



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:22 AM UTC

PDB ID : 8ZP7 / pdb_00008zp7
EMDB ID : EMD-60328
Title : Cryo-EM structure of Cas5-HNH Cascade bound with sDNA, Conf1
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on : 2024-05-29
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

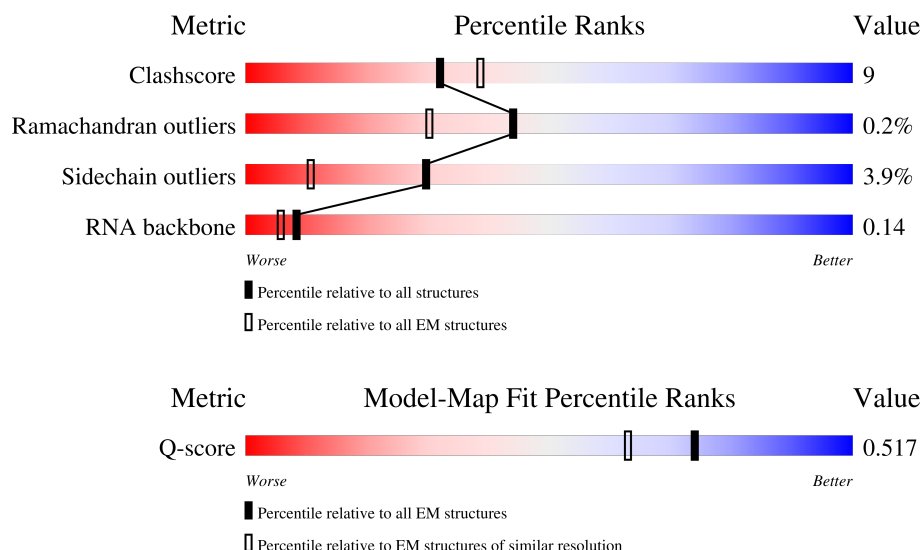
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

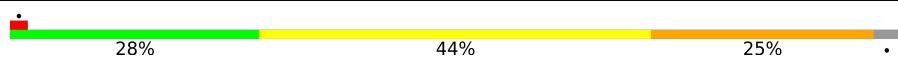
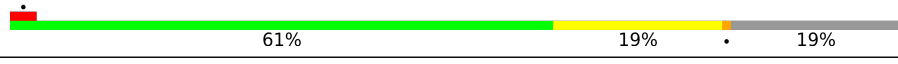
The reported resolution of this entry is 3.00 Å.

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.



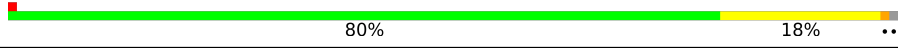
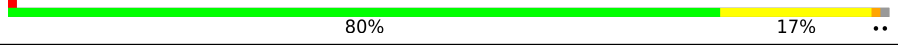
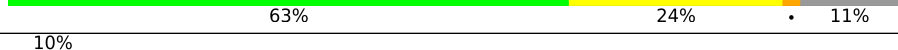
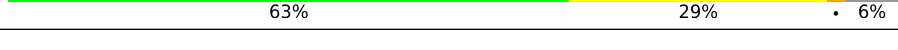
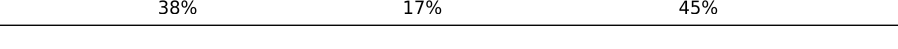
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	61	
2	C	546	
3	E	174	

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Mol	Chain	Length	Quality of chain
4	F	378	
4	G	378	
4	H	378	
4	I	378	
4	J	378	
4	K	378	
5	B	388	
6	D	272	
7	M	60	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27540 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	59	Total	C	N	O	P	0	0
			1258	562	225	413	58		

- Molecule 2 is a protein called CRISPR-associated protein Cse1 (CRISPR_cse1).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	443	Total	C	N	O	S	0	0
			3495	2246	597	633	19		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP A0A1V6F8D1
C	-9	HIS	-	expression tag	UNP A0A1V6F8D1
C	-8	HIS	-	expression tag	UNP A0A1V6F8D1
C	-7	HIS	-	expression tag	UNP A0A1V6F8D1
C	-6	HIS	-	expression tag	UNP A0A1V6F8D1
C	-5	HIS	-	expression tag	UNP A0A1V6F8D1
C	-4	HIS	-	expression tag	UNP A0A1V6F8D1
C	-3	HIS	-	expression tag	UNP A0A1V6F8D1
C	-2	HIS	-	expression tag	UNP A0A1V6F8D1
C	-1	HIS	-	expression tag	UNP A0A1V6F8D1
C	0	HIS	-	expression tag	UNP A0A1V6F8D1
C	1	VAL	-	expression tag	UNP A0A1V6F8D1

- Molecule 3 is a protein called CRISPR-associated protein Cse2 (CRISPR_cse2).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	165	Total	C	N	O	S	0	0
			1352	875	238	233	6		

- Molecule 4 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	368	Total	C	N	O	S	0	0
			2819	1782	489	536	12		
4	H	375	Total	C	N	O	S	0	0
			2878	1812	503	551	12		
4	I	373	Total	C	N	O	S	0	0
			2854	1800	498	544	12		
4	J	374	Total	C	N	O	S	0	0
			2845	1794	496	543	12		
4	K	350	Total	C	N	O	S	0	0
			2701	1708	474	508	11		
4	G	255	Total	C	N	O	S	0	0
			1927	1220	336	363	8		

- Molecule 5 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	344	Total	C	N	O	S	0	0
			2701	1704	499	481	17		

- Molecule 6 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	256	Total	C	N	O	S	0	0
			2039	1309	365	361	4		

- Molecule 7 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	33	Total	C	N	O	P	0	0
			669	319	119	198	33		

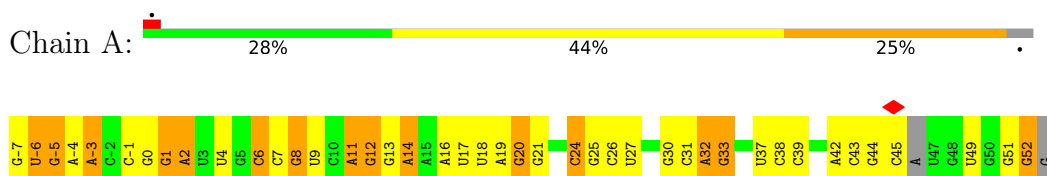
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	Mg	0
			1	1	
8	B	1	Total	Mg	0
			1	1	

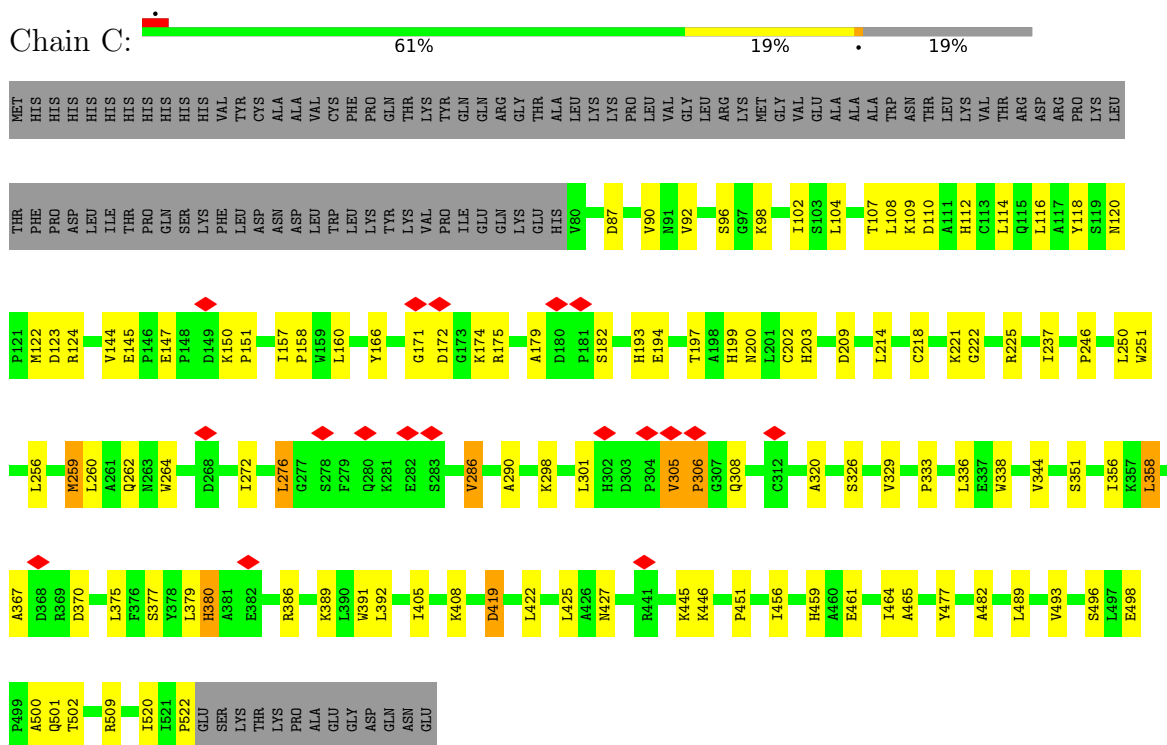
3 Residue-property plots

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

- Molecule 1: RNA (61-MER)

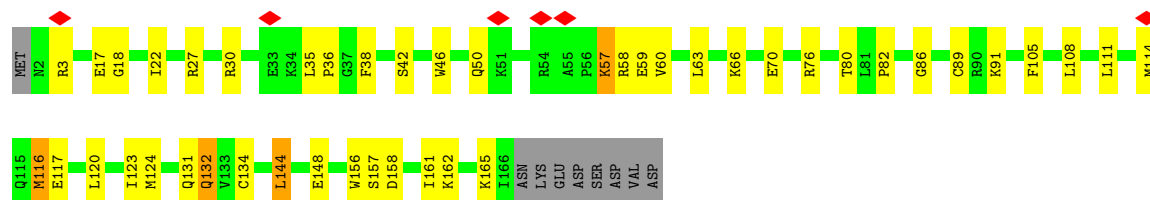


- Molecule 2: CRISPR-associated protein Cse1 (CRISPR_cse1)

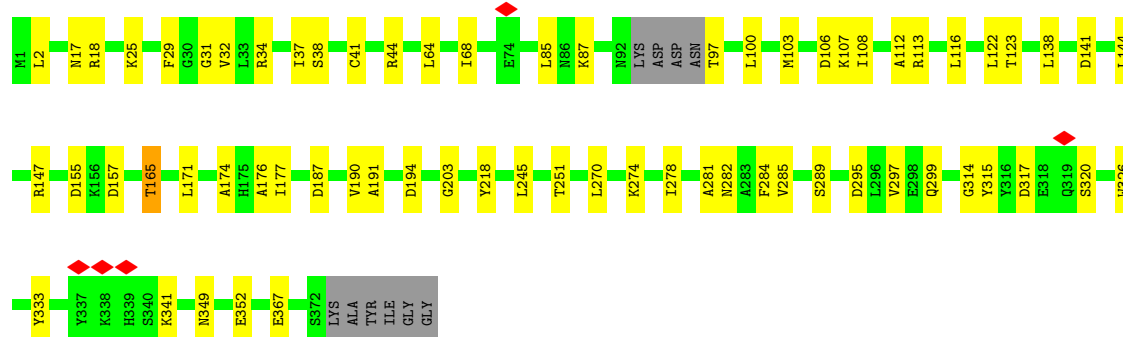
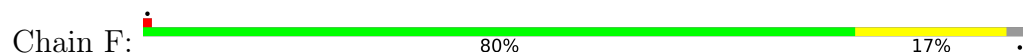


- Molecule 3: CRISPR-associated protein Cse2 (CRISPR_cse2)

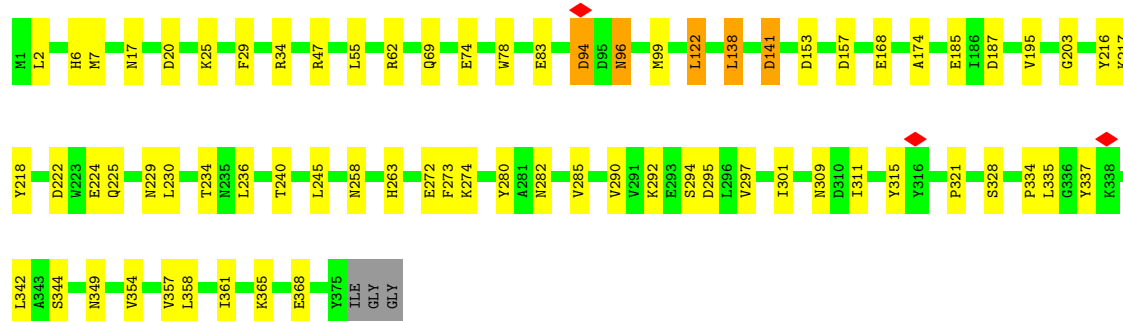
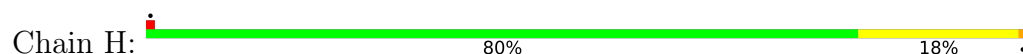




