:ND2	1:A:126:GLU:O	2.45	0.49
1:A:673:LEU:CD2	1:A:693:ILE:HG23	2.42	0.49
1:A:830:GLU:O	1:A:831:ILE:HD13	2.13	0.49
1:A:561:THR:O	1:A:564:ILE:HB	2.13	0.49
1:A:196:VAL:O	1:A:259:ASN:ND2	2.33	0.49
3:D:43:LEU:HD13	3:D:169:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:MET:HB3	3:D:121:THR:OG1	2.12	0.49
1:A:86:VAL:HG13	1:A:130:LEU:HD23	1.94	0.49
1:A:926:VAL:O	1:A:926:VAL:HG13	2.13	0.49
3:D:228:ARG:CZ	3:D:231:LEU:HD23	2.43	0.49
4:P:19:DA:H4'	4:P:20:DG:OP2	2.13	0.48
2:C:139:ILE:HD12	2:C:207:LEU:CD2	2.44	0.48
5:T:13:DC:H2''	5:T:14:DG:C8	2.48	0.48
1:A:360:PRO:HG3	1:A:559:LEU:HB3	1.94	0.48
1:A:796:LYS:O	1:A:800:LEU:HG	2.14	0.48
2:C:159:LEU:O	2:C:169:THR:HA	2.14	0.48
2:C:284:TYR:O	2:C:290:LEU:HD12	2.13	0.48
1:A:189:ALA:CB	3:D:212:LEU:HD22	2.44	0.48
1:A:471:LEU:HD12	1:A:499:ARG:HA	1.95	0.48
1:A:564:ILE:HG23	1:A:785:ALA:CB	2.43	0.48
2:B:283:LEU:CG	2:B:290:LEU:HD21	2.43	0.48
2:C:54:VAL:O	2:C:231:ILE:HB	2.14	0.48
2:B:303:GLU:N	2:C:105:ARG:O	2.46	0.48
3:D:185:LEU:O	3:D:187:LEU:N	2.46	0.48
1:A:21:LEU:HD23	1:A:21:LEU:C	2.38	0.48
6:F:33:MET:HB3	6:F:34:PRO:HD2	1.96	0.48
2:B:122:TRP:CZ2	2:B:224:ARG:HB2	2.49	0.48
3:D:105:GLY:O	3:D:109:TYR:HB2	2.13	0.48
2:C:158:MET:C	2:C:194:ILE:HG23	2.39	0.47
1:A:775:LYS:HA	1:A:782:PHE:CD1	2.49	0.47
2:C:271:ALA:CB	2:C:321:VAL:HG11	2.42	0.47
3:D:145:LEU:O	3:D:149:CYS:HB2	2.14	0.47
1:A:870:ASP:OD2	1:A:872:LYS:HB2	2.14	0.47
1:A:483:GLU:OE1	3:D:21:ILE:HD12	2.15	0.47
1:A:817:ASN:HD21	1:A:891:LEU:HD11	1.80	0.47
2:B:128:PHE:CZ	2:B:216:VAL:HG13	2.48	0.47
1:A:318:ARG:NH1	1:A:322:ASP:OD2	2.48	0.47
2:B:14:LEU:HD21	2:B:79:CYS:SG	2.54	0.47
2:C:150:ASP:H	2:C:156:ASN:CG	2.22	0.47
2:B:362:MET:HE2	3:D:185:LEU:CD2	2.44	0.47
1:A:21:LEU:CD1	1:A:209:ASP:HB3	2.45	0.47
1:A:576:ARG:O	1:A:580:GLY:N	2.47	0.47
2:C:194:ILE:HD11	2:C:241:PHE:HB2	1.97	0.47
6:F:18:VAL:HG11	6:F:48:LEU:HD13	1.97	0.47
1:A:109:TYR:HB3	1:A:114:PRO:HA	1.97	0.47
1:A:559:LEU:HD22	1:A:561:THR:H	1.79	0.47
2:B:3:PHE:CE1	2:B:90:VAL:HB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:GLY:HA2	3:D:185:LEU:HD12	1.97	0.46
3:D:52:LEU:HA	3:D:77:PRO:O	2.16	0.46
2:B:78:ILE:HD11	2:C:273:LEU:HD11	1.97	0.46
3:D:36:VAL:CG1	3:D:168:ALA:HB1	2.42	0.46
1:A:922:ASP:O	2:C:362:MET:HE2	2.16	0.46
2:B:362:MET:HE2	3:D:185:LEU:HD23	1.97	0.46
2:C:150:ASP:O	2:C:156:ASN:OD1	2.33	0.46
1:A:105:TYR:CE1	1:A:114:PRO:HG3	2.50	0.46
1:A:357:PRO:HG2	1:A:566:ASN:HB2	1.96	0.46
1:A:559:LEU:HD13	1:A:561:THR:C	2.39	0.46
2:B:5:VAL:HG23	2:B:88:ILE:HG12	1.98	0.46
1:A:215:ILE:HG23	1:A:448:VAL:HG11	1.98	0.46
1:A:909:ALA:O	1:A:913:ALA:HB3	2.16	0.46
2:C:281:VAL:CG2	2:C:294:ALA:HB2	2.32	0.46
3:D:14:GLU:CD	3:D:163:GLY:HA3	2.41	0.46
3:D:108:ASP:CG	3:D:120:LYS:HB3	2.41	0.46
2:C:259:GLY:O	2:C:263:LEU:HB2	2.15	0.46
2:C:279:ARG:O	2:C:319:PHE:O	2.34	0.46
1:A:609:PHE:CE2	1:A:610:GLN:NE2	2.84	0.46
1:A:757:ASN:ND2	1:A:759:SER:OG	2.49	0.46
6:F:19:ASP:HB2	6:F:51:TRP:HE1	1.80	0.46
1:A:665:ASP:HB2	1:A:747:LEU:HD13	1.98	0.45
1:A:788:THR:HG22	1:A:822:HIS:CD2	2.51	0.45
2:B:281:VAL:HG22	2:B:294:ALA:HB2	1.97	0.45
1:A:711:ALA:CB	1:A:719:GLU:HB3	2.46	0.45
2:C:20:PRO:HB2	2:C:51:MET:HE2	1.98	0.45
2:B:344:VAL:O	2:B:344:VAL:HG22	2.16	0.45
2:C:67:ALA:HB1	2:C:113:ALA:CB	2.46	0.45
3:D:210:SER:O	3:D:211:LYS:C	2.58	0.45
1:A:21:LEU:HD11	1:A:209:ASP:HB3	1.98	0.45
1:A:286:MET:HE1	1:A:294:LYS:CE	2.47	0.45
2:C:51:MET:SD	2:C:51:MET:C	2.99	0.45
3:D:10:VAL:HG13	3:D:96:VAL:O	2.15	0.45
4:P:10:DC:H2'	4:P:11:DT:H72	1.97	0.45
1:A:559:LEU:HD13	1:A:559:LEU:O	2.17	0.45
1:A:697:LEU:HD13	1:A:736:ILE:HD13	1.98	0.45
5:T:14:DG:C2'	5:T:15:DT:H72	2.46	0.45
1:A:782:PHE:CD2	1:A:786:VAL:HG23	2.50	0.45
1:A:904:ASP:OD2	1:A:904:ASP:N	2.49	0.45
2:C:179:VAL:O	2:C:357:ALA:HA	2.17	0.45
2:C:225:ALA:HB3	2:C:232:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:20:DG:H2"	5:T:21:DT:C6	2.52	0.45
6:F:25:VAL:HG22	6:F:40:VAL:HG11	1.98	0.45
1:A:561:THR:HA	1:A:564:ILE:HD12	1.99	0.45
1:A:770:GLN:O	1:A:774:LEU:HD22	2.17	0.45
1:A:65:ILE:HG23	1:A:267:CYS:CB	2.46	0.44
1:A:441:VAL:CG2	1:A:501:LEU:HB3	2.46	0.44
1:A:515:VAL:O	1:A:554:PHE:HD1	1.99	0.44
3:D:14:GLU:OE2	3:D:163:GLY:CA	2.63	0.44
3:D:33:ILE:HD13	3:D:51:TYR:HA	1.99	0.44
1:A:515:VAL:O	1:A:554:PHE:CD1	2.70	0.44
1:A:899:MET:O	1:A:902:LEU:CD1	2.63	0.44
3:D:10:VAL:HG12	3:D:11:LEU:N	2.33	0.44
1:A:913:ALA:C	1:A:916:GLU:OE1	2.61	0.44
1:A:50:LEU:HA	1:A:53:PHE:HB3	2.00	0.44
1:A:430:ILE:HD12	1:A:514:GLY:HA3	1.99	0.44
1:A:922:ASP:HA	2:C:174:GLY:O	2.18	0.44
3:D:122:ASN:HB3	3:D:127:VAL:HG21	1.99	0.44
3:D:156:ASN:HA	3:D:159:ARG:HG2	2.00	0.44
2:B:21:LEU:N	2:B:21:LEU:HD12	2.32	0.44
2:C:3:PHE:CZ	2:C:90:VAL:HB	2.53	0.44
2:C:158:MET:O	2:C:194:ILE:HA	2.17	0.44
1:A:318:ARG:N	1:A:319:PRO:HD2	2.33	0.44
3:D:107:MET:HE2	3:D:121:THR:CB	2.48	0.44
3:D:177:ALA:O	3:D:181:GLY:CA	2.65	0.44
1:A:51:VAL:HG21	1:A:545:ASP:HB3	2.00	0.44
1:A:407:CYS:SG	1:A:562:LEU:HB2	2.58	0.44
1:A:623:LEU:CD2	1:A:634:LEU:HD21	2.47	0.44
2:B:29:ILE:HD12	2:B:111:LEU:HB3	1.99	0.44
2:C:215:ARG:O	2:C:226:HIS:N	2.51	0.44
3:D:210:SER:O	3:D:212:LEU:HG	2.18	0.44
2:C:216:VAL:HA	2:C:225:ALA:HA	1.99	0.44
1:A:91:ASN:O	1:A:95:GLN:HG2	2.17	0.44
1:A:389:GLU:OE2	1:A:702:LEU:HD13	2.17	0.44
1:A:787:MET:HE3	1:A:800:LEU:HD12	2.00	0.44
1:A:894:HIS:CA	1:A:898:LEU:HD21	2.48	0.44
2:C:285:VAL:HG22	2:C:310:TYR:CD2	2.53	0.44
3:D:17:GLY:CA	3:D:62:ALA:HB2	2.47	0.44
3:D:87:MET:HE2	3:D:118:ILE:HG21	1.98	0.44
1:A:777:HIS:O	1:A:778:TYR:CD2	2.70	0.43
2:C:289:GLN:C	2:C:308:VAL:HG22	2.43	0.43
3:D:163:GLY:HA2	3:D:167:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:O	1:A:238:GLN:OE1	2.36	0.43
1:A:436:MET:SD	1:A:504:VAL:O	2.75	0.43
1:A:784:ALA:CB	1:A:823:PHE:HB3	2.45	0.43
2:B:3:PHE:HE2	2:B:88:ILE:HD11	1.83	0.43
