



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:43 PM UTC

PDB ID : 9GDA / pdb_00009gda
EMDB ID : EMD-51259
Title : RNAP-TopoI complex on duplex scaffold
Authors : Vidmar, V.; Weixlbaumer, A.; Lamour, V.
Deposited on : 2024-08-05
Resolution : 2.70 Å (reported)
Based on initial models : 6alh, 4rul

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:

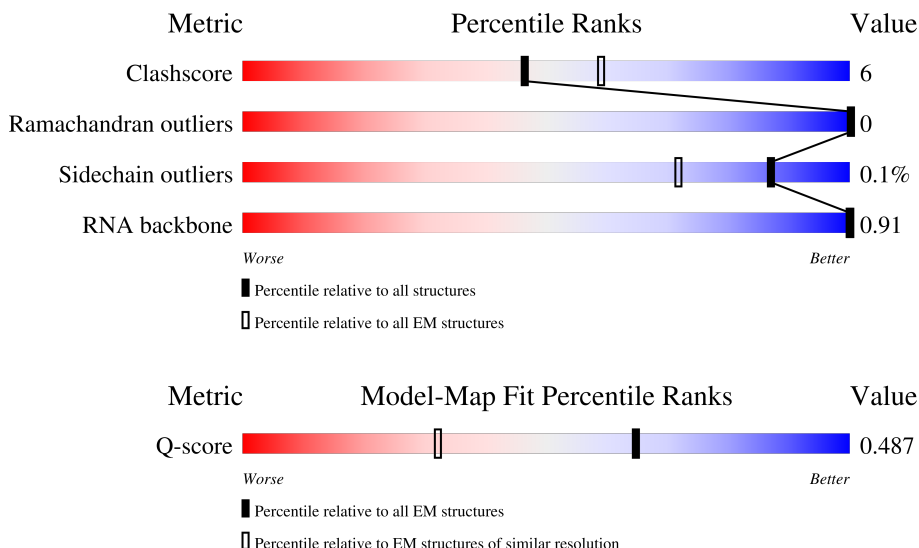
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.70 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	329	
1	B	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
3	D	1415	<div><div></div><div>81%13%5%</div></div>
4	E	91	<div><div></div><div>92%7%</div></div>
5	F	896	<div><div></div><div>78%16%6%</div></div>
6	N	39	<div><div></div><div>10%46%44%10%</div></div>
7	R	14	<div><div></div><div>7%36%43%21%</div></div>
8	T	39	<div><div></div><div>64%33%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 33857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1803	1122	320	355	6		
1	B	232	Total	C	N	O	S	0	0
			1799	1120	319	354	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10577	6636	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1342	Total	C	N	O	S	0	0
			10433	6553	1861	1969	50		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	LEU	-	expression tag	UNP P0A8T7
D	1411	GLU	-	expression tag	UNP P0A8T7
D	1412	VAL	-	expression tag	UNP P0A8T7
D	1413	LEU	-	expression tag	UNP P0A8T7
D	1414	PHE	-	expression tag	UNP P0A8T7
D	1415	GLN	-	expression tag	UNP P0A8T7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a protein called DNA topoisomerase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	846	Total	C	N	O	S	0	0
			6700	4195	1194	1274	37		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	GLY	-	expression tag	UNP P06612
F	-29	PRO	-	expression tag	UNP P06612
F	-28	TRP	-	expression tag	UNP P06612
F	-27	SER	-	expression tag	UNP P06612
F	-26	HIS	-	expression tag	UNP P06612
F	-25	PRO	-	expression tag	UNP P06612
F	-24	GLN	-	expression tag	UNP P06612
F	-23	PHE	-	expression tag	UNP P06612
F	-22	GLU	-	expression tag	UNP P06612
F	-21	LYS	-	expression tag	UNP P06612
F	-20	GLY	-	expression tag	UNP P06612
F	-19	GLY	-	expression tag	UNP P06612
F	-18	GLY	-	expression tag	UNP P06612
F	-17	SER	-	expression tag	UNP P06612
F	-16	GLY	-	expression tag	UNP P06612
F	-15	GLY	-	expression tag	UNP P06612
F	-14	GLY	-	expression tag	UNP P06612
F	-13	SER	-	expression tag	UNP P06612
F	-12	GLY	-	expression tag	UNP P06612
F	-11	GLY	-	expression tag	UNP P06612
F	-10	SER	-	expression tag	UNP P06612
F	-9	ALA	-	expression tag	UNP P06612
F	-8	TRP	-	expression tag	UNP P06612
F	-7	SER	-	expression tag	UNP P06612
F	-6	HIS	-	expression tag	UNP P06612
F	-5	PRO	-	expression tag	UNP P06612
F	-4	GLN	-	expression tag	UNP P06612
F	-3	PHE	-	expression tag	UNP P06612
F	-2	GLU	-	expression tag	UNP P06612
F	-1	LYS	-	expression tag	UNP P06612
F	0	HIS	-	expression tag	UNP P06612

- Molecule 6 is a DNA chain called non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	39	Total	C	N	O	P	0	0
			804	382	149	234	39		

- Molecule 7 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	11	Total	C	N	O	P	0	0
			235	104	42	78	11		

- Molecule 8 is a DNA chain called template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	39	Total	C	N	O	P	0	0
			791	375	141	236	39		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

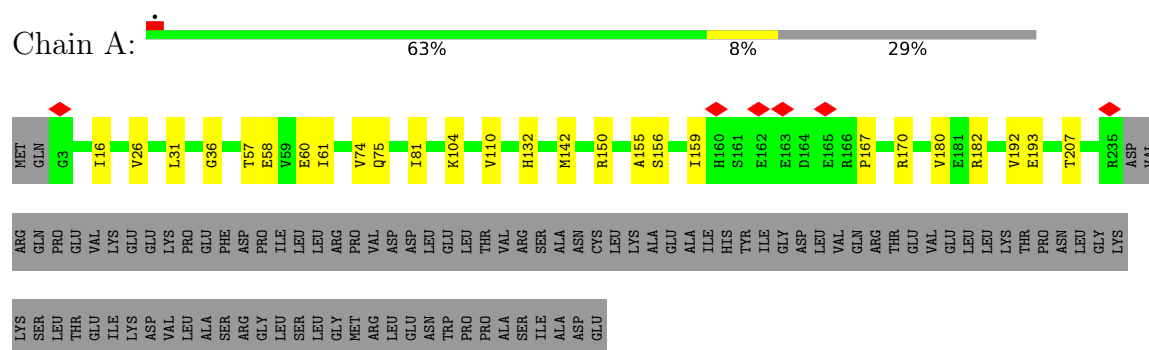
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	
10	F	3	Total	Zn	0
			3	3	

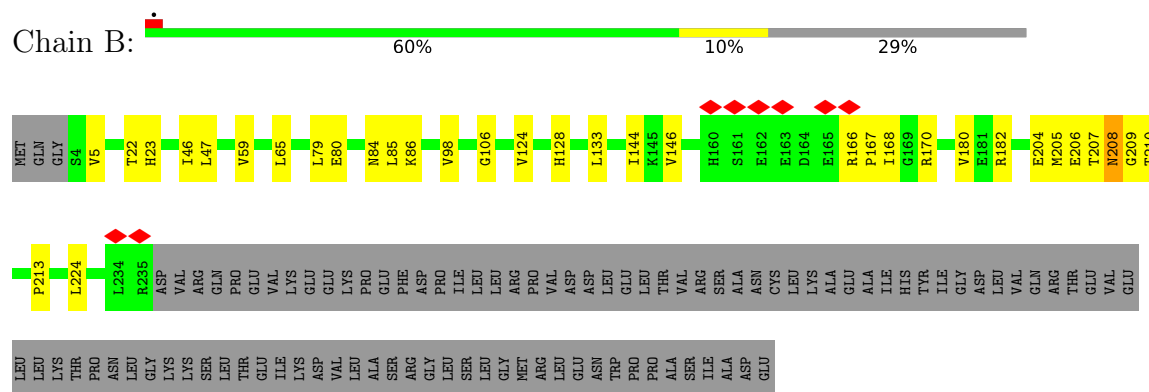
3 Residue-property plots [i](#)

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.

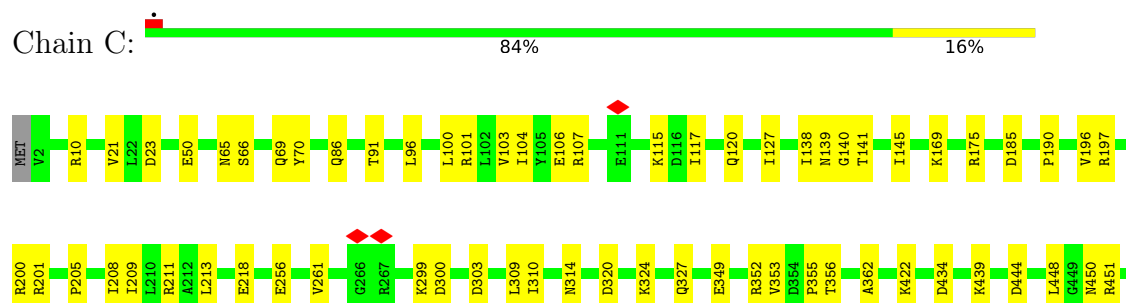
- Molecule 1: DNA-directed RNA polymerase subunit alpha