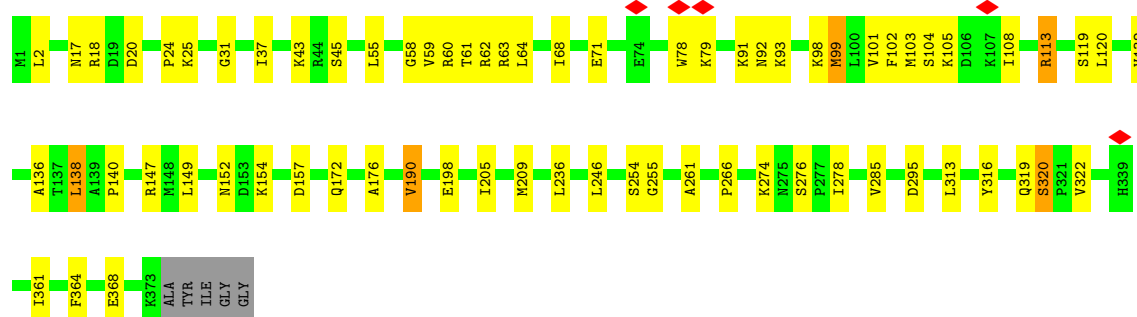
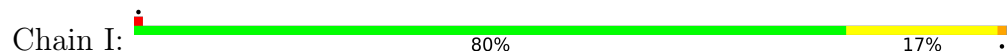
• Molecule 4: CRISPR system Cascade subunit CasC



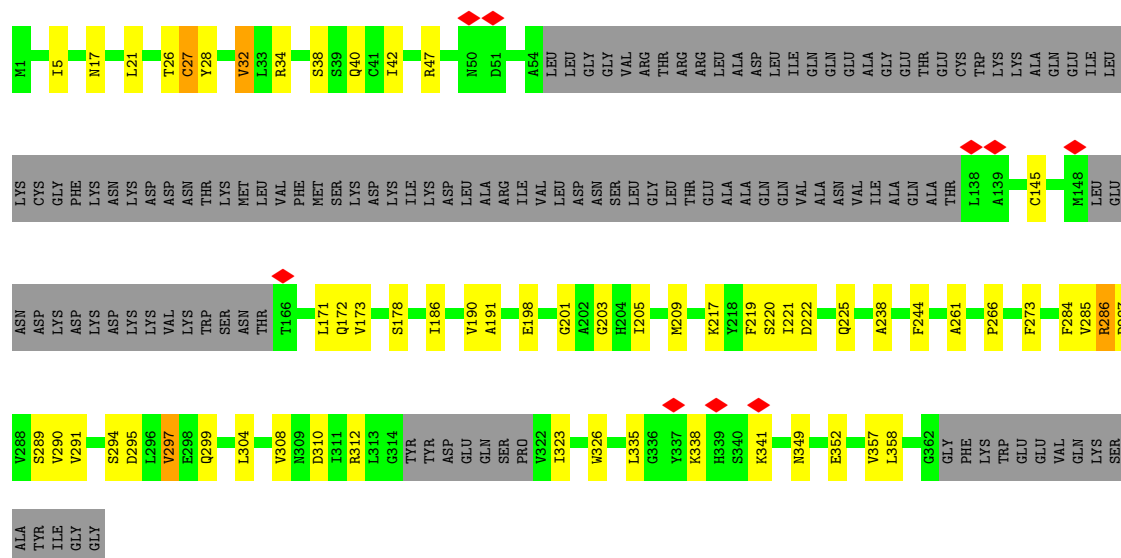
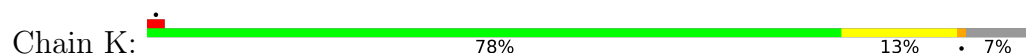
• Molecule 4: CRISPR system Cascade subunit CasC