4:P:20:DG:C8	4:P:21:DT:H73	2.53	0.43
2:B:33:LEU:HD12	2:B:75:PHE:CD2	2.51	0.43
2:C:3:PHE:CE1	2:C:90:VAL:HB	2.54	0.43
1:A:131:LEU:HA	1:A:167:PHE:O	2.19	0.43
2:C:14:LEU:HD23	2:C:79:CYS:HB2	2.01	0.43
2:C:335:ASN:O	2:C:352:ALA:HB3	2.19	0.43
1:A:314:ARG:O	1:A:318:ARG:HB2	2.19	0.43
1:A:345:MET:SD	1:A:374:LEU:HD22	2.58	0.43
1:A:459:ILE:HG23	1:A:484:ILE:HD11	2.00	0.43
2:B:34:LEU:HB3	2:B:45:THR:HB	2.00	0.43
2:B:254:LYS:HB2	2:B:340:LEU:HB2	2.00	0.43
1:A:429:GLN:O	1:A:539:THR:N	2.48	0.43
2:B:132:GLN:NE2	2:B:227:VAL:HG13	2.34	0.43
2:C:122:TRP:CE2	2:C:222:ASN:HB2	2.53	0.43
2:B:364:MET:HE3	3:D:181:GLY:O	2.19	0.43
2:C:41:THR:HG23	2:C:57:VAL:H	1.84	0.43
1:A:255:GLU:HG3	3:D:214:VAL:HG22	2.00	0.43
1:A:593:ASP:CG	1:A:777:HIS:CE1	2.96	0.43
2:C:144:PHE:CE2	2:C:326:ASP:HB3	2.53	0.43
5:T:14:DG:H2'	5:T:15:DT:H72	2.00	0.43
1:A:654:ARG:HG3	1:A:683:ILE:HD11	2.01	0.42
1:A:773:TRP:CZ2	1:A:777:HIS:CD2	3.07	0.42
1:A:894:HIS:CG	1:A:897:ALA:HB3	2.54	0.42
2:B:87:GLU:O	2:B:101:SER:HA	2.18	0.42
3:D:228:ARG:NH1	3:D:231:LEU:HD23	2.33	0.42
1:A:12:HIS:CD2	1:A:42:THR:O	2.72	0.42
2:B:108:LEU:HD12	2:C:273:LEU:HD21	2.01	0.42
2:C:158:MET:HE2	2:C:160:PHE:CE1	2.54	0.42
3:D:9:ILE:HG23	3:D:36:VAL:O	2.19	0.42
1:A:910:ASP:O	1:A:914:LYS:CB	2.67	0.42
2:C:14:LEU:HD21	2:C:79:CYS:SG	2.59	0.42
3:D:16:THR:O	3:D:28:HIS:ND1	2.51	0.42
3:D:217:ALA:CA	3:D:221:GLU:OE1	2.67	0.42
1:A:421:MET:HB3	1:A:422:TYR:CD1	2.54	0.42
1:A:894:HIS:HB2	1:A:897:ALA:HB3	2.02	0.42
3:D:54:PRO:HG2	3:D:74:LEU:HD23	2.01	0.42
1:A:662:SER:O	1:A:682:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:331:LEU:HD11	2:C:351:ASP:HB2	2.00	0.42
3:D:176:LEU:O	3:D:180:GLY:HA3	2.19	0.42
1:A:371:ALA:HA	1:A:376:ILE:HD12	2.00	0.42
1:A:427:VAL:HG22	1:A:517:ILE:HG12	2.00	0.42
1:A:452:PRO:HA	4:P:19:DA:N1	2.35	0.42
2:B:47:THR:HG22	2:B:116:PHE:CE1	2.54	0.42
1:A:400:PRO:O	1:A:401:ASP:C	2.62	0.42
2:C:30:LEU:HD21	2:C:49:LEU:CD1	2.49	0.42
2:C:148:HIS:HA	2:C:197:ARG:CZ	2.48	0.42
1:A:58:HIS:HE1	3:D:235:LYS:HB3	1.80	0.42
2:B:184:ILE:HG21	2:B:188:LEU:HD22	2.02	0.42
2:C:151:VAL:O	2:C:153:TYR:N	2.52	0.42
2:C:252:PRO:HB3	2:C:340:LEU:C	2.45	0.42
2:C:288:ASN:HA	2:C:308:VAL:O	2.19	0.42
1:A:775:LYS:HA	1:A:782:PHE:HD1	1.84	0.42
2:C:34:LEU:O	2:C:44:LEU:HA	2.20	0.42
2:C:196:PRO:O	2:C:200:VAL:HG12	2.19	0.42
1:A:90:ASN:C	1:A:90:ASN:HD22	2.28	0.42
1:A:870:ASP:OD1	1:A:873:LYS:CD	2.68	0.42
1:A:441:VAL:O	1:A:445:VAL:HG23	2.20	0.41
1:A:647:MET:HE2	1:A:751:PHE:CE1	2.55	0.41
1:A:823:PHE:CZ	1:A:833:TYR:HA	2.55	0.41
2:B:292:ILE:HD11	2:B:306:LEU:HD13	2.01	0.41
3:D:15:THR:HA	3:D:31:ILE:HG12	2.01	0.41
3:D:108:ASP:OD1	3:D:121:THR:N	2.53	0.41
1:A:668:TRP:HB3	1:A:744:ILE:HG13	2.02	0.41
1:A:869:THR:HG23	1:A:874:LEU:CD1	2.50	0.41
1:A:279:PRO:HG3	1:A:552:VAL:HG21	2.03	0.41
1:A:295:ARG:HE	1:A:345:MET:HE1	1.85	0.41
2:C:351:ASP:OD2	2:C:354:SER:HB2	2.20	0.41
3:D:83:ALA:HB2	3:D:114:LEU:HD21	2.01	0.41
5:T:5:DG:H2''	5:T:6:DA:C8	2.55	0.41
1:A:463:ILE:HD11	1:A:481:LEU:HD21	2.01	0.41
1:A:782:PHE:CD2	1:A:782:PHE:C	2.97	0.41
2:C:222:ASN:HD22	2:C:235:LYS:HG2	1.85	0.41
6:F:44:GLN:HB3	6:F:48:LEU:CD1	2.47	0.41
1:A:673:LEU:CD2	1:A:697:LEU:HD23	2.49	0.41
3:D:65:VAL:HG11	4:P:21:DT:C6	2.56	0.41
4:P:20:DG:C2'	4:P:21:DT:OP2	2.63	0.41
1:A:40:ALA:HA	1:A:65:ILE:HB	2.02	0.41
1:A:105:TYR:CZ	1:A:529:TYR:CD2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:PHE:O	1:A:755:GLY:N	2.52	0.41
1:A:875:ASN:O	1:A:878:VAL:HB	2.21	0.41
1:A:918:ILE:HG23	2:C:278:PHE:HA	2.02	0.41
2:B:283:LEU:HD11	2:B:290:LEU:HD21	2.01	0.41
2:B:362:MET:HE3	2:B:362:MET:HB2	1.84	0.41
1:A:39:LEU:HD22	1:A:40:ALA:N	2.35	0.41
1:A:431:ILE:HG23	1:A:433:PHE:CE2	2.54	0.41
1:A:593:ASP:CG	1:A:777:HIS:NE2	2.79	0.41
1:A:848:ALA:CB	1:A:873:LYS:HB3	2.51	0.41
2:B:283:LEU:CD1	2:B:290:LEU:HD21	2.51	0.41
2:B:364:MET:CG	3:D:182:GLN:HA	2.50	0.41
1:A:776:ALA:CA	1:A:779:PRO:CD	2.93	0.41
2:B:282:ARG:NH2	2:B:295:ASN:HD22	2.19	0.41
2:B:365:ARG:NH2	3:D:40:ASN:O	2.54	0.41
2:C:1:MET:HB3	2:C:92:LEU:HB3	2.03	0.41
2:C:16:GLN:HE22	2:C:205:ARG:C	2.28	0.41
3:D:122:ASN:CB	3:D:127:VAL:HG21	2.50	0.41
1:A:784:ALA:HB1	1:A:823:PHE:CB	2.49	0.41
1:A:875:ASN:HB3	1:A:878:VAL:HG23	2.02	0.41
2:B:364:MET:HG3	3:D:182:GLN:HA	2.02	0.41
2:C:256:LEU:HD22	2:C:338:MET:HB2	2.03	0.41
3:D:37:GLU:HB3	3:D:44:THR:OG1	2.21	0.41
1:A:340:TYR:CZ	1:A:344:VAL:HG21	2.56	0.40
1:A:559:LEU:CD1	1:A:561:THR:N	2.78	0.40
2:C:67:ALA:HB1	2:C:113:ALA:HB2	2.03	0.40
1:A:324:ARG:HB3	1:A:369:LEU:HD12	2.03	0.40
1:A:782:PHE:O	1:A:783:MET:C	2.64	0.40
1:A:883:ILE:HD11	1:A:895:ARG:O	2.22	0.40
3:D:19:ASN:O	3:D:24:HIS:HA	2.22	0.40
3:D:229:LEU:HD13	3:D:241:TRP:HB3	2.02	0.40
1:A:47:LEU:HB3	1:A:50:LEU:HB2	2.02	0.40
1:A:197:VAL:HA	1:A:256:ALA:HA	2.01	0.40
1:A:527:PRO:HD3	1:A:541:PHE:CZ	2.56	0.40
1:A:922:ASP:OD1	1:A:922:ASP:N	2.55	0.40
2:B:272:ILE:HD13	2:C:78:ILE:N	2.37	0.40
1:A:785:ALA:O	1:A:788:THR:OG1	2.27	0.40
1:A:911:GLN:OE1	2:C:150:ASP:HA	2.21	0.40
2:B:64:GLU:HG2	2:B:65:PRO:HD2	2.03	0.40
2:C:168:ARG:NE	2:C:244:TYR:OH	2.54	0.40
6:F:28:LYS:HE3	6:F:37:ALA:CB	2.48	0.40
1:A:344:VAL:O	1:A:348:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:HA	1:A:637:LEU:HD12	2.04	0.40
1:A:900:ASN:ND2	1:A:900:ASN:C	2.79	0.40
3:D:108:ASP:HA	3:D:120:LYS:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	925/927 (100%)	862 (93%)	59 (6%)	4 (0%)	30	67
2	B	364/366 (100%)	350 (96%)	14 (4%)	0	100	100
2	C	364/366 (100%)	342 (94%)	20 (6%)	2 (0%)	24	63
3	D	225/243 (93%)	211 (94%)	12 (5%)	2 (1%)	14	51
6	F	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	1932/1958 (99%)	1817 (94%)	107 (6%)	8 (0%)	31	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	182	GLN
3	D	186	PRO
1	A	3	GLU
1	A	576	ARG
2	C	189	PRO
2	C	363	PRO
1	A	829	GLY
1	A	337	PHE