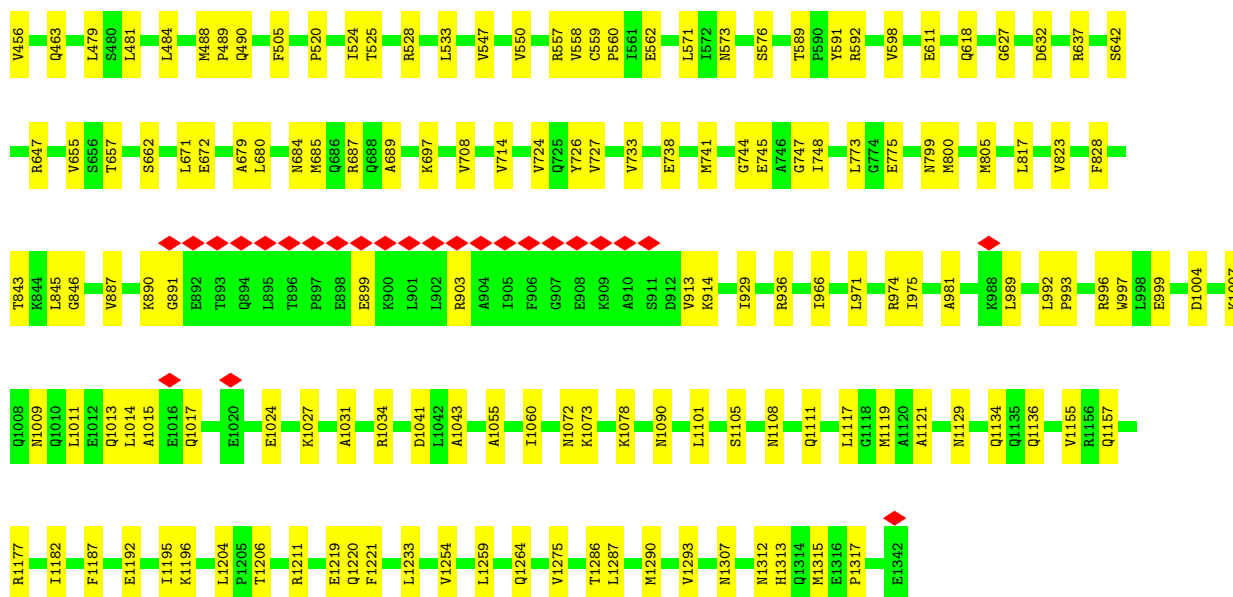


- Molecule 1: DNA-directed RNA polymerase subunit alpha



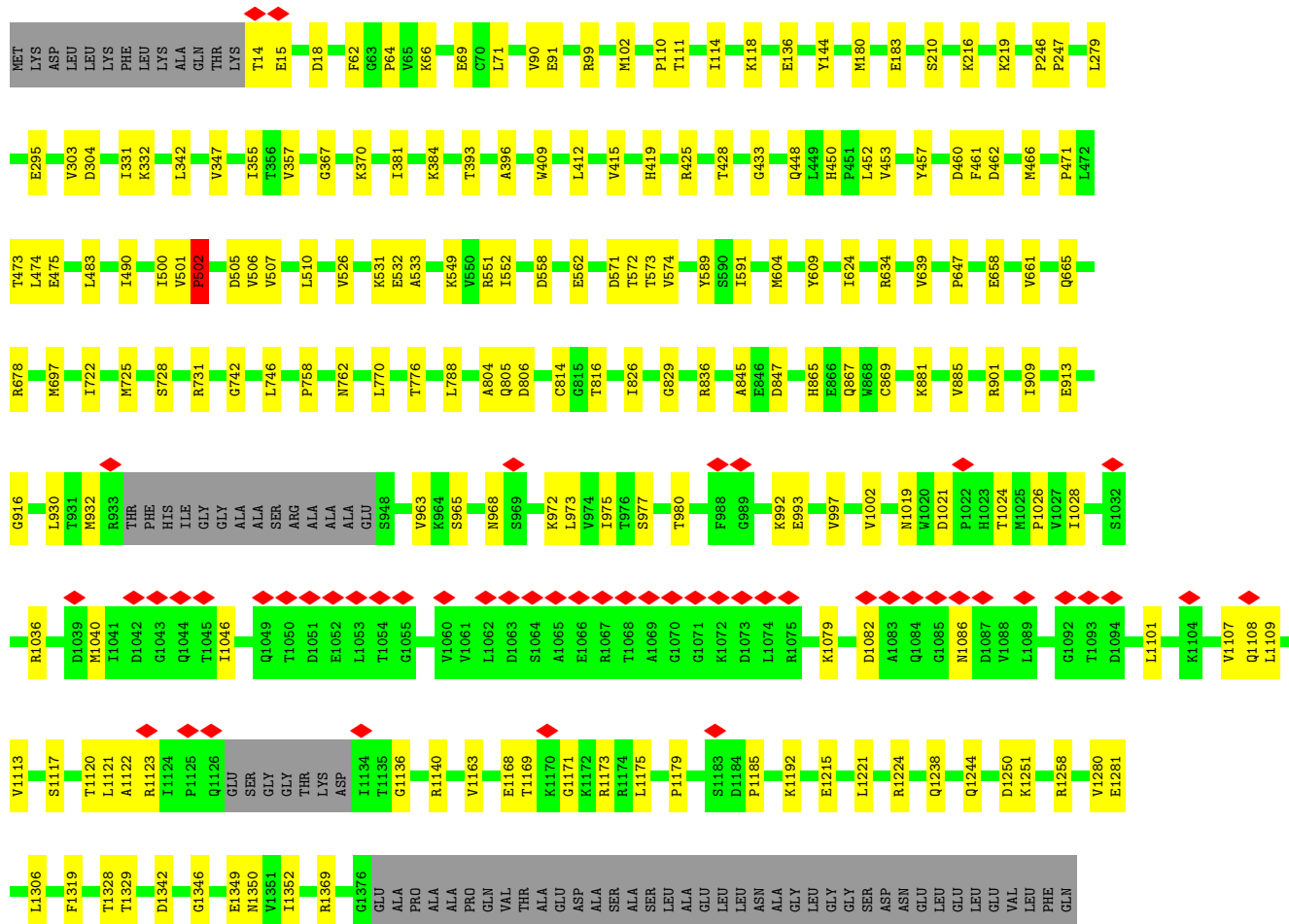
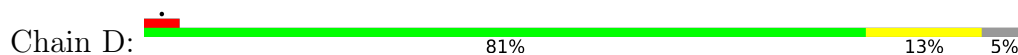
- Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



- Molecule 8: template DNA strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	80.680	Depositor
Minimum map value	-2.970	Depositor
Average map value	0.016	Depositor
Map value standard deviation	1.156	Depositor
Recommended contour level	0.724	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83900005, 0.83900005, 0.83900005	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/1825	0.29	0/2473
1	B	0.32	0/1821	0.37	2/2468 (0.1%)
2	C	0.41	0/10746	0.32	0/14499
3	D	0.42	3/10590 (0.0%)	0.38	5/14298 (0.0%)
4	E	0.33	0/711	0.23	0/956
5	F	0.44	0/6832	0.32	0/9218
6	N	0.58	0/902	0.93	5/1391 (0.4%)
7	R	0.72	0/261	0.93	0/405
8	T	0.68	0/884	0.90	1/1360 (0.1%)
All	All	0.43	3/34572 (0.0%)	0.40	13/47068 (0.0%)

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
8	T	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	PRO	N-CA	17.61	1.67	1.47
3	D	501	VAL	C-N	8.32	1.44	1.33
3	D	502	PRO	C-O	-5.11	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	VAL	CA-C-N	16.99	137.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	VAL	C-N-CA	16.99	137.23	119.90
6	N	24	DC	O5'-C5'-C4'	-7.34	99.79	110.80
1	B	208	ASN	N-CA-C	-7.14	101.63	110.41
3	D	502	PRO	CA-N-CD	-6.82	102.45	112.00
3	D	502	PRO	N-CA-C	-6.53	100.84	111.15
6	N	10	DG	O3'-P-O5'	5.69	112.53	104.00
6	N	12	DC	C4'-C3'-O3'	5.49	118.23	110.00
1	B	208	ASN	CB-CA-C	5.48	122.14	110.19
6	N	24	DC	P-O5'-C5'	5.45	128.17	120.00
6	N	11	DT	P-O3'-C3'	-5.45	112.03	120.20
8	T	16	DG	C4'-C3'-O3'	5.25	117.87	110.00
3	D	502	PRO	CB-CA-C	5.07	118.00	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	T	28	DG	Sidechain