• Molecule 4: CRISPR system Cascade subunit CasC



Chain J: 76% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	15.977	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.667	Depositor
Recommended contour level	2.58	Depositor
Map size ($\text{\AA}$)	290.88, 290.88, 290.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/1405	0.37	0/2187
2	C	0.22	0/3596	0.57	1/4901 (0.0%)
3	E	0.26	0/1382	0.68	2/1862 (0.1%)
4	F	0.20	0/2875	0.46	1/3900 (0.0%)
4	G	0.22	0/1967	0.54	0/2670
4	H	0.19	0/2934	0.46	2/3977 (0.1%)
4	I	0.19	0/2911	0.47	2/3949 (0.1%)
4	J	0.20	0/2901	0.51	1/3937 (0.0%)
4	K	0.19	0/2752	0.49	1/3726 (0.0%)
5	B	0.20	0/2769	0.51	1/3759 (0.0%)
6	D	0.20	0/2095	0.58	1/2845 (0.0%)
7	M	0.26	0/748	0.48	0/1150
All	All	0.20	0/28335	0.51	12/38863 (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
2	C	0	1
5	B	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	57	LYS	CA-CB-CG	6.47	127.03	114.10
4	I	99	MET	CB-CG-SD	5.66	129.67	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	145	PRO	CA-N-CD	-5.59	104.17	112.00
4	H	321	PRO	CA-N-CD	-5.42	104.41	112.00
4	H	292	LYS	CB-CG-CD	5.41	123.75	111.30
2	C	276	LEU	CA-CB-CG	5.37	135.10	116.30
4	K	228	LYS	CA-CB-CG	5.32	124.73	114.10
4	J	158	LYS	CB-CG-CD	5.26	123.39	111.30
4	F	341	LYS	CB-CG-CD	5.22	123.30	111.30
3	E	116	MET	CA-CB-CG	5.18	124.46	114.10
4	I	198	GLU	CA-CB-CG	5.09	124.28	114.10
6	D	37	MET	CB-CG-SD	5.07	127.90	112.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	24	ALA	Peptide
2	C	305	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1258	0	638	32	0
2	C	3495	0	3405	65	0
3	E	1352	0	1387	31	0
4	F	2819	0	2745	46	0
4	G	1927	0	1854	40	0
4	H	2878	0	2805	47	0
4	I	2854	0	2766	47	0
4	J	2845	0	2746	53	0
4	K	2701	0	2651	35	0
5	B	2701	0	2679	69	0
6	D	2039	0	1995	61	0
7	M	669	0	372	11	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
All	All	27540	0	26043	460	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (460) 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)
5:B:358:ARG:HH12	6:D:97:GLN:HE22	1.29	0.78
4:F:2:LEU:HB2	4:F:274:LYS:O	1.87	0.74
4:I:2:LEU:HB2	4:I:274:LYS:O	1.89	0.72
5:B:212:MET:HE1	5:B:250:ARG:HG2	1.70	0.72
2:C:305:VAL:HG22	2:C:306:PRO:HD2	1.73	0.70
4:K:189:PHE:O	6:D:110:LYS:NZ	2.24	0.70
2:C:202:CYS:SG	5:B:121:ARG:NH2	2.65	0.70
5:B:207:ILE:HD11	5:B:251:GLU:HB3	1.75	0.69
2:C:246:PRO:HB3	2:C:351:SER:HB3	1.75	0.69
2:C:222:GLY:HA2	2:C:225:ARG:HD2	1.75	0.68
5:B:315:ARG:HB2	5:B:319:LYS:HG3	1.77	0.67
6:D:7:LEU:HB2	6:D:82:ILE:HB	1.77	0.67
4:G:34:ARG:NH2	4:G:284:PHE:O	2.28	0.66
6:D:253:GLY:O	6:D:256:LYS:NZ	2.28	0.66
5:B:8:LEU:HD22	5:B:151:LEU:HD13	1.79	0.65
1:A:-4:A:H2'	1:A:-3:A:H8	1.62	0.64
4:J:69:GLN:HE22	4:J:76:GLU:HA	1.63	0.64
4:J:2:LEU:HB2	4:J:274:LYS:O	1.98	0.64
4:F:29:PHE:HB3	4:F:34:ARG:HG3	1.81	0.63
5:B:20:GLY:HA2	5:B:31:THR:HA	1.81	0.63
2:C:122:MET:HG2	2:C:405:ILE:HG12	1.79	0.63
2:C:272:ILE:H	2:C:290:ALA:HB2	1.64	0.62
5:B:345:MET:HB3	5:B:349:ARG:HH11	1.64	0.62
4:G:26:THR:O	5:B:79:TRP:NE1	2.32	0.62
4:G:27:CYS:SG	4:G:28:TYR:N	2.73	0.62
1:A:33:G:N2	6:D:165:SER:O	2.33	0.62
2:C:110:ASP:O	2:C:112:HIS:ND1	2.31	0.61
5:B:72:ILE:HB	5:B:209:PRO:HG2	1.83	0.61
4:K:32:VAL:HG21	4:K:287:PRO:HG3	1.82	0.61
6:D:66:LEU:HD22	6:D:85:GLN:HE22	1.64	0.61
6:D:166:THR:HG23	6:D:168:ASP:H	1.65	0.61
4:I:295:ASP:HB3	4:J:286:ARG:HB3	1.83	0.61
1:A:24:C:H5'	4:J:40:GLN:HB2	1.82	0.61
4:K:96:ASN:C	4:K:96:ASN:HD22	2.08	0.61
2:C:333:PRO:HG2	2:C:336:LEU:HD11	1.81	0.61
1:A:49:U:OP2	6:D:254:LYS:NZ	2.34	0.61
4:J:155:ASP:OD1	4:J:156:LYS:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:8:LEU:HD23	5:B:141:LEU:HB2	1.83	0.60
4:J:17:ASN:HB3	4:J:25:LYS:HD2	1.82	0.60
4:K:95:ASP:OD1	4:K:95:ASP:N	2.35	0.60
4:I:20:ASP:N	4:I:20:ASP:OD1	2.34	0.60
5:B:358:ARG:NH2	6:D:97:GLN:OE1	2.30	0.60
1:A:8:G:O2'	4:F:18:ARG:NH2	2.34	0.60
4:H:94:ASP:N	4:H:94:ASP:OD1	2.35	0.60
1:A:21:G:H2'	4:J:148:MET:HG2	1.83	0.60
4:H:195:VAL:HG21	4:I:63:ARG:HB2	1.84	0.60
4:G:191:ALA:HB3	4:G:203:GLY:HA3	1.84	0.59
5:B:37:LYS:HA	5:B:68:MET:HE1	1.84	0.59
4:H:29:PHE:HB3	4:H:34:ARG:HG3	1.84	0.59
4:I:64:LEU:HD11	4:I:103:MET:HE2	1.84	0.59
4:F:37:ILE:HB	4:F:176:ALA:HB3	1.84	0.59
4:H:74:GLU:N	4:H:74:GLU:OE1	2.35	0.59
7:M:46:DC:N3	7:M:47:DA:N6	2.50	0.59
3:E:57:LYS:HD2	3:E:58:ARG:N	2.17	0.59
1:A:52:G:OP1	6:D:62:LYS:NZ	2.35	0.59
6:D:66:LEU:HD21	6:D:261:GLY:H	1.68	0.59
2:C:520:ILE:HD13	2:C:522:PRO:HD2	1.85	0.58
1:A:-6:U:H3	5:B:52:ARG:HH21	1.52	0.58
2:C:147:GLU:N	2:C:147:GLU:OE2	2.37	0.58
4:I:274:LYS:HE3	4:I:278:ILE:HG12	1.85	0.58
2:C:118:TYR:HB2	2:C:124:ARG:HG3	1.86	0.58
4:J:60:ARG:HG2	4:J:100:LEU:HD22	1.86	0.58
4:J:293:GLU:N	4:J:293:GLU:OE2	2.35	0.58
4:K:345:ARG:HH21	4:K:347:ILE:HG21	1.69	0.58
4:F:31:GLY:HA3	4:G:290:VAL:HG21	1.85	0.58
4:H:187:ASP:OD1	4:I:25:LYS:NZ	2.37	0.57
2:C:120:ASN:HB3	2:C:123:ASP:HB2	1.86	0.57
6:D:23:LYS:H	6:D:23:LYS:HD2	1.70	0.57
5:B:37:LYS:NZ	5:B:213:ASP:OD2	2.37	0.57
5:B:229:ILE:O	5:B:230:HIS:ND1	2.37	0.57
5:B:248:ILE:HD12	5:B:250:ARG:HH12	1.69	0.57
6:D:111:GLU:OE2	6:D:113:ASN:ND2	2.37	0.57
3:E:17:GLU:OE1	3:E:17:GLU:N	2.38	0.57
3:E:50:GLN:HG2	5:B:278:TYR:HB2	1.86	0.57
4:F:187:ASP:OD1	4:H:25:LYS:NZ	2.33	0.57
4:J:94:ASP:OD1	4:J:94:ASP:N	2.38	0.57
4:K:7:MET:HG2	4:K:217:LYS:HB2	1.87	0.57
4:K:34:ARG:NH2	4:K:284:PHE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:93:LYS:NZ	7:M:33:DA:OP2	2.37	0.56
4:J:323:ILE:HG12	4:J:360:TYR:HE2	1.70	0.56
3:E:50:GLN:O	5:B:279:ASN:ND2	2.38	0.56
4:J:273:PHE:HD1	4:J:323:ILE:HD11	1.69	0.56
4:K:154:LYS:NZ	7:M:24:DA:OP2	2.38	0.56
4:G:47:ARG:HD3	4:G:145:CYS:HB2	1.87	0.56
5:B:10:LEU:HD11	5:B:44:LEU:HD21	1.88	0.56
5:B:295:HIS:HE1	6:D:56:SER:HA	1.70	0.56
1:A:17:U:OP1	4:I:43:LYS:NZ	2.37	0.56
4:G:34:ARG:NH1	4:G:178:SER:O	2.38	0.56
6:D:41:SER:OG	6:D:44:ARG:NH1	2.39	0.56
4:F:106:ASP:OD1	4:F:106:ASP:N	2.37	0.56
4:H:96:ASN:OD1	4:H:96:ASN:N	2.39	0.56
5:B:35:PRO:HD2	5:B:70:VAL:HG11	1.88	0.56
5:B:276:ALA:HB2	5:B:316:ALA:HB1	1.86	0.56
6:D:122:LEU:HB3	6:D:236:LEU:HB3	1.88	0.56
4:J:103:MET:O	4:J:107:LYS:NZ	2.40	0.55
4:K:39:SER:HB2	4:K:173:VAL:HG13	1.88	0.55
2:C:123:ASP:OD2	2:C:221:LYS:NZ	2.34	0.55
4:F:297:VAL:HG23	4:H:285:VAL:HG11	1.88	0.55
4:H:297:VAL:HG23	4:I:285:VAL:HG11	1.88	0.55
4:G:201:GLY:HA3	7:M:44:DG:H8	1.70	0.55
5:B:33:ASP:OD1	5:B:33:ASP:N	2.39	0.55
4:I:37:ILE:HB	4:I:176:ALA:HB3	1.89	0.55
4:K:186:ILE:HD12	4:K:186:ILE:H	1.72	0.55
4:K:154:LYS:H	4:K:154:LYS:HD2	1.72	0.55
3:E:161:ILE:HG23	3:E:165:LYS:HE3	1.88	0.55
5:B:354:ASP:OD1	5:B:354:ASP:N	2.37	0.55
4:F:68:ILE:HD13	4:F:116:LEU:HD21	1.89	0.54
4:I:295:ASP:OD1	4:I:295:ASP:N	2.39	0.54
4:G:47:ARG:HH11	4:G:145:CYS:HB2	1.72	0.54
3:E:30:ARG:HD2	5:B:342:GLY:HA3	1.89	0.54
4:J:68:ILE:O	4:J:72:ALA:HB2	2.06	0.54
4:G:171:LEU:HD11	4:G:219:PHE:HD2	1.71	0.54
6:D:129:ASN:OD1	6:D:129:ASN:N	2.40	0.54
4:I:108:ILE:HG23	4:I:132:VAL:HG22	1.89	0.54
6:D:139:MET:HE2	6:D:142:GLN:HG3	1.87	0.54
3:E:158:ASP:O	3:E:162:LYS:NZ	2.38	0.54
4:G:349:ASN:HB3	4:G:352:GLU:HG2	1.89	0.54
1:A:6:C:O2'	4:F:41:CYS:SG	2.64	0.54
2:C:459:HIS:HD2	2:C:489:LEU:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:58:GLY:H	4:I:105:LYS:HB2	1.71	0.54
4:K:187:ASP:OD1	4:K:187:ASP:N	2.40	0.54
4:G:190:VAL:HG12	4:G:205:ILE:HG23	1.89	0.54
4:J:58:GLY:HA2	4:J:104:SER:HB2	1.90	0.54
4:K:34:ARG:NH1	4:K:179:THR:O	2.41	0.54
5:B:24:ALA:HB1	5:B:29:ARG:HA	1.90	0.54
4:I:101:VAL:HG13	4:I:149:LEU:HD22	1.90	0.53
2:C:344:VAL:HG13	2:C:377:SER:HB3	1.89	0.53
4:G:285:VAL:HG21	5:B:198:ARG:HD2	1.90	0.53
4:F:295:ASP:N	4:F:295:ASP:OD1	2.41	0.53
4:H:141:ASP:OD1	4:H:141:ASP:N	2.34	0.53
2:C:214:LEU:HD13	2:C:218:CYS:HB3	1.91	0.53
4:I:266:PRO:O	4:J:315:TYR:OH	2.21	0.53
4:K:2:LEU:HB3	4:K:274:LYS:O	2.08	0.53
4:K:163:SER:OG	4:K:164:ASN:N	2.38	0.53
5:B:70:VAL:HG22	5:B:139:VAL:HG22	1.90	0.53
4:H:69:GLN:HG3	4:H:78:TRP:HB2	1.90	0.53
4:K:20:ASP:N	4:K:20:ASP:OD1	2.40	0.53
3:E:27:ARG:HA	3:E:66:LYS:HD2	1.91	0.52
4:H:185:GLU:OE2	4:H:185:GLU:N	2.42	0.52
4:I:55:LEU:HB3	4:I:140:PRO:HG2	1.92	0.52
4:J:92:ASN:ND2	4:J:94:ASP:O	2.41	0.52
4:K:8:ILE:O	4:K:267:ASP:N	2.42	0.52
4:H:203:GLY:O	4:I:62:ARG:NH1	2.42	0.52
6:D:70:ASP:OD2	6:D:125:ARG:NH2	2.41	0.52
1:A:21:G:OP2	4:I:18:ARG:NH2	2.42	0.52
4:F:282:ASN:HA	4:F:285:VAL:HG23	1.91	0.52
6:D:193:GLN:HB3	6:D:231:LEU:HB3	1.91	0.52
4:H:153:ASP:HB2	7:M:42:DA:H5''	1.91	0.52
4:I:102:PHE:HB3	4:I:147:ARG:HG2	1.91	0.52
6:D:77:ASP:N	6:D:77:ASP:OD1	2.39	0.52
2:C:104:LEU:O	2:C:108:LEU:HB2	2.10	0.52
4:I:261:ALA:HB3	4:J:174:ALA:HB2	1.92	0.52
6:D:8:LEU:HD23	6:D:105:ALA:HB3	1.91	0.52
1:A:-7:G:H4'	5:B:46:ALA:HB2	1.90	0.52
4:F:34:ARG:NH1	4:F:284:PHE:O	2.38	0.52
5:B:311:VAL:O	5:B:349:ARG:N	2.39	0.52
2:C:145:GLU:OE1	2:C:264:TRP:NE1	2.41	0.52
4:F:367:GLU:OE2	4:F:367:GLU:N	2.42	0.52
5:B:295:HIS:CE1	6:D:57:PRO:HD3	2.45	0.52
4:F:315:TYR:OH	4:G:266:PRO:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:104:SER:H	4:I:136:ALA:HB1	1.75	0.52
4:J:64:LEU:HD22	4:J:85:LEU:HD11	1.92	0.52
2:C:166:TYR:OH	2:C:276:LEU:HD13	2.10	0.51
6:D:73:ILE:HG13	6:D:81:ILE:HD11	1.92	0.51
2:C:182:SER:OG	2:C:326:SER:OG	2.23	0.51
3:E:57:LYS:HD2	3:E:58:ARG:H	1.74	0.51
5:B:199:TRP:CE2	5:B:202:GLU:HB3	2.46	0.51
6:D:34:ARG:HA	6:D:34:ARG:NH1	2.26	0.51
2:C:370:ASP:OD1	2:C:370:ASP:N	2.39	0.51
4:G:273:PHE:HZ	4:G:357:VAL:HG13	1.74	0.51
4:I:91:LYS:NZ	7:M:35:DT:OP1	2.44	0.51
6:D:37:MET:HE1	6:D:95:CYS:HA	1.93	0.51
4:J:146:GLY:H	4:J:169:ALA:HB2	1.75	0.51
5:B:339:LEU:HD12	5:B:364:LYS:HG3	1.91	0.51
6:D:187:GLN:NE2	6:D:237:GLU:OE2	2.42	0.51
1:A:4:U:H4'	4:F:147:ARG:HA	1.92	0.51
4:H:334:PRO:HG2	4:H:337:TYR:HE1	1.76	0.51
6:D:28:ILE:HD11	6:D:197:VAL:HG12	1.93	0.51
6:D:240:ASP:N	6:D:240:ASP:OD1	2.43	0.50
3:E:132:GLN:HA	3:E:132:GLN:NE2	2.26	0.50
1:A:1:G:OP2	4:G:40:GLN:NE2	2.45	0.50
4:G:32:VAL:HG12	4:G:34:ARG:HE	1.77	0.50
5:B:248:ILE:HB	5:B:250:ARG:HH22	1.77	0.50
4:K:37:ILE:HB	4:K:176:ALA:HB3	1.93	0.50
5:B:307:THR:OG1	5:B:308:VAL:N	2.43	0.50
1:A:-4:A:H2'	1:A:-3:A:C8	2.45	0.50
4:I:119:SER:OG	4:I:120:LEU:N	2.45	0.50
2:C:464:ILE:HG12	2:C:482:ALA:HB1	1.93	0.49
4:H:258:ASN:HA	4:I:172:GLN:HG2	1.94	0.49
4:J:55:LEU:HD22	4:J:140:PRO:HG2	1.94	0.49
4:H:2:LEU:HB3	4:H:274:LYS:O	2.11	0.49
3:E:63:LEU:HD22	3:E:117:GLU:HB3	1.94	0.49
4:G:17:ASN:HD22	4:G:38:SER:H	1.61	0.49
3:E:60:VAL:HG23	3:E:144:LEU:HD23	1.94	0.49
4:J:39:SER:HA	4:J:42:ILE:HD12	1.95	0.49
4:F:144:LEU:HD22	4:F:171:LEU:HB2	1.95	0.49
1:A:-1:C:H1'	5:B:85:VAL:HG13	1.94	0.49
2:C:179:ALA:HB3	2:C:298:LYS:HD2	1.95	0.49
4:J:7:MET:HG2	4:J:269:ILE:HG12	1.95	0.48
4:G:221:ILE:HD11	4:G:244:PHE:CD2	2.47	0.48
4:K:3:ILE:HG23	4:K:221:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:289:SER:O	4:G:299:GLN:NE2	2.46	0.48
6:D:164:SER:O	6:D:164:SER:OG	2.31	0.48
2:C:250:LEU:HD11	2:C:391:TRP:HE3	1.79	0.48
4:F:317:ASP:OD2	4:F:320:SER:OG	2.29	0.48
4:H:309:ASN:HB2	4:H:342:LEU:HD11	1.95	0.48
4:K:274:LYS:HD3	4:K:322:VAL:HG21	1.94	0.48
2:C:92:VAL:HG11	2:C:114:LEU:HD13	1.95	0.48
6:D:10:ASP:HB3	6:D:104:ALA:HB2	1.95	0.48
4:F:285:VAL:HG11	4:G:297:VAL:HG23	1.95	0.48
4:J:16:LEU:HD13	4:J:37:ILE:HD11	1.94	0.48
4:F:155:ASP:OD1	4:F:155:ASP:N	2.47	0.48
4:H:365:LYS:N	4:H:368:GLU:OE1	2.47	0.48
4:K:256:LYS:O	6:D:166:THR:OG1	2.32	0.48
5:B:7:THR:HG22	5:B:142:GLN:HG2	1.96	0.48
2:C:147:GLU:OE1	2:C:150:LYS:HG3	2.14	0.48
