



Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 04:25 PM JST

PDB ID : 9KDN / pdb_00009kdn
EMDB ID : EMD-62282
Title : The structure of 1 ACTD bound to RNA polymerase II elongation complex with 2 CTG repeats.
Authors : Xu, J.; Zhao, W.; Zhu, L.
Deposited on : 2024-11-03
Resolution : 2.96 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

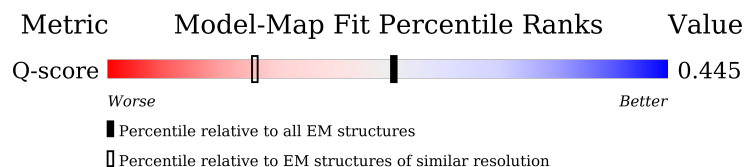
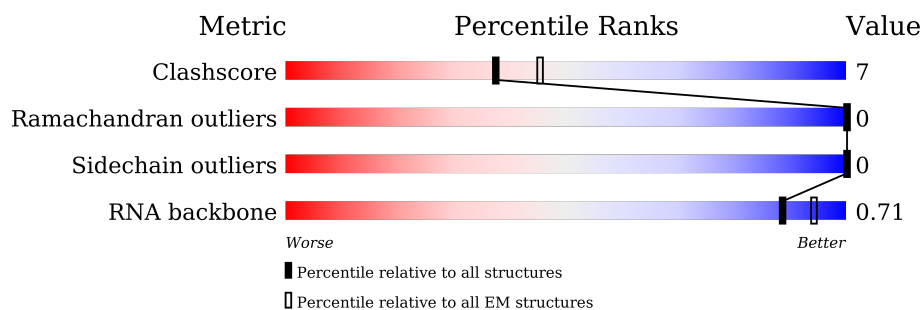
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	11	
14	N	46	
15	P	12	
16	T	46	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33014 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1418	Total	C	N	O	S	0	0
			11153	7029	1947	2115	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0
			9378	5929	1638	1756	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1332	823	238	269	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a protein called Actinomycin D.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	11	Total	C	N	O	0	0
			90	62	12	16		

- Molecule 14 is a DNA chain called NTS(non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	19	Total	C	N	O	P	0	0
			389	186	72	112	19		

- Molecule 15 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*AP*AP*GP*AP*GP*UP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	11	Total	C	N	O	P	0	0
			234	105	43	75	11		

- Molecule 16 is a DNA chain called TS(template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	31	Total	C	N	O	P	0	0
			631	304	104	192	31		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

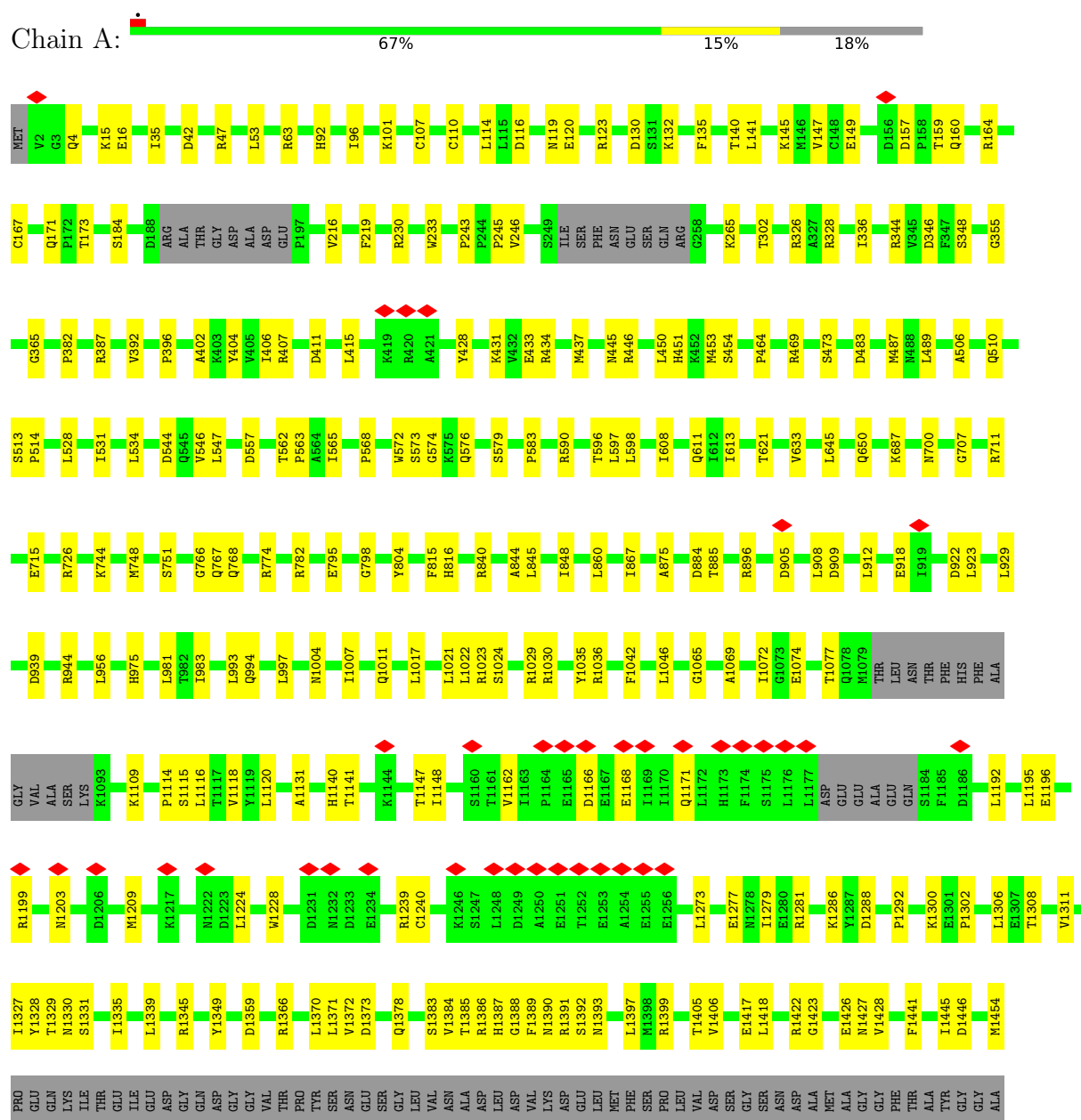
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

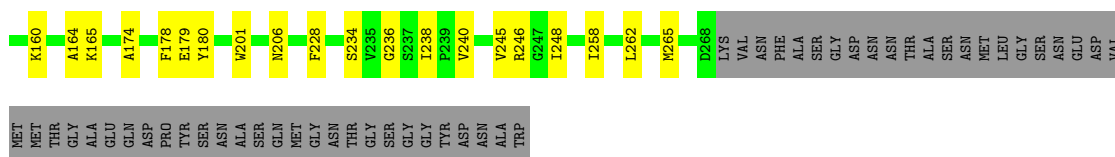
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

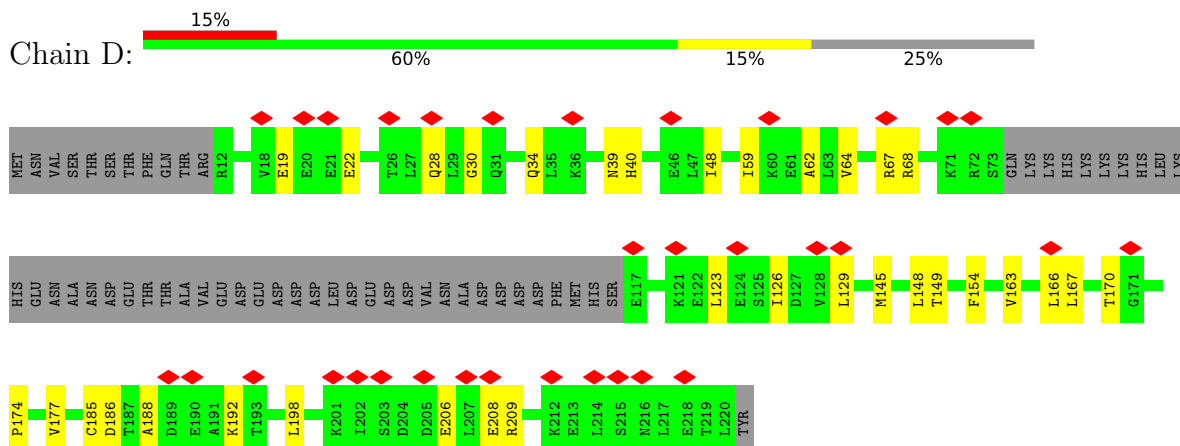
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

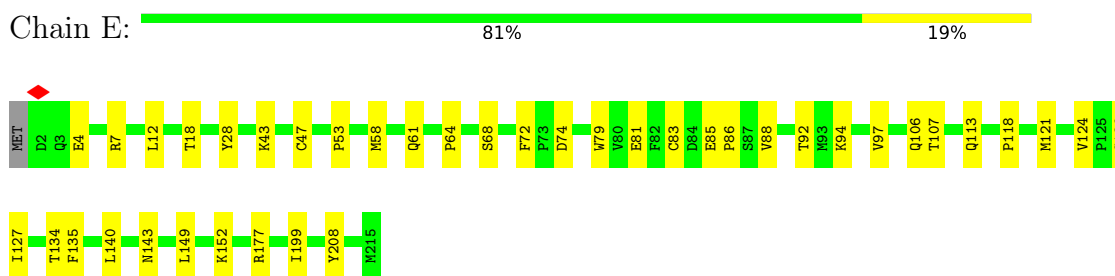




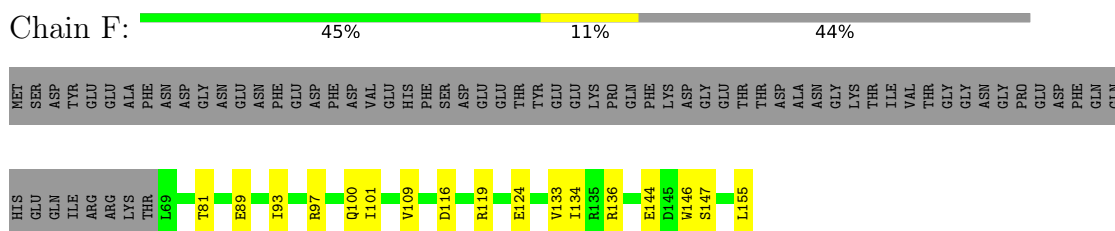
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



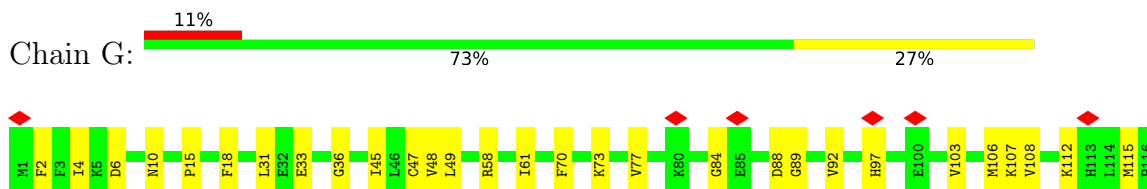
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

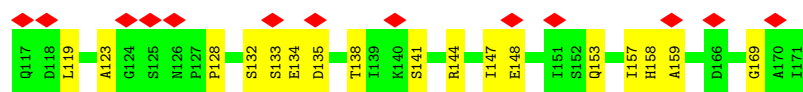


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

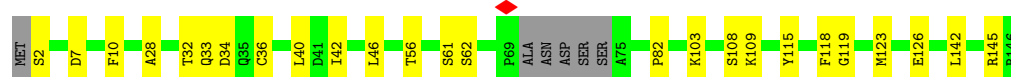
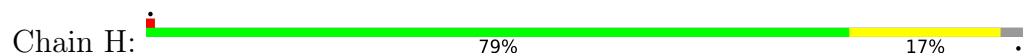