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	1803	0	1830	15	0
1	B	1799	0	1827	23	0
2	C	10577	0	10591	139	0
3	D	10433	0	10654	127	0
4	E	709	0	719	4	0
5	F	6700	0	6645	94	0
6	N	804	0	440	21	0
7	R	235	0	121	9	0
8	T	791	0	438	9	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
10	F	3	0	0	0	0
All	All	33857	0	33265	411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (411) 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)
3:D:502:PRO:N	3:D:502:PRO:CA	1.67	1.37
5:F:270:GLU:HB3	5:F:414:THR:HB	1.60	0.83
5:F:220:TRP:HB2	5:F:248:PRO:HG2	1.64	0.79
2:C:975:ILE:HD11	2:C:1014:LEU:CD1	2.17	0.75
2:C:738:GLU:HA	2:C:741:MET:HE2	1.68	0.73
5:F:842:SER:HG	5:F:849:THR:HG1	1.33	0.72
6:N:19:DA:H2''	6:N:20:DT:H2'	1.71	0.72
2:C:975:ILE:HD11	2:C:1014:LEU:HD11	1.71	0.72
3:D:210:SER:OG	8:T:5:DG:OP1	2.08	0.72
1:B:167:PRO:HD2	1:B:170:ARG:HE	1.54	0.71
3:D:502:PRO:N	3:D:502:PRO:C	2.47	0.71
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.24	0.70
5:F:776:ALA:N	6:N:11:DT:OP1	2.25	0.69
5:F:310:ARG:NH1	5:F:384:GLU:OE2	2.26	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
2:C:657:THR:HG22	2:C:1187:PHE:HB2	1.76	0.68
2:C:481:LEU:HD11	5:F:737:LYS:H	1.58	0.67
2:C:1293:VAL:HG21	2:C:1315:MET:HG3	1.77	0.66
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.76	0.66
5:F:661:ARG:NH1	5:F:666:GLY:O	2.26	0.66
5:F:403:MET:HE2	5:F:433:GLY:O	1.97	0.65
5:F:221:GLU:OE1	5:F:237:GLN:NE2	2.29	0.65
3:D:425:ARG:HB2	3:D:466:MET:HE2	1.78	0.65
5:F:110:THR:OG1	5:F:136:ARG:NH1	2.31	0.64
5:F:309:GLN:HA	5:F:320:MET:HE2	1.79	0.64
5:F:511:ARG:NH1	5:F:520:GLU:OE2	2.27	0.64
1:B:180:VAL:HA	1:B:207:THR:HG22	1.79	0.64
3:D:490:ILE:HD11	3:D:609:TYR:CD1	2.33	0.63
5:F:227:THR:OG1	5:F:460:THR:OG1	2.16	0.63
2:C:314:ASN:O	2:C:352:ARG:NH1	2.32	0.63
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.79	0.63
2:C:444:ASP:O	2:C:450:ASN:ND2	2.31	0.62
5:F:135:SER:HB3	5:F:154:PRO:HB2	1.80	0.62
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.81	0.62
6:N:12:DC:H3'	6:N:13:DC:H5''	1.80	0.62
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.31	0.62
1:B:65:LEU:HG	1:B:168:ILE:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:3:ARG:NH2	4:E:55:GLU:OE1	2.33	0.61
5:F:821:ASP:OD1	5:F:825:ASN:N	2.33	0.61
3:D:805:GLN:NE2	3:D:806:ASP:OD1	2.33	0.61
3:D:1028:ILE:HG22	3:D:1120:THR:HG22	1.83	0.61
6:N:12:DC:H3'	6:N:13:DC:C5'	2.31	0.60
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.83	0.60
2:C:211:ARG:NH1	2:C:356:THR:OG1	2.35	0.60
5:F:493:ARG:NH2	5:F:551:ASP:OD2	2.35	0.60
5:F:744:ARG:NH1	6:N:9:DC:OP2	2.35	0.60
6:N:23:DT:H4'	6:N:24:DC:OP2	2.01	0.60
2:C:1155:VAL:HG12	2:C:1157:GLN:H	1.65	0.59
3:D:1101:LEU:HD11	3:D:1107:VAL:HG21	1.85	0.59
5:F:347:TYR:CD2	5:F:433:GLY:HA2	2.37	0.59
1:A:182:ARG:NH1	2:C:1090:ASN:O	2.35	0.59
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.85	0.59
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.84	0.59
2:C:197:ARG:NH1	2:C:201:ARG:O	2.36	0.59
3:D:450:HIS:HD2	3:D:452:LEU:H	1.51	0.59
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.36	0.58
3:D:453:VAL:HG12	3:D:457:TYR:CD2	2.38	0.58
3:D:1109:LEU:HD13	3:D:1121:LEU:HD21	1.86	0.58
3:D:1036:ARG:HH21	3:D:1079:LYS:HE3	1.69	0.58
5:F:718:MET:HG2	5:F:729:MET:HG3	1.85	0.58
2:C:197:ARG:HD3	2:C:200:ARG:HA	1.85	0.58
3:D:500:ILE:HG13	3:D:500:ILE:O	2.04	0.58
2:C:1014:LEU:HD12	2:C:1014:LEU:C	2.29	0.57
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.36	0.57
5:F:478:SER:N	5:F:481:SER:OG	2.37	0.57
3:D:18:ASP:OD1	3:D:1369:ARG:NH2	2.36	0.57
1:A:16:ILE:HG12	1:A:26:VAL:HG12	1.85	0.57
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.86	0.57
3:D:453:VAL:HG12	3:D:457:TYR:HD2	1.69	0.57
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.87	0.57
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.86	0.57
1:B:86:LYS:NZ	3:D:532:GLU:OE2	2.36	0.57
3:D:558:ASP:OD1	3:D:562:GLU:N	2.36	0.57
2:C:1313:HIS:HB2	3:D:474:LEU:HD12	1.86	0.57
5:F:616:PHE:HA	5:F:636:LEU:HG	1.86	0.57
5:F:669:MET:HG2	5:F:683:CYS:HA	1.87	0.57
2:C:1014:LEU:HD12	2:C:1015:ALA:N	2.20	0.57
2:C:528:ARG:NH2	2:C:576:SER:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:VAL:HG22	3:D:725:MET:HE1	1.86	0.56
2:C:1315:MET:HB2	3:D:473:THR:HG21	1.86	0.56
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.86	0.56
5:F:310:ARG:HB3	5:F:383:MET:HE1	1.86	0.56
5:F:462:VAL:HG12	5:F:463:GLU:H	1.70	0.56
2:C:557:ARG:NH2	2:C:611:GLU:OE1	2.33	0.56
5:F:9:GLU:OE1	5:F:9:GLU:N	2.38	0.56
3:D:977:SER:OG	3:D:980:THR:OG1	2.20	0.56
2:C:598:VAL:HA	2:C:627:GLY:O	2.06	0.56
3:D:572:THR:HG22	3:D:573:THR:H	1.71	0.56
3:D:502:PRO:HB3	3:D:506:VAL:HG12	1.88	0.55
3:D:1082:ASP:OD1	3:D:1086:ASN:N	2.37	0.55
2:C:1073:LYS:NZ	7:R:14:G:OP1	2.27	0.55
8:T:5:DG:H2''	8:T:6:DA:C8	2.41	0.55
2:C:1134:GLN:OE1	2:C:1136:GLN:NE2	2.33	0.55
2:C:632:ASP:HA	2:C:647:ARG:HE	1.71	0.55
2:C:680:LEU:O	2:C:684:ASN:ND2	2.37	0.55
3:D:722:ILE:HA	3:D:725:MET:HE3	1.88	0.55
7:R:7:G:H2'	7:R:8:C:H6	1.72	0.55
5:F:722:MET:HG2	5:F:727:LYS:HG2	1.87	0.55
6:N:19:DA:C2'	6:N:20:DT:H2'	2.36	0.55
3:D:533:ALA:HB1	3:D:574:VAL:HG13	1.87	0.55
2:C:637:ARG:HA	2:C:642:SER:HA	1.89	0.55
2:C:975:ILE:HD11	2:C:1014:LEU:HD13	1.87	0.55
5:F:38:PRO:O	5:F:173:ARG:NH2	2.40	0.54
8:T:27:DG:H2''	8:T:28:DG:OP1	2.08	0.54
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.54
3:D:450:HIS:CD2	3:D:452:LEU:H	2.24	0.54
5:F:80:GLU:OE2	5:F:82:HIS:NE2	2.40	0.54
1:B:166:ARG:HG2	1:B:170:ARG:HD2	1.88	0.54
2:C:1290:MET:HE2	3:D:347:VAL:HG11	1.89	0.54
2:C:120:GLN:OE1	2:C:490:GLN:N	2.29	0.54
2:C:1313:HIS:HB2	3:D:474:LEU:CD1	2.38	0.53
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.89	0.53
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.91	0.53
6:N:20:DT:H4'	6:N:21:DC:OP1	2.08	0.53
3:D:814:CYS:SG	3:D:816:THR:HG23	2.48	0.53
2:C:91:THR:OG1	2:C:138:ILE:O	2.17	0.53
2:C:1031:ALA:O	2:C:1034:ARG:HG3	2.09	0.53
3:D:639:VAL:CG2	3:D:725:MET:HE1	2.39	0.53
5:F:291:GLN:HA	5:F:480:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:VAL:HG22	2:C:117:ILE:HG22	1.90	0.52
2:C:434:ASP:HB3	2:C:439:LYS:HG3	1.92	0.52
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.91	0.52
3:D:572:THR:HG22	3:D:573:THR:N	2.24	0.52
5:F:209:ARG:HH22	5:F:528:ASP:CG	2.17	0.52
2:C:887:VAL:HB	2:C:913:VAL:HG13	1.91	0.52
3:D:901:ARG:O	3:D:1251:LYS:NZ	2.42	0.52
1:B:59:VAL:HG22	1:B:144:ILE:HG22	1.91	0.52
5:F:760:GLU:OE2	5:F:802:ARG:NH2	2.42	0.52
3:D:885:VAL:HG12	3:D:1258:ARG:HD2	1.91	0.52
5:F:462:VAL:HG12	5:F:463:GLU:N	2.25	0.52
1:B:205:MET:HG2	1:B:213:PRO:HB3	1.92	0.51
1:B:106:GLY:H	1:B:133:LEU:HD23	1.75	0.51
3:D:66:LYS:HG3	3:D:69:GLU:HB2	1.92	0.51
3:D:357:VAL:HG22	3:D:461:PHE:CE2	2.45	0.51