4:F:108:ILE:O	4:F:112:ALA:HB3	2.13	0.48
4:F:314:GLY:O	4:G:349:ASN:ND2	2.47	0.48
2:C:262:GLN:O	2:C:386:ARG:NH2	2.47	0.48
1:A:0:G:H22	5:B:124:THR:HG23	1.79	0.48
4:J:156:LYS:NZ	4:J:160:VAL:O	2.47	0.48
5:B:326:ARG:HG3	5:B:352:PRO:HD2	1.96	0.47
6:D:2:ILE:HG13	6:D:114:PRO:HD3	1.96	0.47
6:D:9:ILE:HG21	6:D:25:LEU:HD11	1.96	0.47
2:C:408:LYS:HE2	2:C:465:ALA:HB1	1.94	0.47
4:F:141:ASP:OD1	4:F:141:ASP:N	2.46	0.47
4:H:273:PHE:HZ	4:H:357:VAL:HG13	1.80	0.47
4:K:156:LYS:NZ	4:K:157:ASP:O	2.47	0.47
2:C:92:VAL:HG12	2:C:116:LEU:HD23	1.96	0.47
2:C:456:ILE:HD13	2:C:493:VAL:HG21	1.96	0.47
4:H:62:ARG:HH22	7:M:38:DC:H4'	1.79	0.47
4:K:282:ASN:HA	4:K:285:VAL:HG23	1.96	0.47
5:B:23:GLU:HG3	5:B:30:ARG:HD2	1.96	0.47
4:F:349:ASN:HB3	4:F:352:GLU:HB3	1.96	0.47
5:B:8:LEU:HD13	5:B:151:LEU:HB3	1.96	0.47
1:A:2:A:H62	7:M:49:DT:H3	1.62	0.47
2:C:108:LEU:HD21	2:C:160:LEU:HD12	1.96	0.47
4:F:285:VAL:HG12	4:G:295:ASP:HB2	1.96	0.47
4:H:263:HIS:NE2	4:I:172:GLN:OE1	2.36	0.47
5:B:228:GLU:OE1	5:B:249:ARG:NH1	2.36	0.47
2:C:451:PRO:HB3	4:G:21:LEU:HB2	1.96	0.47
3:E:42:SER:O	3:E:46:TRP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:133:ARG:HH21	6:D:156:ARG:HD3	1.79	0.47
1:A:32:A:C6	6:D:196:TRP:HB2	2.50	0.47
4:H:138:LEU:HD22	4:H:138:LEU:HA	1.79	0.47
5:B:374:ARG:NH1	6:D:15:PRO:O	2.38	0.47
2:C:501:GLN:O	3:E:157:SER:OG	2.29	0.47
5:B:173:ARG:HH22	5:B:196:GLN:HB3	1.79	0.47
4:H:7:MET:HE2	4:H:217:LYS:HD2	1.96	0.46
6:D:255:ALA:HB1	6:D:258:PHE:HB2	1.95	0.46
5:B:346:THR:OG1	5:B:347:THR:N	2.43	0.46
2:C:197:THR:H	2:C:199:HIS:CE1	2.33	0.46
4:F:295:ASP:OD2	4:F:333:TYR:OH	2.26	0.46
4:J:6:HIS:HB3	4:J:216:TYR:HE1	1.80	0.46
4:I:368:GLU:OE2	4:I:368:GLU:N	2.46	0.46
4:J:282:ASN:HA	4:J:285:VAL:HG23	1.97	0.46
4:I:92:ASN:OD1	4:I:92:ASN:N	2.42	0.46
5:B:134:ASP:OD1	5:B:198:ARG:NH1	2.48	0.46
3:E:76:ARG:HB3	3:E:134:CYS:HB2	1.96	0.46
1:A:-4:A:P	5:B:29:ARG:HH21	2.38	0.46
2:C:171:GLY:O	2:C:175:ARG:NH2	2.46	0.46
2:C:172:ASP:OD1	2:C:172:ASP:N	2.41	0.46
2:C:367:ALA:HB1	2:C:461:GLU:HG3	1.97	0.46
4:J:198:GLU:OE2	4:J:198:GLU:N	2.34	0.46
4:K:80:LYS:NZ	4:K:118:ASN:OD1	2.48	0.46
6:D:191:LEU:HD21	6:D:194:LEU:HD22	1.97	0.46
1:A:11:A:O2'	4:F:190:VAL:O	2.32	0.46
1:A:24:C:O2'	4:J:41:CYS:SG	2.62	0.46
2:C:194:GLU:OE1	5:B:25:LYS:HG2	2.16	0.46
3:E:27:ARG:HD3	3:E:70:GLU:HG3	1.97	0.46
3:E:148:GLU:HB3	4:G:291:VAL:HG12	1.98	0.46
1:A:20:G:H5'	4:I:255:GLY:HA2	1.98	0.46
4:I:99:MET:HE3	4:I:99:MET:HA	1.98	0.46
5:B:274:THR:OG1	5:B:275:ARG:N	2.49	0.46
2:C:87:ASP:OD1	2:C:87:ASP:N	2.49	0.45
2:C:237:ILE:HG23	2:C:329:VAL:HG11	1.98	0.45
4:J:295:ASP:OD1	4:J:295:ASP:N	2.47	0.45
4:K:109:LYS:HA	4:K:109:LYS:HD3	1.80	0.45
2:C:379:LEU:HD12	2:C:422:LEU:HD11	1.98	0.45
4:F:103:MET:SD	4:F:108:ILE:HB	2.57	0.45
4:F:174:ALA:HB2	4:G:261:ALA:HB3	1.98	0.45
4:I:157:ASP:OD1	4:I:157:ASP:N	2.49	0.45
5:B:282:GLU:OE2	5:B:285:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:68:ARG:NE	6:D:262:LEU:HB3	2.32	0.45
4:I:71:GLU:OE1	4:I:113:ARG:NE	2.45	0.45
4:J:37:ILE:HB	4:J:176:ALA:HB3	1.97	0.45
2:C:356:ILE:HA	2:C:356:ILE:HD13	1.84	0.45
3:E:105:PHE:HA	3:E:123:ILE:HD11	1.98	0.45
4:F:177:ILE:HD11	4:F:281:ALA:HB1	1.99	0.45
2:C:358:LEU:H	2:C:358:LEU:HG	1.50	0.45
2:C:427:ASN:OD1	2:C:427:ASN:N	2.50	0.45
4:H:99:MET:HE3	4:H:99:MET:HB2	1.81	0.45
4:J:21:LEU:HD22	5:B:375:GLY:HA3	1.99	0.45
2:C:445:LYS:HE2	2:C:446:LYS:HZ1	1.80	0.45
3:E:38:PHE:CG	5:B:338:MET:HG3	2.51	0.45
4:J:157:ASP:OD1	4:J:157:ASP:N	2.50	0.45
5:B:298:CYS:SG	5:B:299:MET:N	2.89	0.45
4:I:152:ASN:OD1	4:I:154:LYS:N	2.44	0.45
4:J:47:ARG:HH12	4:J:60:ARG:HH21	1.64	0.45
6:D:93:ASP:O	6:D:97:GLN:HB3	2.17	0.45
6:D:130:ALA:HB1	6:D:159:LEU:HB3	1.99	0.45
2:C:209:ASP:OD1	2:C:209:ASP:N	2.49	0.44
4:H:294:SER:OG	4:H:295:ASP:N	2.50	0.44
4:G:222:ASP:OD1	4:G:225:GLN:HB3	2.17	0.44
4:G:304:LEU:O	4:G:308:VAL:HG23	2.16	0.44
5:B:309:GLN:HE22	5:B:337:THR:HG23	1.81	0.44
1:A:-6:U:H1'	1:A:-4:A:H1'	2.00	0.44
4:H:230:LEU:HD22	4:H:236:LEU:HD23	1.99	0.44
4:H:335:LEU:HD23	4:H:335:LEU:HA	1.85	0.44
4:G:172:GLN:HE22	4:G:220:SER:HB3	1.81	0.44
4:I:361:ILE:HG22	4:I:364:PHE:HE2	1.83	0.44
4:J:124:GLU:CD	4:J:124:GLU:H	2.26	0.44
6:D:146:THR:OG1	6:D:148:GLU:OE2	2.29	0.44
2:C:375:LEU:HD12	2:C:425:LEU:HD12	1.99	0.44
4:H:20:ASP:OD1	4:H:20:ASP:N	2.44	0.44
4:I:64:LEU:O	4:I:68:ILE:HG12	2.18	0.44
4:G:198:GLU:OE2	4:G:198:GLU:N	2.35	0.44
6:D:62:LYS:HA	6:D:62:LYS:HD2	1.78	0.44
6:D:131:SER:HB2	6:D:156:ARG:HG2	2.00	0.44
2:C:251:TRP:HA	2:C:389:LYS:O	2.17	0.44
3:E:3:ARG:HD3	3:E:3:ARG:HA	1.77	0.44
4:H:174:ALA:HB3	4:H:218:TYR:HB3	1.98	0.44
4:J:141:ASP:OD1	4:J:141:ASP:N	2.49	0.44
4:F:295:ASP:HB2	4:H:285:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:231:LYS:HB2	4:J:231:LYS:HE2	1.74	0.44
3:E:80:THR:HG23	3:E:82:PRO:HD2	2.00	0.44
4:F:270:LEU:HG	4:F:326:TRP:HE3	1.83	0.44
4:I:254:SER:O	4:I:254:SER:OG	2.34	0.44
4:J:109:LYS:O	4:J:113:ARG:HG3	2.17	0.44
4:K:21:LEU:HD22	6:D:25:LEU:HD12	1.99	0.44
4:G:5:ILE:HB	4:G:219:PHE:HB2	2.00	0.44
1:A:30:G:O2'	4:K:41:CYS:SG	2.70	0.44
4:F:32:VAL:HG23	4:F:34:ARG:HE	1.83	0.44
4:J:38:SER:HB3	4:J:40:GLN:HG2	2.00	0.44
4:J:266:PRO:O	4:K:315:TYR:OH	2.31	0.44
2:C:445:LYS:HE2	2:C:445:LYS:HB2	1.68	0.44
4:J:40:GLN:HG2	4:J:40:GLN:H	1.58	0.44
5:B:248:ILE:HB	5:B:250:ARG:NH2	2.33	0.43
1:A:37:U:H6	1:A:38:C:H5	1.65	0.43
4:G:310:ASP:O	4:G:312:ARG:N	2.50	0.43
2:C:308:GLN:HB2	2:C:320:ALA:HA	1.99	0.43
4:F:194:ASP:OD2	4:H:47:ARG:NH2	2.45	0.43
4:H:297:VAL:O	4:H:301:ILE:HG13	2.19	0.43
4:K:71:GLU:N	4:K:71:GLU:OE1	2.51	0.43
5:B:71:ARG:HB2	5:B:190:LEU:HD22	1.99	0.43
5:B:184:ASN:OD1	5:B:184:ASN:N	2.47	0.43
5:B:293:MET:SD	5:B:293:MET:N	2.78	0.43
1:A:20:G:H22	7:M:31:DC:H5	1.66	0.43
4:F:174:ALA:HB3	4:F:218:TYR:HB3	2.00	0.43
4:J:59:VAL:H	4:J:104:SER:HA	1.82	0.43
2:C:262:GLN:OE1	2:C:386:ARG:NE	2.52	0.43
4:H:222:ASP:HB3	4:H:225:GLN:HB3	2.00	0.43
4:J:67:LEU:O	4:J:71:GLU:HG3	2.19	0.43
4:K:96:ASN:C	4:K:96:ASN:ND2	2.76	0.43
2:C:286:VAL:HB	2:C:290:ALA:HB3	2.01	0.43
4:G:209:MET:HE2	4:G:209:MET:HB3	1.90	0.43
1:A:12:G:O2'	1:A:14:A:OP1	2.36	0.43
2:C:498:GLU:O	2:C:509:ARG:NH1	2.51	0.43
4:K:150:GLU:HA	4:K:151:PRO:HD3	1.81	0.43
5:B:362:LEU:HA	5:B:365:ARG:HG2	2.00	0.43
2:C:90:VAL:HB	2:C:102:ILE:HD12	2.00	0.43
4:H:83:GLU:HG2	4:H:122:LEU:HD11	2.00	0.43
4:J:289:SER:O	4:J:299:GLN:NE2	2.39	0.43
4:J:311:ILE:HD13	4:J:311:ILE:HA	1.91	0.43
6:D:91:ASP:N	6:D:91:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-5:G:H3'	5:B:20:GLY:HA3	2.01	0.42
2:C:107:THR:HA	2:C:114:LEU:HD21	2.00	0.42
4:F:289:SER:O	4:F:299:GLN:NE2	2.44	0.42
4:H:282:ASN:HA	4:H:285:VAL:HG23	2.00	0.42
4:I:24:PRO:HD2	4:I:209:MET:HE2	2.01	0.42
4:G:338:LYS:HA	4:G:338:LYS:HD3	1.85	0.42
6:D:61:GLN:NE2	6:D:63:THR:OG1	2.52	0.42
6:D:162:ASP:OD1	6:D:162:ASP:N	2.44	0.42
1:A:16:A:O2'	4:I:60:ARG:NH1	2.42	0.42
2:C:446:LYS:HE2	2:C:446:LYS:N	2.34	0.42
3:E:82:PRO:HG3	3:E:156:TRP:CD1	2.54	0.42
4:F:113:ARG:HD2	4:F:113:ARG:HA	1.76	0.42
4:H:311:ILE:O	4:H:315:TYR:HB2	2.18	0.42
4:I:93:LYS:HB2	4:I:98:LYS:HE2	2.02	0.42
6:D:122:LEU:N	6:D:236:LEU:O	2.46	0.42
6:D:139:MET:HE1	6:D:147:ILE:H	1.83	0.42
2:C:500:ALA:HB1	2:C:502:THR:HG23	2.00	0.42
3:E:57:LYS:HE3	3:E:59:GLU:HB2	2.01	0.42
4:F:274:LYS:HD2	4:F:278:ILE:HG12	2.01	0.42
4:I:190:VAL:HG22	4:I:205:ILE:HG12	2.00	0.42
2:C:380:HIS:NE2	2:C:419:ASP:OD1	2.46	0.42
3:E:131:GLN:N	3:E:131:GLN:OE1	2.52	0.42
4:K:138:LEU:HD12	4:K:138:LEU:HA	1.87	0.42
4:G:286:ARG:HD2	4:G:286:ARG:HA	1.46	0.42
5:B:125:LEU:HD22	5:B:125:LEU:HA	1.90	0.42
2:C:116:LEU:HD23	2:C:116:LEU:HA	1.92	0.42
4:F:165:THR:O	4:F:165:THR:OG1	2.37	0.42
4:I:136:ALA:O	4:I:138:LEU:N	2.52	0.42
4:F:17:ASN:HB3	4:F:25:LYS:HG3	2.02	0.42
4:F:191:ALA:O	4:F:203:GLY:N	2.44	0.42
4:I:78:TRP:CD1	4:I:79:LYS:HG3	2.55	0.42
4:K:1:MET:HE3	4:K:1:MET:N	2.35	0.42
4:G:286:ARG:HA	4:G:287:PRO:HD2	1.97	0.42
5:B:277:ASP:OD1	5:B:280:ASN:ND2	2.29	0.42
4:H:55:LEU:HD13	4:H:240:THR:HA	2.02	0.42
3:E:18:GLY:O	3:E:22:ILE:HG23	2.19	0.42
4:K:33:LEU:HB2	6:D:76:ASN:HA	2.02	0.42
5:B:290:ARG:NE	5:B:325:LEU:O	2.41	0.42
4:H:290:VAL:HG21	4:I:31:GLY:HA3	2.02	0.42
4:H:349:ASN:ND2	4:I:313:LEU:O	2.53	0.42
4:F:64:LEU:HB3	4:F:85:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:64:LEU:HD12	4:F:64:LEU:HA	1.79	0.41
4:F:100:LEU:HD23	4:F:100:LEU:HA	1.84	0.41
4:H:168:GLU:O	4:H:229:ASN:ND2	2.53	0.41
4:H:272:GLU:OE1	4:H:280:TYR:OH	2.33	0.41
4:H:358:LEU:HD23	4:H:361:ILE:HD12	2.02	0.41
6:D:68:ARG:HH22	6:D:127:ARG:N	2.17	0.41
2:C:193:HIS:H	2:C:225:ARG:NH1	2.18	0.41
3:E:108:LEU:HD22	3:E:116:MET:HE1	2.02	0.41
4:J:56:LEU:HD12	4:J:56:LEU:HA	1.93	0.41
4:H:245:LEU:HD23	4:H:354:VAL:HG22	2.01	0.41
2:C:112:HIS:CE1	2:C:151:PRO:HG3	2.56	0.41
4:H:195:VAL:HG13	4:I:61:THR:HG21	2.02	0.41
5:B:358:ARG:HH22	6:D:97:GLN:CD	2.25	0.41
7:M:46:DC:H2'	7:M:47:DA:C8	2.55	0.41
7:M:49:DT:H6	7:M:49:DT:H2'	1.69	0.41
4:F:107:LYS:HD2	4:F:107:LYS:HA	1.84	0.41
4:I:319:GLN:HB3	4:I:320:SER:H	1.64	0.41
4:J:34:ARG:NH1	4:J:284:PHE:O	2.54	0.41
4:G:326:TRP:CD2	4:G:335:LEU:HB2	2.55	0.41
1:A:33:G:C2	6:D:167:PRO:HD3	2.56	0.41
4:J:55:LEU:HB3	4:J:140:PRO:HG2	2.01	0.41
6:D:51:PHE:HB3	6:D:97:GLN:HE21	1.85	0.41
3:E:120:LEU:O	3:E:124:MET:HG3	2.21	0.41
4:G:42:ILE:HG21	4:G:217:LYS:HZ3	1.86	0.41
2:C:157:ILE:HG23	2:C:158:PRO:HD3	2.03	0.41
4:J:29:PHE:HB3	4:J:34:ARG:HG3	2.03	0.41
4:J:246:LEU:HD23	4:J:246:LEU:HA	1.91	0.41
4:K:62:ARG:HG3	4:K:100:LEU:HG	2.03	0.41
5:B:290:ARG:HH21	5:B:326:ARG:HE	1.68	0.41
4:J:61:THR:HG21	4:J:67:LEU:HD11	2.02	0.41
4:G:341:LYS:HA	4:G:341:LYS:HD2	1.76	0.41
5:B:313:TYR:HE1	5:B:349:ARG:HG2	1.86	0.41
3:E:86:GLY:HA2	3:E:89:CYS:HB2	2.02	0.40
3:E:120:LEU:HD23	3:E:120:LEU:HA	1.87	0.40
4:H:224:GLU:OE2	4:H:224:GLU:N	2.36	0.40
4:J:361:ILE:HD13	4:J:361:ILE:HA	1.91	0.40
5:B:229:ILE:HD12	5:B:229:ILE:HA	1.86	0.40
6:D:139:MET:SD	6:D:146:THR:OG1	2.79	0.40
6:D:266:LEU:HD13	6:D:266:LEU:HA	1.91	0.40
2:C:108:LEU:HD12	2:C:108:LEU:HA	1.85	0.40
3:E:63:LEU:HA	3:E:66:LYS:HZ3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:6:HIS:HB3	4:H:216:TYR:HE1	1.87	0.40
4:F:87:LYS:HE3	4:F:122:LEU:HG	2.02	0.40
1:A:6:C:C5	1:A:8:G:H5''	2.55	0.40
2:C:174:LYS:HE2	2:C:174:LYS:HB2	1.98	0.40
2:C:256:LEU:HA	2:C:259:MET:HB2	2.04	0.40
4:I:246:LEU:HD23	4:I:246:LEU:HA	1.97	0.40
6:D:20:PRO:HB2	6:D:102:PHE:HE1	1.86	0.40
6:D:194:LEU:HD12	6:D:194:LEU:HA	1.87	0.40
3:E:22:ILE:HD12	3:E:36:PRO:HB2	2.03	0.40
4:J:68:ILE:O	4:J:72:ALA:CB	2.70	0.40
4:G:238:ALA:HB1	4:G:358:LEU:HD22	2.04	0.40
5:B:69:GLY:HA3	5:B:190:LEU:HD11	2.03	0.40
6:D:51:PHE:HB2	6:D:94:TYR:HE1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	C	441/546 (81%)	395 (90%)	44 (10%)	2 (0%)	24	60
3	E	163/174 (94%)	156 (96%)	7 (4%)	0	100	100
4	F	364/378 (96%)	343 (94%)	21 (6%)	0	100	100
4	G	247/378 (65%)	234 (95%)	13 (5%)	0	100	100
4	H	373/378 (99%)	350 (94%)	23 (6%)	0	100	100
4	I	371/378 (98%)	341 (92%)	29 (8%)	1 (0%)	36	70
4	J	372/378 (98%)	337 (91%)	33 (9%)	2 (0%)	24	60
4	K	344/378 (91%)	318 (92%)	26 (8%)	0	100	100
5	B	339/388 (87%)	315 (93%)	23 (7%)	1 (0%)	36	70
6	D	252/272 (93%)	232 (92%)	19 (8%)	1 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3266/3648 (90%)	3021 (92%)	238 (7%)	7 (0%)	44	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	306	PRO
4	J	151	PRO
2	C	301	LEU
5	B	87	ALA
4	I	322	VAL
6	D	235	VAL
4	J	139	ALA

