



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:44 PM UTC

PDB ID : 8ZM3 / pdb_00008zm3
EMDB ID : EMD-60235
Title : Cryo-EM strcuture of Cas5-HNH Cascade,apo-Conf2
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on : 2024-05-22
Resolution : 3.10 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:

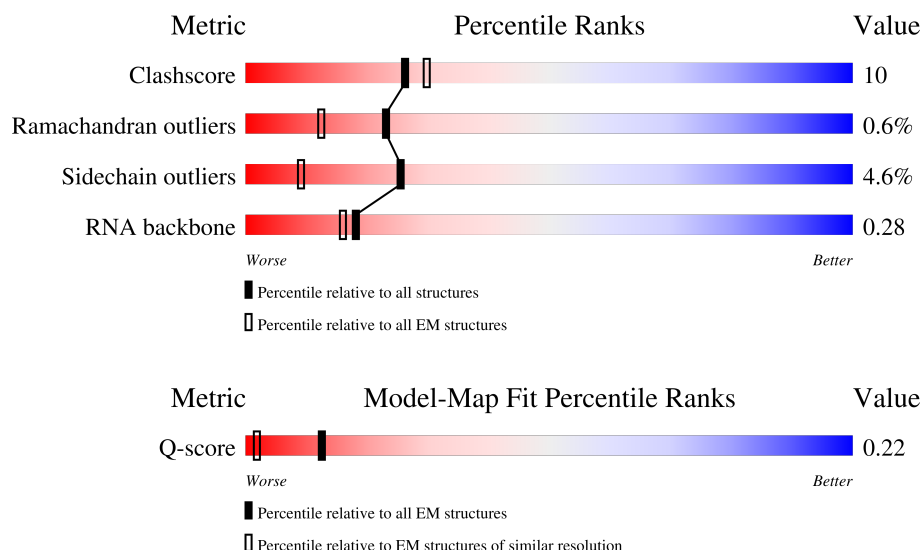
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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.



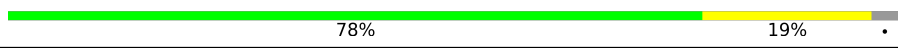
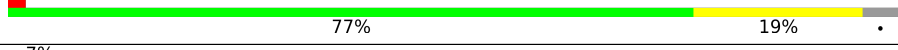
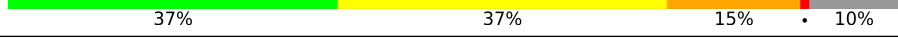
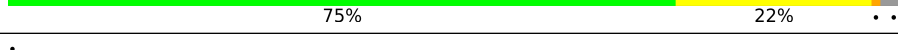
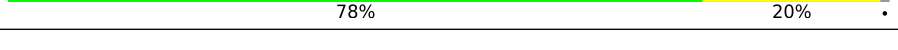
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	535	
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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26938 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	442	Total	C	N	O	S	0	0
			3476	2233	594	630	19		

- 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	367	Total	C	N	O	S	0	0
			2799	1772	485	530	12		
4	H	367	Total	C	N	O	S	0	0
			2833	1787	495	539	12		
4	I	364	Total	C	N	O	S	0	0
			2781	1760	484	525	12		
4	J	367	Total	C	N	O	S	0	0
			2804	1772	488	532	12		
4	K	341	Total	C	N	O	S	0	0
			2624	1660	463	490	11		
4	G	251	Total	C	N	O	S	0	0
			1919	1222	334	355	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	378	Total	C	N	O	S	0	0
			2955	1866	546	522	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	268	Total	C	N	O	S	0	0
			2135	1369	383	379	4		

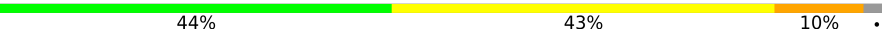
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	
7	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.

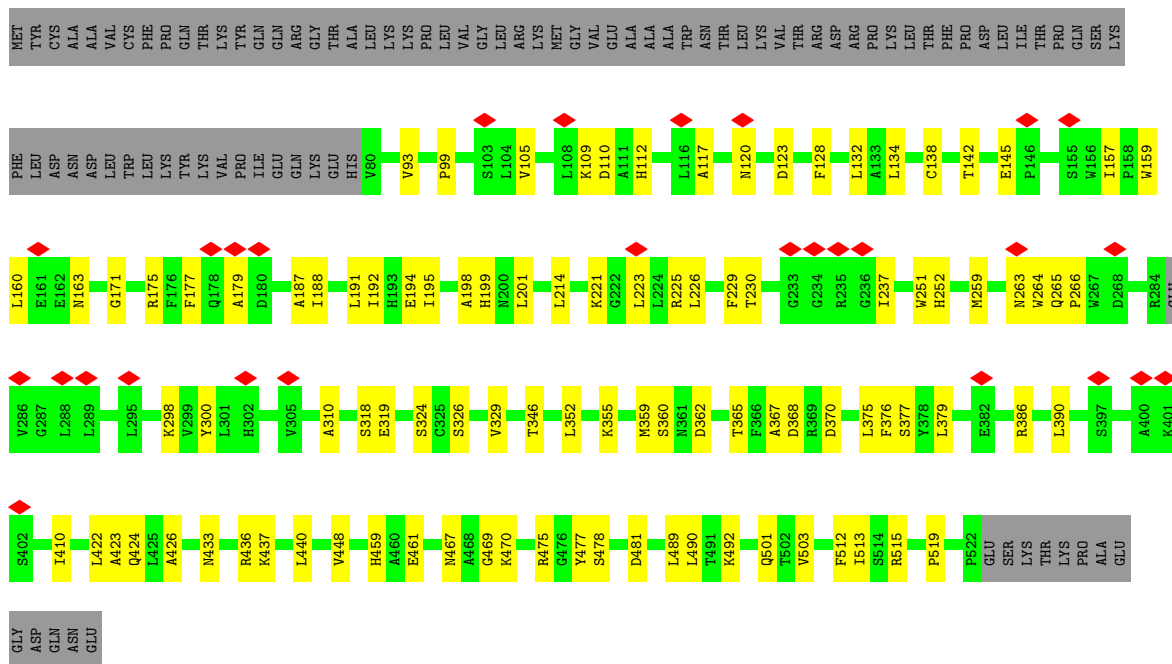
• Molecule 1: RNA (61-MER)

Chain A: 



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

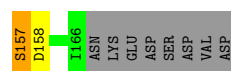
Chain C: 



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

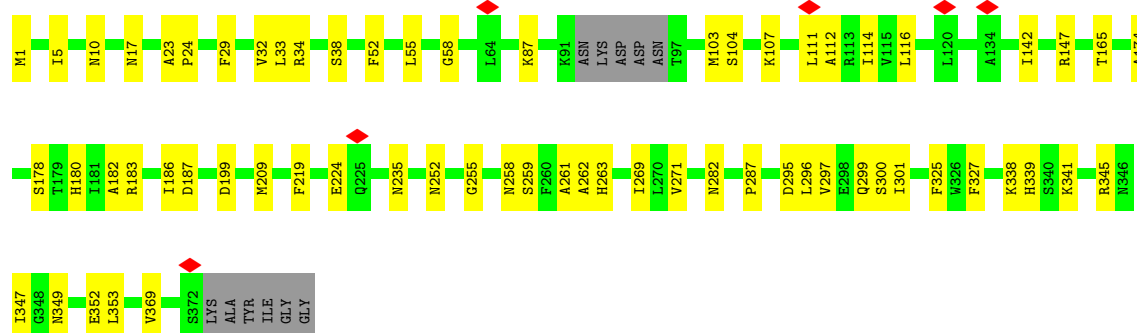
Chain E: 





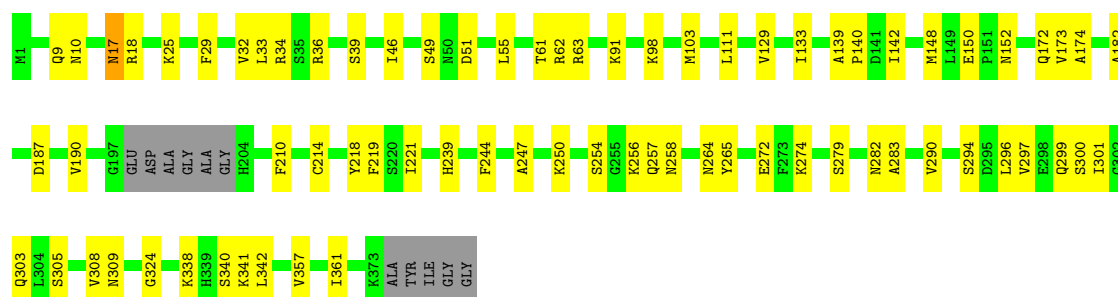
• Molecule 4: CRISPR system Cascade subunit CasC

Chain F: 80% 17%



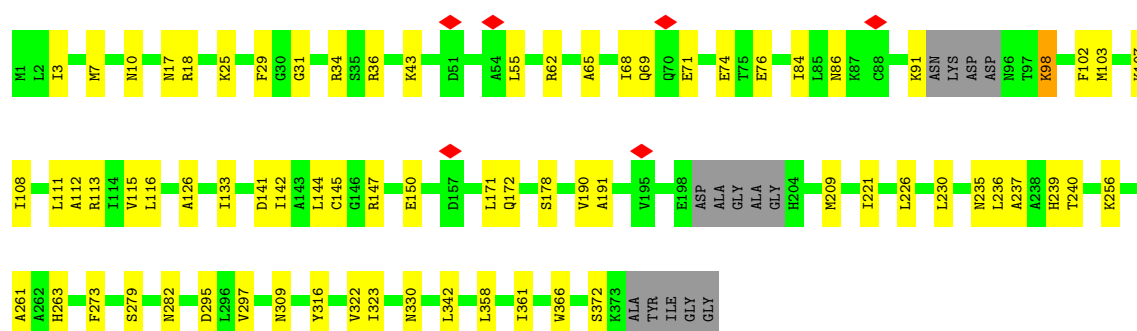
• Molecule 4: CRISPR system Cascade subunit CasC