3:D:975:ILE:HD12	3:D:997:VAL:HG11	1.91	0.51
2:C:300:ASP:HB3	2:C:309:LEU:HD11	1.93	0.51
2:C:525:THR:HG21	2:C:687:ARG:CD	2.40	0.51
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.92	0.51
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.92	0.51
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.10	0.51
2:C:169:LYS:NZ	2:C:190:PRO:O	2.38	0.51
1:A:150:ARG:NH1	1:B:5:VAL:O	2.43	0.51
3:D:572:THR:HG21	3:D:589:TYR:OH	2.11	0.51
5:F:268:VAL:HA	5:F:415:VAL:HG22	1.92	0.51
3:D:460:ASP:OD1	3:D:460:ASP:N	2.44	0.50
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.94	0.50
2:C:451:ARG:NH2	2:C:547:VAL:HG13	2.27	0.50
3:D:1238:GLN:NE2	3:D:1250:ASP:OD1	2.33	0.50
3:D:1349:GLU:OE1	3:D:1349:GLU:N	2.38	0.50
5:F:79:TRP:NE1	5:F:565:ASP:OD1	2.32	0.50
7:R:5:C:H2'	7:R:6:C:H6	1.77	0.50
2:C:196:VAL:HG21	2:C:209:ILE:HD12	1.94	0.50
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.42	0.50
3:D:102:MET:HG2	3:D:246:PRO:HD3	1.94	0.50
2:C:1011:LEU:HD23	2:C:1014:LEU:HD21	1.93	0.50
5:F:609:ARG:HB2	5:F:616:PHE:CZ	2.47	0.50
2:C:971:LEU:O	2:C:975:ILE:HG12	2.11	0.49
2:C:996:ARG:NH1	2:C:999:GLU:OE1	2.44	0.49
5:F:473:PRO:HD2	5:F:653:THR:HG22	1.93	0.49
1:B:47:LEU:HB3	1:B:180:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:ARG:HH22	2:C:547:VAL:HG13	1.76	0.49
2:C:727:VAL:HG23	2:C:773:LEU:HD23	1.94	0.49
7:R:5:C:H2'	7:R:6:C:C6	2.47	0.49
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.95	0.49
6:N:6:DG:C8	6:N:7:DT:H72	2.46	0.49
7:R:7:G:H2'	7:R:8:C:C6	2.47	0.49
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.41	0.49
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.94	0.49
2:C:1219:GLU:OE1	3:D:634:ARG:NH1	2.37	0.49
2:C:65:ASN:OD1	2:C:107:ARG:NH1	2.46	0.49
5:F:825:ASN:HD22	5:F:849:THR:HG21	1.78	0.49
5:F:218:GLU:OE2	5:F:468:GLN:NE2	2.37	0.48
3:D:1026:PRO:HA	3:D:1122:ALA:HB3	1.93	0.48
3:D:1109:LEU:HG	3:D:1113:VAL:HB	1.94	0.48
5:F:108:LEU:HD13	5:F:120:ALA:HB1	1.96	0.48
2:C:989:LEU:O	2:C:997:TRP:NE1	2.46	0.48
1:B:208:ASN:OD1	1:B:210:THR:HG23	2.13	0.48
2:C:1101:LEU:HD12	3:D:505:ASP:OD1	2.14	0.48
2:C:1315:MET:HG2	2:C:1317:PRO:HD3	1.95	0.48
3:D:71:LEU:HB2	3:D:90:VAL:HG21	1.96	0.48
5:F:415:VAL:HB	5:F:422:LEU:HD11	1.95	0.48
5:F:610:THR:HG22	5:F:615:VAL:HG22	1.96	0.48
6:N:35:DC:H2''	6:N:36:DA:C8	2.49	0.48
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.49	0.48
1:A:60:GLU:OE2	1:A:170:ARG:NH1	2.47	0.48
2:C:1119:MET:HG3	2:C:1204:LEU:HD13	1.95	0.48
3:D:847:ASP:OD1	3:D:847:ASP:N	2.47	0.48
2:C:10:ARG:CZ	2:C:697:LYS:HD3	2.44	0.48
3:D:1136:GLY:HA2	3:D:1140:ARG:HB2	1.95	0.48
2:C:1259:LEU:HD23	2:C:1264:GLN:HB3	1.96	0.48
3:D:963:VAL:HB	3:D:980:THR:HG23	1.95	0.48
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.96	0.47
5:F:100:ALA:O	5:F:133:ARG:NH2	2.47	0.47
2:C:213:LEU:HD22	2:C:422:LYS:HG2	1.97	0.47
6:N:21:DC:H3'	6:N:22:DT:H5''	1.95	0.47
1:A:192:VAL:HG13	1:A:193:GLU:HG2	1.95	0.47
5:F:227:THR:HG1	5:F:460:THR:HG1	1.55	0.47
5:F:347:TYR:CE2	5:F:433:GLY:HA2	2.50	0.47
5:F:236:LEU:HB2	5:F:422:LEU:HD13	1.96	0.47
8:T:9:DC:C2'	8:T:10:DT:H71	2.44	0.47
2:C:975:ILE:CD1	2:C:1014:LEU:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:THR:HG21	3:D:303:VAL:HB	1.96	0.47
3:D:342:LEU:HD13	3:D:1352:ILE:HG23	1.95	0.47
5:F:403:MET:CE	5:F:433:GLY:O	2.61	0.47
3:D:216:LYS:HA	3:D:219:LYS:HE2	1.97	0.47
3:D:665:GLN:OE1	3:D:678:ARG:NH2	2.43	0.47
3:D:1120:THR:O	3:D:1121:LEU:HD12	2.15	0.47
5:F:740:ARG:NH2	5:F:749:ALA:O	2.37	0.47
2:C:50:GLU:OE1	2:C:70:TYR:OH	2.28	0.47
4:E:25:ARG:HH21	4:E:68:GLU:CD	2.22	0.47
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.97	0.47
1:A:180:VAL:HA	1:A:207:THR:HG22	1.96	0.47
1:B:79:LEU:HD21	3:D:526:VAL:HG21	1.97	0.47
2:C:843:THR:OG1	2:C:846:GLY:O	2.28	0.47
5:F:228:THR:OG1	5:F:232:GLU:N	2.48	0.47
2:C:560:PRO:CB	3:D:776:THR:HG21	2.45	0.46
2:C:890:LYS:HG2	2:C:914:LYS:HB2	1.97	0.46
5:F:832:SER:O	5:F:836:LYS:N	2.49	0.46
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.55	0.46
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.97	0.46
3:D:742:GLY:O	3:D:762:ASN:HB3	2.16	0.46
2:C:520:PRO:HG3	2:C:714:VAL:HG11	1.97	0.46
3:D:788:LEU:HB3	3:D:932:MET:HE1	1.98	0.46
5:F:347:TYR:HD2	5:F:433:GLY:HA2	1.80	0.46
6:N:18:DG:H5''	6:N:19:DA:H5'	1.96	0.46
3:D:14:THR:OG1	3:D:15:GLU:N	2.48	0.46
5:F:6:VAL:HG22	5:F:107:TYR:HB2	1.97	0.46
5:F:369:ARG:NH1	5:F:370:PRO:O	2.49	0.46
2:C:550:VAL:HG21	3:D:776:THR:HG22	1.98	0.46
2:C:817:LEU:HD12	2:C:1078:LYS:HB3	1.98	0.46
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.47	0.46
2:C:70:TYR:HA	2:C:100:LEU:HD23	1.96	0.46
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	1.98	0.46
6:N:10:DG:C8	6:N:11:DT:H72	2.51	0.46
5:F:743:LEU:HD12	5:F:745:ASN:H	1.80	0.46
3:D:647:PRO:HG3	3:D:697:MET:HA	1.98	0.46
5:F:707:PRO:HG2	5:F:720:LEU:HD22	1.97	0.45
5:F:728:TYR:HB3	6:N:15:DA:C2	2.51	0.45
2:C:256:GLU:HB3	2:C:261:VAL:HG22	1.98	0.45
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.97	0.45
1:A:167:PRO:HD2	1:A:170:ARG:HE	1.80	0.45
2:C:562:GLU:OE1	2:C:662:SER:OG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:187:ILE:HD11	5:F:529:ARG:HG3	1.98	0.45
2:C:744:GLY:O	2:C:1017:GLN:HG3	2.17	0.45
2:C:1129:ASN:OD1	2:C:1177:ARG:NH1	2.49	0.45
5:F:671:SER:HB3	5:F:679:LYS:HE2	1.98	0.45
2:C:805:MET:HE1	2:C:1221:PHE:CE1	2.52	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.99	0.45
3:D:1040:MET:HG3	3:D:1046:ILE:HG12	1.99	0.45
5:F:104:ASP:OD1	5:F:105:HIS:N	2.50	0.45
3:D:355:ILE:HD13	3:D:466:MET:HE3	1.98	0.45
3:D:549:LYS:NZ	3:D:571:ASP:OD1	2.49	0.45
8:T:7:DA:C8	8:T:8:DT:H72	2.51	0.45
8:T:9:DC:H2'	8:T:10:DT:H71	1.98	0.45
2:C:208:ILE:HG23	2:C:362:ALA:HB1	1.99	0.45
5:F:629:ARG:HD2	5:F:631:LYS:HE3	1.98	0.45
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.82	0.45
3:D:965:SER:HB2	3:D:973:LEU:HD11	1.98	0.45
3:D:393:THR:HG23	3:D:396:ALA:H	1.82	0.45
3:D:804:ALA:O	3:D:916:GLY:HA3	2.16	0.45
5:F:817:ALA:HB2	5:F:860:TRP:CZ2	2.52	0.45
2:C:488:MET:HE3	2:C:489:PRO:HD2	1.99	0.44
5:F:718:MET:HG3	5:F:730:ALA:C	2.42	0.44
2:C:1121:ALA:HB2	2:C:1182:ILE:HD12	1.98	0.44
2:C:1211:ARG:HD2	2:C:1220:GLN:NE2	2.32	0.44
5:F:454:ASN:O	5:F:457:ASP:HB2	2.17	0.44
5:F:756:VAL:HG21	5:F:808:PRO:HD3	1.98	0.44
5:F:234:LEU:HD13	5:F:451:PRO:HD2	1.98	0.44
1:A:156:SER:O	1:A:159:ILE:HG12	2.17	0.44
2:C:23:ASP:OD1	2:C:23:ASP:N	2.51	0.44
3:D:64:PRO:HG3	3:D:91:GLU:O	2.17	0.44
3:D:483:LEU:HD23	4:E:16:ARG:HD3	2.00	0.44
5:F:162:VAL:O	5:F:166:GLN:HG2	2.17	0.44
5:F:617:LEU:HB2	5:F:634:ILE:HB	1.99	0.44
6:N:24:DC:H2''	6:N:25:DG:H8	1.82	0.44
2:C:66:SER:HB2	2:C:479:LEU:HD11	2.00	0.44
2:C:689:ALA:HB2	2:C:1233:LEU:HD23	1.99	0.44
2:C:899:GLU:O	2:C:903:ARG:HG2	2.18	0.44
2:C:1101:LEU:O	3:D:731:ARG:HG2	2.17	0.44