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	
2	C	370/470 (79%)	354 (96%)	16 (4%)	26	60
3	E	143/153 (94%)	137 (96%)	6 (4%)	26	61
4	F	295/313 (94%)	286 (97%)	9 (3%)	35	68
4	G	199/313 (64%)	191 (96%)	8 (4%)	28	62
4	H	302/313 (96%)	292 (97%)	10 (3%)	33	67
4	I	297/313 (95%)	287 (97%)	10 (3%)	32	66
4	J	293/313 (94%)	278 (95%)	15 (5%)	21	55
4	K	285/313 (91%)	277 (97%)	8 (3%)	38	70
5	B	282/322 (88%)	269 (95%)	13 (5%)	24	58
6	D	213/238 (90%)	204 (96%)	9 (4%)	26	61
All	All	2679/3061 (88%)	2575 (96%)	104 (4%)	30	62

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	96	SER
2	C	98	LYS
2	C	109	LYS
2	C	144	VAL
2	C	200	ASN
2	C	203	HIS
2	C	259	MET
2	C	260	LEU
2	C	286	VAL
2	C	338	TRP
2	C	358	LEU
2	C	380	HIS
2	C	392	LEU
2	C	419	ASP
2	C	477	TYR
2	C	496	SER
3	E	35	LEU
3	E	91	LYS
3	E	111	LEU
3	E	114	MET
3	E	132	GLN
3	E	144	LEU
4	F	38	SER
4	F	44	ARG
4	F	97	THR
4	F	123	THR
4	F	138	LEU
4	F	157	ASP
4	F	165	THR
4	F	245	LEU
4	F	251	THR
4	H	17	ASN
4	H	94	ASP
4	H	96	ASN
4	H	122	LEU
4	H	138	LEU
4	H	141	ASP
4	H	157	ASP
4	H	234	THR
4	H	328	SER
4	H	344	SER
4	I	17	ASN
4	I	45	SER

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Mol	Chain	Res	Type
4	I	59	VAL
4	I	113	ARG
4	I	138	LEU
4	I	190	VAL
4	I	236	LEU
4	I	276	SER
4	I	316	TYR
4	I	320	SER
4	J	18	ARG
4	J	20	ASP
4	J	49	SER
4	J	74	GLU
4	J	102	PHE
4	J	119	SER
4	J	145	CYS
4	J	163	SER
4	J	251	THR
4	J	289	SER
4	J	290	VAL
4	J	294	SER
4	J	328	SER
4	J	340	SER
4	J	369	VAL
4	K	3	ILE
4	K	88	CYS
4	K	96	ASN
4	K	100	LEU
4	K	323	ILE
4	K	328	SER
4	K	338	LYS
4	K	341	LYS
4	G	27	CYS
4	G	32	VAL
4	G	173	VAL
4	G	186	ILE
4	G	286	ARG
4	G	294	SER
4	G	297	VAL
4	G	323	ILE
5	B	8	LEU
5	B	50	ILE
5	B	60	LEU

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Mol	Chain	Res	Type
5	B	125	LEU
5	B	136	SER
5	B	159	VAL
5	B	235	VAL
5	B	237	PHE
5	B	253	VAL
5	B	299	MET
5	B	306	THR
5	B	311	VAL
5	B	347	THR
6	D	41	SER
6	D	63	THR
6	D	135	HIS
6	D	154	HIS
6	D	166	THR
6	D	225	LEU
6	D	245	LEU
6	D	264	SER
6	D	266	LEU

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

Mol	Chain	Res	Type
2	C	120	ASN
2	C	178	GLN
2	C	384	ASN
2	C	459	HIS
2	C	474	ASN
4	F	252	ASN
4	F	257	GLN
4	F	339	HIS
4	H	257	GLN
4	H	309	ASN
4	I	69	GLN
4	I	225	GLN
4	J	50	ASN
4	J	69	GLN
4	J	92	ASN
4	J	135	GLN
4	J	152	ASN
4	J	263	HIS
4	J	309	ASN

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Mol	Chain	Res	Type
4	K	15	ASN
4	K	82	GLN
4	K	92	ASN
4	K	135	GLN
4	G	17	ASN
4	G	172	GLN
4	G	252	ASN
4	G	258	ASN
5	B	206	GLN
5	B	222	HIS
6	D	30	ASN
6	D	61	GLN
6	D	220	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/61 (93%)	30 (52%)	0

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-6	U
1	A	-5	G
1	A	-3	A
1	A	1	G
1	A	2	A
1	A	6	C
1	A	7	C
1	A	8	G
1	A	9	U
1	A	11	A
1	A	12	G
1	A	13	G
1	A	14	A
1	A	18	U
1	A	19	A
1	A	20	G
1	A	24	C
1	A	25	G
1	A	26	C

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Mol	Chain	Res	Type
1	A	27	U
1	A	31	C
1	A	32	A
1	A	33	G
1	A	39	C
1	A	42	A
1	A	43	C
1	A	44	G
1	A	45	C
1	A	51	G
1	A	52	G

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 2 ligands modelled in this entry, 2 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.

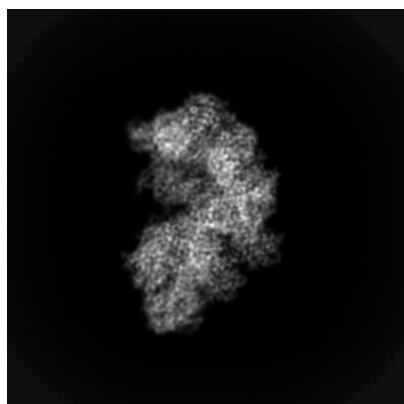
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60328. These allow visual inspection of the internal detail of the map and identification of artifacts.