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

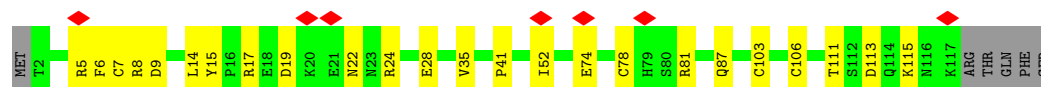
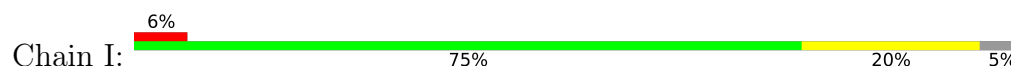




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



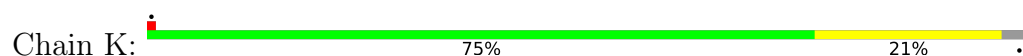
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



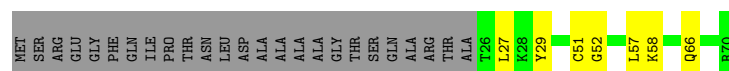
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

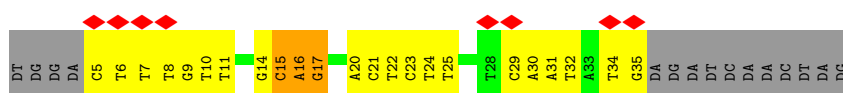


- Molecule 13: Actinomycin D



- Molecule 14: NTS(non-template strand)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.93, 0.93, 0.93	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, PXZ, MG, SAR, MVA, DVA