3:D:591:ILE:HD11	3:D:604:MET:HA	1.99	0.44
5:F:830:ARG:NH2	5:F:843:GLU:OE2	2.41	0.44
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.99	0.44
2:C:592:ARG:HG3	2:C:655:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.99	0.44
3:D:370:LYS:HG2	3:D:409:TRP:CZ3	2.52	0.44
2:C:724:VAL:HG12	2:C:775:GLU:O	2.17	0.44
3:D:1169:THR:HB	6:N:37:DG:OP1	2.18	0.44
5:F:592:MET:SD	5:F:607:GLY:HA3	2.58	0.44
7:R:8:C:H2'	7:R:9:G:H8	1.82	0.44
2:C:992:LEU:O	2:C:997:TRP:NE1	2.51	0.44
5:F:660:ARG:HD2	5:F:681:HIS:CE1	2.52	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.18	0.44
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.99	0.44
3:D:1163:VAL:HG13	3:D:1175:LEU:HD21	2.00	0.43
5:F:65:GLY:O	5:F:69:ASN:ND2	2.37	0.43
8:T:4:DT:H2''	8:T:5:DG:C8	2.53	0.43
3:D:930:LEU:HA	3:D:1244:GLN:HG3	2.00	0.43
5:F:408:TYR:CZ	5:F:429:LEU:HD13	2.53	0.43
5:F:609:ARG:HD3	5:F:616:PHE:CE2	2.53	0.43
6:N:12:DC:C4	6:N:13:DC:N4	2.86	0.43
2:C:205:PRO:HG2	2:C:355:PRO:HD3	1.99	0.43
2:C:1041:ASP:OD1	2:C:1041:ASP:N	2.50	0.43
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.52	0.43
5:F:220:TRP:CZ3	5:F:468:GLN:HB2	2.53	0.43
2:C:993:PRO:HG2	2:C:996:ARG:HG2	2.00	0.43
3:D:1168:GLU:OE2	3:D:1173:ARG:NE	2.40	0.43
7:R:6:C:H2'	7:R:7:G:H8	1.83	0.43
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.00	0.43
3:D:975:ILE:HG22	3:D:977:SER:H	1.82	0.43
2:C:975:ILE:HA	2:C:975:ILE:HD13	1.81	0.43
5:F:20:TYR:HB2	5:F:147:ILE:HD12	2.00	0.43
5:F:415:VAL:HB	5:F:422:LEU:CD1	2.47	0.43
3:D:1215:GLU:OE2	3:D:1224:ARG:NH2	2.33	0.43
5:F:636:LEU:HD22	5:F:674:ILE:HG22	2.00	0.43
7:R:6:C:H2'	7:R:7:G:C8	2.54	0.43
3:D:419:HIS:NE2	3:D:471:PRO:O	2.38	0.43
5:F:774:ASP:OD1	5:F:775:GLY:N	2.52	0.43
2:C:1286:THR:O	2:C:1290:MET:HG3	2.19	0.43
5:F:647:GLU:OE1	5:F:654:ASN:ND2	2.38	0.42
2:C:558:VAL:HG13	2:C:573:ASN:HB3	2.02	0.42
3:D:507:VAL:HG12	3:D:728:SER:OG	2.19	0.42
3:D:746:LEU:HG	3:D:758:PRO:HG3	2.02	0.42
5:F:796:LEU:HB2	5:F:799:GLU:HG3	2.01	0.42
3:D:118:LYS:NZ	3:D:136:GLU:OE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:HIS:CE1	1:B:204:GLU:HG3	2.54	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.42
3:D:658:GLU:HA	3:D:661:VAL:HG22	2.01	0.42
1:B:98:VAL:HG12	1:B:146:VAL:HB	2.00	0.42
5:F:225:SER:HB2	5:F:462:VAL:HB	2.01	0.42
1:B:206:GLU:OE1	3:D:531:LYS:NZ	2.38	0.42
5:F:376:MET:O	5:F:379:SER:OG	2.34	0.42
2:C:845:LEU:HD23	2:C:891:GLY:HA2	2.01	0.42
3:D:144:TYR:CE1	3:D:180:MET:HE3	2.54	0.42
3:D:1179:PRO:HD3	3:D:1185:PRO:HA	2.02	0.42
3:D:1280:VAL:HG12	3:D:1281:GLU:N	2.34	0.42
5:F:269:LEU:HD23	5:F:414:THR:O	2.19	0.42
5:F:720:LEU:HD12	5:F:728:TYR:O	2.20	0.42
8:T:36:DG:H2''	8:T:37:DA:C8	2.55	0.42
2:C:96:LEU:HD22	2:C:127:ILE:HD11	2.02	0.42
3:D:1319:PHE:CE1	3:D:1342:ASP:HB2	2.55	0.42
6:N:36:DA:H2''	6:N:37:DG:C8	2.55	0.42
1:B:182:ARG:HH12	1:B:204:GLU:CD	2.28	0.41
2:C:320:ASP:N	2:C:320:ASP:OD1	2.53	0.41
3:D:1021:ASP:HB3	3:D:1024:THR:HB	2.00	0.41
5:F:793:ARG:HH22	5:F:799:GLU:CD	2.27	0.41
2:C:324:LYS:O	2:C:327:GLN:HG3	2.20	0.41
2:C:349:GLU:O	2:C:353:VAL:HG23	2.20	0.41
2:C:745:GLU:O	2:C:974:ARG:NH1	2.53	0.41
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.55	0.41
3:D:552:ILE:HG21	3:D:589:TYR:CD1	2.55	0.41
8:T:22:DC:H2'	8:T:23:DC:H6	1.85	0.41
3:D:279:LEU:HD13	3:D:295:GLU:HB3	2.02	0.41
2:C:805:MET:HE3	2:C:805:MET:HB2	1.95	0.41
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	2.01	0.41
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	2.02	0.41
3:D:826:ILE:HD13	3:D:992:LYS:HA	2.01	0.41
5:F:128:GLY:O	5:F:134:TYR:OH	2.22	0.41
5:F:644:ASN:ND2	5:F:647:GLU:HG3	2.35	0.41
2:C:21:VAL:HG21	2:C:592:ARG:CZ	2.51	0.41
2:C:975:ILE:HD12	2:C:975:ILE:HG23	1.78	0.41
2:C:697:LYS:O	2:C:799:ASN:ND2	2.43	0.41
3:D:829:GLY:HA2	3:D:993:GLU:HG2	2.02	0.41
5:F:384:GLU:H	5:F:384:GLU:HG2	1.71	0.41
5:F:728:TYR:HE2	5:F:730:ALA:HB2	1.86	0.41
6:N:13:DC:H2''	6:N:14:DT:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.90	0.41
2:C:672:GLU:OE1	2:C:672:GLU:N	2.38	0.41
3:D:332:LYS:HD3	3:D:1329:THR:HG23	2.03	0.41
2:C:104:ILE:HD13	2:C:484:LEU:HB3	2.03	0.41
2:C:671:LEU:HD11	2:C:679:ALA:HB1	2.01	0.41
3:D:968:ASN:HA	3:D:1117:SER:O	2.20	0.41
1:B:84:ASN:O	1:B:128:HIS:HE1	2.04	0.41
2:C:106:GLU:HG3	2:C:115:LYS:HB3	2.02	0.41
2:C:218:GLU:HG2	2:C:299:LYS:HA	2.03	0.41
2:C:745:GLU:HG2	2:C:747:GLY:H	1.85	0.41
2:C:1105:SER:HB2	3:D:731:ARG:HG3	2.02	0.41
2:C:1196:LYS:HB3	2:C:1206:THR:HG23	2.03	0.41
3:D:1002:VAL:HB	3:D:1019:ASN:HB3	2.02	0.41
2:C:69:GLN:OE1	2:C:101:ARG:NH1	2.44	0.41
2:C:618:GLN:NE2	3:D:770:LEU:HD13	2.36	0.41
3:D:384:LYS:HD2	3:D:415:VAL:HG12	2.02	0.41
6:N:12:DC:C5	6:N:13:DC:N4	2.89	0.41
7:R:8:C:H2'	7:R:9:G:C8	2.55	0.41
2:C:890:LYS:HE3	2:C:913:VAL:O	2.21	0.40
5:F:406:ALA:H	5:F:434:TRP:HD1	1.69	0.40
5:F:487:GLU:OE1	5:F:497:TYR:OH	2.23	0.40
1:A:75:GLN:HB3	1:A:132:HIS:HB2	2.03	0.40
2:C:139:ASN:C	2:C:141:THR:H	2.28	0.40
2:C:748:ILE:HG21	2:C:966:ILE:HG22	2.03	0.40
2:C:800:MET:HE3	2:C:828:PHE:CE2	2.56	0.40
2:C:823:VAL:HG22	2:C:1060:ILE:HG23	2.03	0.40
2:C:981:ALA:O	2:C:1007:LYS:NZ	2.54	0.40
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.21	0.40
5:F:16:THR:O	5:F:19:LYS:HB2	2.20	0.40
1:A:74:VAL:HG11	1:A:81:ILE:HD11	2.03	0.40
1:A:155:ALA:O	1:A:159:ILE:HG23	2.22	0.40
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.22	0.40
2:C:1009:ASN:O	2:C:1013:GLN:HG2	2.21	0.40
3:D:428:THR:HG23	3:D:433:GLY:HA3	2.03	0.40
3:D:968:ASN:OD1	3:D:972:LYS:N	2.54	0.40
5:F:521:LYS:O	5:F:525:ILE:HG12	2.20	0.40
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.03	0.40
3:D:331:ILE:HG22	3:D:1328:THR:HG21	2.03	0.40
3:D:885:VAL:O	3:D:1258:ARG:NH1	2.51	0.40
3:D:1171:GLY:HA2	3:D:1192:LYS:HG2	2.02	0.40
5:F:606:MET:HE2	5:F:606:MET:HB3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:842:SER:OG	5:F:849:THR:OG1	2.13	0.40
1:A:61:ILE:HG12	1:A:142:MET:HG3	2.02	0.40
1:B:80:GLU:HG3	3:D:551:ARG:HH21	1.86	0.40
3:D:845:ALA:HB3	3:D:881:LYS:HG2	2.04	0.40
6:N:37:DG:H2"	6:N:38:DA:C8	2.56	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	231/329 (70%)	229 (99%)	2 (1%)	0	100	100
1	B	230/329 (70%)	227 (99%)	3 (1%)	0	100	100
2	C	1339/1342 (100%)	1321 (99%)	18 (1%)	0	100	100
3	D	1336/1415 (94%)	1323 (99%)	13 (1%)	0	100	100
4	E	88/91 (97%)	88 (100%)	0	0	100	100
5	F	842/896 (94%)	820 (97%)	22 (3%)	0	100	100
All	All	4066/4402 (92%)	4008 (99%)	58 (1%)	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	200/286 (70%)	200 (100%)	0	100	100
1	B	200/286 (70%)	200 (100%)	0	100	100
2	C	1156/1157 (100%)	1155 (100%)	1 (0%)	88	96
3	D	1124/1176 (96%)	1123 (100%)	1 (0%)	88	96
4	E	74/75 (99%)	74 (100%)	0	100	100
5	F	718/754 (95%)	717 (100%)	1 (0%)	88	96
All	All	3472/3734 (93%)	3469 (100%)	3 (0%)	87	96