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	765/765 (100%)	690 (90%)	75 (10%)	7	24
2	B	313/313 (100%)	265 (85%)	48 (15%)	3	12
2	C	313/313 (100%)	261 (83%)	52 (17%)	2	10
3	D	189/200 (94%)	173 (92%)	16 (8%)	10	29
6	F	47/47 (100%)	38 (81%)	9 (19%)	1	8
All	All	1627/1638 (99%)	1427 (88%)	200 (12%)	7	17

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	LEU
1	A	39	LEU
1	A	54	TYR
1	A	84	LEU
1	A	90	ASN
1	A	99	LEU
1	A	100	LEU
1	A	123	GLU
1	A	124	LEU
1	A	141	ARG
1	A	144	LEU
1	A	154	CYS
1	A	168	LEU
1	A	171	ILE
1	A	172	ARG
1	A	179	GLU
1	A	188	LEU
1	A	190	GLU
1	A	224	THR
1	A	225	LEU
1	A	249	LEU
1	A	262	GLU

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	329	LEU
1	A	342	LEU
1	A	349	GLN
1	A	351	SER
1	A	352	LYS
1	A	362	ARG
1	A	369	LEU
1	A	378	ASP
1	A	385	ASP
1	A	387	LEU
1	A	404	VAL
1	A	407	CYS
1	A	414	VAL
1	A	431	ILE
1	A	436	MET
1	A	456	VAL
1	A	481	LEU
1	A	494	LEU
1	A	497	MET
1	A	544	SER
1	A	554	PHE
1	A	557	LEU
1	A	559	LEU
1	A	578	LYS
1	A	599	MET
1	A	606	THR
1	A	614	ARG
1	A	643	LEU
1	A	658	ARG
1	A	695	GLN
1	A	697	LEU
1	A	707	MET
1	A	715	LYS
1	A	723	GLN
1	A	743	LYS
1	A	749	GLU
1	A	757	ASN
1	A	774	LEU
1	A	782	PHE
1	A	787	MET
1	A	822	HIS

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Mol	Chain	Res	Type
1	A	868	ARG
1	A	872	LYS
1	A	876	ARG
1	A	898	LEU
1	A	899	MET
1	A	900	ASN
1	A	902	LEU
1	A	920	GLN
1	A	923	LEU
1	A	926	VAL
2	B	5	VAL
2	B	11	LEU
2	B	12	LYS
2	B	14	LEU
2	B	16	GLN
2	B	21	LEU
2	B	42	LEU
2	B	64	GLU
2	B	88	ILE
2	B	97	MET
2	B	103	ARG
2	B	108	LEU
2	B	119	LEU
2	B	123	GLN
2	B	125	GLU
2	B	138	LEU
2	B	143	GLN
2	B	165	GLU
2	B	170	VAL
2	B	176	ARG
2	B	177	LEU
2	B	182	MET
2	B	188	LEU
2	B	195	VAL
2	B	200	VAL
2	B	201	ILE
2	B	204	MET
2	B	207	LEU
2	B	216	VAL
2	B	233	THR
2	B	236	LEU
2	B	237	VAL