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	0.15	0/11352	0.30	0/15350
2	B	0.12	0/9563	0.29	0/12900
3	C	0.12	0/2124	0.29	0/2879
4	D	0.10	0/1340	0.28	0/1797
5	E	0.11	0/1788	0.28	0/2406
6	F	0.11	0/717	0.27	0/967
7	G	0.11	0/1367	0.32	0/1844
8	H	0.11	0/1139	0.26	0/1544
9	I	0.10	0/962	0.31	0/1295
10	J	0.11	0/578	0.26	0/775
11	K	0.11	0/942	0.26	0/1272
12	L	0.11	0/361	0.33	0/478
13	M	0.28	0/26	0.40	0/30
14	N	0.35	0/435	0.70	1/666 (0.2%)
15	P	0.09	0/261	0.22	0/404
16	T	0.30	0/704	0.65	4/1084 (0.4%)
All	All	0.14	0/33659	0.31	5/45691 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	31	DT	P-O3'-C3'	-8.05	108.12	120.20
16	T	16	DA	P-O3'-C3'	-7.90	108.36	120.20
16	T	14	DG	P-O3'-C3'	-6.53	110.40	120.20
16	T	17	DG	P-O3'-C3'	-6.11	111.03	120.20
16	T	15	DC	P-O3'-C3'	-5.43	112.06	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11153	0	11228	174	0
2	B	9378	0	9366	127	0
3	C	2086	0	2045	35	0
4	D	1332	0	1353	22	0
5	E	1752	0	1776	24	0
6	F	705	0	731	12	0
7	G	1339	0	1357	29	0
8	H	1120	0	1086	18	0
9	I	944	0	899	16	0
10	J	569	0	585	11	0
11	K	924	0	934	20	0
12	L	359	0	381	7	0
13	M	90	0	84	11	0
14	N	389	0	216	9	0
15	P	234	0	120	3	0
16	T	631	0	355	23	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	33014	0	32516	474	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 7.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.58	0.84
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.15	0.79
1:A:469:ARG:NH2	2:B:991:GLY:O	2.16	0.78
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.70	0.74
1:A:700:ASN:O	9:I:115:LYS:NZ	2.22	0.72
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.29	0.72
13:M:1:THR:HG23	14:N:32:DG:H2''	1.70	0.71
7:G:84:GLY:N	7:G:147:ILE:O	2.22	0.71
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.72	0.69
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.66	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.68
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.27	0.67
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.25	0.67
9:I:74:GLU:OE1	9:I:81:ARG:NH2	2.28	0.67
2:B:928:ARG:NH1	2:B:929:THR:O	2.28	0.67
2:B:996:ARG:NH1	3:C:174:ALA:O	2.22	0.66
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.29	0.66
9:I:28:GLU:HG3	9:I:35:VAL:HG22	1.77	0.66
3:C:22:LEU:HG	3:C:25:VAL:HG11	1.76	0.66
5:E:106:GLN:HG2	5:E:107:THR:HG23	1.78	0.66
1:A:140:THR:HG23	1:A:141:LEU:HD12	1.78	0.65
2:B:244:LEU:HD22	2:B:362:PRO:HB2	1.79	0.65
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.78	0.65
9:I:19:ASP:OD2	9:I:24:ARG:NH1	2.30	0.65
1:A:355:GLY:O	1:A:469:ARG:NH1	2.30	0.65
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.30	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.30	0.65
2:B:307:ASP:OD2	2:B:392:ARG:NH1	2.30	0.64
1:A:1109:LYS:NZ	13:M:9:PRO:O	2.30	0.63
14:N:35:DG:H2''	14:N:36:DA:C8	2.34	0.63
1:A:1115:SER:OG	1:A:1330:ASN:OD1	2.15	0.63
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.14	0.63
2:B:487:THR:OG1	2:B:777:ALA:O	2.17	0.63
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.32	0.62
1:A:1166:ASP:OD2	1:A:1239:ARG:NH1	2.32	0.62
1:A:344:ARG:NH1	16:T:21:DC:OP1	2.27	0.62
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.79	0.62
2:B:165:VAL:HB	2:B:448:ILE:HD13	1.81	0.62
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.31	0.62
1:A:473:SER:OG	1:A:650:GLN:NE2	2.32	0.62
14:N:30:DC:H42	16:T:17:DG:H1	1.45	0.62
2:B:287:ARG:NH1	2:B:321:GLY:O	2.33	0.62
2:B:792:MET:SD	2:B:857:ARG:NH2	2.73	0.61
13:M:11:MVA:HG12	13:M:11:MVA:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:VAL:HG13	3:C:40:GLU:HB2	1.83	0.61
7:G:115:MET:HG2	7:G:119:LEU:HD23	1.82	0.60
9:I:22:ASN:HB2	9:I:24:ARG:HH11	1.67	0.60
10:J:48:ARG:NH1	10:J:49:MET:SD	2.74	0.60
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.83	0.60
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.84	0.60
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.83	0.60
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.82	0.60
1:A:840:ARG:HD2	1:A:1384:VAL:O	2.02	0.59
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.35	0.59
4:D:48:ILE:HD11	7:G:4:ILE:HD11	1.85	0.59
1:A:896:ARG:HD2	1:A:1030:ARG:HH11	1.67	0.59
2:B:104:GLU:OE2	2:B:120:ARG:NH2	2.32	0.59
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.38	0.59
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.30	0.59
4:D:59:ILE:HD11	7:G:77:VAL:HG11	1.83	0.59
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.84	0.59
2:B:309:GLN:HE22	9:I:52:ILE:HD11	1.68	0.59
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.83	0.59
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.36	0.59
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.36	0.59
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.84	0.59
9:I:5:ARG:HG3	9:I:14:LEU:HD12	1.85	0.59
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.84	0.59
1:A:844:ALA:HA	1:A:1389:PHE:CD1	2.38	0.59
1:A:744:LYS:HG3	1:A:748:MET:HE2	1.85	0.58
6:F:116:ASP:HB3	6:F:119:ARG:HG2	1.85	0.58
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.86	0.58
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.28	0.58
4:D:126:ILE:HD13	4:D:149:THR:HG21	1.86	0.58
16:T:8:DT:H2''	16:T:9:DG:H5'	1.85	0.58
2:B:61:ASP:OD2	2:B:246:LYS:NZ	2.35	0.57
3:C:75:MET:O	3:C:246:ARG:NH2	2.32	0.57
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.85	0.57
2:B:304:ASP:HB3	2:B:307:ASP:HB2	1.85	0.57
1:A:451:HIS:O	1:A:454:SER:OG	2.20	0.57
1:A:782:ARG:NH2	2:B:699:GLU:O	2.36	0.57
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.85	0.57
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.87	0.57
2:B:638:PHE:HB2	2:B:741:CYS:HB3	1.87	0.56
3:C:262:LEU:HD12	3:C:265:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:LYS:NZ	4:D:198:LEU:O	2.34	0.56
5:E:121:MET:HE1	5:E:134:THR:HG21	1.87	0.56
1:A:402:ALA:HA	1:A:434:ARG:HA	1.86	0.56
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.88	0.56
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.87	0.56
10:J:1:MET:HA	10:J:56:LEU:HB2	1.86	0.56
16:T:24:DT:H2'	16:T:25:DT:H71	1.87	0.56
1:A:407:ARG:HH21	1:A:411:ASP:HB3	1.70	0.56
2:B:463:THR:OG1	2:B:465:ASN:OD1	2.19	0.56
7:G:133:SER:OG	7:G:134:GLU:OE1	2.22	0.56
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.88	0.56
2:B:214:ALA:HB3	2:B:498:THR:HG22	1.88	0.56
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.88	0.56
16:T:30:DA:C8	16:T:30:DA:H5''	2.41	0.55
4:D:167:LEU:O	4:D:170:THR:OG1	2.19	0.55
2:B:232:SER:O	2:B:261:ARG:NH1	2.38	0.55
2:B:868:MET:N	2:B:868:MET:SD	2.79	0.55
1:A:336:ILE:HG13	1:A:1405:THR:HG21	1.88	0.55
1:A:981:LEU:HD11	1:A:1042:PHE:HB2	1.89	0.55
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.37	0.55
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.39	0.55
16:T:15:DC:H2''	16:T:16:DA:C8	2.41	0.55
2:B:237:VAL:HG13	2:B:257:LYS:HG2	1.89	0.55
2:B:773:MET:HE1	2:B:987:LYS:HE3	1.89	0.54
1:A:562:THR:O	1:A:576:GLN:NE2	2.40	0.54
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.31	0.54
11:K:77:THR:OG1	11:K:81:TYR:O	2.26	0.54
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.26	0.54
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.72	0.54
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.89	0.54
11:K:102:LYS:NZ	11:K:106:GLU:OE2	2.37	0.54
2:B:1122:ARG:N	16:T:22:DT:OP1	2.41	0.54
1:A:1386:ARG:O	1:A:1391:ARG:HG2	2.08	0.54
2:B:101:MET:HE2	2:B:109:THR:HG22	1.90	0.54
2:B:857:ARG:NH1	16:T:24:DT:OP1	2.38	0.54
1:A:63:ARG:NE	1:A:63:ARG:O	2.41	0.54
1:A:939:ASP:OD2	1:A:1023:ARG:NE	2.32	0.54
7:G:132:SER:OG	7:G:135:ASP:OD1	2.26	0.54
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.72	0.53
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.91	0.53
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.88	0.53
1:A:147:VAL:HG13	1:A:149:GLU:HG2	1.88	0.53
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.90	0.53
14:N:31:DT:H2"	14:N:32:DG:C8	2.42	0.53
1:A:119:ASN:O	1:A:123:ARG:NH1	2.41	0.53
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.47	0.53
2:B:911:ILE:HG13	2:B:912:ILE:HG13	1.91	0.53
3:C:245:VAL:HG13	11:K:102:LYS:HE2	1.90	0.53
5:E:47:CYS:HA	5:E:53:PRO:HA	1.91	0.52
8:H:123:MET:HE2	8:H:142:LEU:HD13	1.92	0.52
1:A:404:TYR:HB2	1:A:433:GLU:HB3	1.92	0.52
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.42	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HA	1.90	0.52
2:B:722:ASP:OD1	2:B:722:ASP:N	2.42	0.52
12:L:27:LEU:HD13	12:L:58:LYS:HZ1	1.74	0.52
7:G:97:HIS:O	7:G:112:LYS:N	2.41	0.52
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.92	0.52
1:A:514:PRO:HB3	1:A:875:ALA:HB3	1.91	0.52
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.41	0.52
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.90	0.52
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.91	0.52
14:N:42:DG:N2	16:T:5:DC:O2	2.35	0.52
1:A:596:THR:OG1	1:A:598:LEU:O	2.21	0.52
2:B:901:PRO:HA	2:B:949:VAL:HG13	1.91	0.52
3:C:48:SER:OG	12:L:66:GLN:OE1	2.28	0.52
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.37	0.52
5:E:152:LYS:HB3	5:E:199:ILE:HB	1.92	0.52
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.93	0.51
1:A:1392:SER:O	1:A:1399:ARG:HD3	2.10	0.51
2:B:919:SER:OG	2:B:922:GLU:OE2	2.27	0.51
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.91	0.51
2:B:881:ASN:O	2:B:934:LYS:NZ	2.43	0.51
14:N:34:DT:H2"	14:N:35:DG:H5"	1.91	0.51
1:A:782:ARG:NH2	2:B:701:ILE:O	2.35	0.51
8:H:108:SER:OG	8:H:109:LYS:N	2.44	0.51
2:B:600:LEU:HB3	2:B:615:MET:SD	2.49	0.51
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.26	0.51
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.93	0.51
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.93	0.51
7:G:88:ASP:OD1	7:G:89:GLY:N	2.44	0.51
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:SER:HB3	3:C:160:LYS:HG2	1.92	0.51
1:A:579:SER:HB3	1:A:611:GLN:HA	1.92	0.50
3:C:55:THR:HG1	3:C:152:GLU:H	1.58	0.50
1:A:557:ASP:N	1:A:557:ASP:OD1	2.45	0.50
1:A:1148:ILE:N	1:A:1196:GLU:O	2.45	0.50
10:J:7:CYS:HA	10:J:49:MET:HG3	1.93	0.50
3:C:89:GLU:HG2	3:C:90:ASP:H	1.77	0.50
5:E:28:TYR:HA	5:E:64:PRO:HA	1.93	0.50
2:B:51:PHE:HB2	2:B:173:MET:HE3	1.94	0.50
1:A:1385:THR:HG21	13:M:2:DVA:CG1	2.42	0.50
2:B:643:ASP:OD2	2:B:654:ARG:NH2	2.45	0.50
3:C:6:PRO:O	11:K:104:ASN:ND2	2.44	0.50
7:G:138:THR:O	7:G:141:SER:OG	2.29	0.50
13:M:6:PXZ:N2	14:N:32:DG:H2'	2.26	0.50
2:B:289:LEU:HD22	2:B:356:LEU:HD13	1.93	0.50
3:C:10:ILE:HA	3:C:20:PHE:HA	1.94	0.49
3:C:66:ARG:NH2	3:C:143:LEU:O	2.32	0.49
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.94	0.49
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.27	0.49
7:G:153:GLN:HG3	7:G:158:HIS:CD2	2.47	0.49
1:A:1378:GLN:OE1	5:E:177:ARG:NH1	2.46	0.49
2:B:59:LEU:HD11	2:B:170:LEU:HD22	1.94	0.49
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.94	0.49
13:M:3:PRO:HG2	16:T:16:DA:C5'	2.42	0.49
1:A:157:ASP:OD1	1:A:160:GLN:NE2	2.45	0.49
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.47	0.49
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.47	0.49
4:D:62:ALA:HB2	7:G:49:LEU:HD13	1.95	0.49
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.28	0.49
2:B:360:PHE:HZ	2:B:378:LEU:HD13	1.76	0.49
1:A:908:LEU:HA	1:A:1029:ARG:HH12	1.77	0.49
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.95	0.49
11:K:53:ASP:OD1	11:K:54:ARG:N	2.46	0.49
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.77	0.49
1:A:573:SER:OG	8:H:119:GLY:O	2.16	0.49
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.95	0.49
2:B:895:ASP:HB2	12:L:27:LEU:HD11	1.95	0.49
1:A:445:ASN:OD1	1:A:446:ARG:N	2.46	0.49
2:B:459:TYR:OH	2:B:465:ASN:ND2	2.37	0.49
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.48	0.48
2:B:510:LYS:HB3	2:B:513:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:2:SER:HA	8:H:62:SER:HB3	1.96	0.48
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.48
1:A:265:LYS:NZ	1:A:302:THR:OG1	2.42	0.48
1:A:583:PRO:HD3	1:A:645:LEU:HD13	1.95	0.48
2:B:311:LEU:O	2:B:315:LYS:HG2	2.12	0.48
3:C:148:ARG:HG2	3:C:149:LYS:H	1.78	0.48
5:E:18:THR:HG22	5:E:143:ASN:HB2	1.94	0.48
2:B:343:ILE:HB	2:B:348:ARG:HE	1.77	0.48
4:D:64:VAL:HG12	4:D:129:LEU:HD11	1.96	0.48
8:H:2:SER:N	8:H:61:SER:OG	2.47	0.48
1:A:1030:ARG:HH21	1:A:1035:TYR:HH	1.57	0.48
7:G:92:VAL:HG11	7:G:107:LYS:HZ2	1.79	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
2:B:1129:ARG:HG2	16:T:20:DA:O5'	2.14	0.48
14:N:30:DC:H2''	14:N:31:DT:C6	2.49	0.48
16:T:31:DA:H2''	16:T:32:DT:C5	2.49	0.48
1:A:1345:ARG:NE	1:A:1373:ASP:OD1	2.38	0.48
2:B:644:GLU:OE1	2:B:644:GLU:N	2.45	0.48
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.47
3:C:71:PRO:HG3	10:J:13:VAL:HG21	1.96	0.47
11:K:114:LEU:H	11:K:114:LEU:HD23	1.78	0.47