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

Mol	Chain	Res	Type
2	C	589	THR
3	D	502	PRO
5	F	736	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	137	ASN
1	B	37	HIS
1	B	66	HIS
1	B	128	HIS
2	C	330	HIS
2	C	518	ASN
2	C	573	ASN
2	C	761	GLN
2	C	808	ASN
2	C	1256	GLN
2	C	1264	GLN
3	D	364	HIS
3	D	450	HIS
3	D	469	HIS
3	D	489	ASN
3	D	1019	ASN
3	D	1259	GLN
5	F	333	ASN
5	F	374	ASN
5	F	469	HIS
5	F	681	HIS

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Mol	Chain	Res	Type
5	F	719	HIS
5	F	825	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	10/14 (71%)	0	0

There are no RNA backbone outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

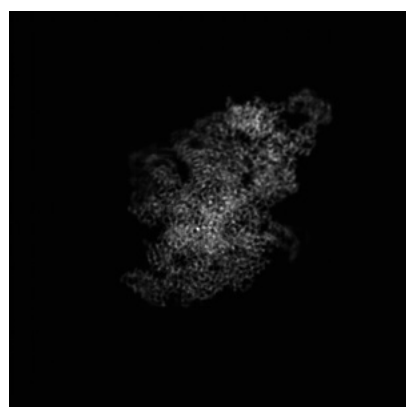
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51259. These allow visual inspection of the internal detail of the map and identification of artifacts.

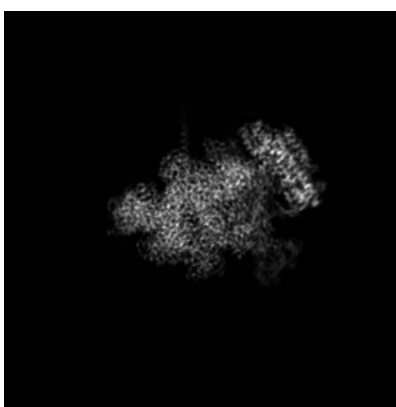
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

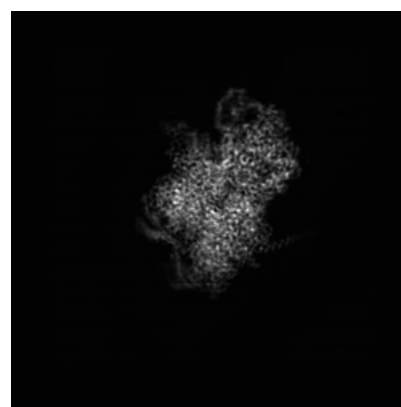
6.1.1 Primary map



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: 180



Y Index: 180

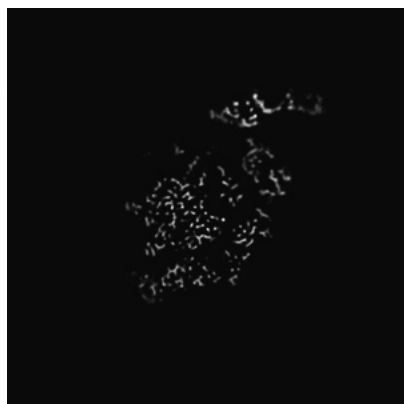


Z Index: 180

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: 191



Y Index: 180

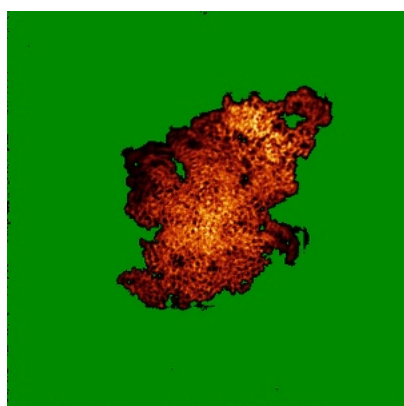


Z Index: 155

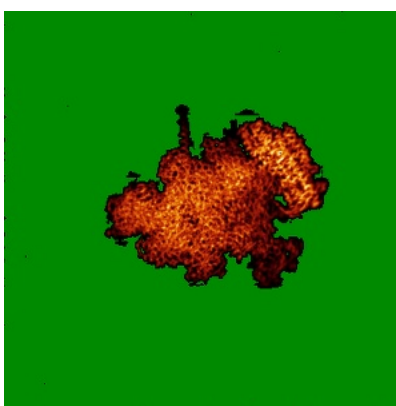
The images above show the largest variance slices of the map in three orthogonal directions.

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

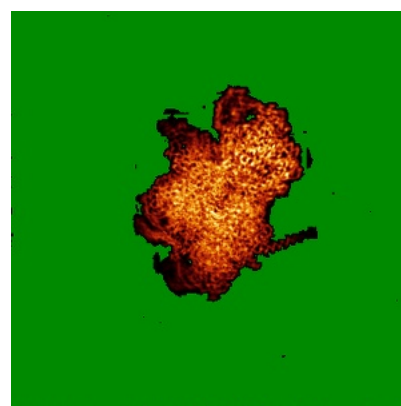
6.4.1 Primary map



X



Y

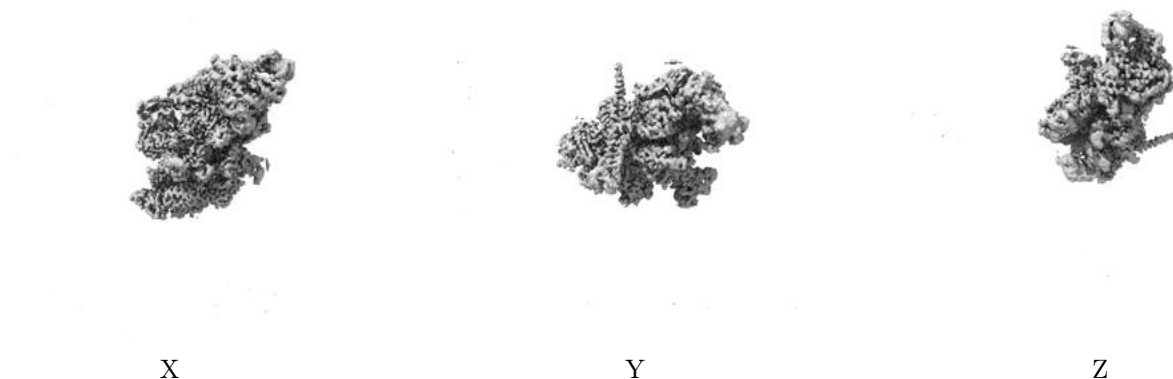


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.724. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