Chain H: 78% 19%



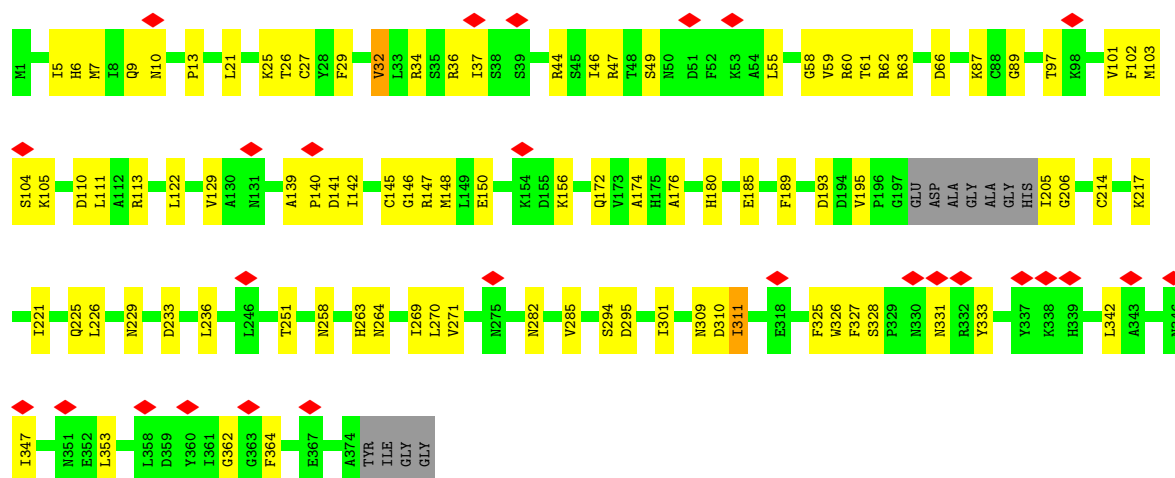
• Molecule 4: CRISPR system Cascade subunit CasC

Chain I: 77% 19%

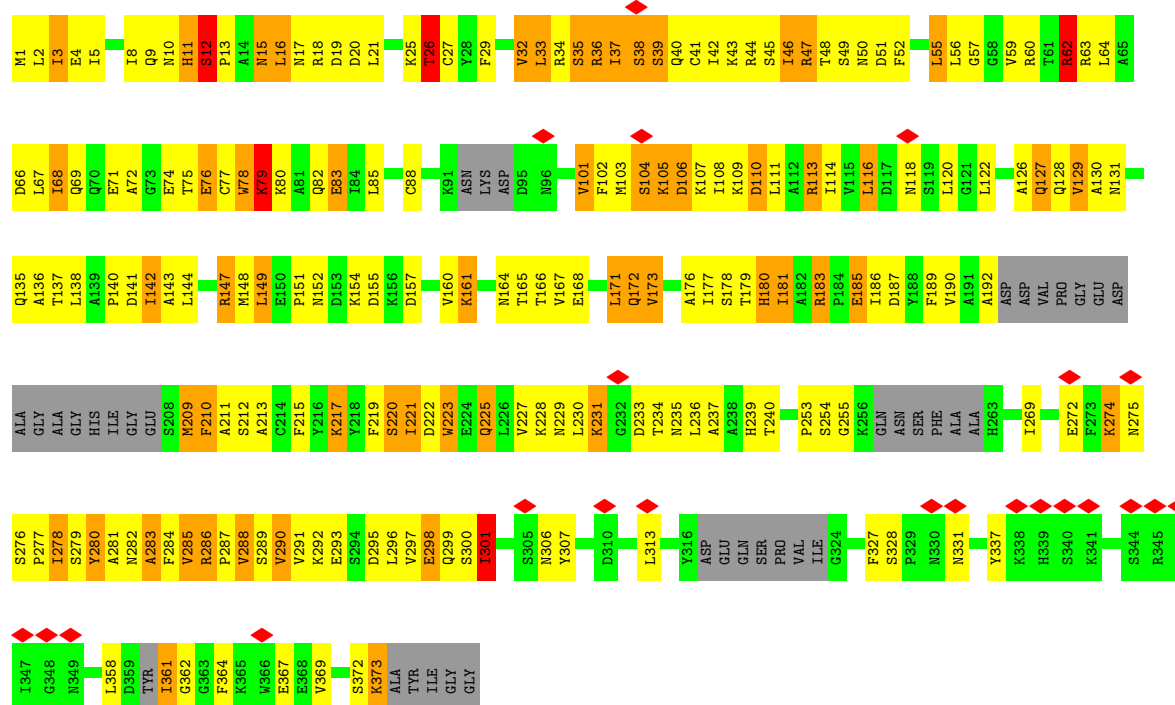


• Molecule 4: CRISPR system Cascade subunit CasC

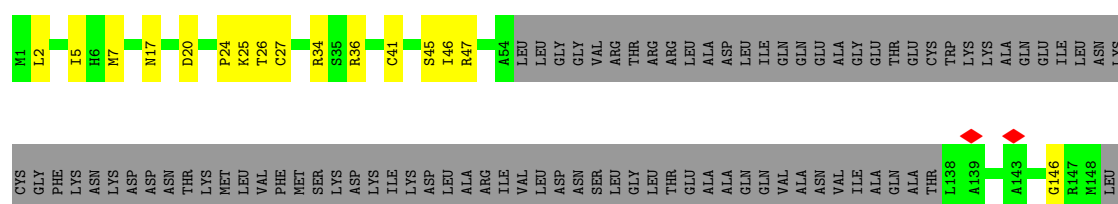
Chain J: 7% 72% 24%

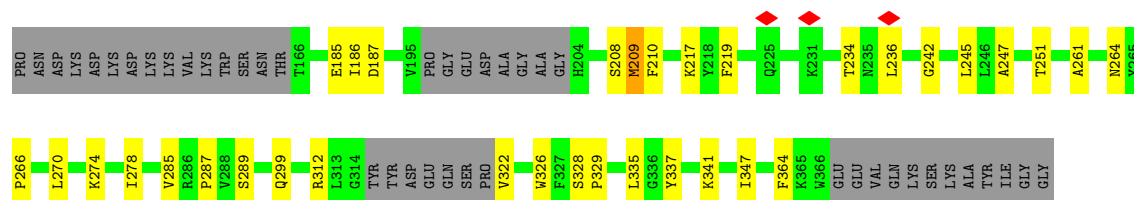


• Molecule 4: CRISPR system Cascade subunit CasC

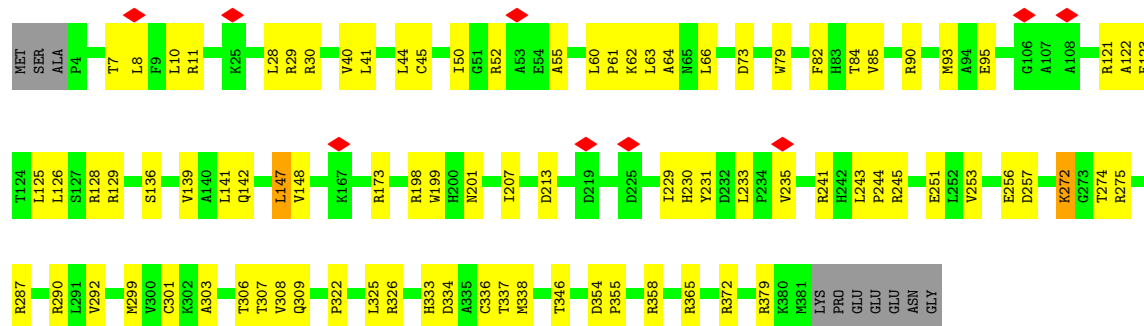


• Molecule 4: CRISPR system Cascade subunit CasC

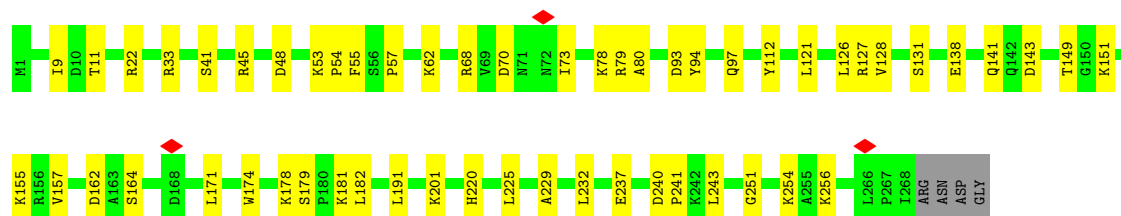
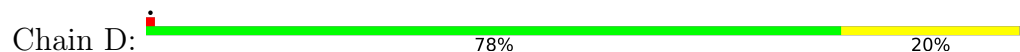




• Molecule 5: CRISPR system Cascade subunit CasD



• Molecule 6: CRISPR-associated endoribonuclease Cse3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS 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	2.467	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.00549	Depositor
Map size ($\text{\AA}$)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	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	0.16	0/1405	0.43	0/2187
2	C	0.23	0/3575	0.50	0/4871
3	E	0.31	0/1382	0.59	1/1862 (0.1%)
4	F	0.23	0/2854	0.48	2/3872 (0.1%)
4	G	0.25	0/1960	0.51	2/2658 (0.1%)
4	H	0.18	0/2888	0.43	0/3913
4	I	0.26	0/2836	0.57	1/3848 (0.0%)
4	J	0.20	0/2858	0.51	0/3876
4	K	0.67	0/2670	1.17	29/3609 (0.8%)
5	B	0.25	0/3028	0.53	2/4107 (0.0%)
6	D	0.23	0/2193	0.52	0/2976
All	All	0.30	0/27649	0.60	37/37779 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	129	VAL	N-CA-C	-15.75	97.21	112.96
4	K	280	TYR	N-CA-C	-11.56	99.51	112.57
4	K	39	SER	N-CA-C	-11.24	99.61	113.20
4	K	235	ASN	N-CA-C	-10.70	99.40	111.71
4	K	181	ILE	N-CA-C	-10.12	96.53	109.58
4	K	19	ASP	N-CA-C	9.12	120.82	108.23
4	K	225	GLN	N-CA-C	-8.75	101.21	114.16
4	K	80	LYS	N-CA-C	-8.20	103.42	113.50
4	K	66	ASP	N-CA-C	-8.02	102.52	111.82
4	G	209	MET	CG-SD-CE	-7.92	83.47	100.90
4	K	126	ALA	N-CA-C	-7.40	103.29	111.36
4	K	111	LEU	N-CA-C	-6.94	104.07	112.54
4	K	12	SER	N-CA-C	6.91	121.11	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	253	PRO	CA-N-CD	-6.43	102.99	112.00
4	K	223	TRP	N-CA-C	6.29	124.20	110.80
5	B	303	ALA	N-CA-C	-6.24	102.83	110.31
4	K	138	LEU	N-CA-C	6.19	120.73	111.81
4	K	77	CYS	N-CA-C	6.17	118.22	108.79
4	K	62	ARG	N-CA-C	-6.10	104.00	112.30
4	G	329	PRO	CA-N-CD	-6.04	103.54	112.00
4	K	180	HIS	N-CA-C	6.04	117.41	108.60
4	K	137	THR	N-CA-C	5.83	120.08	113.15
4	K	297	VAL	N-CA-C	-5.82	107.07	112.83
4	K	26	THR	N-CA-C	5.80	118.17	108.02
4	K	301	ILE	N-CA-C	5.79	121.38	109.34
4	K	253	PRO	N-CD-CG	-5.60	94.81	103.20
4	I	98	LYS	CA-CB-CG	5.57	125.23	114.10
4	K	189	PHE	N-CA-C	-5.50	105.37	112.68
5	B	272	LYS	CB-CG-CD	5.49	123.92	111.30
4	F	87	LYS	CA-CB-CG	5.49	125.07	114.10
4	K	128	GLN	N-CA-C	-5.45	106.64	113.72
3	E	85	MET	CG-SD-CE	-5.44	88.93	100.90
4	K	79	LYS	N-CA-C	-5.40	106.57	112.72
4	K	290	VAL	N-CA-C	5.33	115.57	108.27
4	F	341	LYS	CA-CB-CG	5.14	124.37	114.10
4	K	105	LYS	N-CA-C	5.12	117.30	109.62
4	K	11	HIS	N-CA-C	5.05	116.96	109.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	26	0
2	C	3476	0	3376	62	0
3	E	1352	0	1387	25	0
4	F	2799	0	2728	42	0
4	G	1919	0	1852	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2833	0	2771	52	0
4	I	2781	0	2689	46	0
4	J	2804	0	2723	77	0
4	K	2624	0	2582	133	0
5	B	2955	0	2967	63	0
6	D	2135	0	2096	37	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
All	All	26938	0	25809	531	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 10.