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.95	0.47
1:A:707:GLY:HA2	1:A:1281:ARG:HD3	1.96	0.47
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.95	0.47
5:E:118:PRO:HG2	16:T:6:DT:H5'	1.97	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.96	0.47
2:B:978:ASP:OD2	2:B:1094:ARG:NH2	2.47	0.47
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.15	0.47
4:D:148:LEU:HD21	7:G:2:PHE:HE2	1.79	0.47
1:A:909:ASP:HB3	1:A:912:LEU:HG	1.97	0.47
1:A:1386:ARG:HA	1:A:1390:ASN:CB	2.44	0.47
2:B:848:ARG:HH22	2:B:996:ARG:HE	1.62	0.47
2:B:951:GLN:HE21	12:L:57:LEU:HD22	1.77	0.47
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.97	0.47
1:A:4:GLN:NE2	2:B:1159:ARG:H	2.13	0.47
1:A:157:ASP:OD2	1:A:159:THR:OG1	2.32	0.47
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.46	0.47
1:A:922:ASP:OD1	1:A:923:LEU:N	2.48	0.47
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.97	0.47
4:D:174:PRO:HA	4:D:177:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:29:DC:H2''	16:T:30:DA:C5	2.50	0.47
16:T:8:DT:H2''	16:T:9:DG:C8	2.49	0.47
1:A:42:ASP:OD2	1:A:47:ARG:NH1	2.48	0.47
1:A:116:ASP:H	1:A:164:ARG:HH12	1.62	0.47
5:E:126:SER:OG	5:E:127:ILE:N	2.46	0.47
2:B:904:ARG:NH1	12:L:66:GLN:O	2.47	0.47
4:D:126:ILE:HD12	4:D:145:MET:HG3	1.97	0.47
15:P:5:A:H2'	15:P:6:A:C8	2.50	0.47
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.50	0.46
1:A:568:PRO:HD2	8:H:46:LEU:HG	1.97	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.97	0.46
1:A:767:GLN:NE2	1:A:768:GLN:O	2.47	0.46
2:B:819:ALA:O	2:B:1093:GLN:HG3	2.15	0.46
4:D:123:LEU:HA	4:D:126:ILE:HG12	1.98	0.46
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.97	0.46
1:A:130:ASP:OD1	1:A:130:ASP:N	2.47	0.46
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.96	0.46
2:B:936:ASP:OD1	2:B:938:SER:OG	2.21	0.46
10:J:48:ARG:O	10:J:52:THR:OG1	2.27	0.46
1:A:1386:ARG:HG3	1:A:1387:HIS:N	2.31	0.46
2:B:883:LEU:HD21	2:B:928:ARG:HD3	1.97	0.46
2:B:762:ASN:HD21	2:B:984:HIS:HB3	1.80	0.46
5:E:68:SER:O	5:E:72:PHE:N	2.37	0.46
5:E:74:ASP:N	5:E:74:ASP:OD1	2.49	0.46
10:J:58:GLU:O	10:J:62:ARG:HG2	2.15	0.46
16:T:22:DT:H2'	16:T:23:DC:H6	1.81	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.96	0.46
6:F:109:VAL:HG11	6:F:124:GLU:HA	1.98	0.46
3:C:16:ASP:OD1	3:C:16:ASP:N	2.49	0.45
13:M:2:DVA:HA	13:M:3:PRO:HA	1.80	0.45
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.98	0.45
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.16	0.45
6:F:133:VAL:HG12	6:F:147:SER:HA	1.98	0.45
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.16	0.45
9:I:111:THR:HG23	9:I:113:ASP:H	1.82	0.45
1:A:348:SER:HA	1:A:489:LEU:O	2.17	0.45
1:A:994:GLN:OE1	1:A:1023:ARG:NH1	2.49	0.45
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.97	0.45
3:C:234:SER:OG	3:C:238:ILE:O	2.34	0.45
7:G:47:CYS:SG	7:G:48:VAL:N	2.90	0.45
2:B:865:LYS:HG2	2:B:871:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:106:MET:HE3	7:G:157:ILE:HG13	1.98	0.45
1:A:173:THR:OG1	1:A:184:SER:OG	2.23	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.99	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	1.99	0.45
2:B:924:GLU:O	2:B:928:ARG:HB3	2.15	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.52	0.45
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.52	0.45
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.98	0.45
13:M:3:PRO:HB2	16:T:16:DA:O4'	2.17	0.45
1:A:1168:GLU:HA	1:A:1171:GLN:HG3	1.99	0.45
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.57	0.45
3:C:145:CYS:SG	3:C:146:LYS:N	2.90	0.45
5:E:121:MET:HE2	5:E:124:VAL:HG21	1.99	0.45
1:A:396:PRO:HD3	1:A:415:LEU:HB3	1.99	0.44
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.99	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG11	1.99	0.44
6:F:97:ARG:O	6:F:101:ILE:HG12	2.17	0.44
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.81	0.44
1:A:1386:ARG:O	1:A:1390:ASN:HB3	2.17	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.99	0.44
14:N:35:DG:H2''	14:N:36:DA:H8	1.82	0.44
1:A:114:LEU:HD23	1:A:145:LYS:HG3	2.00	0.44
1:A:246:VAL:O	1:A:328:ARG:NH2	2.45	0.44
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.99	0.44
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.99	0.44
1:A:1209:MET:HE3	1:A:1228:TRP:HB2	1.99	0.44
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.53	0.44
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.00	0.44
1:A:1329:THR:HG22	1:A:1331:SER:H	1.82	0.44
2:B:760:ASP:OD1	2:B:760:ASP:N	2.50	0.44
8:H:56:THR:HB	8:H:145:ARG:HG2	1.99	0.44
10:J:17:LYS:HB3	10:J:39:LEU:HD13	2.00	0.44
1:A:120:GLU:HA	1:A:123:ARG:NH2	2.32	0.44
1:A:230:ARG:HD3	1:A:233:TRP:CZ2	2.52	0.44
1:A:1422:ARG:HD3	2:B:1224:PHE:CD2	2.53	0.44
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.53	0.44
5:E:43:LYS:O	5:E:47:CYS:HB3	2.18	0.44
13:M:9:PRO:HA	13:M:10:SAR:HA3	1.71	0.44
1:A:528:LEU:O	1:A:531:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.00	0.44
1:A:114:LEU:O	1:A:164:ARG:NH2	2.51	0.44
1:A:597:LEU:HD23	8:H:115:TYR:CZ	2.52	0.44
7:G:31:LEU:C	7:G:33:GLU:H	2.26	0.44
1:A:528:LEU:HB3	1:A:751:SER:HB3	2.00	0.43
1:A:885:THR:HG23	1:A:1024:SER:HB2	2.00	0.43
9:I:15:TYR:OH	9:I:17:ARG:NH2	2.51	0.43
11:K:20:LYS:HG2	11:K:34:THR:HB	2.00	0.43
1:A:101:LYS:HD3	1:A:135:PHE:HE2	1.83	0.43
2:B:796:LEU:HB2	2:B:799:PRO:HG3	2.01	0.43
1:A:544:ASP:N	1:A:544:ASP:OD1	2.51	0.43
1:A:905:ASP:OD1	1:A:905:ASP:N	2.49	0.43
1:A:918:GLU:N	1:A:918:GLU:OE1	2.52	0.43
1:A:1454:MET:SD	1:A:1454:MET:N	2.91	0.43
2:B:72:GLU:HG2	2:B:74:LEU:HD22	2.00	0.43
5:E:135:PHE:HB3	5:E:140:LEU:HD11	2.00	0.43
1:A:132:LYS:NZ	1:A:1417:GLU:OE2	2.42	0.43
1:A:1072:ILE:HD13	1:A:1371:LEU:HD22	2.01	0.43
4:D:22:GLU:HG2	4:D:28:GLN:O	2.18	0.43
13:M:8:DVA:HA	13:M:9:PRO:HA	1.91	0.43
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.52	0.43
4:D:185:CYS:SG	4:D:186:ASP:N	2.92	0.43
8:H:82:PRO:O	11:K:54:ARG:NH2	2.52	0.43
15:P:7:G:H2'	15:P:8:A:C8	2.54	0.43
16:T:6:DT:H2'	16:T:7:DT:H71	2.00	0.43
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.01	0.43
1:A:365:GLY:N	1:A:469:ARG:O	2.29	0.43
1:A:1386:ARG:HA	1:A:1390:ASN:HB3	2.01	0.43
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.84	0.43
2:B:641:GLU:OE2	2:B:654:ARG:NH2	2.51	0.43
2:B:1133:MET:HA	2:B:1136:ASP:OD2	2.19	0.43
3:C:165:LYS:O	11:K:6:ARG:NH2	2.50	0.43
4:D:67:ARG:HH21	4:D:68:ARG:NH1	2.16	0.43
4:D:166:LEU:O	4:D:170:THR:HG23	2.19	0.43
11:K:61:TYR:HB3	11:K:73:LEU:HD13	2.00	0.43
16:T:23:DC:H2'	16:T:24:DT:C6	2.54	0.43
2:B:751:VAL:HG13	2:B:812:LEU:HD22	2.01	0.42
1:A:92:HIS:O	1:A:96:ILE:HG13	2.19	0.42
2:B:906:SER:O	2:B:941:LEU:HD23	2.18	0.42
2:B:986:GLN:NE2	2:B:1022:THR:OG1	2.52	0.42
4:D:154:PHE:CZ	4:D:163:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:THR:OG1	6:F:146:TRP:NE1	2.51	0.42
7:G:103:VAL:O	7:G:106:MET:HG2	2.19	0.42
9:I:7:CYS:HB2	9:I:14:LEU:HD21	2.01	0.42
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.54	0.42
2:B:298:LEU:HD12	9:I:6:PHE:CZ	2.54	0.42
7:G:84:GLY:H	7:G:148:GLU:HA	1.83	0.42
1:A:860:LEU:HD21	1:A:1393:ASN:O	2.18	0.42
1:A:993:LEU:O	1:A:997:LEU:HG	2.19	0.42
1:A:534:LEU:O	1:A:574:GLY:HA3	2.19	0.42
2:B:1041:GLU:OE1	2:B:1041:GLU:N	2.44	0.42
4:D:19:GLU:N	4:D:19:GLU:OE1	2.52	0.42
1:A:1385:THR:HG21	13:M:2:DVA:HG12	2.02	0.42
2:B:953:LEU:O	2:B:964:VAL:HA	2.20	0.42
5:E:12:LEU:HG	5:E:58:MET:HE1	2.01	0.42
2:B:365:THR:HG21	2:B:370:PHE:HB2	2.01	0.42
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.42
2:B:886:LYS:HD2	2:B:940:PRO:HG3	2.01	0.42
7:G:36:GLY:CA	7:G:45:ILE:O	2.67	0.42
15:P:7:G:H2'	15:P:8:A:H8	1.84	0.42
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.02	0.42
3:C:180:TYR:HB3	3:C:228:PHE:CD2	2.55	0.42
3:C:234:SER:HB2	3:C:240:VAL:HB	2.01	0.42
1:A:506:ALA:O	1:A:510:GLN:HG2	2.20	0.42
2:B:954:VAL:HG12	2:B:964:VAL:HG12	2.01	0.42
5:E:94:LYS:HA	5:E:97:VAL:HG12	2.00	0.42
7:G:144:ARG:NH1	7:G:169:GLY:O	2.52	0.42
2:B:496:ARG:NH1	2:B:540:SER:O	2.44	0.41
1:A:944:ARG:NH1	1:A:1292:PRO:HB3	2.34	0.41
1:A:1328:TYR:HD1	5:E:149:LEU:HD11	1.86	0.41
2:B:244:LEU:HD23	2:B:244:LEU:H	1.85	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.02	0.41
16:T:22:DT:H2'	16:T:23:DC:C6	2.55	0.41
1:A:382:PRO:HG3	1:A:428:TYR:CZ	2.55	0.41
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.56	0.41
2:B:581:PHE:N	2:B:624:LEU:O	2.46	0.41
2:B:693:ILE:HG21	2:B:701:ILE:HD13	2.02	0.41
5:E:4:GLU:HA	5:E:7:ARG:HG2	2.02	0.41
1:A:450:LEU:HD13	1:A:1077:THR:HG21	2.02	0.41
1:A:464:PRO:O	11:K:4:PRO:HD3	2.20	0.41
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	2.01	0.41
4:D:30:GLY:O	4:D:34:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:CYS:SG	5:E:88:VAL:HG22	2.61	0.41
11:K:27:ALA:HB3	11:K:74:ARG:HH22	1.85	0.41
12:L:51:CYS:SG	12:L:52:GLY:N	2.93	0.41
1:A:975:HIS:CD2	1:A:1036:ARG:HD2	2.56	0.41
1:A:1288:ASP:OD2	1:A:1300:LYS:HB3	2.20	0.41
1:A:1359:ASP:OD1	1:A:1359:ASP:N	2.47	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:105:SER:HB2	2:B:960:GLY:HA3	2.02	0.41
7:G:15:PRO:HA	7:G:18:PHE:HE2	1.85	0.41
1:A:687:LYS:NZ	1:A:795:GLU:OE1	2.49	0.41
1:A:1192:LEU:HD21	1:A:1239:ARG:HG2	2.02	0.41
2:B:974:PRO:HB3	2:B:980:PHE:HZ	1.84	0.41
3:C:84:ARG:HD3	11:K:11:LEU:HD11	2.03	0.41
4:D:188:ALA:HB2	4:D:208:GLU:HB2	2.02	0.41
16:T:29:DC:H2''	16:T:30:DA:OP1	2.21	0.41
1:A:1004:ASN:OD1	1:A:1007:ILE:HG12	2.20	0.41
1:A:1199:ARG:HG3	1:A:1203:ASN:ND2	2.36	0.41
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.54	0.41
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.56	0.41
1:A:92:HIS:CE1	2:B:1211:ASN:HB3	2.55	0.41
1:A:451:HIS:ND1	1:A:453:MET:HB2	2.36	0.41
1:A:1147:THR:HG21	1:A:1195:LEU:HD23	2.02	0.41
2:B:541:LEU:HD21	2:B:812:LEU:HD21	2.02	0.41
2:B:592:ASN:OD1	2:B:595:ARG:NH1	2.54	0.41
2:B:821:GLN:OE1	2:B:851:PHE:N	2.54	0.41
2:B:899:ILE:HD12	2:B:911:ILE:HG22	2.03	0.41
3:C:142:VAL:HG13	10:J:15:GLY:HA3	2.03	0.41
6:F:155:LEU:H	6:F:155:LEU:HD23	1.86	0.41
8:H:34:ASP:OD1	8:H:34:ASP:N	2.53	0.41
16:T:34:DT:H2''	16:T:35:DG:C8	2.56	0.41
1:A:453:MET:HE3	1:A:513:SER:HB2	2.02	0.41
1:A:483:ASP:HB2	2:B:987:LYS:HG3	2.02	0.41
1:A:1141:THR:OG1	1:A:1273:LEU:HB2	2.21	0.41
16:T:10:DT:H2'	16:T:11:DT:H72	2.03	0.41
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.36	0.40
1:A:944:ARG:HH12	1:A:1292:PRO:HB3	1.86	0.40
8:H:118:PHE:HZ	8:H:123:MET:HE3	1.86	0.40
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.38	0.40
1:A:867:ILE:HG22	5:E:208:TYR:HE1	1.86	0.40
1:A:387:ARG:HH21	1:A:437:MET:HE1	1.85	0.40
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:HG21	9:I:41:PRO:HG3	2.02	0.40
2:B:69:LEU:O	2:B:89:GLU:HA	2.21	0.40
2:B:129:PHE:HB3	2:B:164:LYS:HB2	2.02	0.40
2:B:806:THR:H	2:B:809:MET:HE3	1.87	0.40
8:H:7:ASP:OD1	8:H:7:ASP:N	2.53	0.40
9:I:8:ARG:NH1	9:I:9:ASP:HB2	2.37	0.40
1:A:35:ILE:HG21	1:A:53:LEU:HD23	2.02	0.40
1:A:1140:HIS:NE2	1:A:1277:GLU:OE2	2.54	0.40
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.54	0.40
2:B:839:MET:O	2:B:991:GLY:N	2.46	0.40
7:G:10:ASN:HA	7:G:70:PHE:O	2.21	0.40
1:A:565:ILE:HG21	8:H:46:LEU:HD23	2.04	0.40
1:A:1120:LEU:HD11	1:A:1131:ALA:HB2	2.04	0.40
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	2.04	0.40
2:B:77:HIS:HB2	2:B:79:THR:O	2.21	0.40
2:B:168:GLY:HA2	2:B:450:ALA:HB1	2.04	0.40
2:B:199:MET:SD	2:B:199:MET:N	2.83	0.40
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.25	0.40
6:F:89:GLU:O	6:F:93:ILE:HG12	2.22	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	1408/1733 (81%)	1373 (98%)	35 (2%)	0	100	100
2	B	1164/1224 (95%)	1128 (97%)	36 (3%)	0	100	100
3	C	263/318 (83%)	256 (97%)	7 (3%)	0	100	100
4	D	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
5	E	212/215 (99%)	207 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	85/155 (55%)	83 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
8	H	136/146 (93%)	133 (98%)	3 (2%)	0	100	100
9	I	114/122 (93%)	107 (94%)	7 (6%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
13	M	2/11 (18%)	2 (100%)	0	0	100	100
All	All	3938/4576 (86%)	3832 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1240/1520 (82%)	1240 (100%)	0	100	100
2	B	1022/1061 (96%)	1022 (100%)	0	100	100
3	C	233/274 (85%)	233 (100%)	0	100	100
4	D	148/200 (74%)	148 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	4/4 (100%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3508/4013 (87%)	3508 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	171	GLN
1	A	339	ASN
1	A	399	HIS
1	A	435	HIS
1	A	515	GLN
1	A	611	GLN
1	A	659	HIS
1	A	786	HIS
1	A	877	HIS
1	A	903	ASN
1	A	975	HIS
1	A	1106	ASN
1	A	1203	ASN
1	A	1387	HIS
2	B	110	HIS
2	B	115	GLN
2	B	300	HIS
2	B	357	GLN
2	B	366	GLN
2	B	513	GLN
2	B	951	GLN
2	B	1104	HIS
3	C	195	GLN
4	D	28	GLN
4	D	138	ASN
4	D	200	ASN
5	E	101	GLN
5	E	115	ASN
7	G	96	GLN
7	G	122	ASN
7	G	158	HIS
8	H	11	GLN
8	H	35	GLN
8	H	83	GLN