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Mol	Chain	Res	Type
2	B	250	LYS
2	B	257	GLU
2	B	276	GLU
2	B	283	LEU
2	B	308	VAL
2	B	316	GLU
2	B	319	PHE
2	B	321	VAL
2	B	325	LEU
2	B	327	VAL
2	B	328	LEU
2	B	331	LEU
2	B	332	LYS
2	B	340	LEU
2	B	347	VAL
2	B	360	VAL
2	C	5	VAL
2	C	21	LEU
2	C	29	ILE
2	C	41	THR
2	C	42	LEU
2	C	57	VAL
2	C	64	GLU
2	C	88	ILE
2	C	103	ARG
2	C	107	SER
2	C	110	THR
2	C	118	ASN
2	C	119	LEU
2	C	123	GLN
2	C	125	GLU
2	C	126	VAL
2	C	137	ARG
2	C	138	LEU
2	C	142	THR
2	C	151	VAL
2	C	152	ARG
2	C	167	LEU
2	C	170	VAL
2	C	176	ARG
2	C	188	LEU
2	C	193	VAL

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Mol	Chain	Res	Type
2	C	195	VAL
2	C	200	VAL
2	C	203	LEU
2	C	204	MET
2	C	205	ARG
2	C	207	LEU
2	C	214	LEU
2	C	215	ARG
2	C	216	VAL
2	C	222	ASN
2	C	233	THR
2	C	236	LEU
2	C	237	VAL
2	C	240	ARG
2	C	248	LEU
2	C	276	GLU
2	C	281	VAL
2	C	315	MET
2	C	324	VAL
2	C	325	LEU
2	C	327	VAL
2	C	328	LEU
2	C	347	VAL
2	C	355	GLN
2	C	360	VAL
2	C	366	LEU
3	D	12	ASP
3	D	13	THR
3	D	43	LEU
3	D	78	THR
3	D	87	MET
3	D	103	ASP
3	D	121	THR
3	D	153	GLU
3	D	157	SER
3	D	159	ARG
3	D	162	HIS
3	D	165	LEU
3	D	189	MET
3	D	190	GLU
3	D	204	ARG
3	D	234	LYS

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Mol	Chain	Res	Type
6	F	10	GLN
6	F	13	MET
6	F	17	ASN
6	F	25	VAL
6	F	30	ARG
6	F	35	VAL
6	F	38	GLU
6	F	50	SER
6	F	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	58	HIS
1	A	90	ASN
1	A	106	GLN
1	A	125	ASN
1	A	147	ASN
1	A	161	HIS
1	A	238	GLN
1	A	417	HIS
1	A	429	GLN
1	A	566	ASN
1	A	601	GLN
1	A	656	HIS
1	A	695	GLN
1	A	737	ASN
1	A	777	HIS
1	A	822	HIS
1	A	824	HIS
1	A	894	HIS
1	A	900	ASN
1	A	912	HIS
1	A	920	GLN
2	B	132	GLN
2	B	143	GLN
2	B	191	HIS
2	B	212	ASN
2	B	217	GLN
2	B	221	ASN
2	B	222	ASN

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Mol	Chain	Res	Type
2	B	288	ASN
2	B	295	ASN
2	B	329	ASN
2	C	16	GLN
2	C	61	GLN
2	C	132	GLN
2	C	217	GLN
2	C	222	ASN
2	C	251	ASN
2	C	288	ASN
2	C	329	ASN
2	C	355	GLN
3	D	8	GLN
3	D	47	ASN
3	D	169	GLN
3	D	182	GLN
6	F	59	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

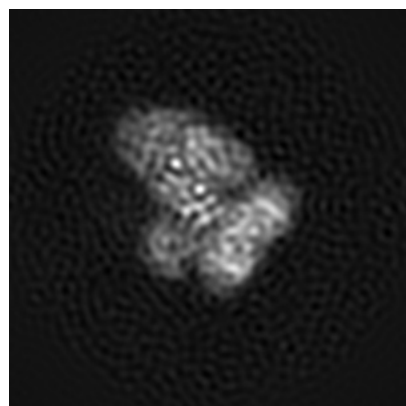
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4141. These allow visual inspection of the internal detail of the map and identification of artifacts.

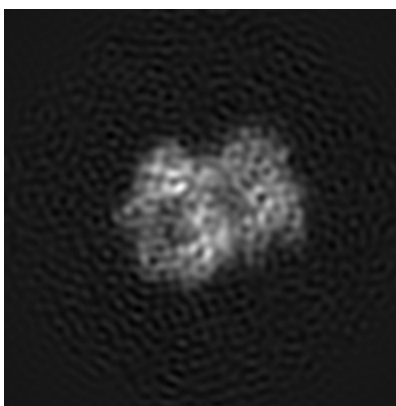
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

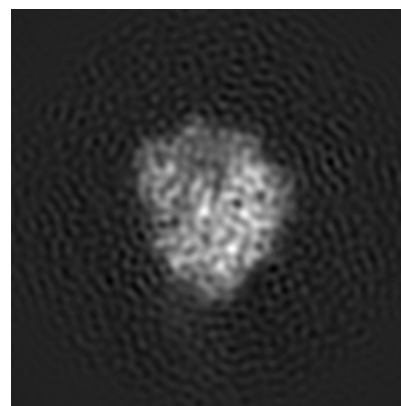
6.1.1 Primary map



X

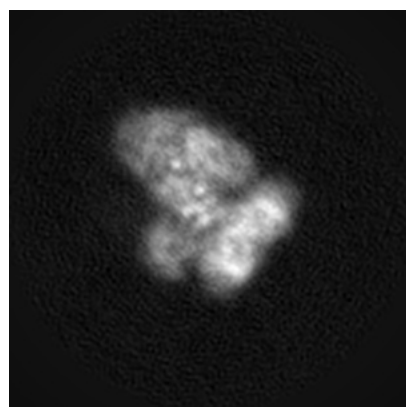


Y

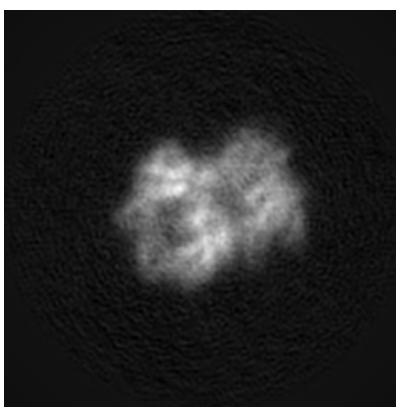


Z

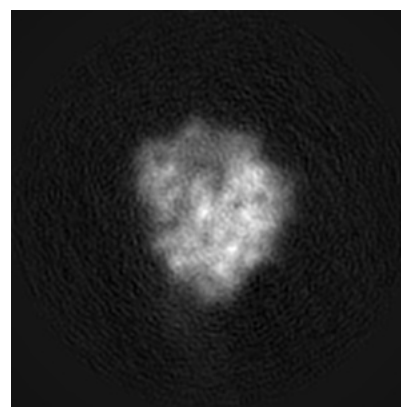
6.1.2 Raw map



X



Y

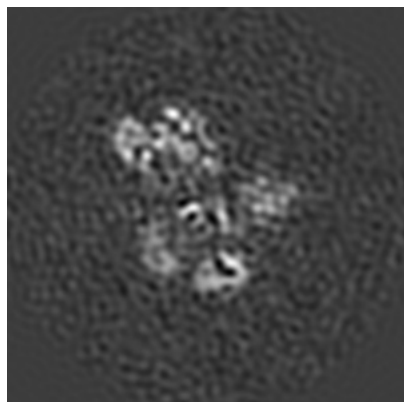


Z

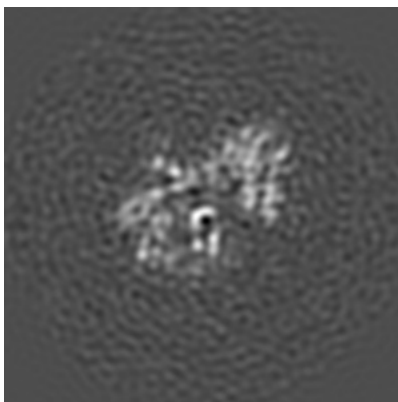
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