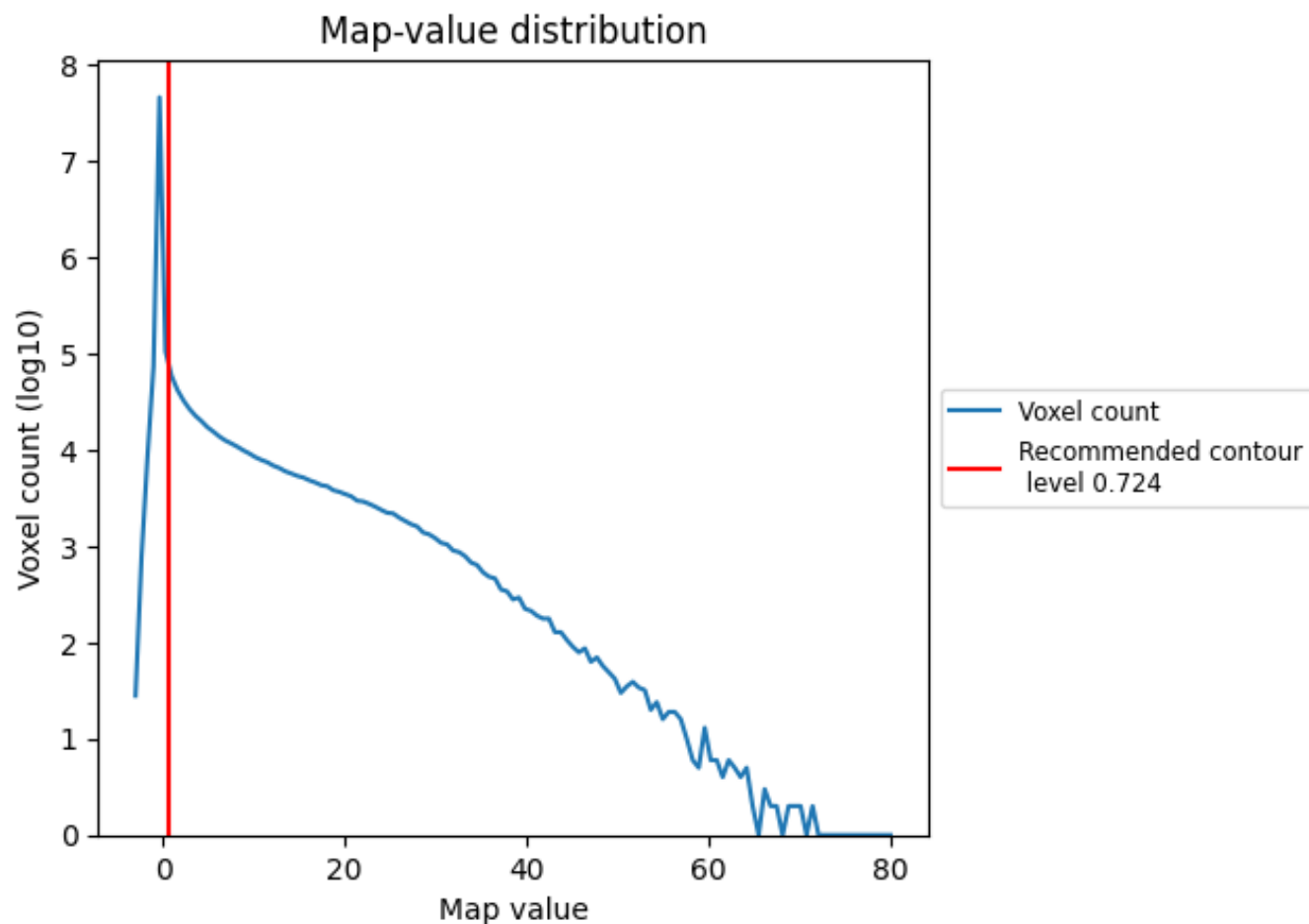
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

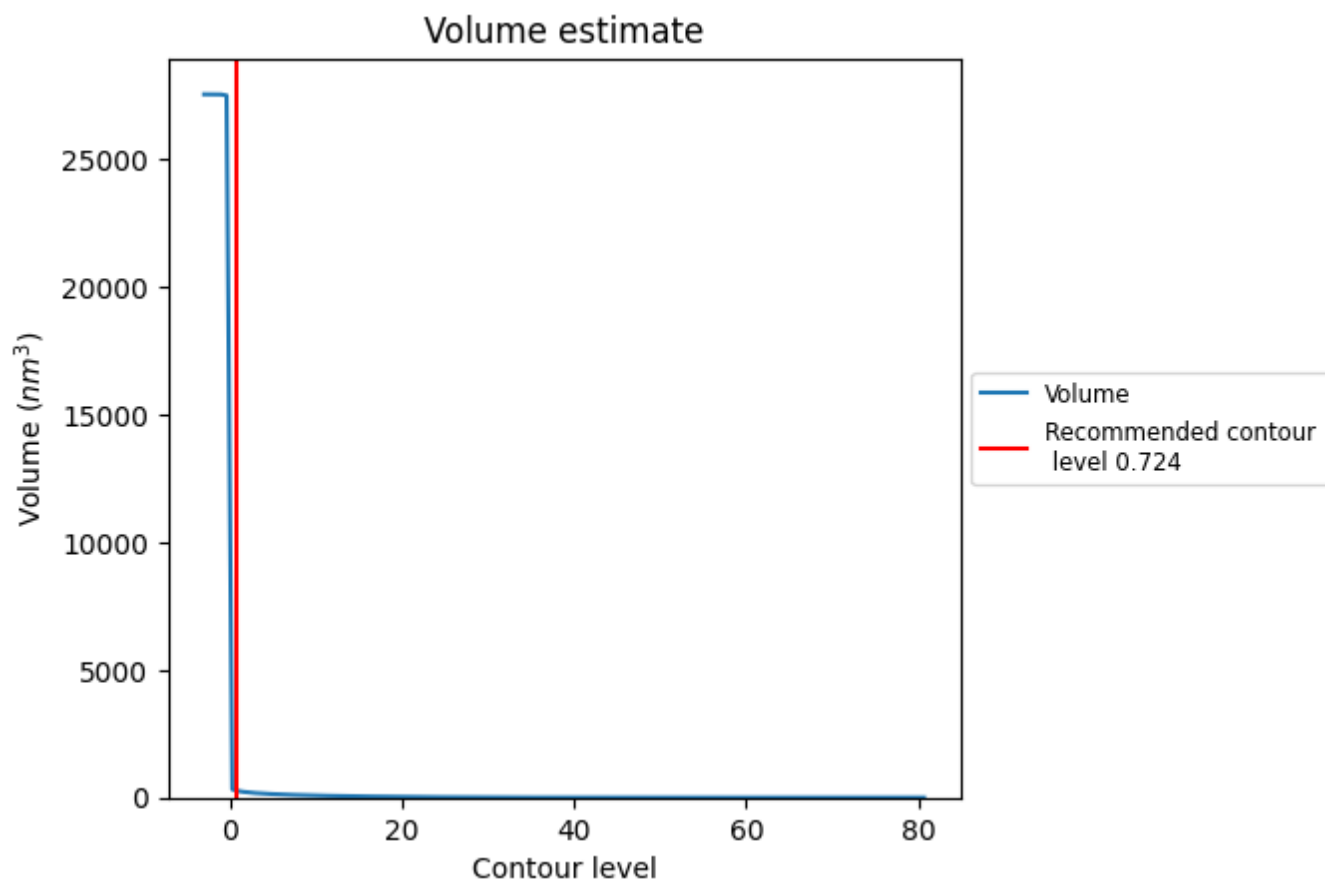
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

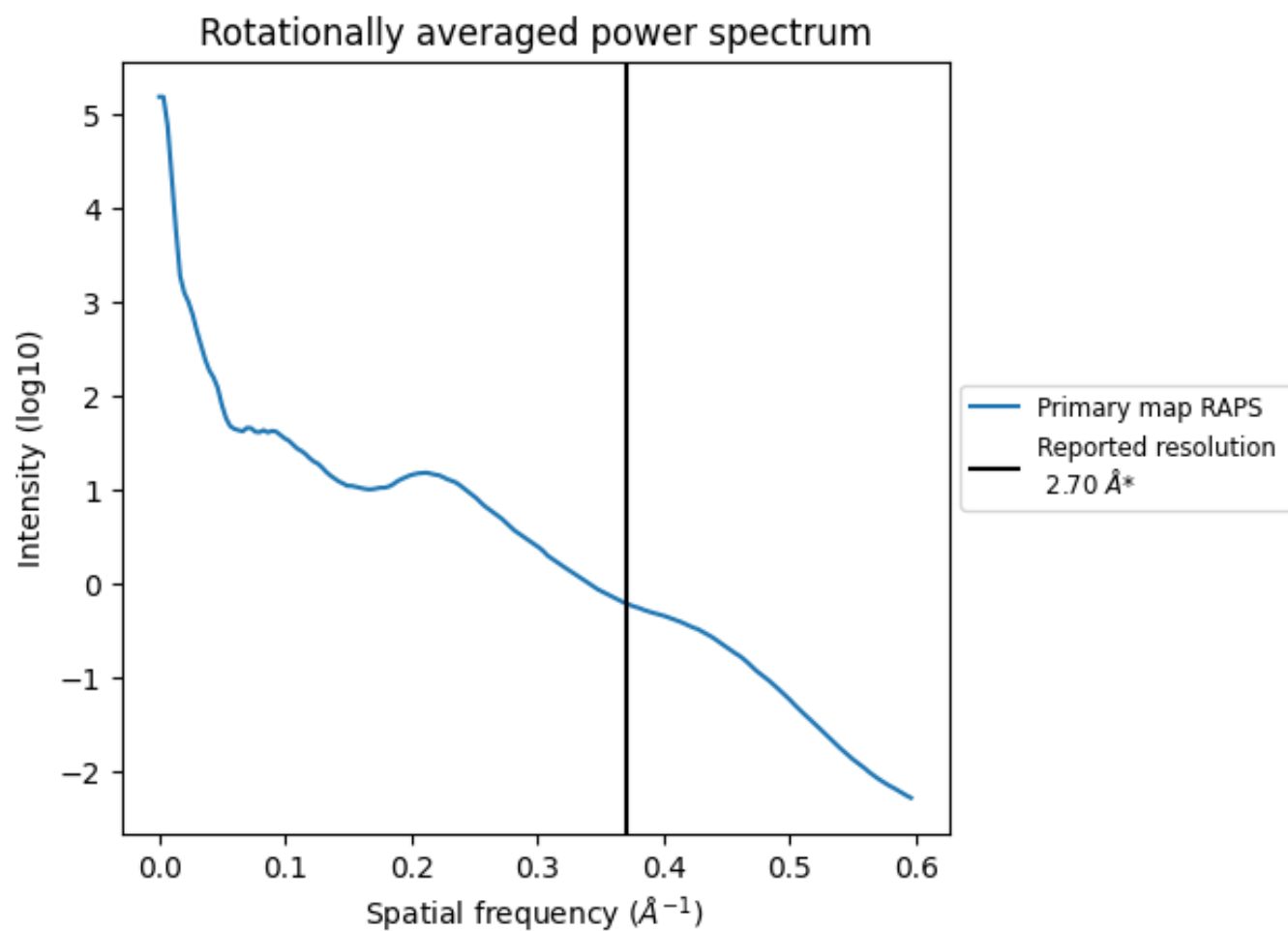
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 254 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 0.370 Å⁻¹