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Mol	Chain	Res	Type
8	H	133	ASN
8	H	139	ASN
9	I	90	GLN
9	I	108	HIS
11	K	29	ASN
11	K	110	ASN
11	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/12 (83%)	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 ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	DVA	M	8	13	4,6,7	0.51	0	6,7,9	0.65	0
13	DVA	M	2	13	4,6,7	0.63	0	6,7,9	0.65	0
13	SAR	M	4	13	4,4,5	1.11	0	1,3,5	2.71	1 (100%)
13	MVA	M	11	13	6,7,8	1.08	1 (16%)	7,8,10	2.07	3 (42%)
13	MVA	M	5	13	6,7,8	0.80	0	7,8,10	1.30	2 (28%)
13	SAR	M	10	13	4,4,5	1.06	0	1,3,5	2.68	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DVA	M	8	13	-	5/5/6/8	-
13	DVA	M	2	13	-	3/5/6/8	-
13	SAR	M	4	13	-	1/1/2/3	-
13	MVA	M	11	13	-	5/6/8/10	-
13	MVA	M	5	13	-	6/6/8/10	-
13	SAR	M	10	13	-	1/1/2/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	11	MVA	O-C	2.57	1.30	1.19

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	11	MVA	O-C-CA	-4.25	112.98	124.83
13	M	4	SAR	O-C-CA	-2.71	117.57	125.42
13	M	10	SAR	O-C-CA	-2.68	117.66	125.42
13	M	5	MVA	CB-CA-N	-2.42	108.01	111.17
13	M	11	MVA	C-CA-N	2.31	118.61	110.88
13	M	11	MVA	CB-CA-C	-2.14	110.36	113.04
13	M	5	MVA	CG1-CB-CA	2.03	114.32	111.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	2	DVA	N-CA-CB-CG2
13	M	2	DVA	C-CA-CB-CG1
13	M	2	DVA	C-CA-CB-CG2
13	M	4	SAR	C-CA-N-CN
13	M	5	MVA	N-CA-CB-CG1
13	M	5	MVA	N-CA-CB-CG2
13	M	5	MVA	C-CA-CB-CG1
13	M	5	MVA	C-CA-CB-CG2
13	M	8	DVA	N-CA-CB-CG1
13	M	8	DVA	N-CA-CB-CG2
13	M	8	DVA	C-CA-CB-CG1
13	M	8	DVA	C-CA-CB-CG2
13	M	10	SAR	C-CA-N-CN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	M	11	MVA	CB-CA-N-CN
13	M	11	MVA	N-CA-CB-CG1
13	M	11	MVA	N-CA-CB-CG2
13	M	11	MVA	C-CA-CB-CG1
13	M	11	MVA	C-CA-CB-CG2
13	M	5	MVA	CB-CA-N-CN
13	M	5	MVA	O-C-CA-CB
13	M	8	DVA	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	8	DVA	1	0
13	M	2	DVA	3	0
13	M	11	MVA	1	0
13	M	10	SAR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

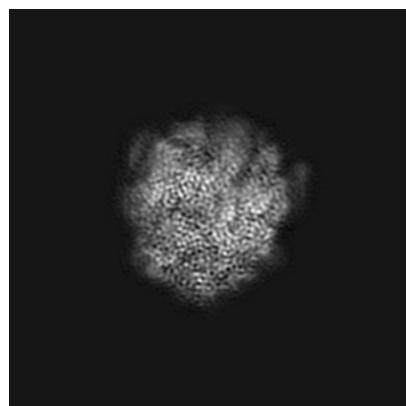
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62282. These allow visual inspection of the internal detail of the map and identification of artifacts.

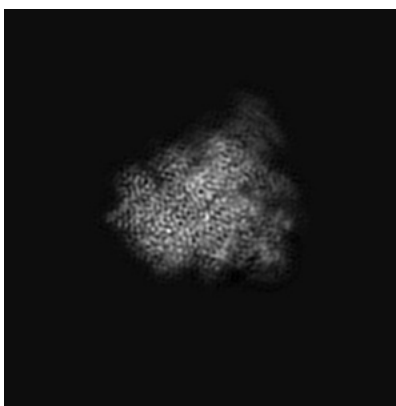
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

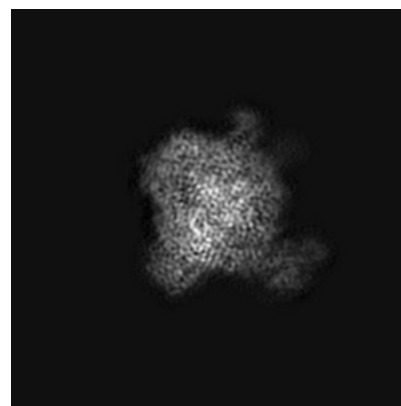
6.1.1 Primary map



X

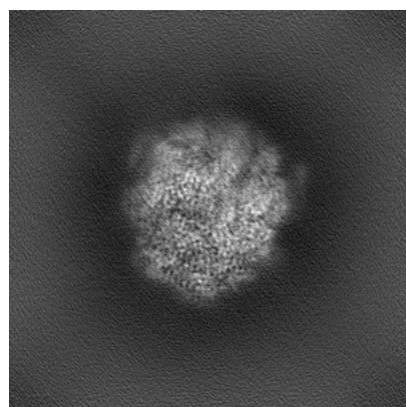


Y

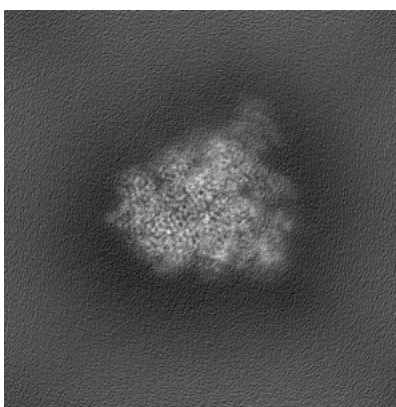


Z

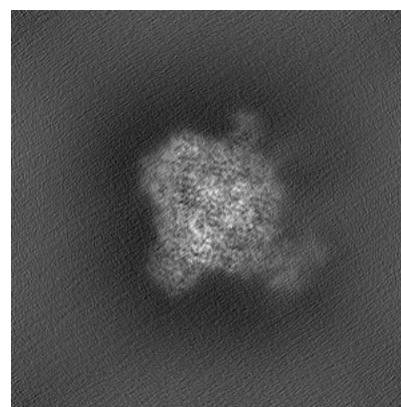
6.1.2 Raw map



X



Y

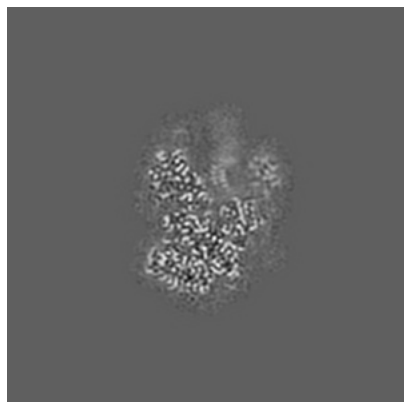


Z

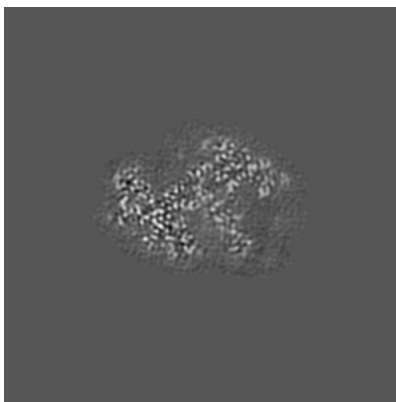
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

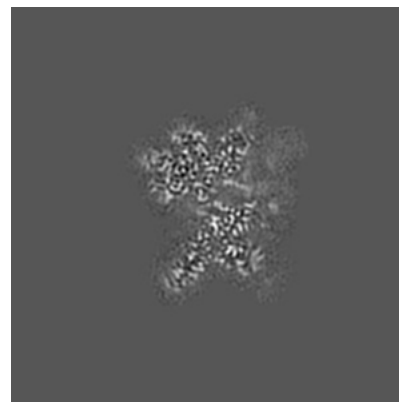
6.2.1 Primary map



X Index: 160

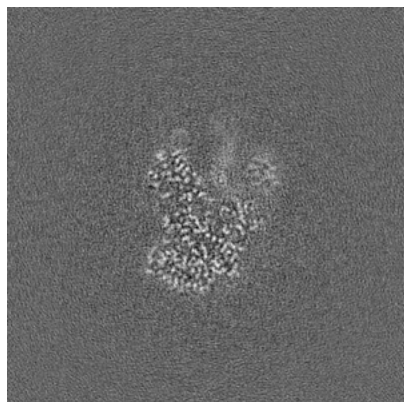


Y Index: 160

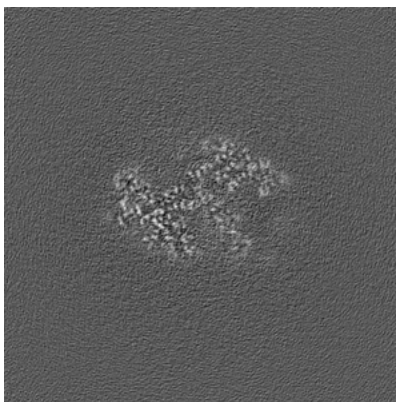


Z Index: 160

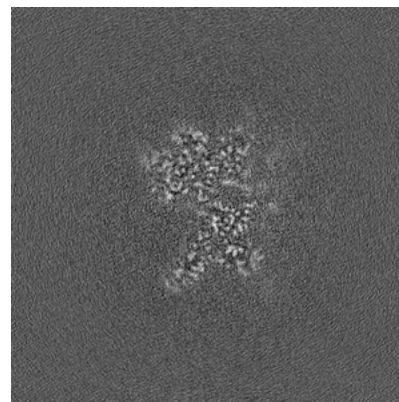
6.2.2 Raw map



X Index: 160



Y Index: 160

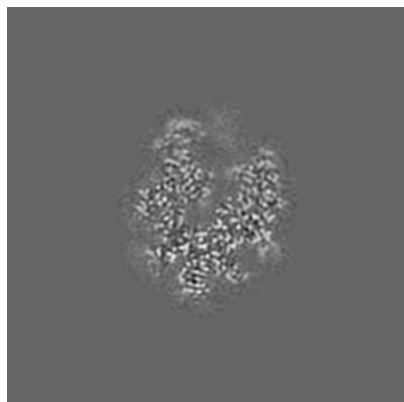


Z Index: 160

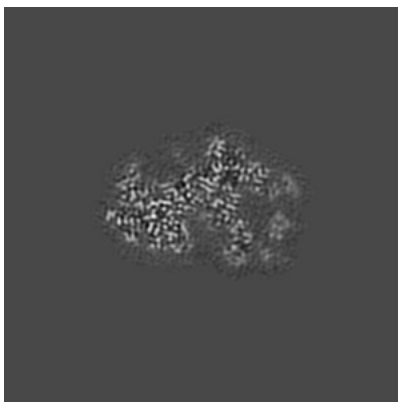
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