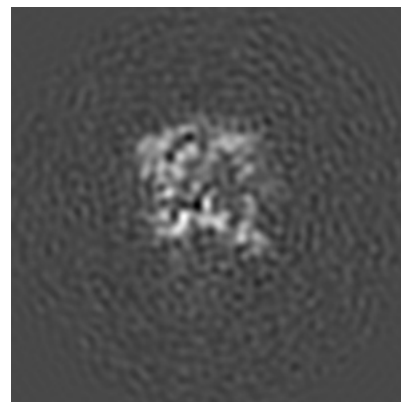
6.2.1 Primary map



X Index: 70

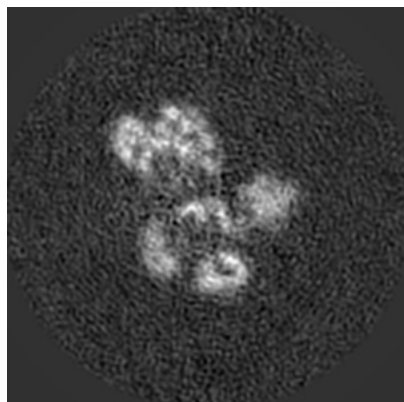


Y Index: 70

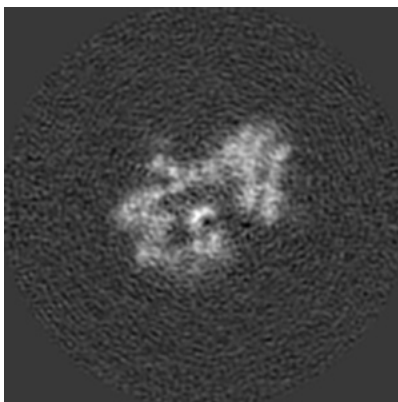


Z Index: 70

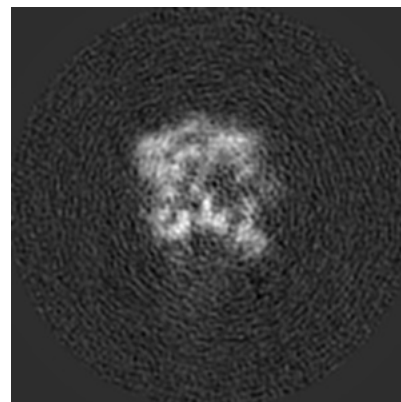
6.2.2 Raw map



X Index: 70



Y Index: 70

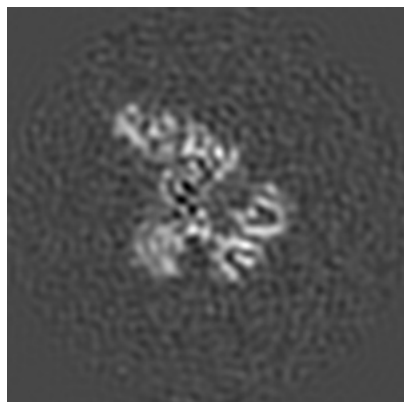


Z Index: 70

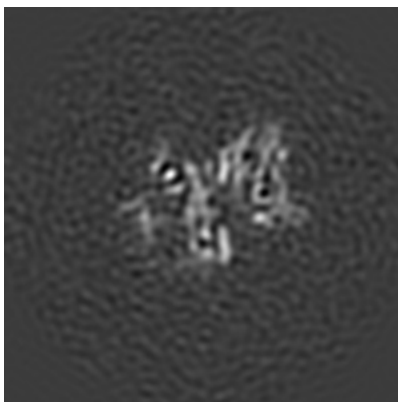
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

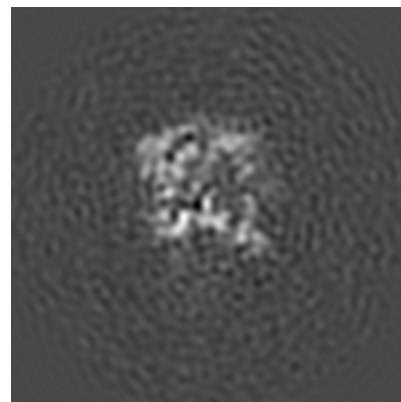
6.3.1 Primary map



X Index: 77

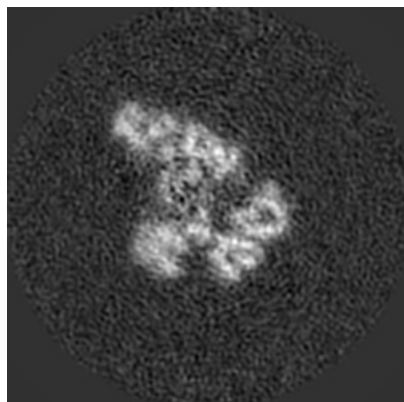


Y Index: 67

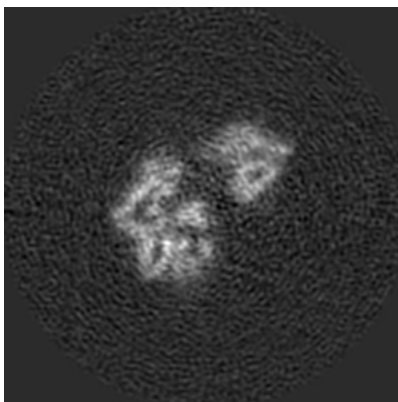


Z Index: 70

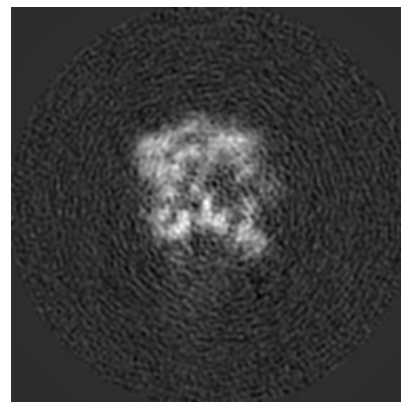
6.3.2 Raw map



X Index: 77



Y Index: 75

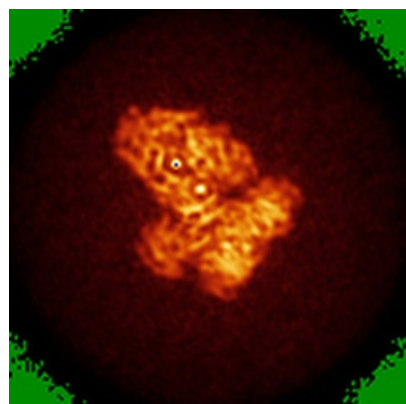


Z Index: 70

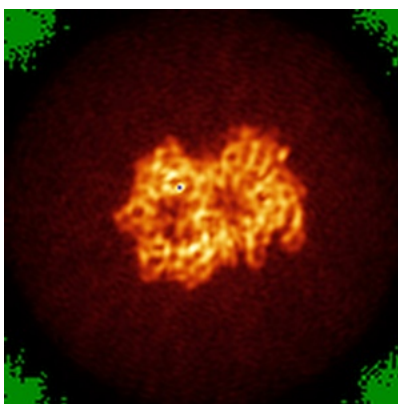
The images above show the largest variance slices of the map in three orthogonal directions.

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

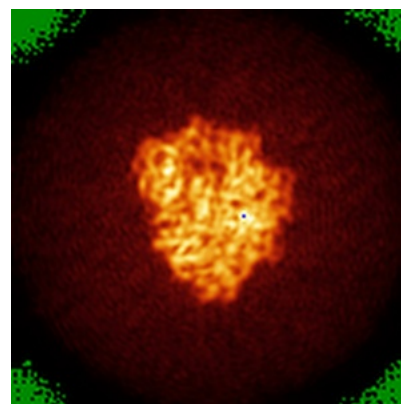
6.4.1 Primary map



X

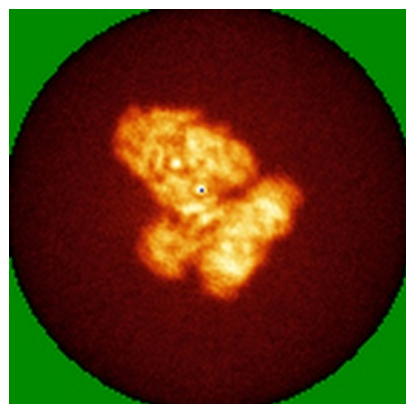


Y

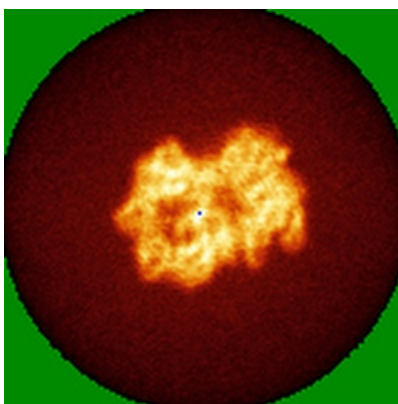


Z

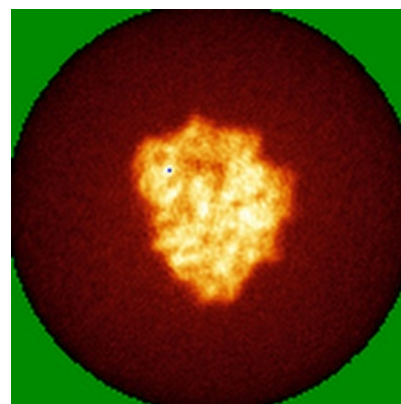
6.4.2 Raw map



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](#)

This section was not generated.