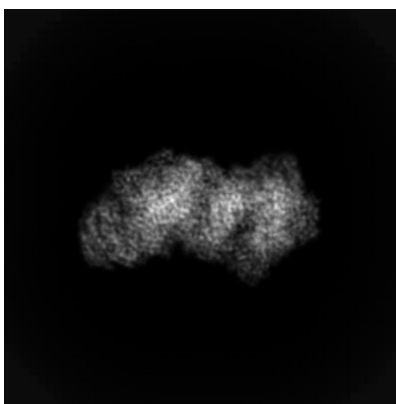
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

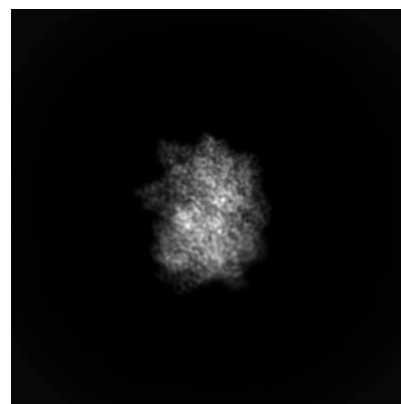
6.1.1 Primary map



X

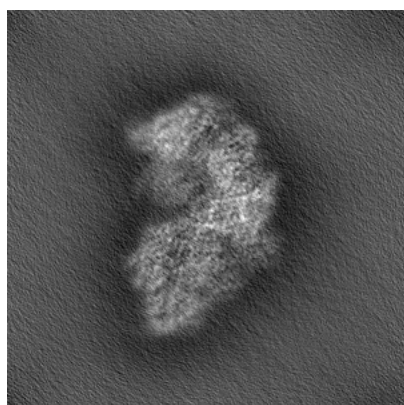


Y

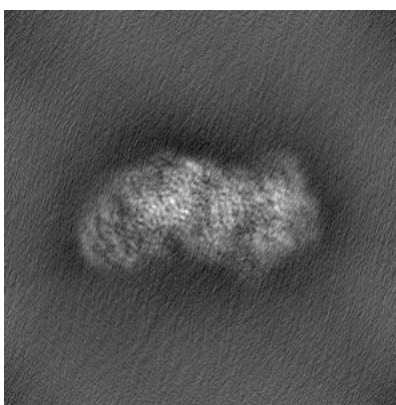


Z

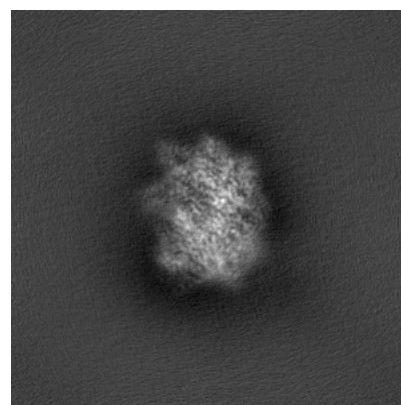
6.1.2 Raw map



X



Y



Z

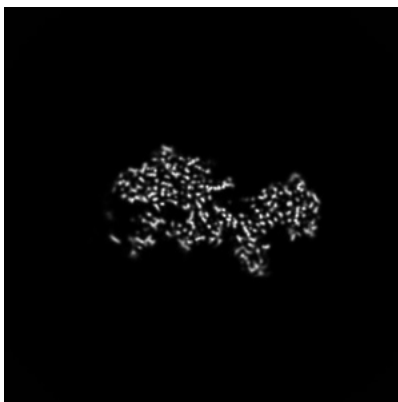
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

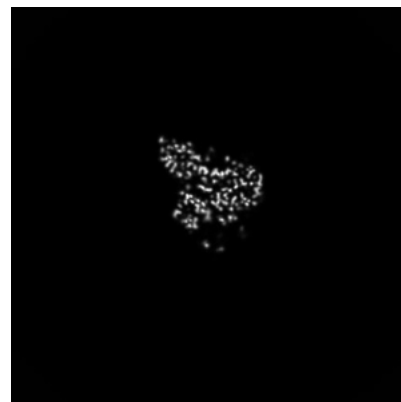
6.2.1 Primary map



X Index: 180

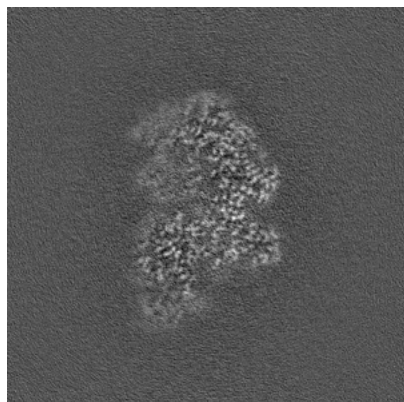


Y Index: 180

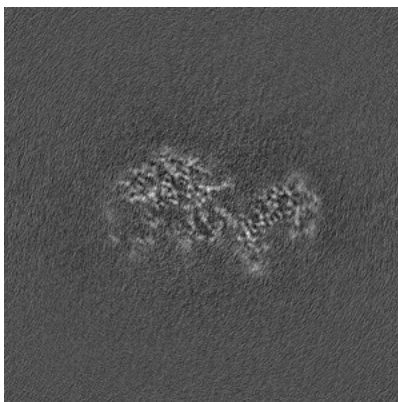


Z Index: 180

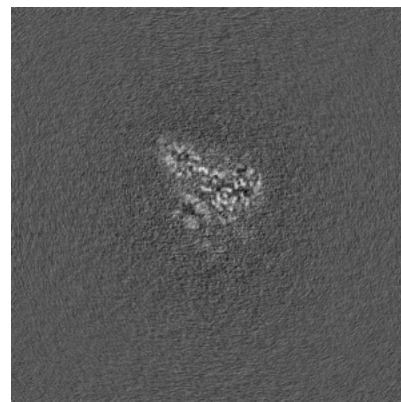
6.2.2 Raw map



X Index: 180



Y Index: 180

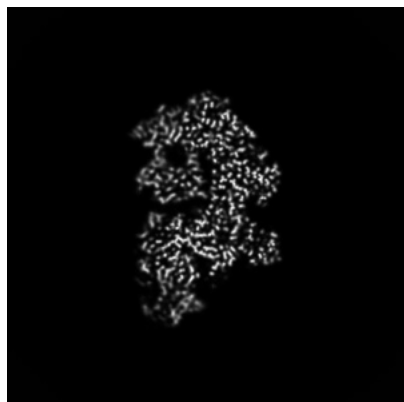


Z Index: 180

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

6.3 Largest variance slices [i](#)

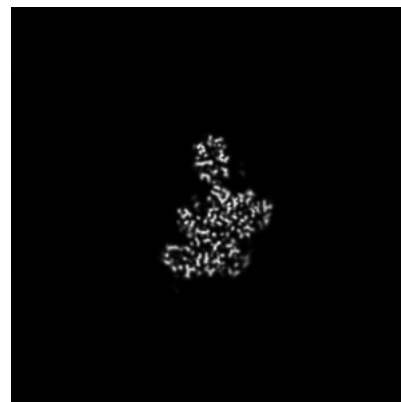
6.3.1 Primary map



X Index: 182

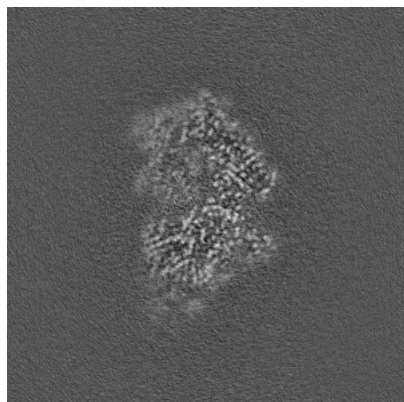


Y Index: 166

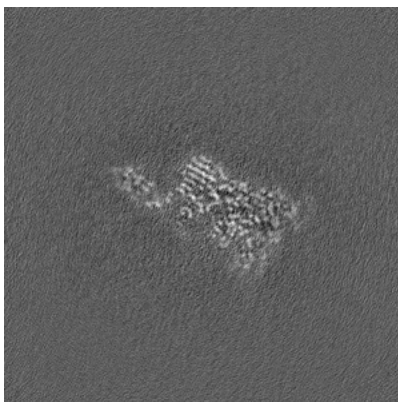


Z Index: 144

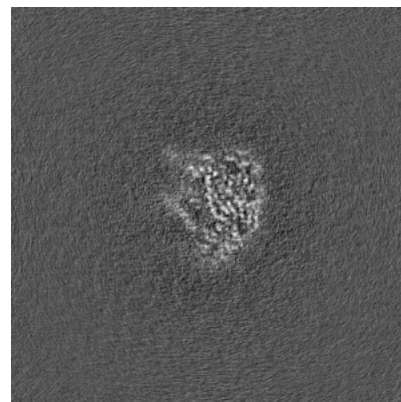
6.3.2 Raw map



X Index: 187



Y Index: 200



Z Index: 165

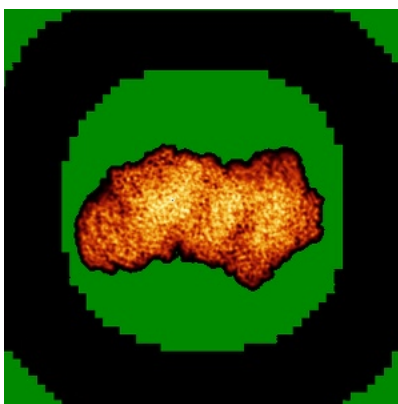
The images above show the largest variance slices of the map in three orthogonal directions.

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

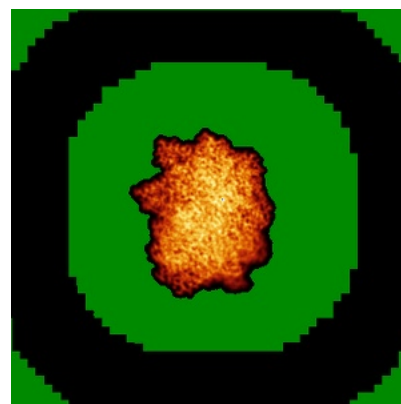
6.4.1 Primary map



X

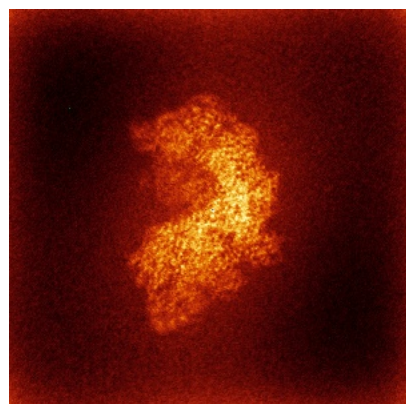


Y

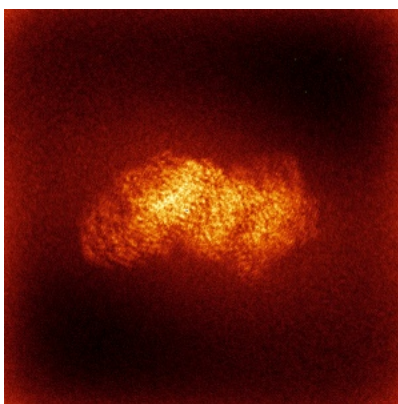


Z

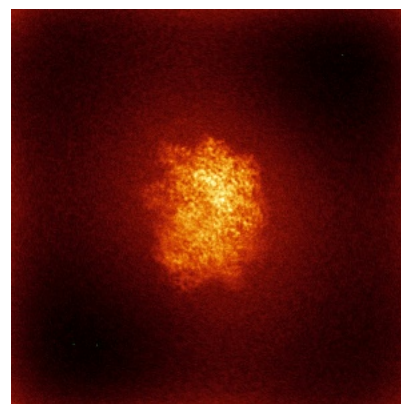
6.4.2 Raw map



X



Y

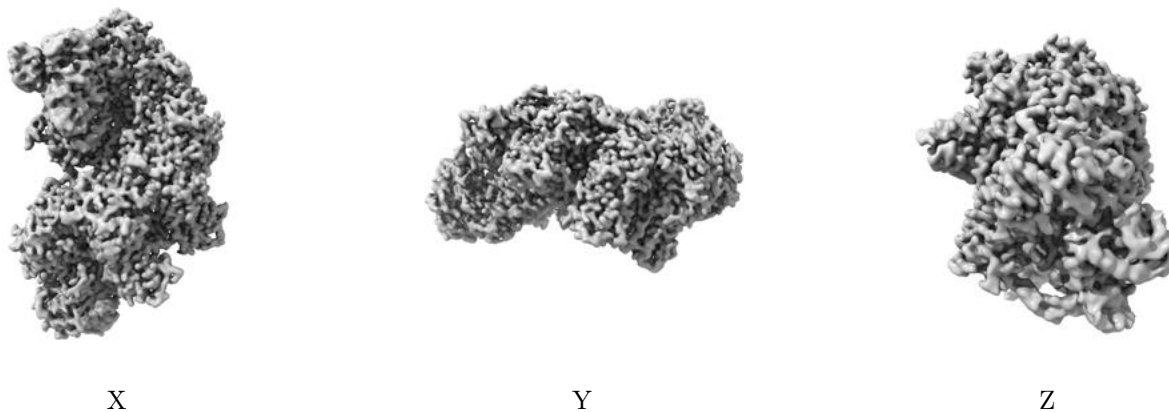


Z

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.