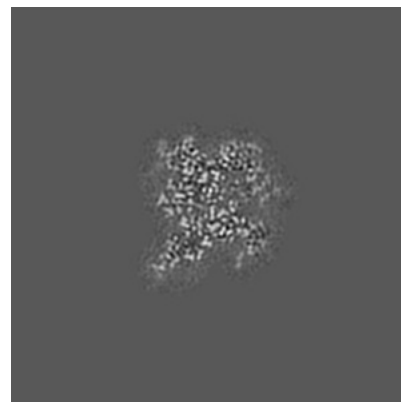
6.3.1 Primary map



X Index: 148

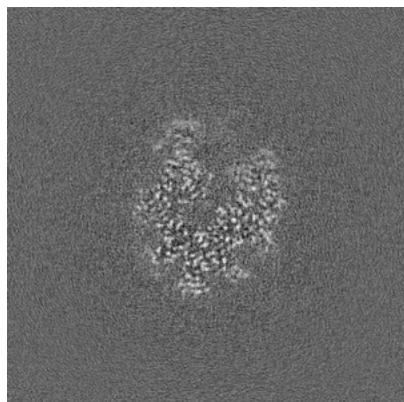


Y Index: 153

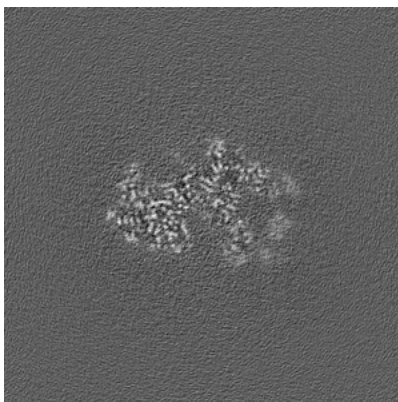


Z Index: 141

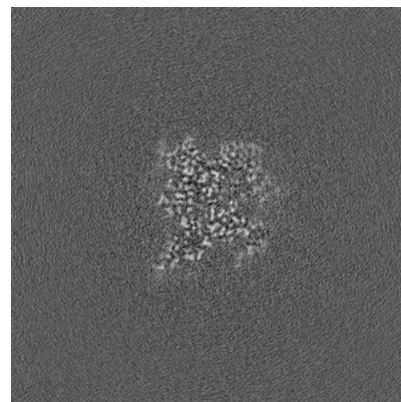
6.3.2 Raw map



X Index: 147



Y Index: 153

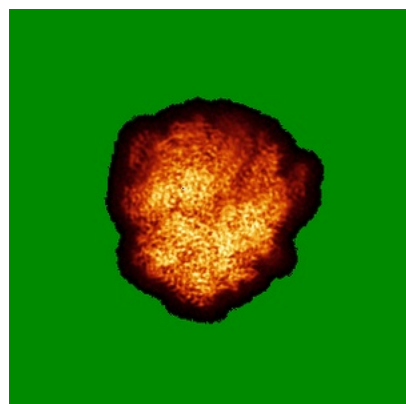


Z Index: 141

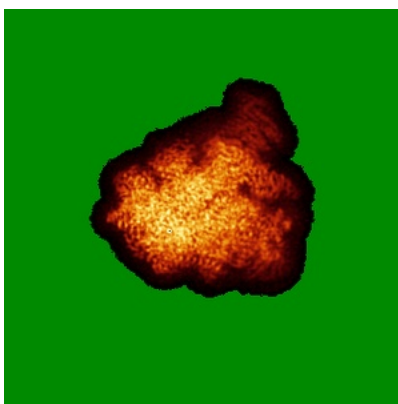
The images above show the largest variance slices of the map in three orthogonal directions.

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

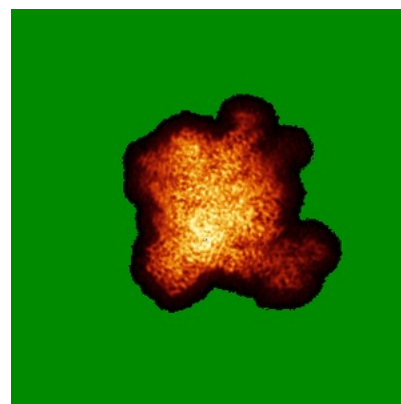
6.4.1 Primary map



X

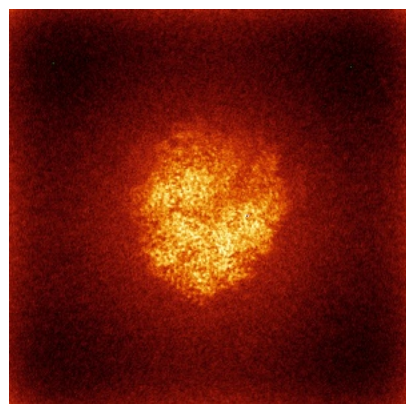


Y

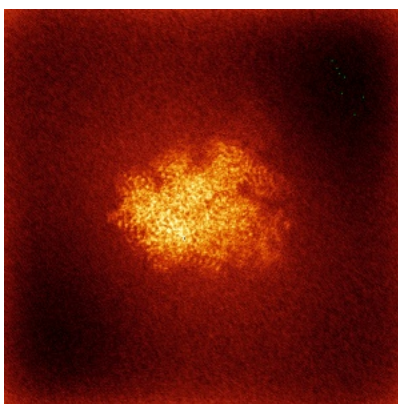


Z

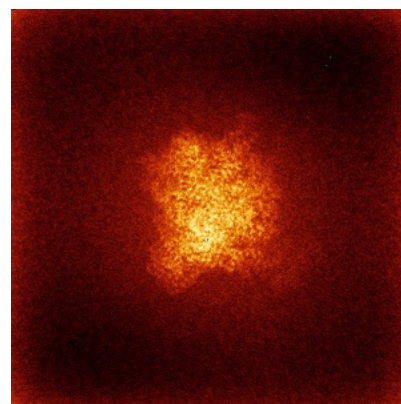
6.4.2 Raw map



X



Y



Z

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

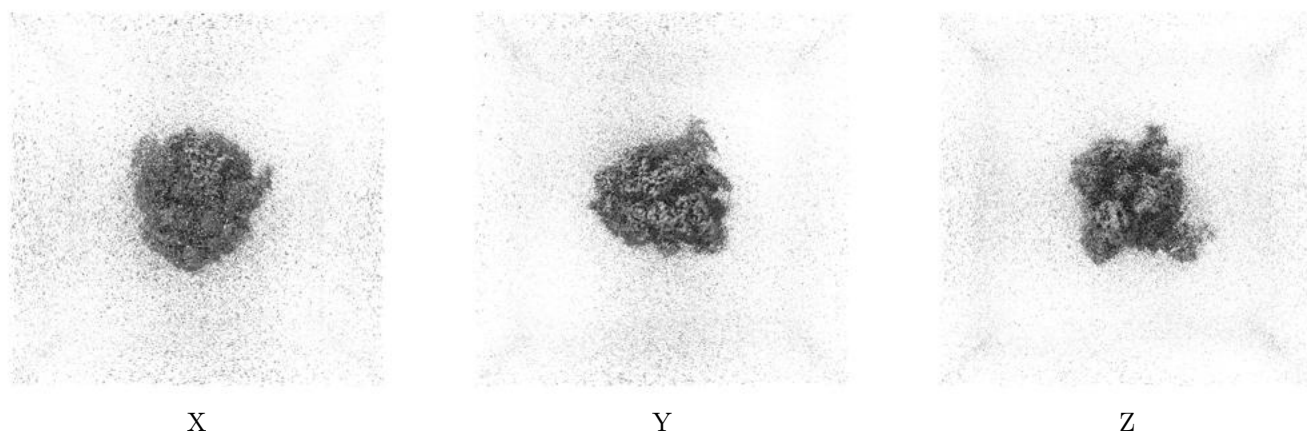
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

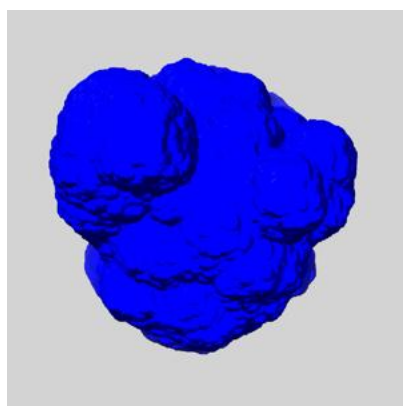
6.6 Mask visualisation [i](#)

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

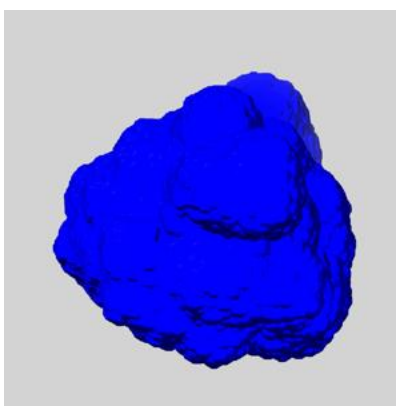
A mask typically either:

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

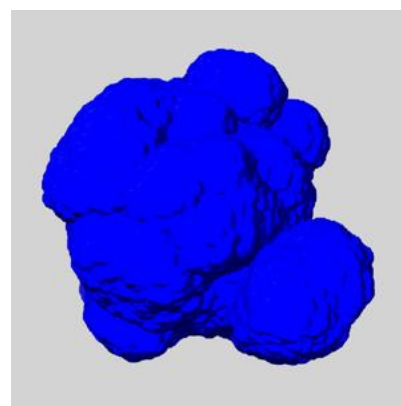
6.6.1 emd_62282_msk_1.map [i](#)