All (531) 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)
4:G:185:GLU:O	4:G:209:MET:HG3	1.27	1.30
4:K:102:PHE:HB3	4:K:147:ARG:HG2	1.50	0.92
4:J:263:HIS:HB2	4:K:279:SER:H	1.39	0.87
1:A:30:G:H4'	4:K:41:CYS:HA	1.57	0.85
4:K:127:GLN:HA	4:K:130:ALA:HB3	1.56	0.85
1:A:42:A:H2	1:A:48:G:H1	1.20	0.83
4:K:17:ASN:HB3	4:K:25:LYS:HG3	1.63	0.80
4:K:147:ARG:HD3	4:K:148:MET:H	1.46	0.80
4:K:236:LEU:HD12	4:K:372:SER:HB3	1.63	0.79
4:J:29:PHE:O	4:J:34:ARG:NH1	2.16	0.78
4:J:62:ARG:HH21	4:J:97:THR:H	1.31	0.77
4:K:15:ASN:HB3	4:K:255:GLY:HA3	1.67	0.77
4:K:239:HIS:CD2	4:K:372:SER:HB2	2.20	0.76
4:K:239:HIS:HD2	4:K:372:SER:HB2	1.52	0.75
4:I:62:ARG:HD2	4:I:98:LYS:HB2	1.69	0.73
4:J:7:MET:HB2	4:J:217:LYS:HB2	1.71	0.73
4:G:41:CYS:O	4:G:45:SER:HB3	1.89	0.72
4:K:298:GLU:OE2	4:K:301:ILE:HD11	1.90	0.72
4:K:60:ARG:HG3	4:K:102:PHE:HB2	1.72	0.72
2:C:237:ILE:HG12	2:C:329:VAL:HG21	1.71	0.70
4:F:252:ASN:ND2	4:F:262:ALA:O	2.24	0.70
4:H:305:SER:O	4:H:309:ASN:ND2	2.25	0.70
4:K:183:ARG:HH21	4:K:213:ALA:HB2	1.57	0.69
2:C:199:HIS:O	5:B:121:ARG:NH2	2.26	0.68
4:K:38:SER:HB2	4:K:41:CYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:A:N1	1:A:48:G:O6	2.27	0.68
2:C:470:LYS:HE2	2:C:477:TYR:HB2	1.75	0.68
4:K:269:ILE:HB	4:K:327:PHE:HB3	1.75	0.68
4:I:68:ILE:HG22	4:I:76:GLU:HG3	1.75	0.67
4:K:298:GLU:OE2	4:K:301:ILE:CD1	2.41	0.67
3:E:151:PRO:HA	3:E:154:ARG:HB2	1.76	0.67
5:B:309:GLN:HE21	5:B:333:HIS:HA	1.59	0.67
4:G:27:CYS:HB3	4:G:36:ARG:HD3	1.75	0.67
5:B:8:LEU:HB3	5:B:148:VAL:HG13	1.76	0.67
4:J:263:HIS:HB2	4:K:279:SER:N	2.10	0.67
5:B:299:MET:HE3	5:B:326:ARG:HD2	1.77	0.67
4:K:71:GLU:HG2	4:K:109:LYS:NZ	2.09	0.66
4:F:33:LEU:HG	4:F:182:ALA:HB3	1.78	0.66
4:J:13:PRO:CG	4:K:29:PHE:HB2	2.25	0.66
4:K:55:LEU:HB3	4:K:140:PRO:HG2	1.76	0.66
1:A:-4:A:H2'	1:A:-3:A:H8	1.61	0.66
4:J:58:GLY:HA2	4:J:104:SER:HA	1.77	0.65
4:H:264:ASN:ND2	4:I:279:SER:OG	2.30	0.65
4:J:5:ILE:HG23	4:J:7:MET:HE3	1.79	0.65
4:K:33:LEU:O	4:K:181:ILE:HA	1.96	0.65
5:B:233:LEU:HB3	5:B:243:LEU:HB3	1.78	0.65
4:J:221:ILE:HD11	4:J:226:LEU:HD22	1.78	0.64
6:D:9:ILE:HB	6:D:80:ALA:HB3	1.79	0.63
4:F:261:ALA:HB3	4:H:174:ALA:HB2	1.81	0.63
4:I:358:LEU:HD23	4:I:361:ILE:HD12	1.81	0.63
4:K:29:PHE:CE2	4:K:285:VAL:HA	2.34	0.63
2:C:123:ASP:OD1	2:C:225:ARG:NH2	2.32	0.62
4:K:176:ALA:HB2	4:K:217:LYS:HG3	1.82	0.62
4:K:183:ARG:NH2	4:K:213:ALA:HB2	2.14	0.62
4:K:27:CYS:HB3	4:K:36:ARG:HD3	1.81	0.62
4:H:290:VAL:HG21	4:I:31:GLY:HA3	1.82	0.62
4:I:10:ASN:ND2	4:J:282:ASN:OD1	2.32	0.62
4:H:9:GLN:NE2	4:H:264:ASN:O	2.32	0.61
4:G:25:LYS:NZ	5:B:82:PHE:O	2.33	0.61
4:K:284:PHE:CZ	4:K:300:SER:HA	2.35	0.61
4:K:101:VAL:HA	4:K:149:LEU:HD21	1.81	0.61
4:I:65:ALA:HA	4:I:68:ILE:HD12	1.82	0.61
2:C:367:ALA:HB1	2:C:461:GLU:HG3	1.83	0.61
4:J:13:PRO:HD3	4:K:29:PHE:CD1	2.36	0.61
3:E:85:MET:HE1	3:E:127:LEU:HD13	1.82	0.61
4:J:37:ILE:HB	4:J:176:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:185:GLU:O	4:G:209:MET:CG	2.23	0.60
4:I:144:LEU:HD11	4:I:240:THR:HG21	1.83	0.60
4:J:328:SER:HB3	4:J:331:ASN:HA	1.82	0.60
4:K:110:ASP:HA	4:K:113:ARG:HB2	1.83	0.60
2:C:120:ASN:ND2	2:C:194:GLU:OE1	2.34	0.60
4:F:282:ASN:OD1	4:G:264:ASN:ND2	2.35	0.60
4:J:263:HIS:HB2	4:K:278:ILE:HA	1.82	0.60
4:K:176:ALA:HB1	4:K:215:PHE:HB3	1.84	0.60
4:J:195:VAL:HG21	4:K:67:LEU:HD11	1.85	0.59
2:C:177:PHE:HB3	2:C:223:LEU:HD13	1.85	0.59
4:J:145:CYS:SG	4:J:146:GLY:N	2.72	0.59
4:J:264:ASN:ND2	4:K:282:ASN:HB2	2.17	0.59
4:K:2:LEU:HD23	4:K:277:PRO:HD3	1.85	0.59
4:G:209:MET:HG2	4:G:210:PHE:N	2.18	0.59
2:C:93:VAL:HA	2:C:99:PRO:HA	1.85	0.59
4:K:74:GLU:HB2	4:K:116:LEU:HD12	1.84	0.59
2:C:138:CYS:O	2:C:142:THR:HB	2.02	0.58
4:H:62:ARG:HD2	4:H:98:LYS:HA	1.85	0.58
4:J:26:THR:O	4:J:36:ARG:NH1	2.36	0.58
4:J:180:HIS:HE1	4:J:214:CYS:H	1.49	0.58
4:K:35:SER:OG	4:K:178:SER:HB2	2.03	0.58
2:C:362:ASP:OD1	2:C:437:LYS:NZ	2.31	0.58
4:J:87:LYS:HZ2	4:J:122:LEU:HB3	1.69	0.58
4:J:233:ASP:OD1	4:J:236:LEU:N	2.33	0.58
4:F:187:ASP:OD1	4:H:25:LYS:NZ	2.34	0.58
5:B:233:LEU:HD22	5:B:243:LEU:HD23	1.85	0.58
4:K:2:LEU:CD2	4:K:277:PRO:HD3	2.34	0.57
5:B:257:ASP:OD1	5:B:257:ASP:N	2.36	0.57
4:F:1:MET:N	4:F:224:GLU:OE1	2.36	0.57
4:K:283:ALA:HB2	4:K:307:TYR:CD2	2.39	0.57
4:I:108:ILE:O	4:I:112:ALA:HB3	2.05	0.57
4:F:147:ARG:NH2	4:F:165:THR:OG1	2.38	0.57
4:I:34:ARG:HG2	4:I:178:SER:HB2	1.86	0.57
6:D:138:GLU:HG3	6:D:151:LYS:HE2	1.87	0.57
2:C:490:LEU:CD2	2:C:513:ILE:HA	2.35	0.57
5:B:10:LEU:HD21	5:B:44:LEU:HD21	1.86	0.57
4:K:37:ILE:HB	4:K:176:ALA:H	1.70	0.57
6:D:171:LEU:HD23	6:D:232:LEU:HD21	1.86	0.57
1:A:23:G:H1'	4:I:191:ALA:HB2	1.87	0.56
4:H:139:ALA:HB3	4:H:142:ILE:HG13	1.87	0.56
4:K:29:PHE:HE2	4:K:284:PHE:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:57:GLY:HA2	4:K:105:LYS:HG2	1.86	0.56
4:G:7:MET:HB3	4:G:217:LYS:HB2	1.87	0.56
4:G:270:LEU:HB2	4:G:326:TRP:HD1	1.70	0.56
5:B:66:LEU:HD23	5:B:141:LEU:HB3	1.87	0.56
4:K:37:ILE:HG13	4:K:176:ALA:HB3	1.88	0.56
4:K:328:SER:HB3	4:K:331:ASN:HA	1.87	0.56
4:G:47:ARG:NH2	4:G:146:GLY:O	2.35	0.56
5:B:90:ARG:HG2	5:B:122:ALA:HB2	1.87	0.56
4:H:29:PHE:HB3	4:H:34:ARG:HG3	1.87	0.55
2:C:171:GLY:O	2:C:175:ARG:NH1	2.37	0.55
5:B:287:ARG:NH2	5:B:306:THR:O	2.40	0.55
4:H:308:VAL:HG12	4:H:342:LEU:HD22	1.89	0.55
4:K:144:LEU:HB3	4:K:171:LEU:HD23	1.89	0.55
4:G:186:ILE:HG12	4:G:209:MET:HB2	1.87	0.55
2:C:459:HIS:HD2	2:C:489:LEU:HD11	1.72	0.55
4:I:141:ASP:O	4:I:145:CYS:HB3	2.07	0.55
4:K:60:ARG:HB2	4:K:102:PHE:HD1	1.72	0.55
4:J:263:HIS:CB	4:K:278:ILE:HA	2.37	0.54
4:G:7:MET:HG2	4:G:219:PHE:HE2	1.72	0.54
4:J:32:VAL:HG23	4:J:34:ARG:NH1	2.23	0.54
6:D:131:SER:OG	6:D:254:LYS:NZ	2.40	0.54
4:F:112:ALA:O	4:F:116:LEU:HB2	2.07	0.54
4:I:144:LEU:HD12	4:I:226:LEU:HD11	1.88	0.54
2:C:478:SER:H	2:C:481:ASP:HB2	1.71	0.54
4:F:259:SER:OG	4:H:39:SER:OG	2.25	0.54
4:J:104:SER:HB3	4:J:142:ILE:HD13	1.89	0.54
4:I:261:ALA:HB3	4:J:174:ALA:HB2	1.89	0.54
4:K:306:ASN:OD1	4:K:337:TYR:OH	2.26	0.54
5:B:207:ILE:HD11	5:B:251:GLU:HB3	1.90	0.54
4:F:10:ASN:ND2	4:H:282:ASN:OD1	2.36	0.53
4:H:283:ALA:O	4:H:303:GLN:NE2	2.41	0.53
5:B:93:MET:HE1	5:B:95:GLU:HB3	1.89	0.53
2:C:436:ARG:NH1	2:C:448:VAL:O	2.41	0.53
4:F:338:LYS:HD2	4:F:339:HIS:N	2.23	0.53
4:K:2:LEU:HB2	4:K:275:ASN:HA	1.90	0.53
4:K:183:ARG:HD2	4:K:211:ALA:HB1	1.90	0.53
5:B:85:VAL:HB	5:B:125:LEU:HB3	1.89	0.53
6:D:240:ASP:HB3	6:D:243:LEU:CB	2.38	0.53
4:F:325:PHE:CD1	4:F:345:ARG:HB3	2.43	0.53
4:H:10:ASN:ND2	4:I:282:ASN:OD1	2.37	0.53
3:E:153:LYS:HA	3:E:156:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:103:MET:HE2	4:H:133:ILE:HG13	1.90	0.53
4:I:18:ARG:HH21	4:I:256:LYS:HE2	1.74	0.53
2:C:318:SER:OG	2:C:319:GLU:N	2.34	0.53
4:F:349:ASN:HB3	4:F:352:GLU:HG3	1.90	0.53
2:C:467:ASN:HB2	2:C:470:LYS:HB3	1.91	0.53
4:J:46:ILE:O	4:J:49:SER:OG	2.25	0.53
4:J:264:ASN:HD22	4:K:282:ASN:HB2	1.74	0.53
2:C:376:PHE:HB3	2:C:426:ALA:HB2	1.90	0.52
4:H:296:LEU:O	4:H:300:SER:OG	2.27	0.52
5:B:29:ARG:HG3	5:B:129:ARG:HG2	1.91	0.52
4:H:111:LEU:HD22	4:H:129:VAL:HG22	1.92	0.52
4:I:69:GLN:NE2	4:I:74:GLU:OE1	2.33	0.52
6:D:57:PRO:O	6:D:62:LYS:NZ	2.43	0.52
2:C:159:TRP:O	2:C:163:ASN:ND2	2.42	0.52
4:K:230:LEU:O	4:K:231:LYS:C	2.52	0.52
6:D:127:ARG:HD3	6:D:229:ALA:HB1	1.91	0.52
1:A:-6:U:OP2	5:B:52:ARG:NH2	2.41	0.52
4:G:187:ASP:N	4:G:208:SER:O	2.31	0.52
4:I:263:HIS:NE2	4:J:172:GLN:OE1	2.42	0.52
4:I:295:ASP:OD1	4:I:297:VAL:N	2.43	0.52
2:C:512:PHE:HA	2:C:515:ARG:HE	1.75	0.52
3:E:19:ASP:HA	3:E:22:ILE:HG22	1.91	0.52
4:H:10:ASN:HA	4:H:214:CYS:HA	1.92	0.52
4:I:358:LEU:HD11	4:I:366:TRP:HE3	1.75	0.52
2:C:201:LEU:HD22	5:B:125:LEU:HD13	1.92	0.51
4:H:91:LYS:HD3	4:H:152:ASN:HD22	1.75	0.51
4:K:171:LEU:HB2	4:K:221:ILE:HG23	1.92	0.51
4:F:271:VAL:HG11	4:F:353:LEU:HD11	1.91	0.51
4:J:193:ASP:OD1	4:J:195:VAL:N	2.39	0.51
4:K:71:GLU:HG2	4:K:109:LYS:HZ2	1.74	0.51
2:C:490:LEU:HD22	2:C:513:ILE:HA	1.93	0.51
4:J:225:GLN:NE2	4:J:229:ASN:OD1	2.44	0.51
4:J:301:ILE:HD13	4:J:333:TYR:HB3	1.93	0.51