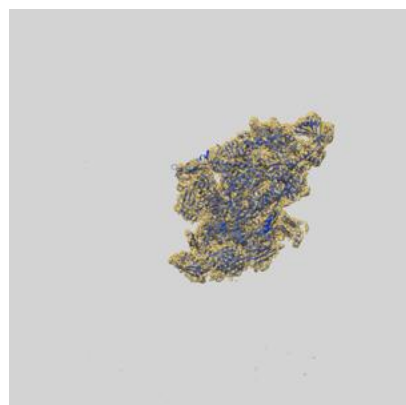
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

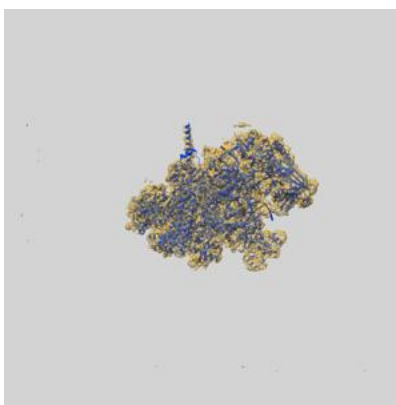
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51259 and PDB model 9GDA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

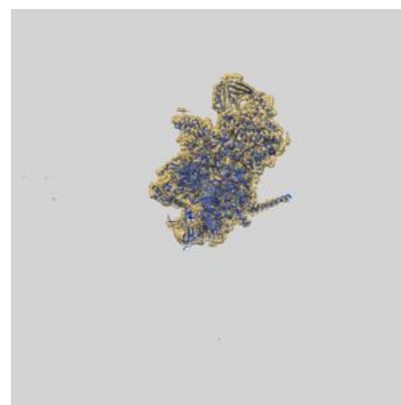
9.1 Map-model overlay [i](#)



X



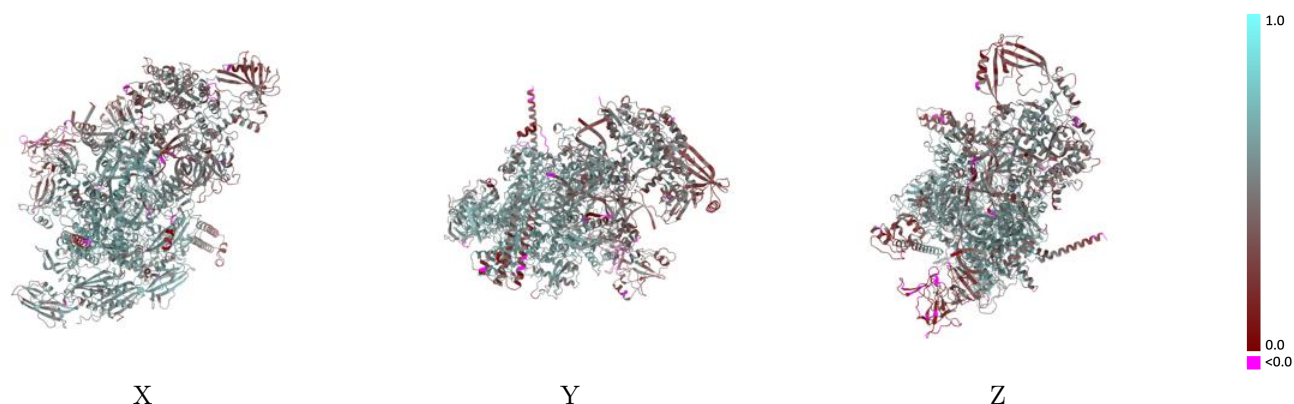
Y



Z

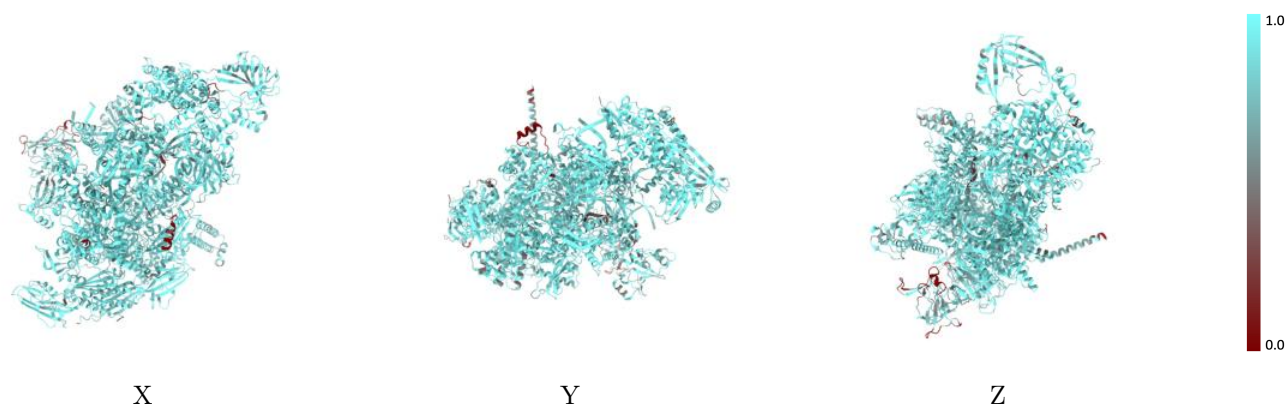
The images above show the 3D surface view of the map at the recommended contour level 0.724 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



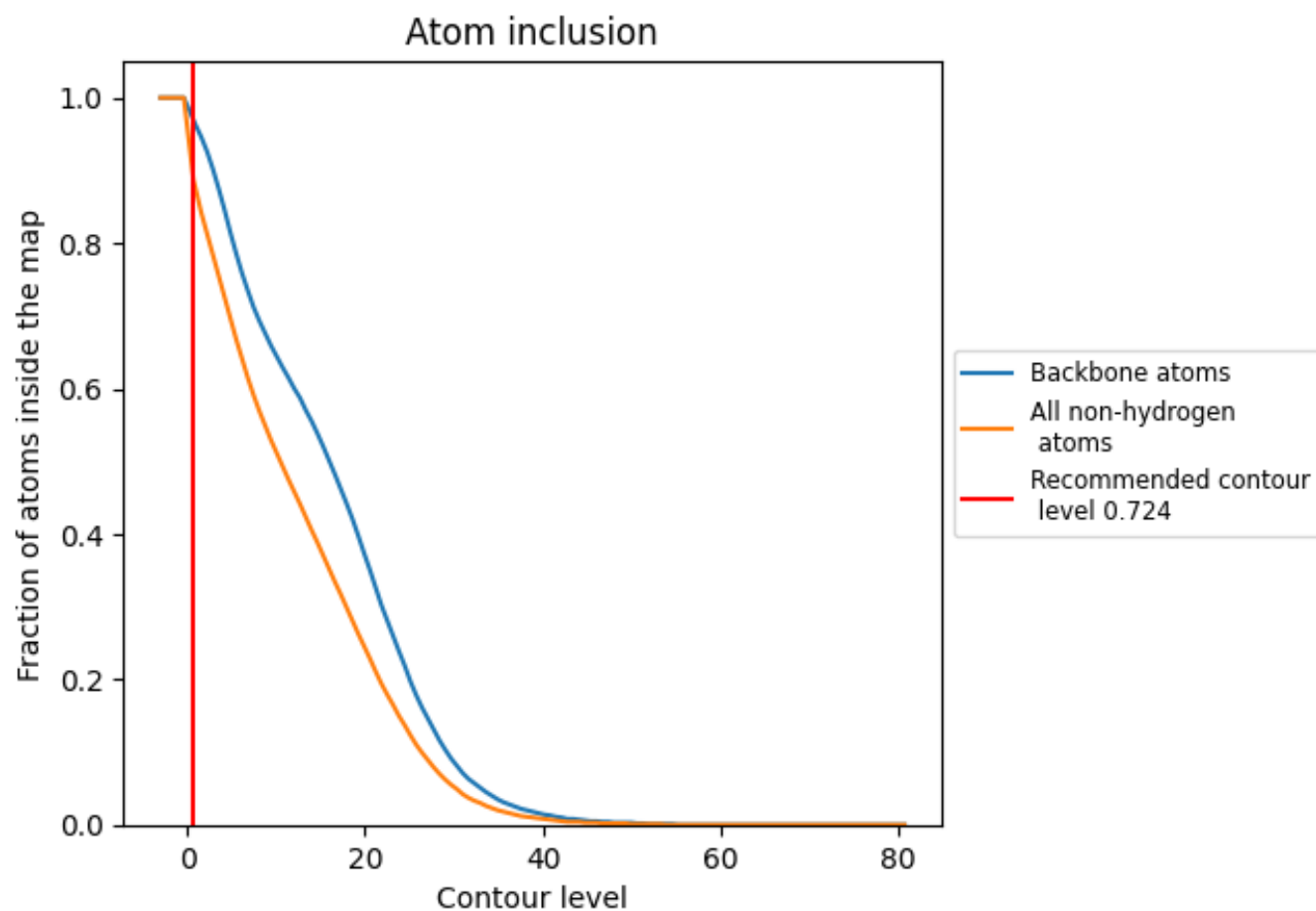
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.724).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.724) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8870</div>	<div><div></div>0.4870</div>
A	<div><div></div>0.9110</div>	<div><div></div>0.5530</div>
B	<div><div></div>0.8750</div>	<div><div></div>0.4890</div>
C	<div><div></div>0.8990</div>	<div><div></div>0.5190</div>
D	<div><div></div>0.8800</div>	<div><div></div>0.5010</div>
E	<div><div></div>0.8480</div>	<div><div></div>0.4780</div>
F	<div><div></div>0.8790</div>	<div><div></div>0.4060</div>
N	<div><div></div>0.8320</div>	<div><div></div>0.3670</div>
R	<div><div></div>0.9060</div>	<div><div></div>0.5050</div>
T	<div><div></div>0.9660</div>	<div><div></div>0.5050</div>

1.0

0.0

<0.0