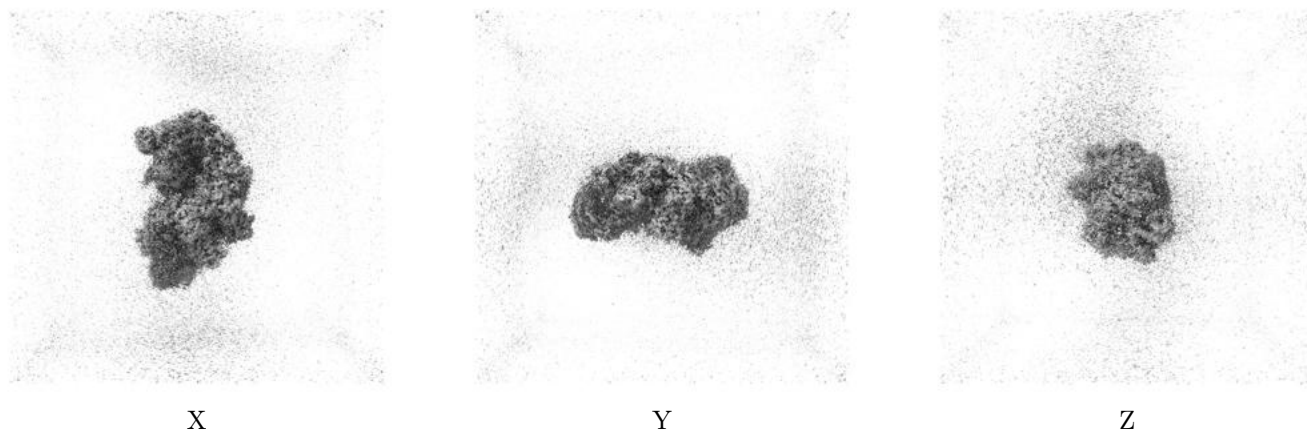
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.58. 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.

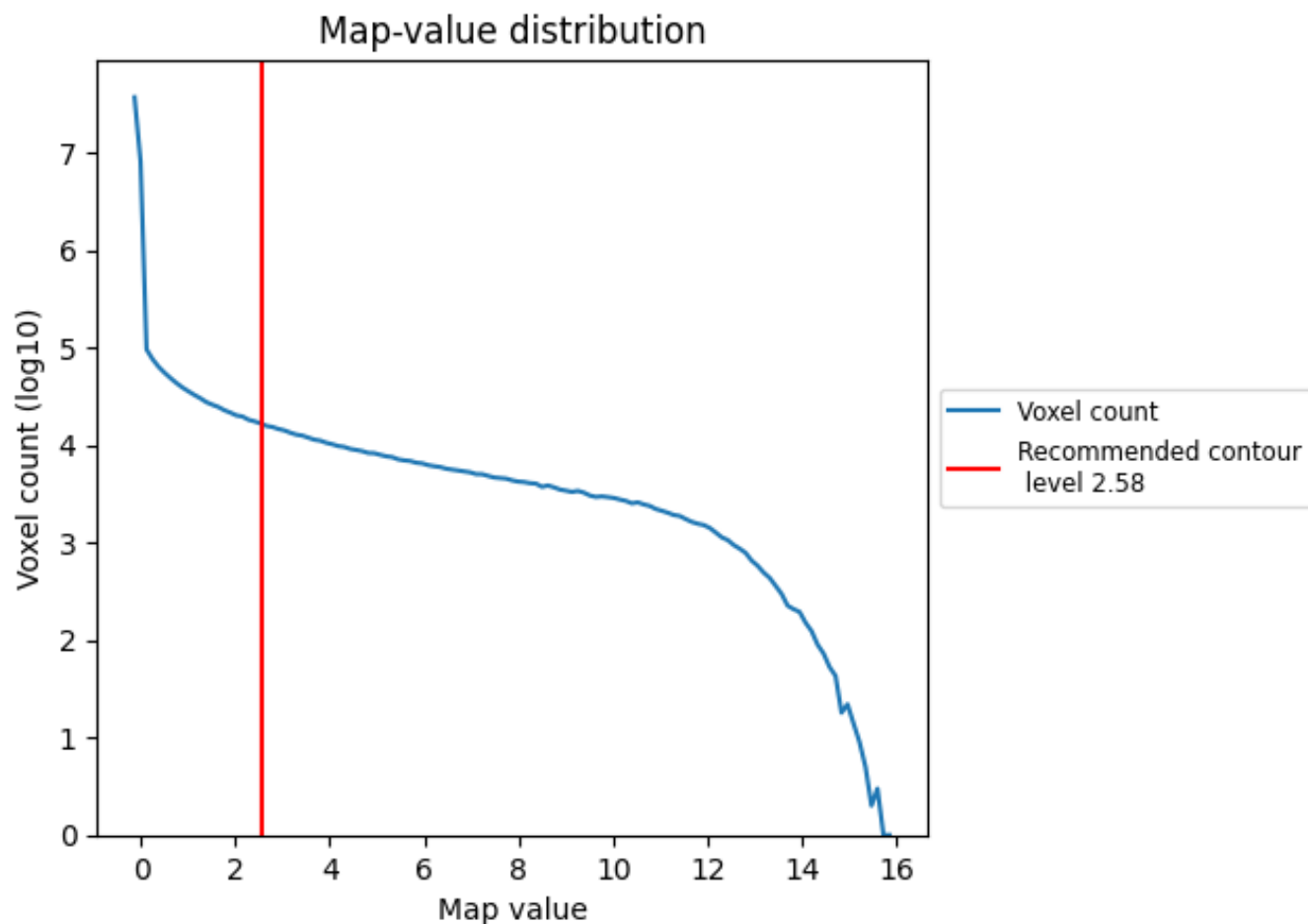
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

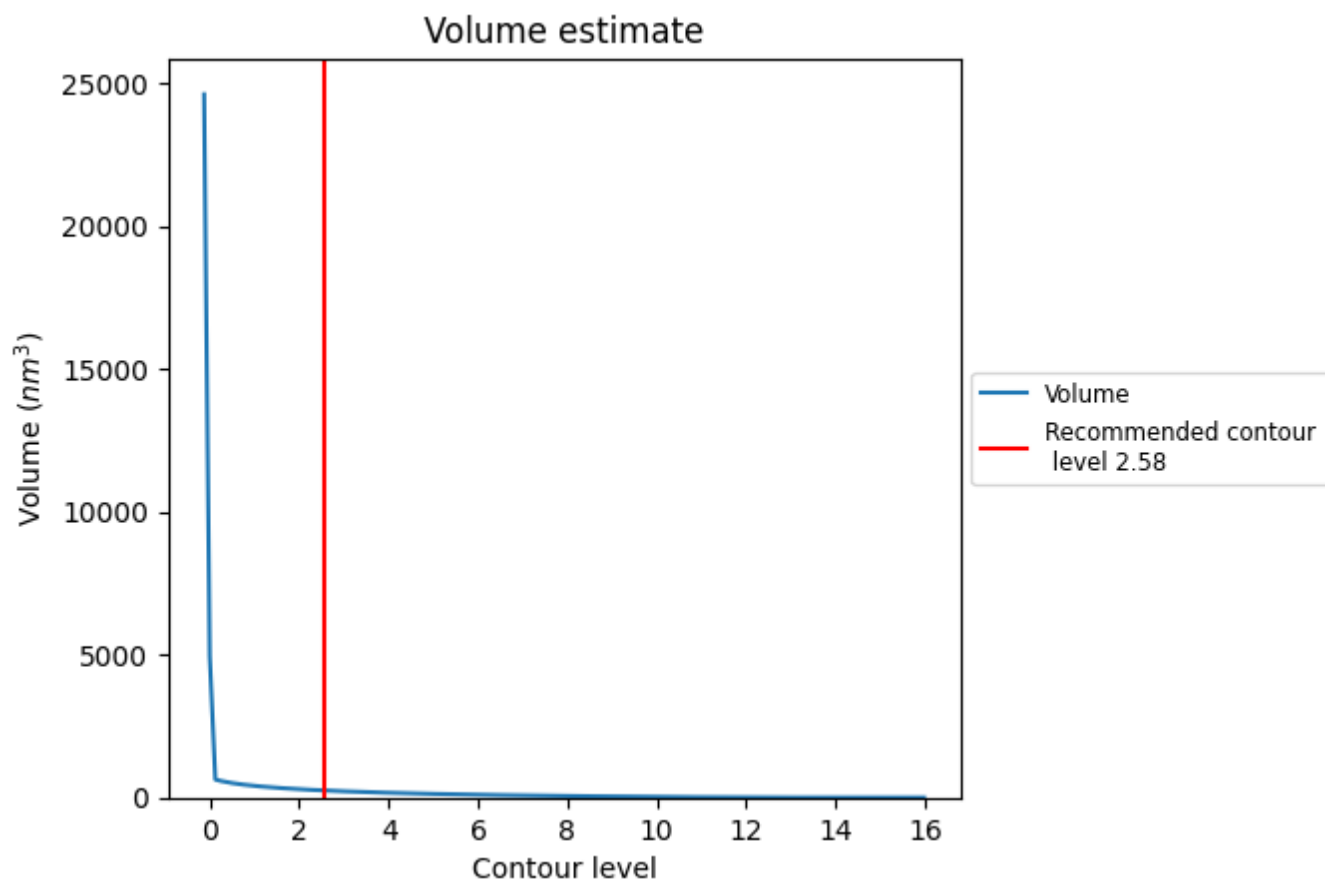
This section contains the results of statistical analysis of the map.

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.

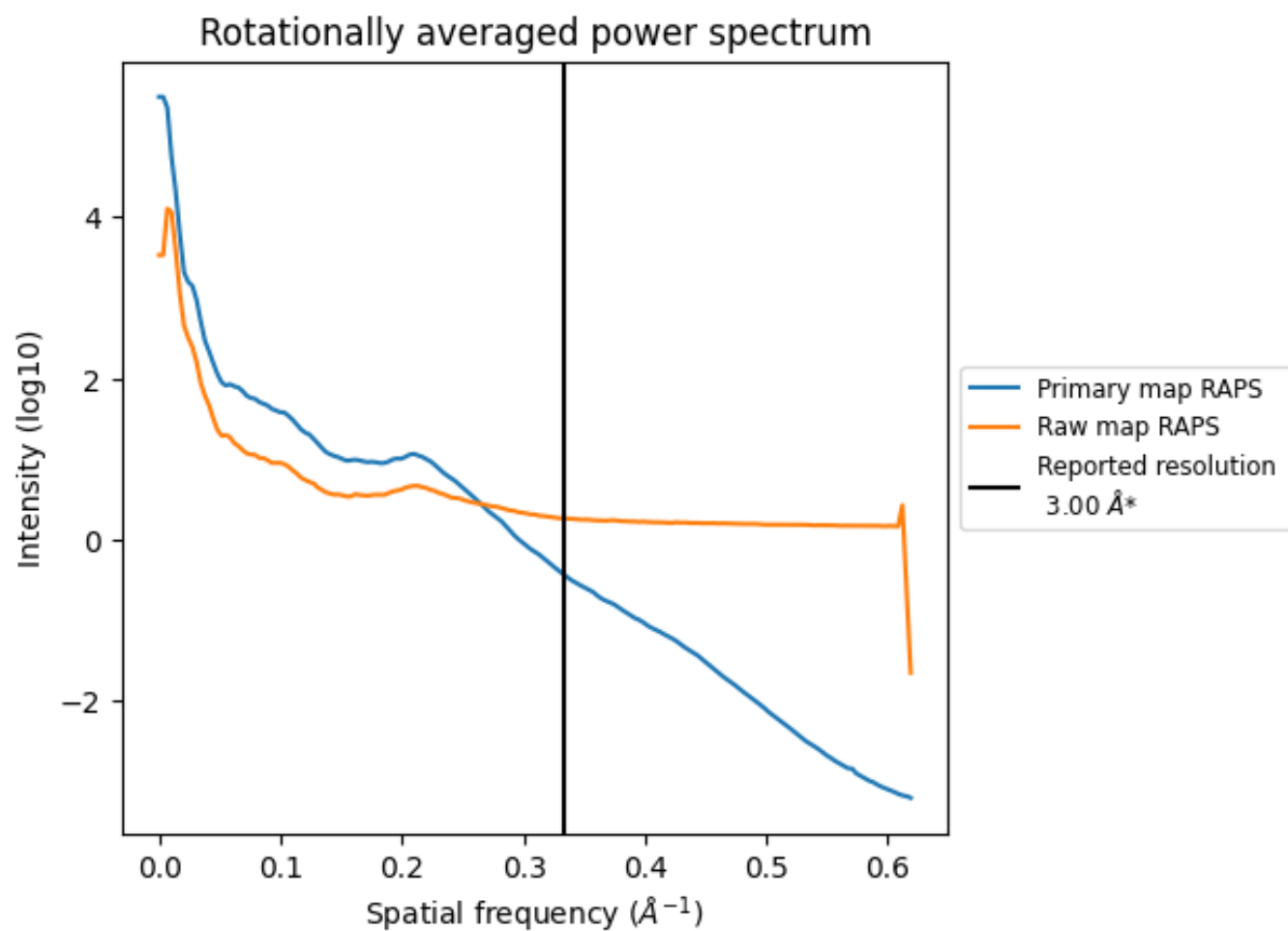
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 223 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 ⓘ