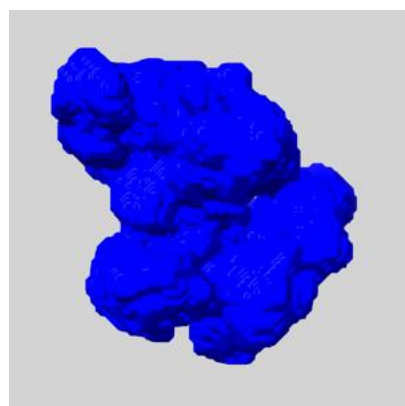
6.6 Mask visualisation [i](#)

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

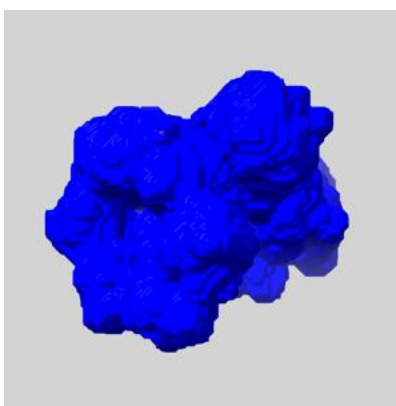
A mask typically either:

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

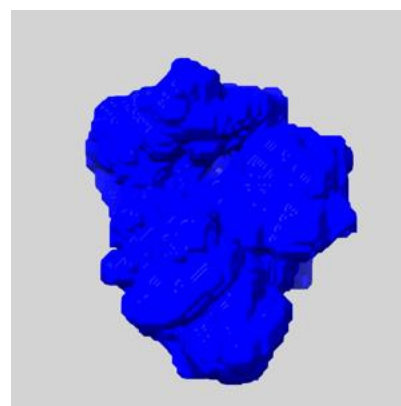
6.6.1 emd_4141_msk_1.map [i](#)



X



Y

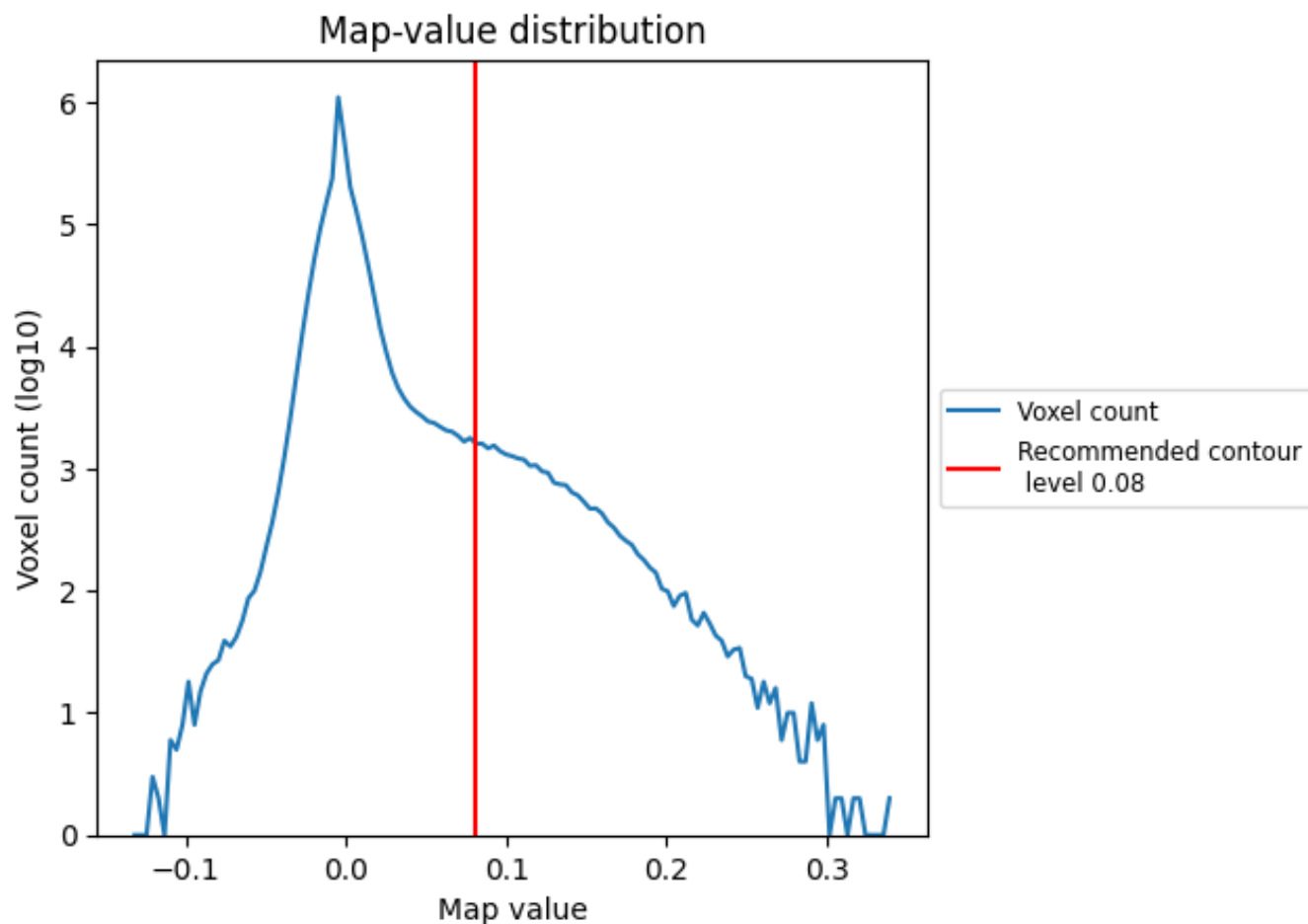


Z

7 Map analysis [i](#)

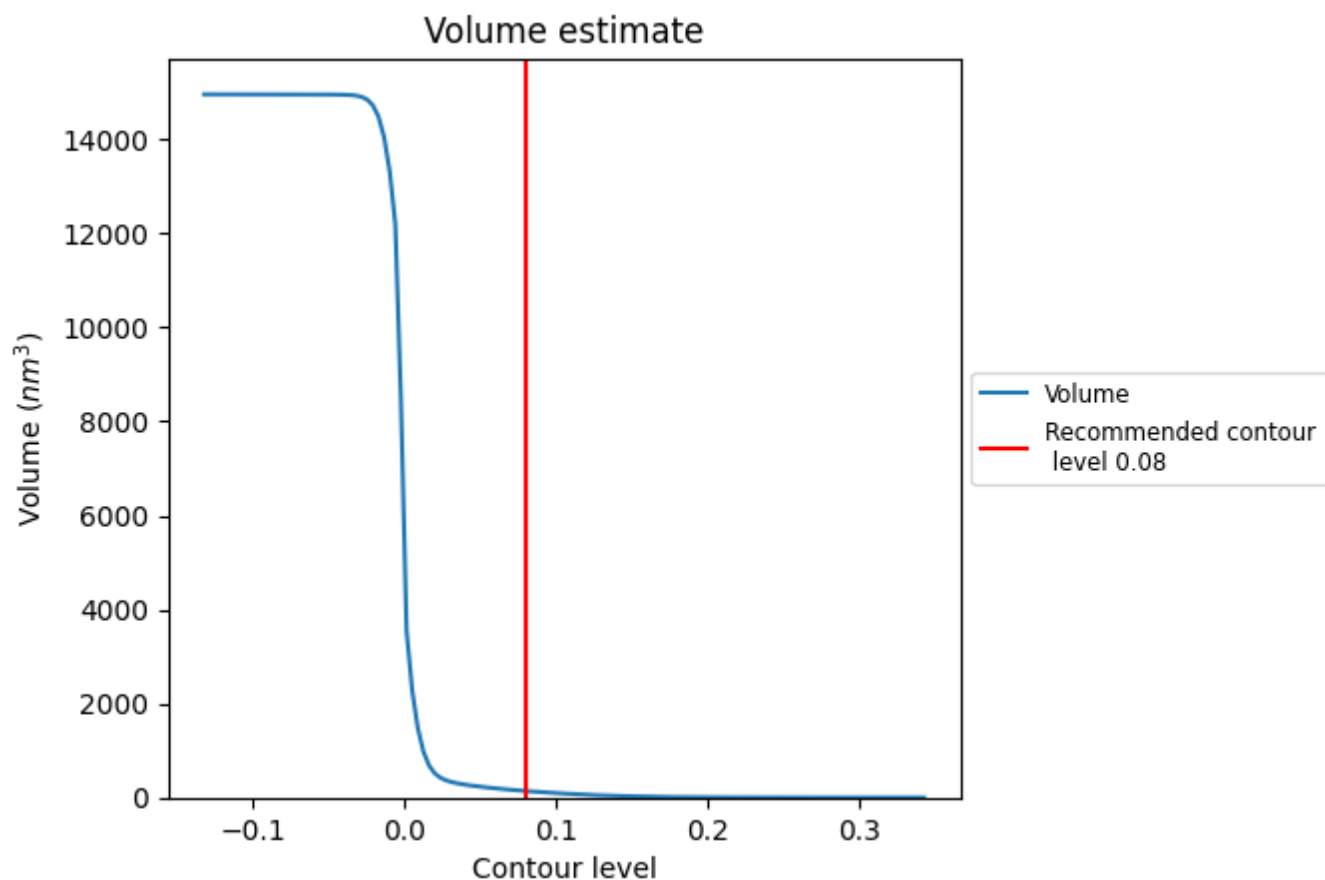
This section contains the results of statistical analysis of the map.