4:G:247:ALA:O	4:G:251:THR:OG1	2.20	0.51
4:K:32:VAL:HG21	4:K:287:PRO:HG3	1.92	0.51
3:E:114:MET:HG3	3:E:115:GLN:HG3	1.93	0.51
4:J:32:VAL:HG23	4:J:34:ARG:HH12	1.75	0.51
5:B:11:ARG:HD2	5:B:173:ARG:HH21	1.75	0.51
3:E:32:ASP:N	3:E:32:ASP:OD1	2.43	0.51
3:E:55:ALA:O	5:B:275:ARG:NH2	2.44	0.51
4:K:42:ILE:HD11	4:K:173:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:78:LYS:O	6:D:79:ARG:NH1	2.44	0.51
2:C:360:SER:O	2:C:360:SER:OG	2.29	0.50
6:D:68:ARG:NH1	6:D:70:ASP:OD2	2.43	0.50
2:C:134:LEU:HD11	2:C:160:LEU:HD21	1.93	0.50
4:H:258:ASN:HA	4:I:172:GLN:HG2	1.93	0.50
4:J:55:LEU:HD22	4:J:140:PRO:HG2	1.94	0.50
4:J:104:SER:OG	4:J:105:LYS:N	2.45	0.50
4:F:5:ILE:HB	4:F:219:PHE:HB2	1.94	0.50
4:K:102:PHE:HE2	4:K:142:ILE:HG23	1.77	0.50
4:K:220:SER:CB	4:K:277:PRO:HB3	2.42	0.50
4:K:230:LEU:HD22	4:K:236:LEU:HD23	1.94	0.50
2:C:226:LEU:O	2:C:230:THR:OG1	2.28	0.50
4:K:42:ILE:HD12	4:K:219:PHE:HE2	1.77	0.50
4:F:263:HIS:HB2	4:H:279:SER:HB2	1.94	0.50
4:I:230:LEU:HD13	4:I:236:LEU:HB3	1.93	0.50
4:J:6:HIS:HB2	4:J:270:LEU:HB3	1.94	0.50
4:G:209:MET:CG	4:G:210:PHE:N	2.75	0.50
5:B:55:ALA:HB1	5:B:60:LEU:HG	1.93	0.50
4:F:103:MET:HA	4:F:142:ILE:HD11	1.94	0.49
4:G:7:MET:HE1	4:G:266:PRO:HB3	1.94	0.49
2:C:110:ASP:O	2:C:112:HIS:ND1	2.46	0.49
2:C:503:VAL:HG22	3:E:157:SER:HB3	1.93	0.49
4:K:104:SER:HB3	4:K:136:ALA:HB1	1.94	0.49
4:G:242:GLY:HA2	4:G:245:LEU:HD12	1.95	0.49
2:C:368:ASP:HA	5:B:30:ARG:HH22	1.77	0.49
4:I:235:ASN:OD1	4:I:372:SER:OG	2.27	0.49
4:K:13:PRO:HG2	4:K:210:PHE:HB2	1.94	0.49
4:G:312:ARG:NH2	4:G:322:VAL:O	2.45	0.49
4:G:24:PRO:HD3	4:G:209:MET:HE3	1.93	0.49
5:B:309:GLN:HE22	5:B:336:CYS:HB2	1.78	0.49
4:I:330:ASN:HD22	4:J:310:ASP:HA	1.78	0.49
4:K:147:ARG:HD3	4:K:148:MET:N	2.22	0.49
1:A:25:G:OP1	4:J:25:LYS:NZ	2.32	0.49
4:G:5:ILE:HB	4:G:219:PHE:HB2	1.94	0.49
4:K:12:SER:O	4:K:16:LEU:HB2	2.13	0.49
1:A:31:C:H41	4:J:205:ILE:HD11	1.78	0.48
2:C:376:PHE:HD1	2:C:422:LEU:HB3	1.77	0.48
3:E:19:ASP:O	3:E:23:LEU:HG	2.12	0.48
4:H:32:VAL:HG23	4:H:34:ARG:HE	1.78	0.48
4:G:337:TYR:CE2	5:B:272:LYS:HG3	2.47	0.48
4:F:338:LYS:HD2	4:F:339:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:55:LEU:CB	4:K:140:PRO:HG2	2.43	0.48
4:K:102:PHE:CE2	4:K:142:ILE:HG23	2.48	0.48
4:K:1:MET:HE1	4:K:361:ILE:HA	1.94	0.48
4:K:47:ARG:HG2	4:K:56:LEU:HD11	1.96	0.48
4:G:285:VAL:HG21	5:B:198:ARG:HD2	1.96	0.48
4:H:18:ARG:HH12	4:H:256:LYS:HD3	1.79	0.48
6:D:121:LEU:HD23	6:D:237:GLU:HG3	1.94	0.48
2:C:501:GLN:NE2	3:E:154:ARG:HA	2.28	0.48
1:A:42:A:N1	1:A:48:G:C6	2.82	0.48
4:K:358:LEU:HG	4:K:364:PHE:HB2	1.94	0.48
1:A:30:G:C4'	4:K:41:CYS:HA	2.39	0.48
3:E:41:PHE:HE2	3:E:58:ARG:HG2	1.78	0.48
4:H:340:SER:O	4:H:341:LYS:NZ	2.45	0.48
4:K:13:PRO:HG3	4:K:211:ALA:O	2.13	0.48
6:D:22:ARG:O	6:D:22:ARG:NH1	2.40	0.48
4:J:13:PRO:HG3	4:K:29:PHE:HB2	1.95	0.48
3:E:27:ARG:HH21	3:E:117:GLU:HG2	1.78	0.48
4:K:72:ALA:HB1	4:K:116:LEU:HD11	1.94	0.48
4:I:102:PHE:HB3	4:I:142:ILE:HD11	1.95	0.47
4:I:171:LEU:HB2	4:I:221:ILE:HD11	1.96	0.47
5:B:274:THR:HG22	5:B:275:ARG:H	1.80	0.47
4:K:15:ASN:HA	4:K:254:SER:O	2.14	0.47
4:K:176:ALA:CB	4:K:215:PHE:HB3	2.44	0.47
1:A:14:A:H8	4:H:18:ARG:HH21	1.62	0.47
2:C:192:ILE:HG22	2:C:194:GLU:H	1.79	0.47
4:I:84:ILE:HG23	4:I:126:ALA:HB2	1.96	0.47
4:H:17:ASN:HD22	4:H:17:ASN:HA	1.58	0.47
4:J:59:VAL:HG22	4:J:61:THR:HG23	1.96	0.47
4:K:17:ASN:HD22	4:K:37:ILE:HD13	1.78	0.47
4:K:34:ARG:NH2	4:K:284:PHE:O	2.47	0.47
5:B:292:VAL:HG22	6:D:220:HIS:CD2	2.49	0.47
4:H:55:LEU:HD21	4:H:239:HIS:CD2	2.50	0.47
4:G:26:THR:O	5:B:79:TRP:NE1	2.47	0.47
5:B:358:ARG:NH2	6:D:97:GLN:O	2.47	0.47
4:J:63:ARG:NH1	4:J:97:THR:OG1	2.48	0.47
4:J:258:ASN:HA	4:K:172:GLN:HE21	1.79	0.47
4:K:68:ILE:HD13	4:K:68:ILE:HA	1.64	0.47
4:F:174:ALA:HB2	4:G:261:ALA:HB3	1.97	0.47
4:H:297:VAL:O	4:H:301:ILE:HG13	2.15	0.47
5:B:308:VAL:HG11	5:B:325:LEU:HD23	1.96	0.47
4:K:49:SER:HB3	4:K:52:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:46:ILE:HA	4:G:251:THR:HG21	1.97	0.46
4:K:282:ASN:O	4:K:284:PHE:N	2.48	0.46
4:K:1:MET:N	4:K:223:TRP:HB2	2.31	0.46
5:B:82:PHE:HZ	5:B:126:LEU:HD22	1.80	0.46
4:H:51:ASP:OD2	4:H:247:ALA:HA	2.15	0.46
4:J:139:ALA:O	4:J:142:ILE:HD12	2.15	0.46
4:J:147:ARG:NH2	4:J:150:GLU:HB2	2.31	0.46
4:K:173:VAL:HG12	4:K:219:PHE:HD2	1.80	0.46
6:D:251:GLY:HA3	6:D:256:LYS:HD3	1.98	0.46
1:A:17:U:O2'	4:H:190:VAL:O	2.34	0.46
4:H:309:ASN:ND2	4:H:342:LEU:HD11	2.30	0.46
4:I:111:LEU:O	4:I:115:VAL:HG12	2.15	0.46
4:G:209:MET:HB3	4:G:209:MET:HE2	1.72	0.46
4:J:111:LEU:HG	4:J:129:VAL:HG22	1.98	0.46
4:K:38:SER:C	4:K:40:GLN:N	2.70	0.46
4:G:234:THR:HG22	4:G:364:PHE:HZ	1.80	0.46
3:E:18:GLY:HA2	4:I:209:MET:HE2	1.98	0.46
3:E:23:LEU:HD21	3:E:40:LEU:HD23	1.96	0.46
4:H:294:SER:OG	4:H:299:GLN:NE2	2.47	0.46
4:J:269:ILE:HB	4:J:327:PHE:HD2	1.81	0.46
5:B:213:ASP:OD1	5:B:245:ARG:NH1	2.49	0.46
6:D:174:TRP:O	6:D:178:LYS:NZ	2.40	0.46
6:D:179:SER:HA	6:D:182:LEU:HD12	1.98	0.46
2:C:225:ARG:HB2	2:C:229:PHE:CD2	2.51	0.46
4:F:186:ILE:HG12	4:F:209:MET:SD	2.55	0.46
4:J:271:VAL:HG12	4:J:325:PHE:HB2	1.97	0.46
4:K:102:PHE:CB	4:K:147:ARG:HG2	2.35	0.46
6:D:45:ARG:NH2	6:D:93:ASP:OD1	2.49	0.46
2:C:390:LEU:HD23	2:C:410:ILE:HD11	1.97	0.46
2:C:440:LEU:HD12	2:C:440:LEU:H	1.80	0.46
4:F:17:ASN:HD22	4:F:38:SER:H	1.63	0.46
4:F:52:PHE:CE1	4:F:55:LEU:HD23	2.51	0.46
4:H:61:THR:HG23	4:H:63:ARG:H	1.79	0.46
4:J:347:ILE:HD12	4:J:353:LEU:HD12	1.98	0.45
5:B:40:VAL:HG21	5:B:139:VAL:HG21	1.98	0.45
4:J:102:PHE:CD2	4:J:146:GLY:HA2	2.51	0.45
5:B:333:HIS:O	5:B:337:THR:OG1	2.27	0.45
4:G:24:PRO:CD	4:G:209:MET:HE3	2.47	0.45
2:C:355:LYS:N	2:C:370:ASP:OD2	2.49	0.45
4:F:258:ASN:HA	4:H:172:GLN:HG2	1.98	0.45
4:J:101:VAL:HB	4:J:103:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:55:LEU:HB3	4:K:140:PRO:CG	2.44	0.45
4:J:309:ASN:HB2	4:J:342:LEU:HD11	1.99	0.45
4:K:27:CYS:HB3	4:K:36:ARG:HB3	1.99	0.45
4:K:282:ASN:O	4:K:283:ALA:C	2.60	0.45
1:A:35:A:H61	6:D:162:ASP:HA	1.81	0.45
3:E:34:LYS:HE2	3:E:36:PRO:HD2	1.99	0.45
4:I:86:ASN:OD1	4:I:86:ASN:N	2.50	0.45
4:J:27:CYS:HB3	4:J:36:ARG:HD3	1.98	0.45
4:K:227:VAL:HG22	4:K:237:ALA:HB1	1.99	0.45
4:K:298:GLU:OE2	4:K:301:ILE:HD12	2.15	0.45
5:B:73:ASP:HB2	5:B:136:SER:HB2	1.98	0.45
4:K:286:ARG:HE	4:K:286:ARG:HB2	1.54	0.45
5:B:334:ASP:OD2	5:B:372:ARG:NH2	2.38	0.45
6:D:48:ASP:O	6:D:94:TYR:OH	2.21	0.45
6:D:178:LYS:HA	6:D:181:LYS:HE2	1.97	0.45
3:E:88:ILE:HD12	3:E:130:HIS:ND1	2.32	0.45
4:K:103:MET:HE2	4:K:103:MET:HB3	1.82	0.45
5:B:121:ARG:NH1	5:B:123:GLU:OE1	2.50	0.45
1:A:30:G:H4'	4:K:41:CYS:CA	2.39	0.45
4:F:297:VAL:O	4:F:301:ILE:HG12	2.16	0.45
4:H:357:VAL:O	4:H:361:ILE:HG12	2.17	0.45
4:K:185:GLU:H	6:D:73:ILE:HD13	1.81	0.45
4:K:373:LYS:HE3	4:K:373:LYS:HB3	1.63	0.45
1:A:1:G:O5'	5:B:84:THR:OG1	2.32	0.44
4:K:3:ILE:H	4:K:3:ILE:HG13	1.42	0.44
4:K:26:THR:CB	6:D:78:LYS:HE2	2.47	0.44
4:K:185:GLU:H	4:K:185:GLU:HG3	1.51	0.44
5:B:41:LEU:HD22	5:B:63:LEU:HD22	1.99	0.44
2:C:359:MET:SD	2:C:360:SER:N	2.90	0.44
4:F:32:VAL:HG21	4:F:287:PRO:HG3	1.99	0.44
4:I:3:ILE:HG22	4:I:273:PHE:CD1	2.53	0.44
4:J:13:PRO:HG2	4:K:29:PHE:HB2	1.97	0.44
4:J:270:LEU:HB2	4:J:326:TRP:CZ3	2.52	0.44
4:K:85:LEU:HD12	4:K:85:LEU:HA	1.88	0.44
4:G:326:TRP:CE2	4:G:335:LEU:HB2	2.52	0.44
2:C:188:ILE:HG13	2:C:191:LEU:HD12	1.99	0.44
4:F:180:HIS:HD2	4:F:183:ARG:NH2	2.16	0.44
4:I:309:ASN:HA	4:I:342:LEU:HD11	2.00	0.44
2:C:105:VAL:HG13	2:C:157:ILE:HD12	1.99	0.44
2:C:300:TYR:HB2	2:C:326:SER:HB3	2.00	0.44
2:C:375:LEU:C	2:C:377:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:33:LEU:HB3	4:H:182:ALA:HB3	1.98	0.44
4:J:66:ASP:OD1	4:J:66:ASP:N	2.50	0.44
5:B:147:LEU:HD12	5:B:147:LEU:HA	1.85	0.44
6:D:141:GLN:HG3	6:D:143:ASP:HB2	2.00	0.44
2:C:501:GLN:HE21	3:E:154:ARG:HG2	1.81	0.44
4:I:103:MET:HG3	4:I:133:ILE:HG23	1.98	0.44
5:B:231:TYR:HA	5:B:244:PRO:HA	1.99	0.44
6:D:178:LYS:HE3	6:D:178:LYS:HB3	1.83	0.44
2:C:221:LYS:HD2	2:C:221:LYS:C	2.43	0.44
4:H:173:VAL:HG22	4:H:219:PHE:HD1	1.83	0.44