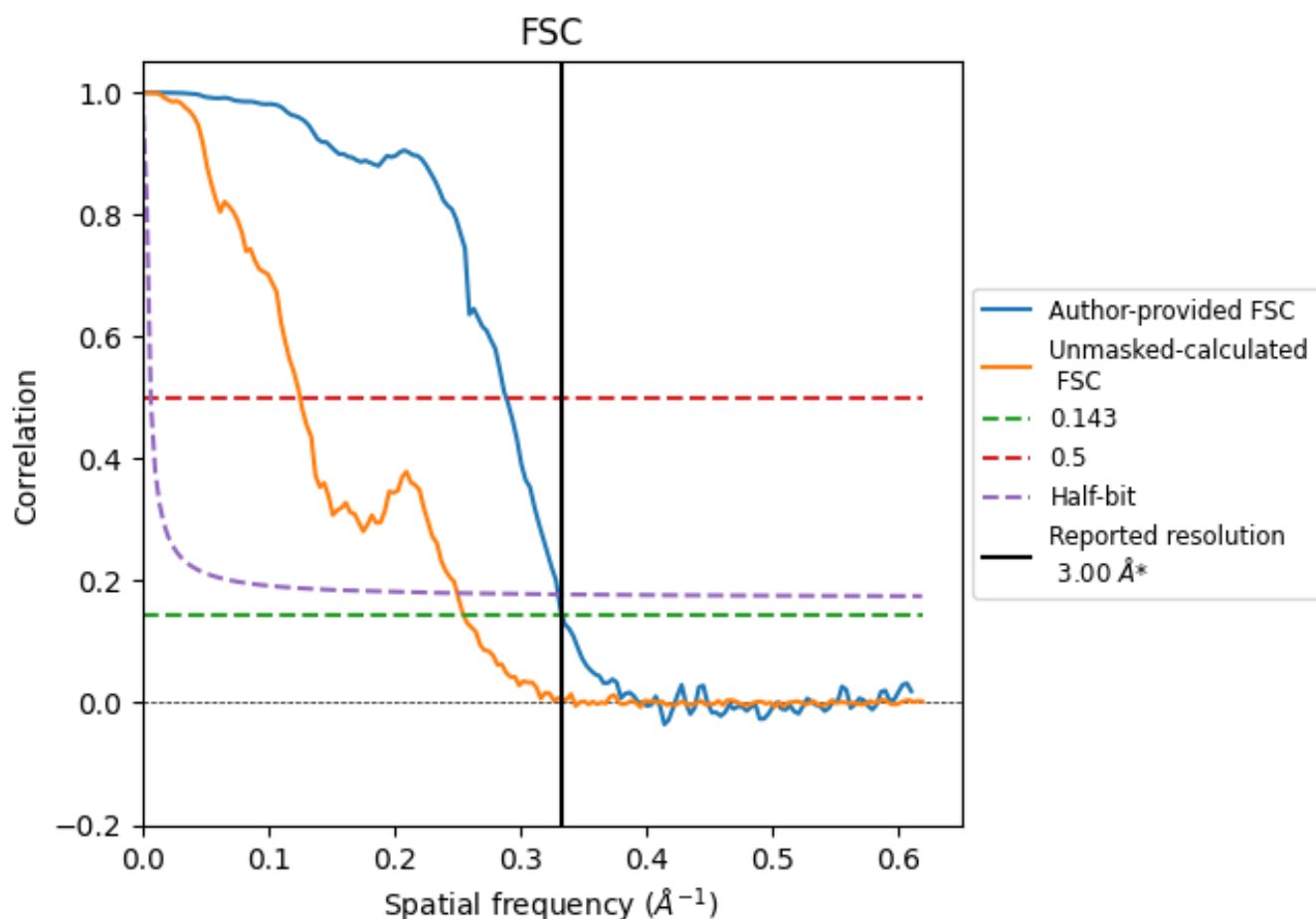


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

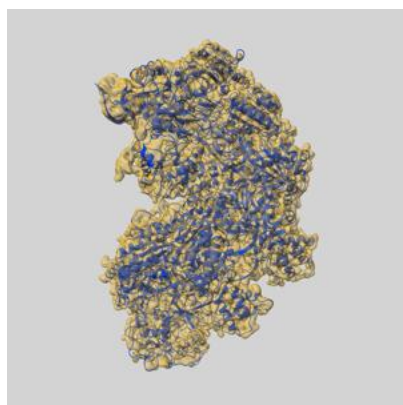
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.46	3.03
Unmasked-calculated*	3.92	7.99	4.00

*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 3.92 differs from the reported value 3.0 by more than 10 %

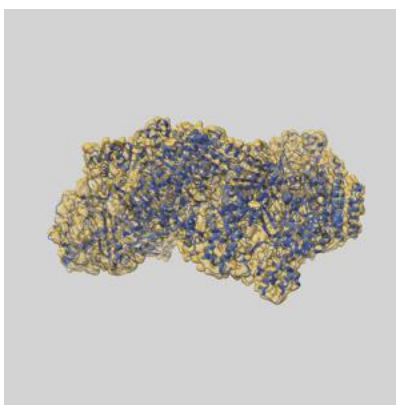
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60328 and PDB model 8ZP7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

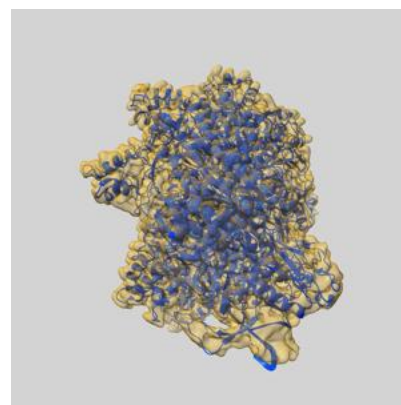
9.1 Map-model overlay [i](#)



X



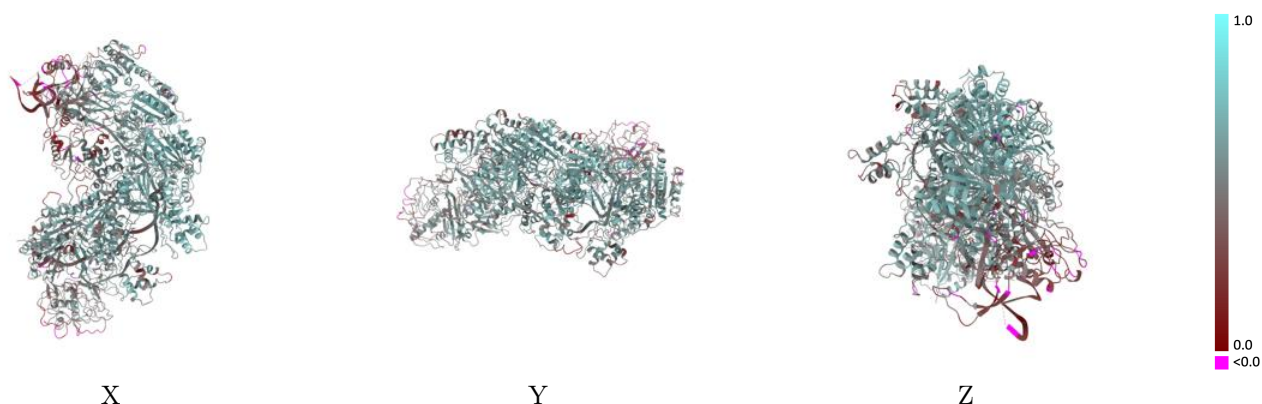
Y



Z

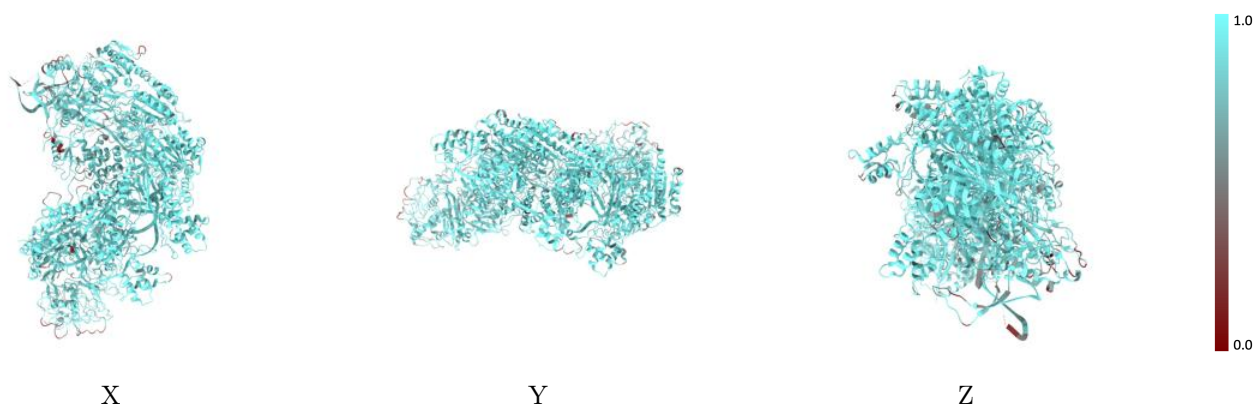
The images above show the 3D surface view of the map at the recommended contour level 2.58 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



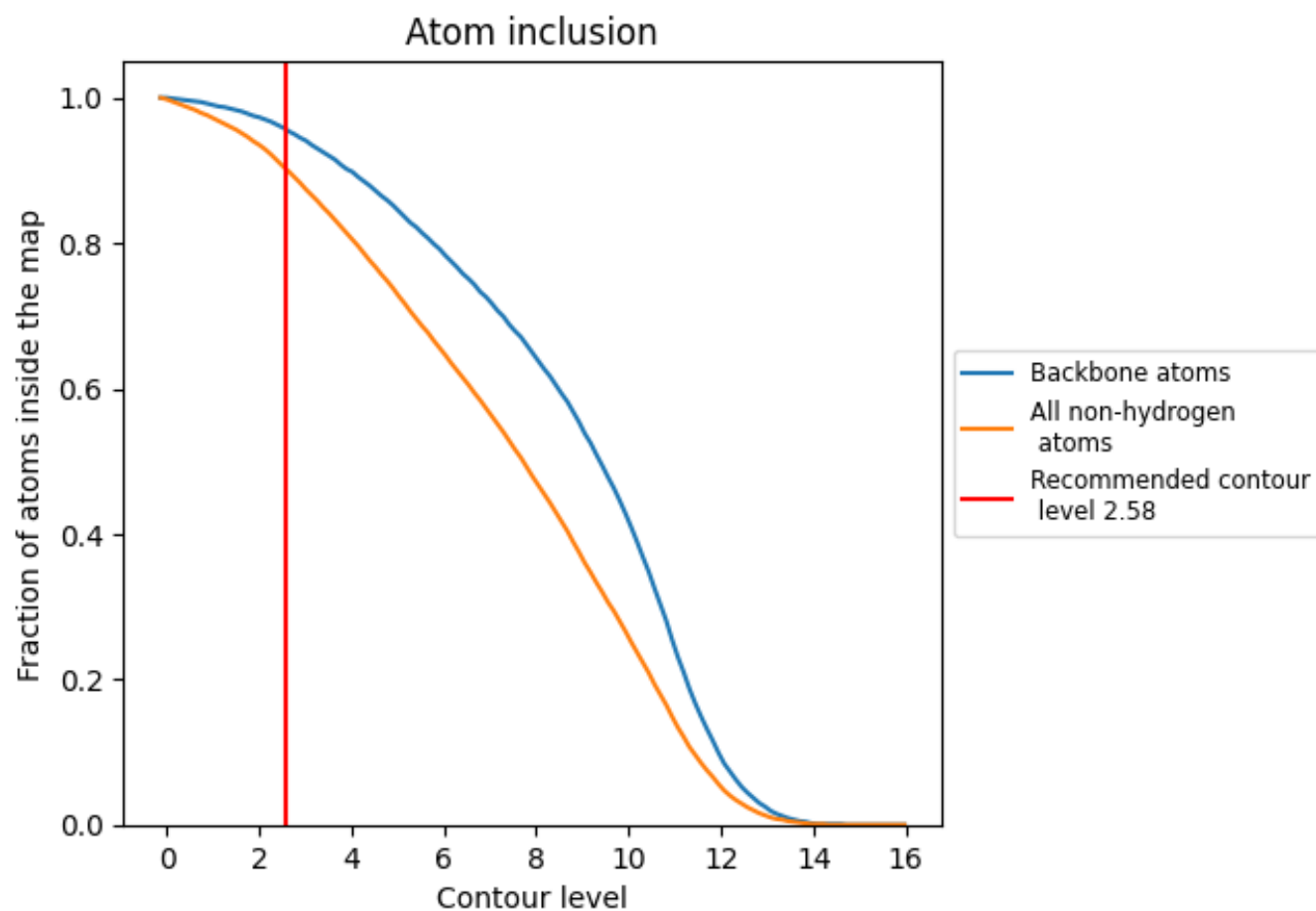
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.58).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (2.58) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.5170
A	0.8670	0.4030
B	0.9010	0.4910
C	0.8680	0.4590
D	0.7610	0.3010
E	0.8760	0.5200
F	0.9300	0.5560
G	0.9180	0.5430
H	0.9580	0.6190
I	0.9450	0.5990
J	0.9290	0.5630
K	0.8980	0.5340
M	0.9600	0.5140