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.

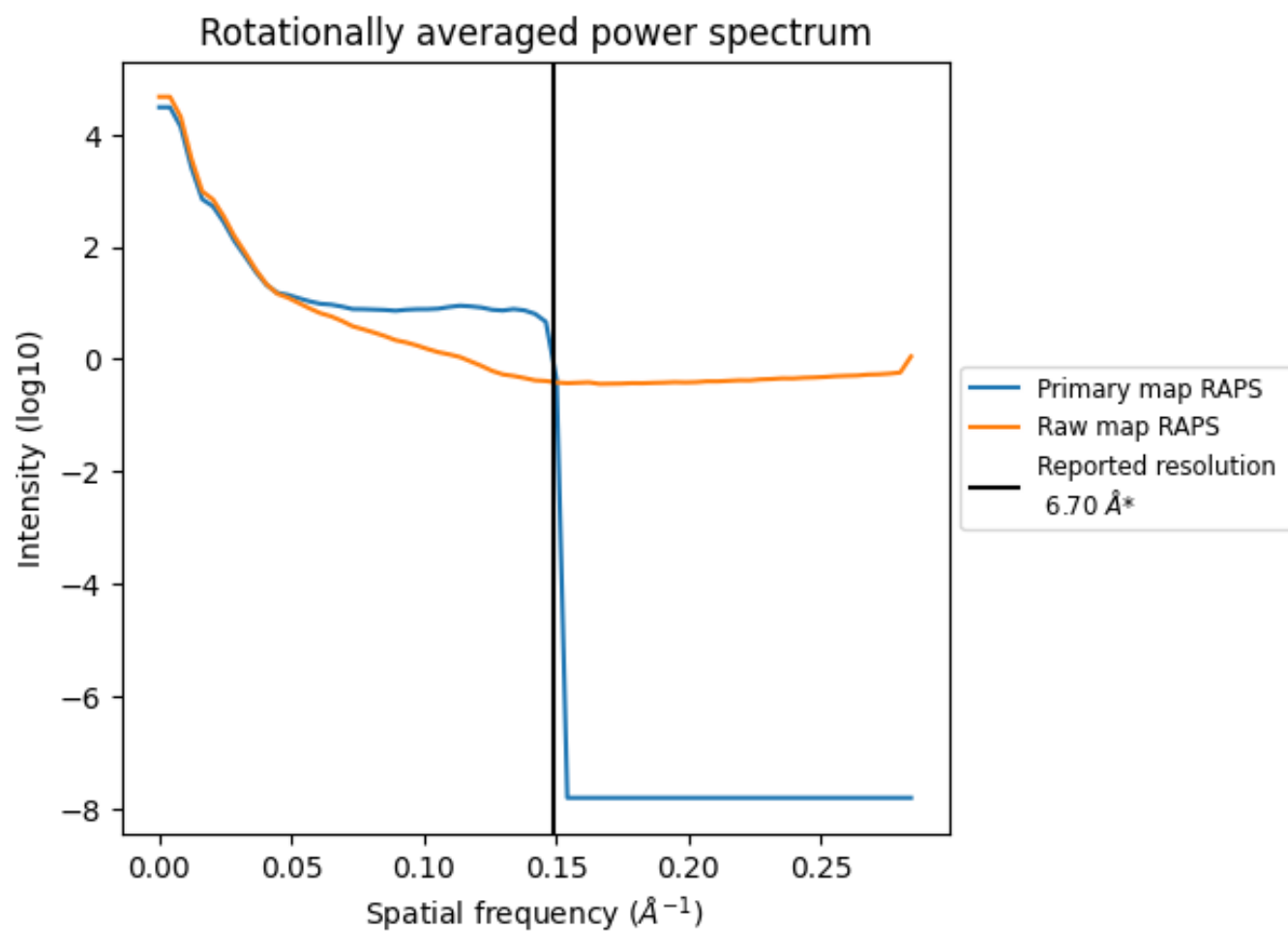
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 126 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 ⓘ