4:I:29:PHE:O	4:I:34:ARG:NH1	2.51	0.44
4:J:110:ASP:HA	4:J:113:ARG:HE	1.82	0.44
4:G:186:ILE:HG13	4:G:209:MET:SD	2.58	0.44
1:A:35:A:H4'	1:A:36:U:H5''	1.99	0.44
1:A:38:C:OP2	6:D:155:LYS:NZ	2.45	0.44
2:C:187:ALA:HA	2:C:324:SER:HA	2.00	0.44
6:D:33:ARG:CZ	6:D:55:PHE:HE2	2.31	0.44
1:A:17:U:OP1	4:I:43:LYS:NZ	2.34	0.43
2:C:179:ALA:HB3	2:C:298:LYS:HB2	1.99	0.43
4:H:148:MET:SD	4:H:150:GLU:HG3	2.58	0.43
4:K:220:SER:HB2	4:K:277:PRO:HB3	2.00	0.43
4:G:289:SER:O	4:G:299:GLN:NE2	2.46	0.43
4:H:250:LYS:HA	4:H:265:TYR:HE1	1.83	0.43
4:J:9:GLN:NE2	4:J:264:ASN:O	2.51	0.43
4:K:279:SER:C	4:K:281:ALA:H	2.25	0.43
1:A:-1:C:O2	5:B:129:ARG:NH2	2.51	0.43
4:F:199:ASP:H	4:H:63:ARG:HH12	1.67	0.43
4:F:235:ASN:HB3	4:F:369:VAL:HG12	1.99	0.43
4:J:147:ARG:HH22	4:J:150:GLU:HB2	1.83	0.43
4:G:312:ARG:HH21	4:G:322:VAL:HG23	1.83	0.43
6:D:149:THR:HG22	6:D:151:LYS:HG2	1.99	0.43
2:C:346:THR:HG22	2:C:352:LEU:HD13	2.01	0.43
3:E:22:ILE:HD13	3:E:22:ILE:HG21	1.83	0.43
4:H:221:ILE:HD11	4:H:244:PHE:CD2	2.54	0.43
4:I:107:LYS:HE2	4:I:107:LYS:HB2	1.71	0.43
4:I:230:LEU:HD12	4:I:237:ALA:HB2	1.99	0.43
4:K:16:LEU:HG	4:K:215:PHE:HE1	1.82	0.43
4:K:38:SER:C	4:K:40:GLN:H	2.24	0.43
4:K:140:PRO:HB3	4:K:240:THR:HG23	1.99	0.43
4:K:287:PRO:O	4:K:288:VAL:C	2.59	0.43
1:A:42:A:C2	1:A:48:G:N1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:PHE:CE1	2:C:423:ALA:HB2	2.53	0.43
4:J:6:HIS:C	4:J:7:MET:HE2	2.44	0.43
4:K:143:ALA:HA	4:K:229:ASN:HD22	1.83	0.43
5:B:199:TRP:NE1	5:B:201:ASN:O	2.52	0.43
1:A:8:G:H5'	4:F:255:GLY:HA2	1.99	0.43
3:E:116:MET:HE3	3:E:116:MET:HB2	1.79	0.43
4:F:24:PRO:HD3	4:F:209:MET:HB2	2.01	0.43
4:F:263:HIS:HD2	4:H:218:TYR:HE2	1.66	0.43
4:J:103:MET:H	4:J:103:MET:HG2	1.63	0.43
4:F:111:LEU:HA	4:F:114:ILE:HG12	2.01	0.43
4:J:101:VAL:HA	4:J:148:MET:O	2.19	0.43
6:D:11:THR:HG23	6:D:22:ARG:HD3	2.00	0.43
4:I:55:LEU:HD21	4:I:239:HIS:HB3	2.00	0.43
4:K:62:ARG:HE	4:K:62:ARG:HB2	1.44	0.43
6:D:126:LEU:HG	6:D:128:VAL:HG22	2.01	0.43
2:C:265:GLN:HA	2:C:266:PRO:HD3	1.91	0.43
4:K:29:PHE:HE2	4:K:284:PHE:C	2.27	0.43
5:B:61:PRO:HA	5:B:64:ALA:HB3	2.00	0.43
1:A:36:U:H4'	6:D:157:VAL:HG11	2.00	0.42
4:H:46:ILE:O	4:H:49:SER:OG	2.36	0.42
4:H:254:SER:HA	4:H:257:GLN:HG3	2.01	0.42
4:J:139:ALA:O	4:J:141:ASP:N	2.52	0.42
4:J:295:ASP:OD1	4:J:295:ASP:N	2.43	0.42
2:C:259:MET:O	2:C:263:ASN:ND2	2.52	0.42
4:F:29:PHE:HB3	4:F:34:ARG:HE	1.83	0.42
4:H:187:ASP:HB2	4:H:210:PHE:HE2	1.84	0.42
4:I:91:LYS:O	4:I:98:LYS:HD3	2.19	0.42
4:J:294:SER:OG	4:J:295:ASP:N	2.52	0.42
4:J:362:GLY:HA3	4:J:364:PHE:CZ	2.53	0.42
4:K:16:LEU:HB3	4:K:17:ASN:H	1.69	0.42
2:C:251:TRP:CZ2	2:C:386:ARG:HG2	2.55	0.42
4:K:16:LEU:HD21	4:K:215:PHE:CE1	2.55	0.42
2:C:492:LYS:HA	2:C:492:LYS:HD3	1.64	0.42
5:B:235:VAL:HB	5:B:241:ARG:HG2	2.01	0.42
2:C:198:ALA:HA	5:B:95:GLU:HB2	2.01	0.42
2:C:370:ASP:OD1	2:C:370:ASP:N	2.38	0.42
4:K:142:ILE:H	4:K:142:ILE:HG12	1.51	0.42
4:K:149:LEU:HD13	4:K:149:LEU:HA	1.54	0.42
4:G:20:ASP:OD2	5:B:128:ARG:NH1	2.52	0.42
4:G:312:ARG:HE	4:G:322:VAL:HG22	1.85	0.42
4:G:341:LYS:HD3	4:G:341:LYS:HA	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:301:CYS:SG	5:B:365:ARG:NH1	2.89	0.42
6:D:48:ASP:OD1	6:D:48:ASP:N	2.51	0.42
4:F:296:LEU:O	4:F:300:SER:OG	2.31	0.42
4:K:192:ALA:HA	6:D:112:TYR:HE1	1.84	0.42
5:B:45:CYS:HA	5:B:50:ILE:HD12	2.02	0.42
6:D:164:SER:O	6:D:164:SER:OG	2.38	0.42
4:H:338:LYS:H	4:H:338:LYS:HG2	1.54	0.42
4:I:323:ILE:H	4:I:323:ILE:HD12	1.85	0.42
5:B:229:ILE:O	5:B:230:HIS:ND1	2.52	0.42
6:D:151:LYS:HB2	6:D:151:LYS:HE3	1.87	0.42
4:F:34:ARG:HB3	4:F:178:SER:HB3	2.01	0.42
4:F:58:GLY:HA2	4:F:104:SER:HA	2.01	0.42
4:K:148:MET:HG3	4:K:166:THR:HG23	2.02	0.42
6:D:191:LEU:HA	6:D:232:LEU:HD23	2.02	0.42
2:C:145:GLU:HG2	2:C:264:TRP:HE1	1.85	0.41
2:C:424:GLN:CD	2:C:519:PRO:HB2	2.45	0.41
2:C:433:ASN:O	2:C:437:LYS:HB2	2.20	0.41
4:F:269:ILE:HD13	4:F:327:PHE:CD2	2.55	0.41
4:J:10:ASN:HB3	4:K:282:ASN:HD21	1.85	0.41
4:J:44:ARG:HD2	4:J:47:ARG:HH21	1.85	0.41
4:J:282:ASN:HA	4:J:285:VAL:HG23	2.01	0.41
4:K:29:PHE:HB3	4:K:34:ARG:HD2	2.02	0.41
4:G:326:TRP:CH2	4:G:328:SER:HB2	2.55	0.41
4:J:263:HIS:N	4:K:279:SER:HB3	2.36	0.41
4:K:283:ALA:HB2	4:K:307:TYR:CE2	2.55	0.41
4:G:337:TYR:CZ	5:B:272:LYS:HG3	2.56	0.41
5:B:84:THR:HG22	5:B:126:LEU:HD23	2.02	0.41
4:J:46:ILE:HA	4:J:251:THR:HG21	2.01	0.41
4:J:185:GLU:OE2	4:K:27:CYS:HA	2.20	0.41
4:K:49:SER:O	4:K:50:ASN:C	2.62	0.41
4:K:313:LEU:HD23	4:K:313:LEU:HA	1.91	0.41
5:B:62:LYS:HE2	5:B:147:LEU:HD11	2.02	0.41
6:D:53:LYS:HE3	6:D:54:PRO:HD2	2.01	0.41
1:A:12:G:O2'	1:A:13:G:H4'	2.19	0.41
3:E:63:LEU:HA	3:E:66:LYS:HE2	2.02	0.41
4:F:23:ALA:HA	4:F:209:MET:HB2	2.01	0.41
4:H:25:LYS:HD2	4:H:36:ARG:NH2	2.36	0.41
4:G:34:ARG:HH22	4:G:287:PRO:HB3	1.85	0.41
4:G:209:MET:CG	4:G:210:PHE:H	2.34	0.41
5:B:338:MET:HE2	5:B:338:MET:HB2	1.86	0.41
1:A:1:G:OP1	4:G:17:ASN:ND2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:116:MET:HE1	3:E:147:TRP:CD1	2.55	0.41
4:I:226:LEU:HA	4:I:226:LEU:HD12	1.53	0.41
4:J:311:ILE:HD13	4:J:311:ILE:HA	1.98	0.41
4:K:274:LYS:HE2	4:K:274:LYS:HB2	1.70	0.41
5:B:253:VAL:HG13	5:B:256:GLU:HG2	2.02	0.41
5:B:290:ARG:NH1	5:B:322:PRO:O	2.51	0.41
4:F:347:ILE:HG22	4:F:349:ASN:H	1.86	0.41
4:J:63:ARG:HD3	4:J:63:ARG:HA	1.92	0.41
4:K:217:LYS:HB2	4:K:217:LYS:HE3	1.64	0.41
2:C:188:ILE:HG12	2:C:214:LEU:HD12	2.01	0.41
3:E:120:LEU:O	3:E:124:MET:HG2	2.21	0.41
4:H:103:MET:HE1	4:H:111:LEU:HD11	2.03	0.41
4:K:27:CYS:SG	4:K:36:ARG:HB3	2.60	0.41
2:C:109:LYS:HB2	2:C:109:LYS:HE3	1.86	0.41
3:E:113:ILE:H	3:E:113:ILE:HD12	1.86	0.41
1:A:24:C:H5"	4:I:190:VAL:O	2.21	0.41
3:E:74:GLU:OE1	3:E:76:ARG:HB2	2.21	0.41
4:H:272:GLU:OE1	4:H:274:LYS:NZ	2.48	0.41
4:I:25:LYS:HB3	4:I:36:ARG:NH2	2.36	0.41
4:J:47:ARG:HH12	4:J:60:ARG:HH21	1.69	0.41
4:J:189:PHE:CZ	4:J:206:GLY:HA3	2.56	0.41
4:K:161:LYS:HA	4:K:161:LYS:HD3	1.55	0.41
4:K:358:LEU:HD12	4:K:358:LEU:HA	1.89	0.41
4:G:236:LEU:HD12	4:G:236:LEU:HA	1.91	0.41
5:B:28:LEU:HD12	5:B:28:LEU:HA	1.93	0.41
6:D:201:LYS:HE2	6:D:225:LEU:HD11	2.03	0.41
2:C:93:VAL:HG12	2:C:117:ALA:HB2	2.02	0.41
4:F:295:ASP:O	4:F:299:GLN:HG3	2.21	0.41
4:H:272:GLU:HG2	4:H:324:GLY:HA3	2.02	0.41
4:J:89:GLY:HA3	4:J:156:LYS:HB3	2.02	0.41
4:K:151:PRO:O	4:K:152:ASN:C	2.63	0.41
5:B:7:THR:HB	5:B:142:GLN:HG3	2.03	0.41
5:B:309:GLN:NE2	5:B:336:CYS:HB2	2.35	0.41
5:B:354:ASP:HA	5:B:355:PRO:HD3	1.96	0.41
2:C:128:PHE:CZ	2:C:132:LEU:HD22	2.56	0.40
2:C:469:GLY:O	2:C:475:ARG:NH2	2.55	0.40
4:I:112:ALA:O	4:I:116:LEU:HG	2.21	0.40
3:E:71:PHE:CZ	3:E:124:MET:HB2	2.56	0.40
4:I:71:GLU:HG3	4:I:113:ARG:HE	1.85	0.40
4:K:79:LYS:H	4:K:79:LYS:HG3	1.60	0.40
4:F:199:ASP:H	4:H:63:ARG:NH1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:142:ILE:HD12	4:I:147:ARG:HB2	2.04	0.40
4:K:16:LEU:CG	4:K:215:PHE:HE1	2.33	0.40
4:K:46:ILE:HD12	4:K:46:ILE:HA	1.86	0.40
4:K:209:MET:HE2	4:K:209:MET:HB2	1.46	0.40
4:G:274:LYS:HG2	4:G:322:VAL:HG11	2.03	0.40
2:C:192:ILE:HG13	2:C:195:ILE:HD12	2.04	0.40
2:C:365:THR:OG1	2:C:433:ASN:OD1	2.37	0.40
4:K:1:MET:H3	4:K:223:TRP:HB2	1.86	0.40
5:B:307:THR:OG1	5:B:308:VAL:N	2.54	0.40
1:A:-4:A:P	5:B:29:ARG:HH21	2.44	0.40
4:F:107:LYS:O	4:F:111:LEU:HB2	2.22	0.40
4:H:55:LEU:HB3	4:H:140:PRO:HG2	2.04	0.40
4:J:21:LEU:HA	5:B:379:ARG:CZ	2.52	0.40
4:K:180:HIS:CD2	4:K:296:LEU:HD22	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	438/535 (82%)	378 (86%)	59 (14%)	1 (0%)	43	73
3	E	163/174 (94%)	156 (96%)	7 (4%)	0	100	100
4	F	363/378 (96%)	337 (93%)	26 (7%)	0	100	100
4	G	241/378 (64%)	223 (92%)	18 (8%)	0	100	100
4	H	363/378 (96%)	332 (92%)	31 (8%)	0	100	100
4	I	358/378 (95%)	324 (90%)	33 (9%)	1 (0%)	36	67
4	J	363/378 (96%)	327 (90%)	36 (10%)	0	100	100
4	K	329/378 (87%)	239 (73%)	75 (23%)	15 (5%)	2	12
5	B	376/388 (97%)	350 (93%)	25 (7%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	266/272 (98%)	248 (93%)	17 (6%)	1 (0%)	30	61
All	All	3260/3637 (90%)	2914 (89%)	327 (10%)	19 (1%)	23	52