X



Y

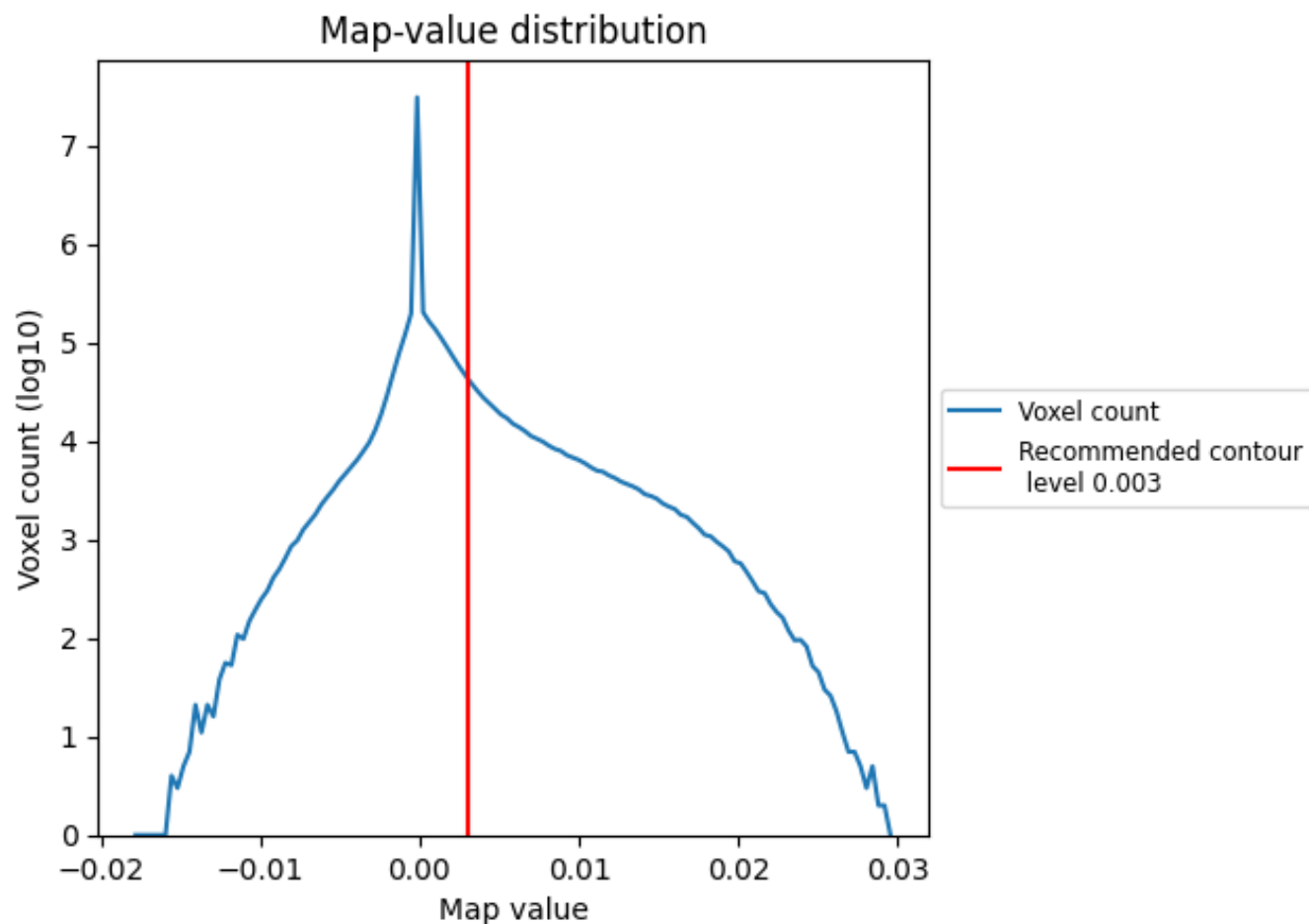


Z

7 Map analysis [i](#)

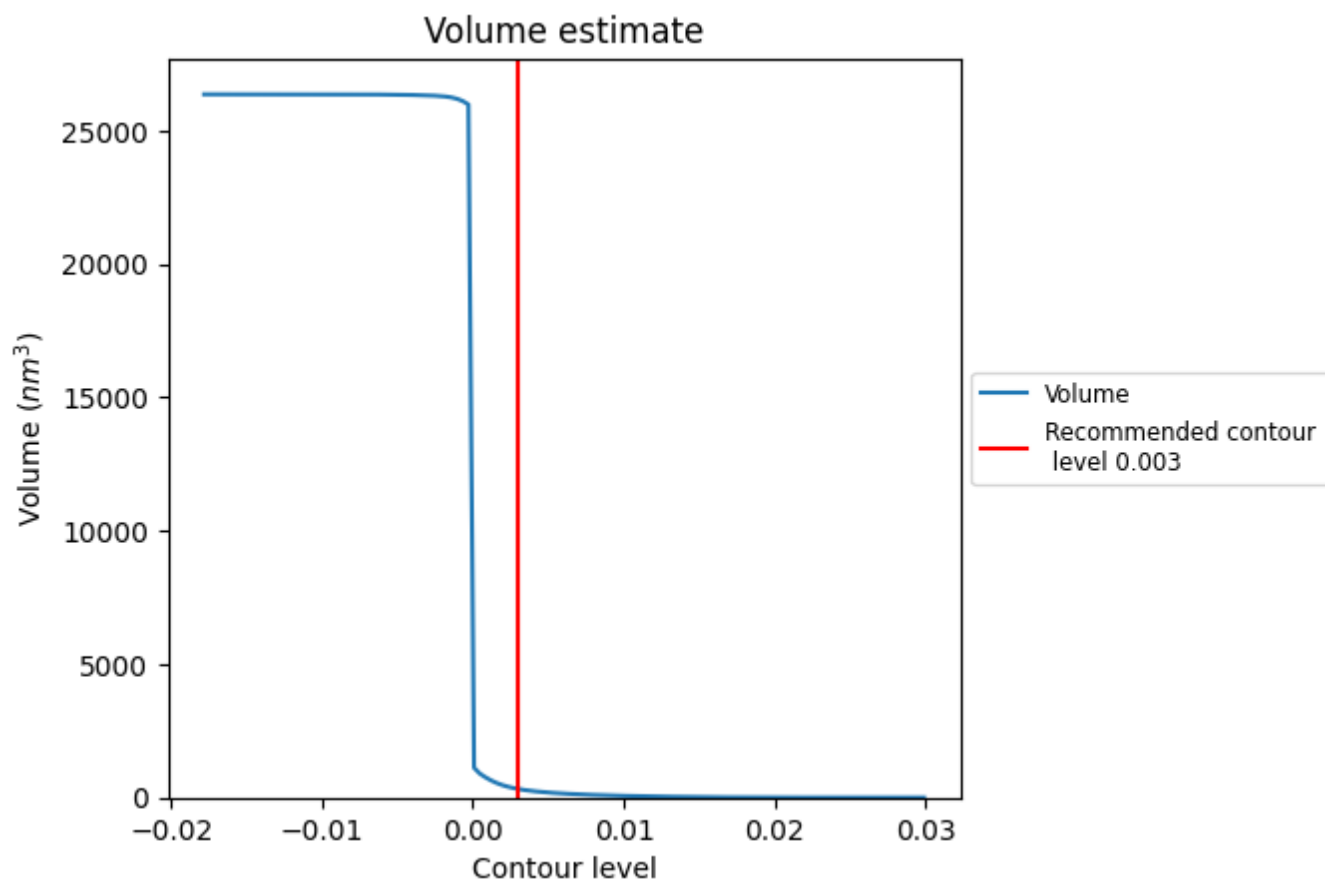
This section contains the results of statistical analysis of the map.

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.

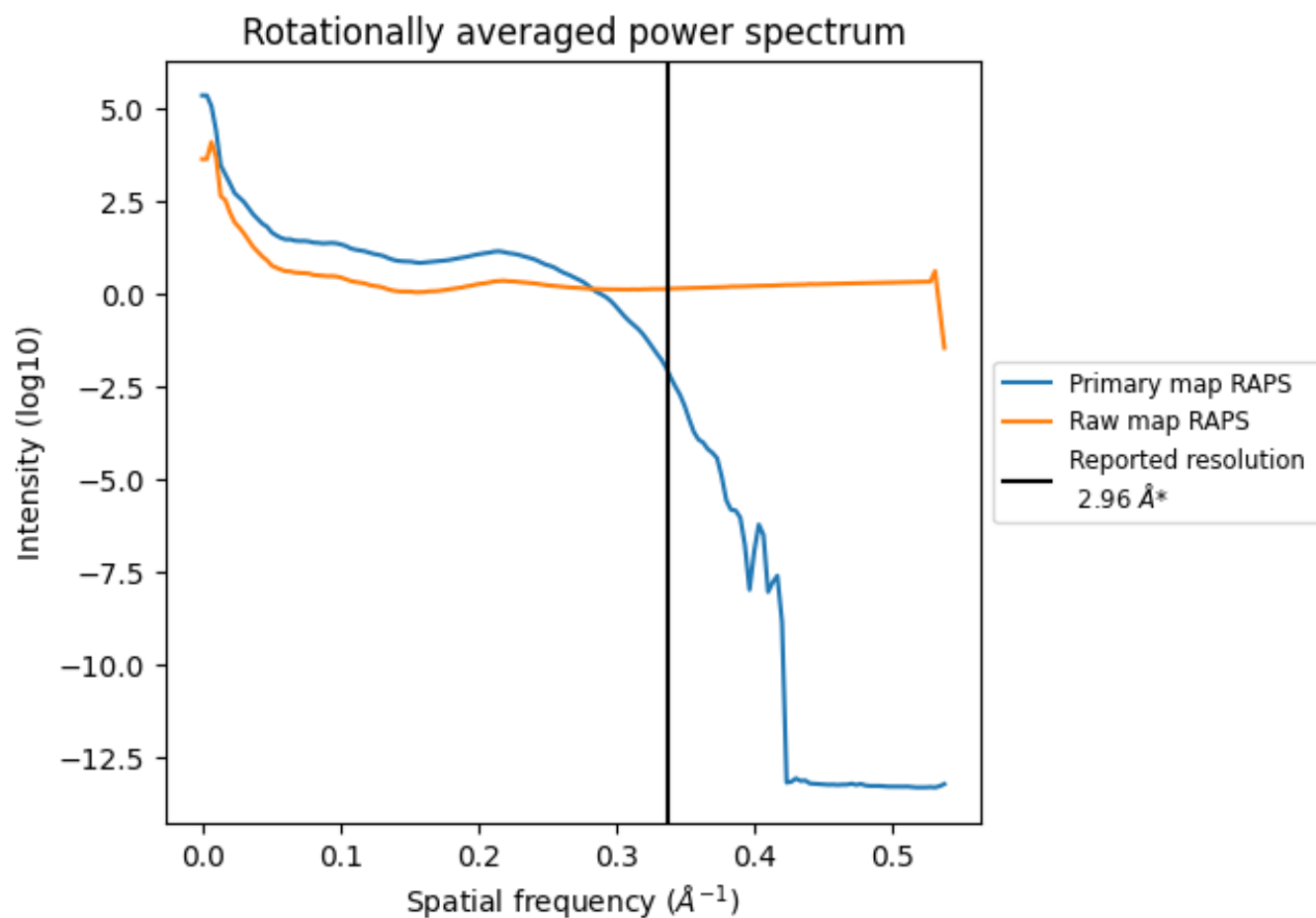
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323 nm^3 ; this corresponds to an approximate mass of 292 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 ⓘ