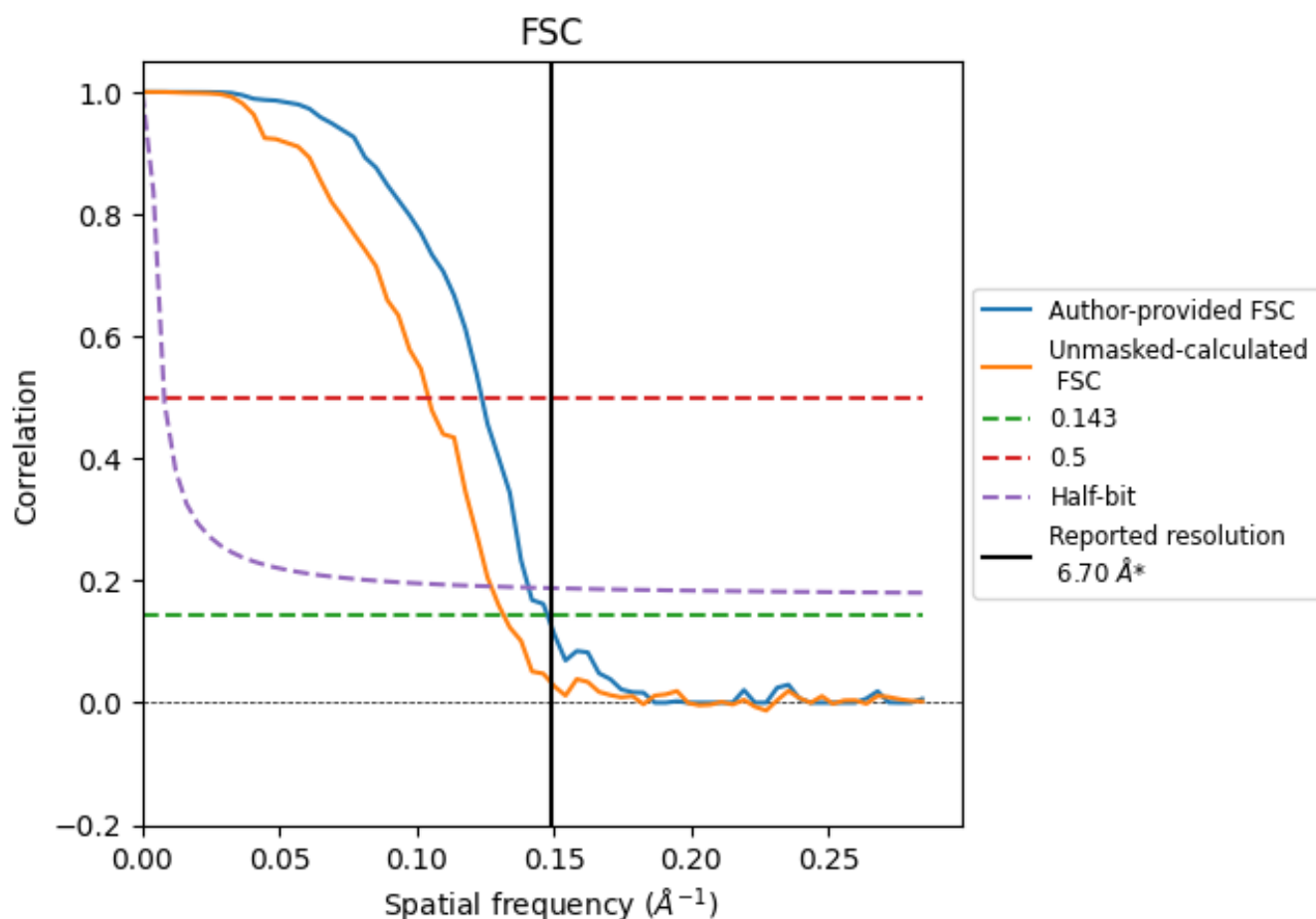


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

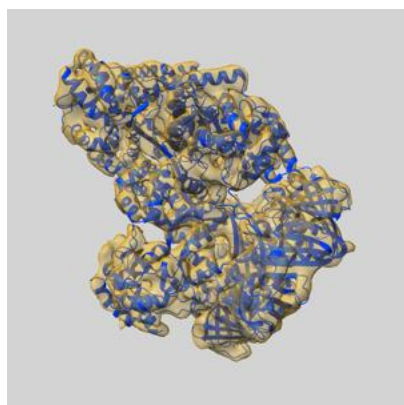
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.78	8.08	7.10
Unmasked-calculated*	7.59	9.59	7.87

*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 7.59 differs from the reported value 6.7 by more than 10 %

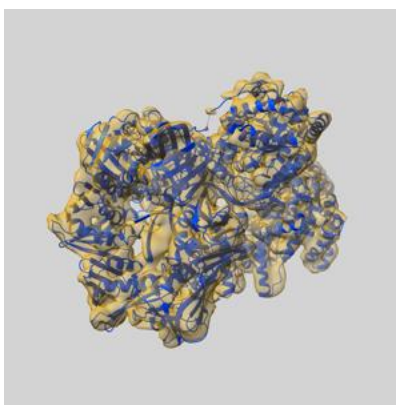
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4141 and PDB model 5M1S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

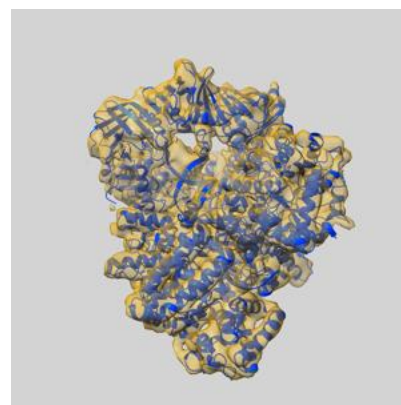
9.1 Map-model overlay [i](#)



X



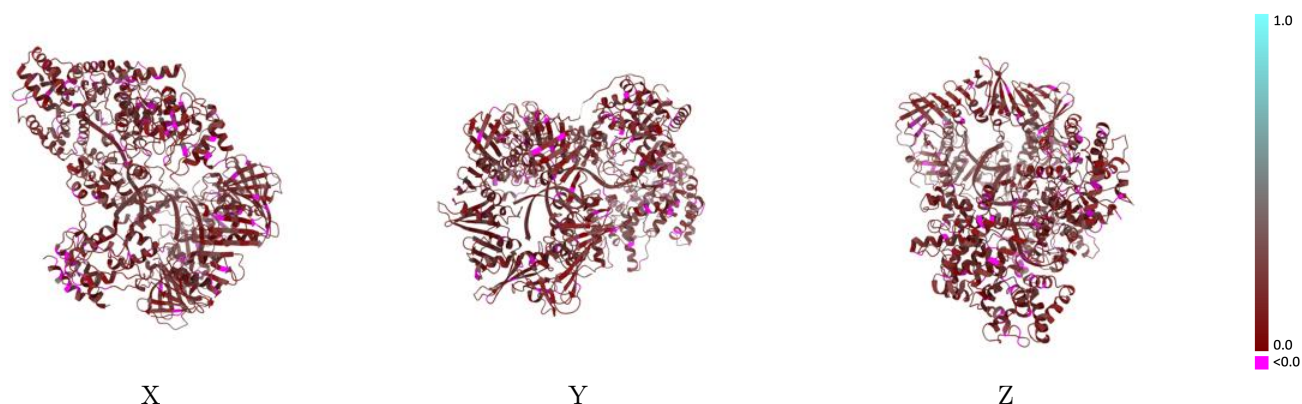
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

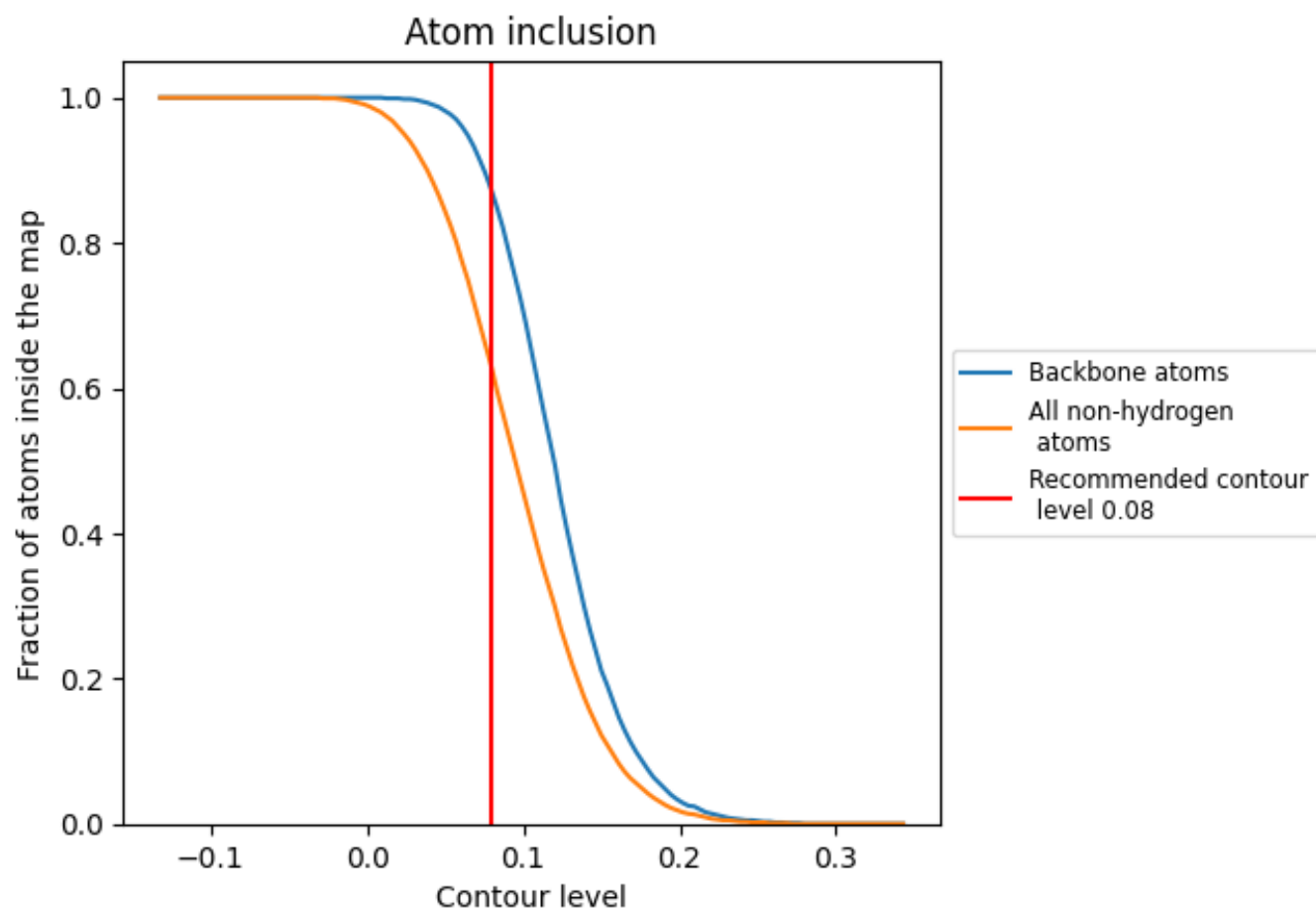


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 63% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.1730
A	0.6310	0.1680
B	0.6140	0.1750
C	0.6440	0.1780
D	0.5810	0.1720
F	0.5590	0.1340
P	0.7460	0.2180
T	0.6560	0.2150

1.0

0.0

<0.0