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	310	ALA
4	I	322	VAL
4	K	20	ASP
4	K	301	ILE
5	B	346	THR
4	K	78	TRP
4	K	283	ALA
4	K	288	VAL
6	D	241	PRO
4	K	76	GLU
4	K	83	GLU
4	K	106	ASP
4	K	231	LYS
4	K	155	ASP
4	K	362	GLY
4	K	118	ASN
4	K	160	VAL
4	K	164	ASN
4	K	369	VAL

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	366/459 (80%)	364 (100%)	2 (0%)	81	85
3	E	143/153 (94%)	139 (97%)	4 (3%)	38	66
4	F	291/313 (93%)	291 (100%)	0	100	100
4	G	199/313 (64%)	196 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	300/313 (96%)	299 (100%)	1 (0%)	86	87
4	I	288/313 (92%)	284 (99%)	4 (1%)	59	76
4	J	291/313 (93%)	289 (99%)	2 (1%)	76	82
4	K	275/313 (88%)	169 (62%)	106 (38%)	0	0
5	B	308/322 (96%)	307 (100%)	1 (0%)	86	87
6	D	223/238 (94%)	222 (100%)	1 (0%)	84	86
All	All	2684/3050 (88%)	2560 (95%)	124 (5%)	25	55

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	252	HIS
2	C	379	LEU
3	E	127	LEU
3	E	153	LYS
3	E	157	SER
3	E	158	ASP
4	H	17	ASN
4	I	7	MET
4	I	17	ASN
4	I	150	GLU
4	I	316	TYR
4	J	32	VAL
4	J	311	ILE
4	K	3	ILE
4	K	4	GLU
4	K	5	ILE
4	K	8	ILE
4	K	9	GLN
4	K	10	ASN
4	K	11	HIS
4	K	12	SER
4	K	15	ASN
4	K	16	LEU
4	K	18	ARG
4	K	21	LEU
4	K	26	THR
4	K	32	VAL
4	K	33	LEU
4	K	35	SER