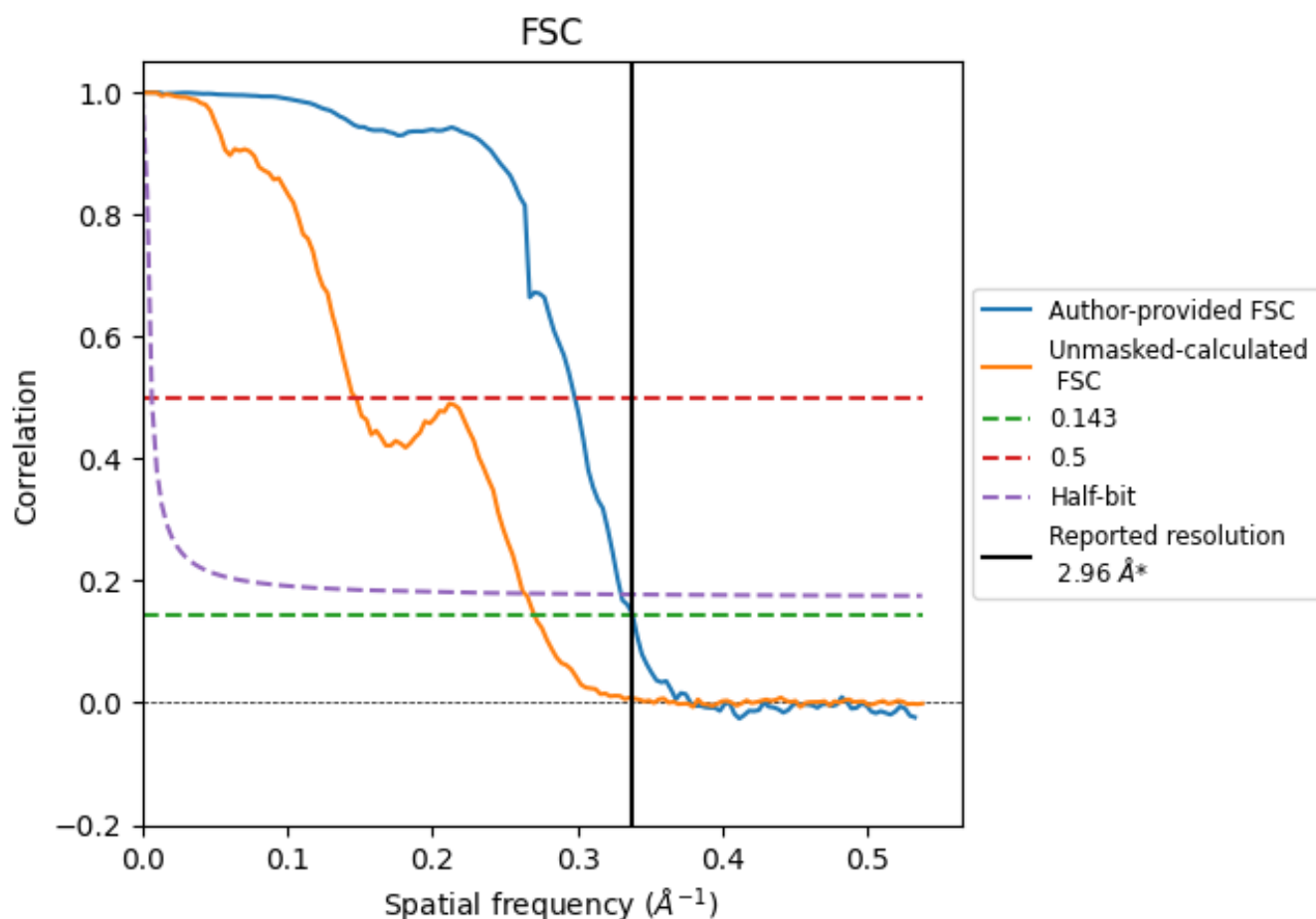


*Reported resolution corresponds to spatial frequency of 0.338 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

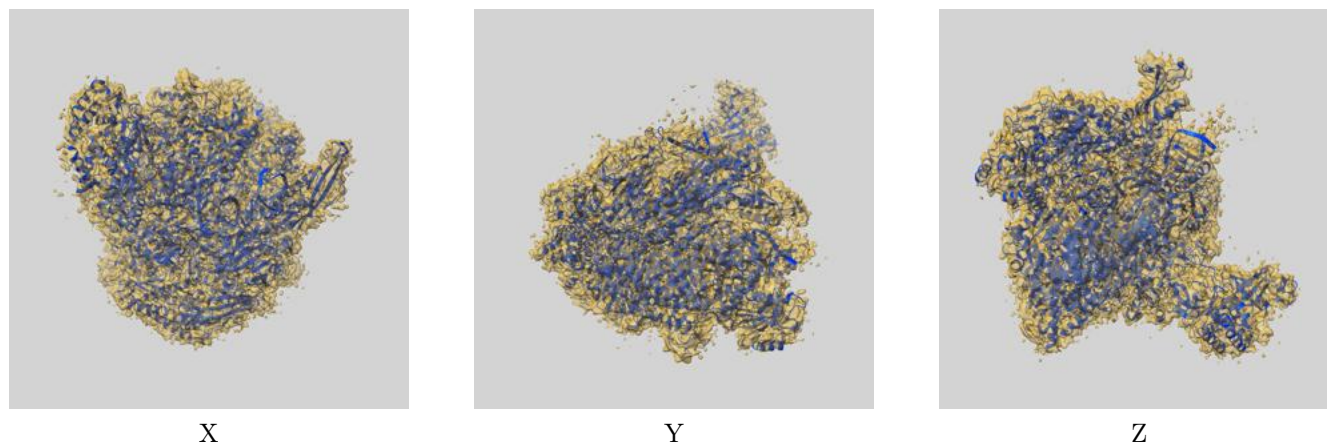
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.35	3.03
Unmasked-calculated*	3.70	6.80	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

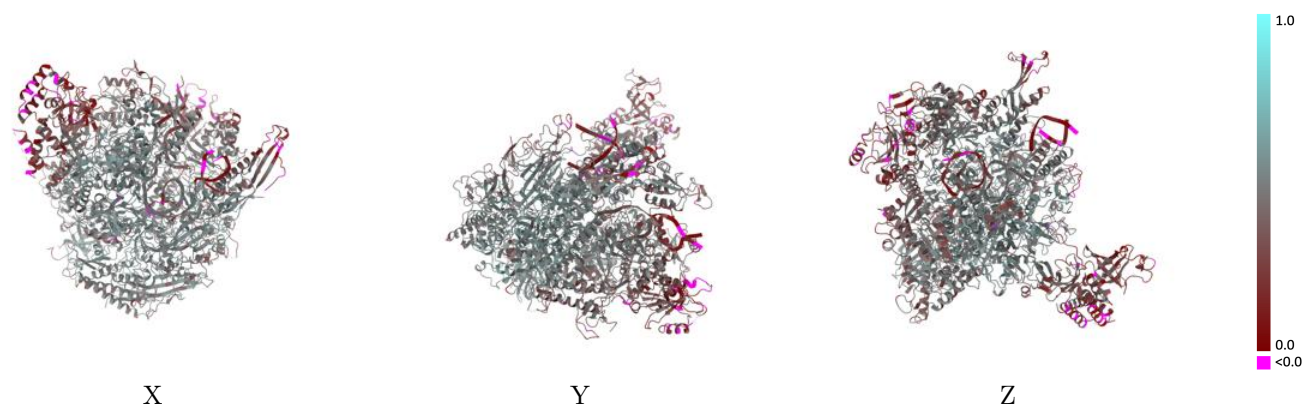
This section contains information regarding the fit between EMDB map EMD-62282 and PDB model 9KDN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



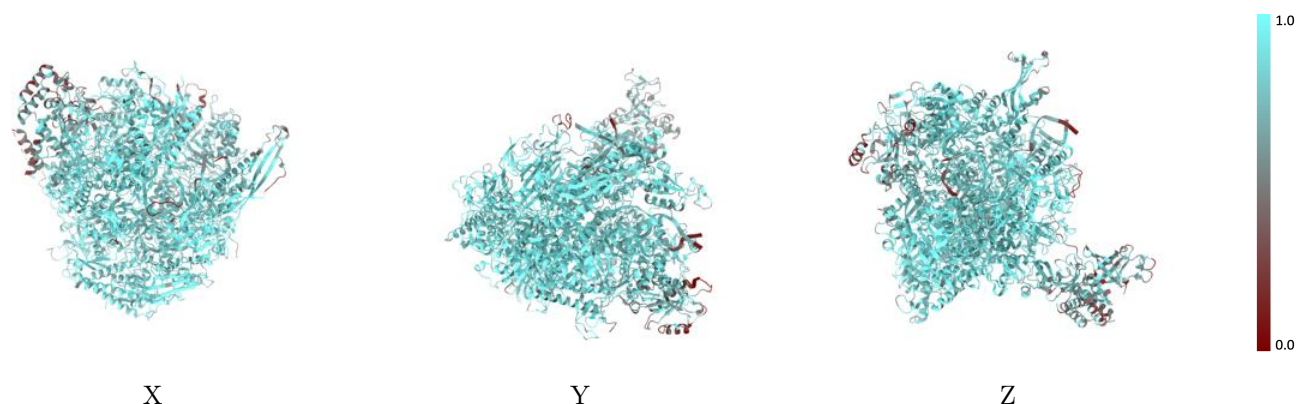
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



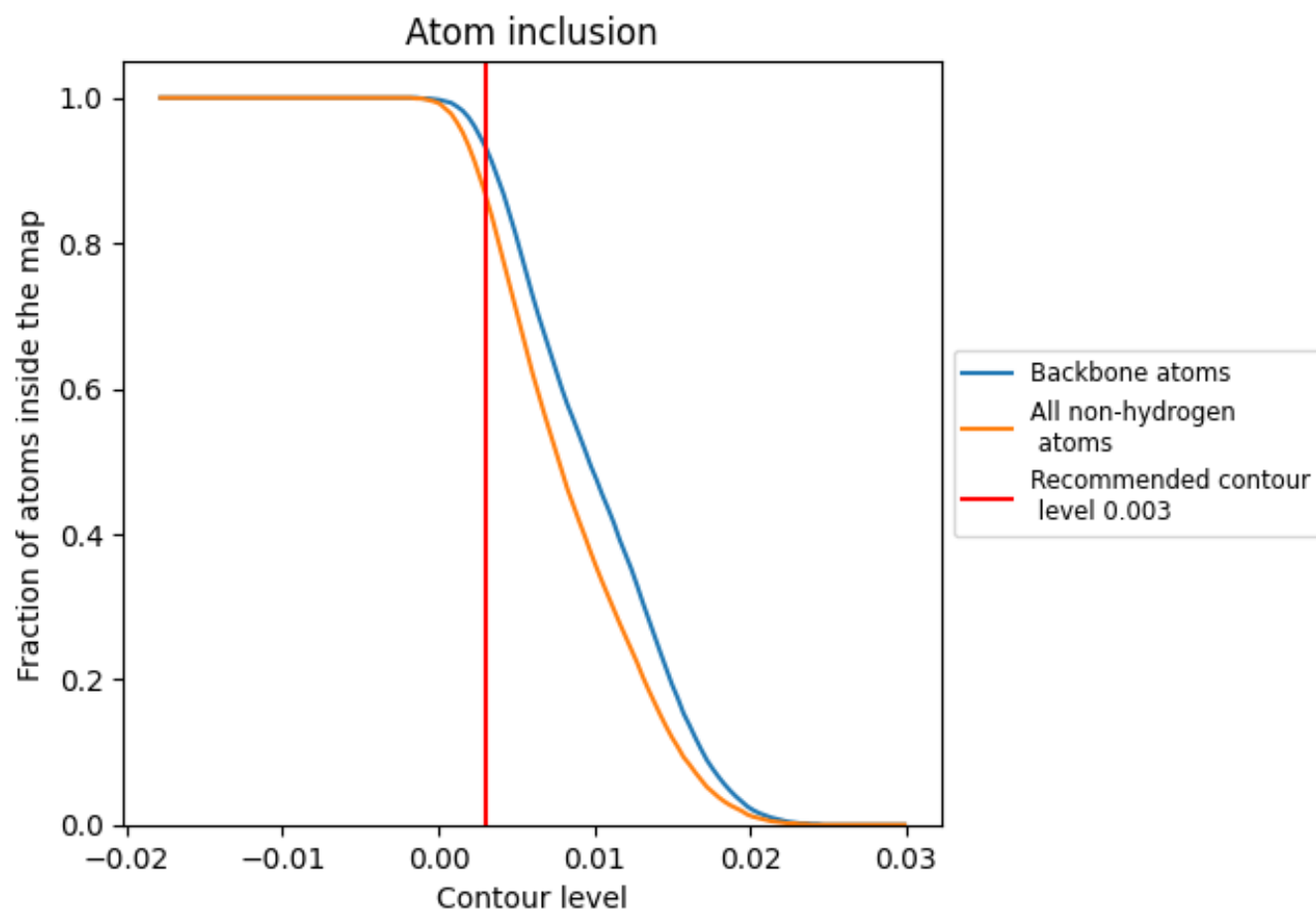
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.003).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.4450
A	 0.8880	 0.4670
B	 0.8970	 0.4730
C	 0.9160	 0.4960
D	 0.6010	 0.2360
E	 0.8920	 0.4260
F	 0.9360	 0.5100
G	 0.7090	 0.3340
H	 0.9200	 0.4980
I	 0.7570	 0.3140
J	 0.9240	 0.5170
K	 0.9220	 0.5050
L	 0.9190	 0.4380
M	 0.8780	 0.3380
N	 0.7330	 0.1540
P	 0.9740	 0.4550
T	 0.7130	 0.2660