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Mol	Chain	Res	Type
4	K	36	ARG
4	K	37	ILE
4	K	38	SER
4	K	39	SER
4	K	43	LYS
4	K	44	ARG
4	K	45	SER
4	K	46	ILE
4	K	47	ARG
4	K	48	THR
4	K	51	ASP
4	K	55	LEU
4	K	59	VAL
4	K	62	ARG
4	K	63	ARG
4	K	64	LEU
4	K	68	ILE
4	K	69	GLN
4	K	75	THR
4	K	76	GLU
4	K	78	TRP
4	K	79	LYS
4	K	82	GLN
4	K	83	GLU
4	K	88	CYS
4	K	101	VAL
4	K	104	SER
4	K	106	ASP
4	K	107	LYS
4	K	108	ILE
4	K	110	ASP
4	K	113	ARG
4	K	114	ILE
4	K	116	LEU
4	K	120	LEU
4	K	122	LEU
4	K	127	GLN
4	K	129	VAL
4	K	131	ASN
4	K	135	GLN
4	K	141	ASP
4	K	142	ILE

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Mol	Chain	Res	Type
4	K	147	ARG
4	K	149	LEU
4	K	154	LYS
4	K	157	ASP
4	K	161	LYS
4	K	165	THR
4	K	167	VAL
4	K	168	GLU
4	K	171	LEU
4	K	172	GLN
4	K	173	VAL
4	K	177	ILE
4	K	179	THR
4	K	183	ARG
4	K	185	GLU
4	K	186	ILE
4	K	187	ASP
4	K	190	VAL
4	K	209	MET
4	K	210	PHE
4	K	212	SER
4	K	217	LYS
4	K	220	SER
4	K	221	ILE
4	K	222	ASP
4	K	225	GLN
4	K	228	LYS
4	K	233	ASP
4	K	234	THR
4	K	272	GLU
4	K	274	LYS
4	K	276	SER
4	K	278	ILE
4	K	280	TYR
4	K	285	VAL
4	K	286	ARG
4	K	289	SER
4	K	290	VAL
4	K	291	VAL
4	K	292	LYS
4	K	293	GLU
4	K	295	ASP

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Mol	Chain	Res	Type
4	K	298	GLU
4	K	299	GLN
4	K	301	ILE
4	K	361	ILE
4	K	367	GLU
4	K	373	LYS
4	G	2	LEU
4	G	278	ILE
4	G	347	ILE
5	B	147	LEU
6	D	41	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	243	ASN
2	C	308	GLN
2	C	501	GLN
3	E	50	GLN
4	F	17	ASN
4	F	239	HIS
4	F	257	GLN
4	F	351	ASN
4	H	252	ASN
4	H	331	ASN
4	I	40	GLN
4	I	225	GLN
4	I	309	ASN
4	I	339	HIS
4	J	10	ASN
4	J	264	ASN
4	J	351	ASN
4	J	370	GLN
4	K	15	ASN
4	K	17	ASN
4	K	69	GLN
4	K	82	GLN
4	K	96	ASN
4	K	131	ASN
4	K	135	GLN
4	K	172	GLN
4	K	225	GLN

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Mol	Chain	Res	Type
4	K	229	ASN
4	K	239	HIS
5	B	22	ASN
5	B	89	GLN
5	B	206	GLN
5	B	309	GLN
5	B	310	HIS
6	D	113	ASN
6	D	135	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/61 (93%)	18 (31%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-4	A
1	A	0	G
1	A	1	G
1	A	6	C
1	A	7	C
1	A	8	G
1	A	11	A
1	A	13	G
1	A	18	U
1	A	19	A
1	A	20	G
1	A	25	G
1	A	29	A
1	A	31	C
1	A	37	U
1	A	44	G
1	A	45	C
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 [i](#)

There are no chain breaks in this entry.

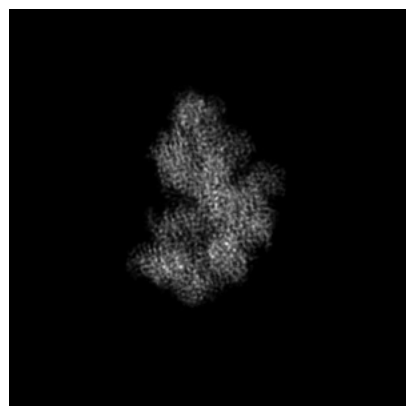
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60235. These allow visual inspection of the internal detail of the map and identification of artifacts.

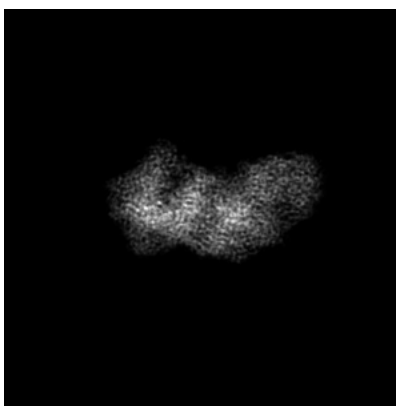
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

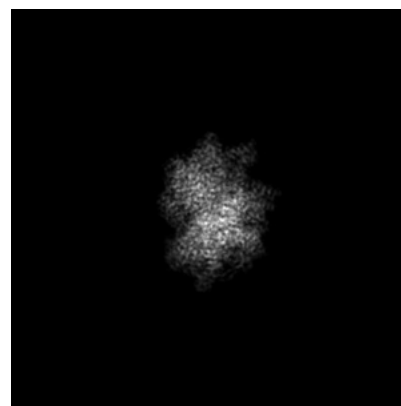
6.1.1 Primary map



X

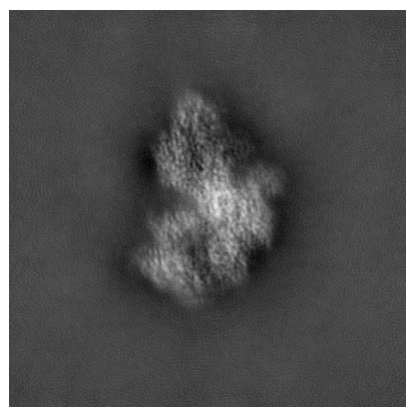


Y

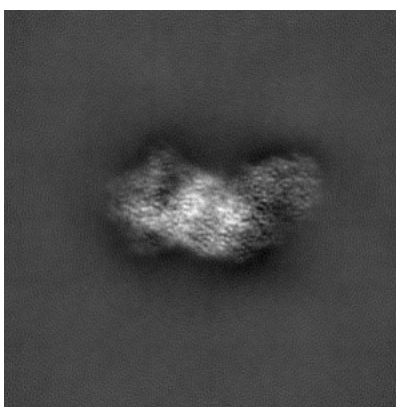


Z

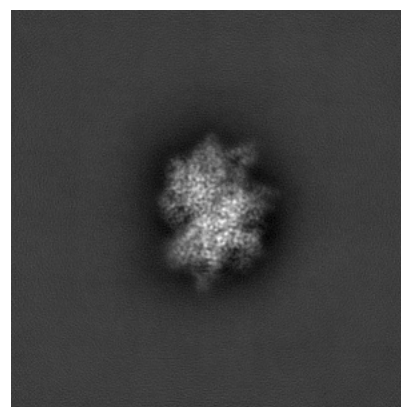
6.1.2 Raw map



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: 200

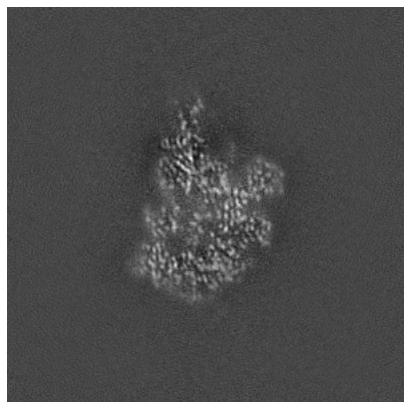


Y Index: 200

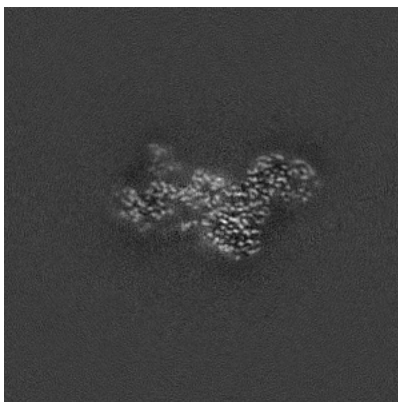


Z Index: 200

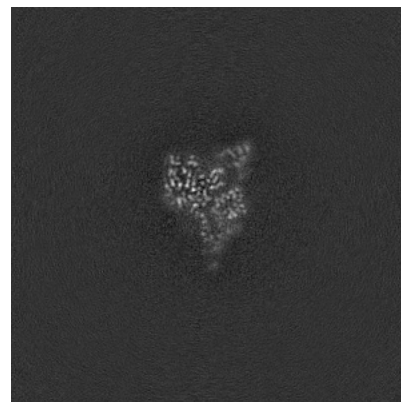
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

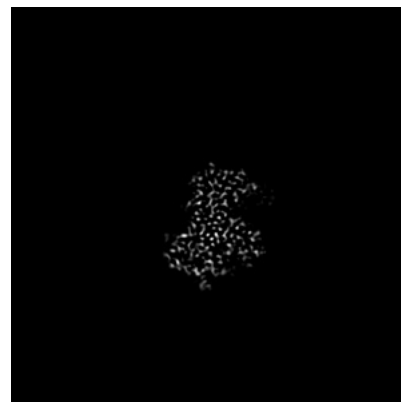
6.3.1 Primary map



X Index: 197

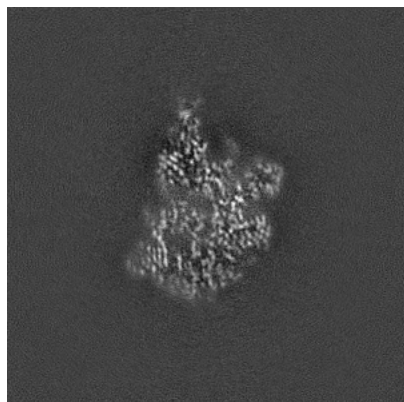


Y Index: 206

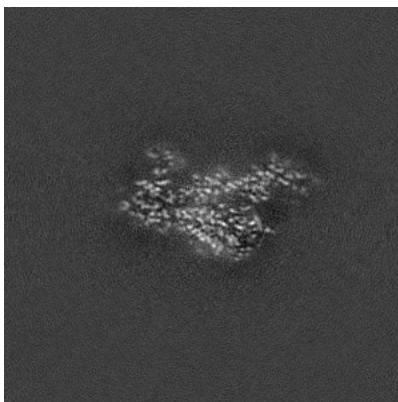


Z Index: 142

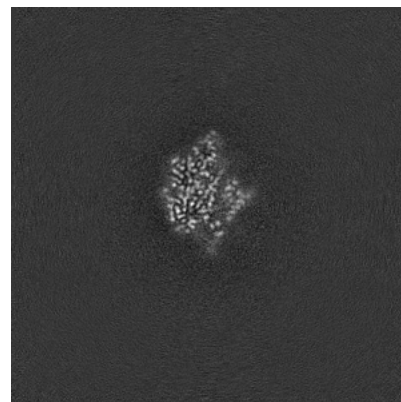
6.3.2 Raw map



X Index: 197



Y Index: 208

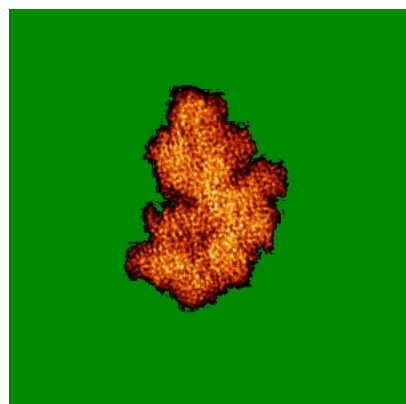


Z Index: 217

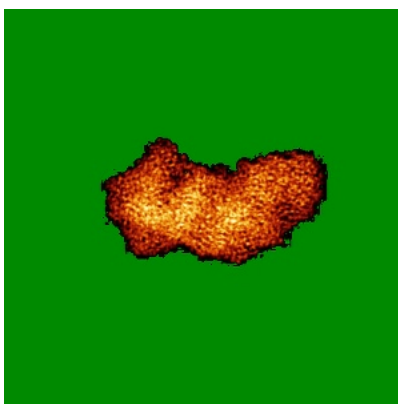
The images above show the largest variance slices of the map in three orthogonal directions.

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

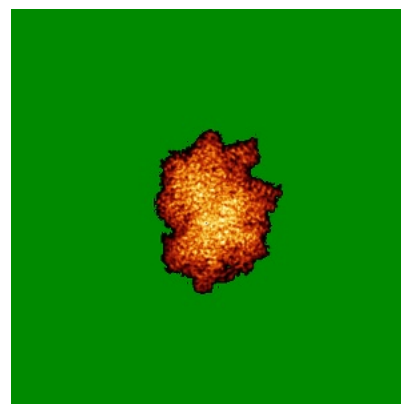
6.4.1 Primary map



X

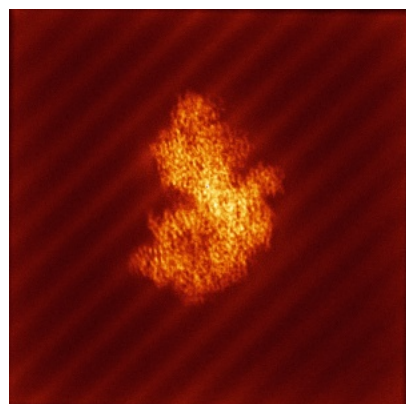


Y

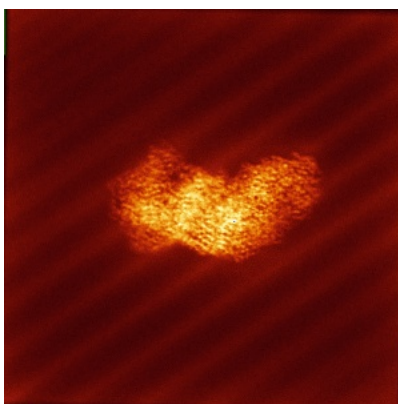


Z

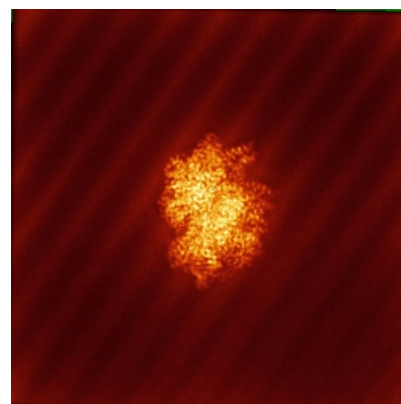
6.4.2 Raw map



X



Y

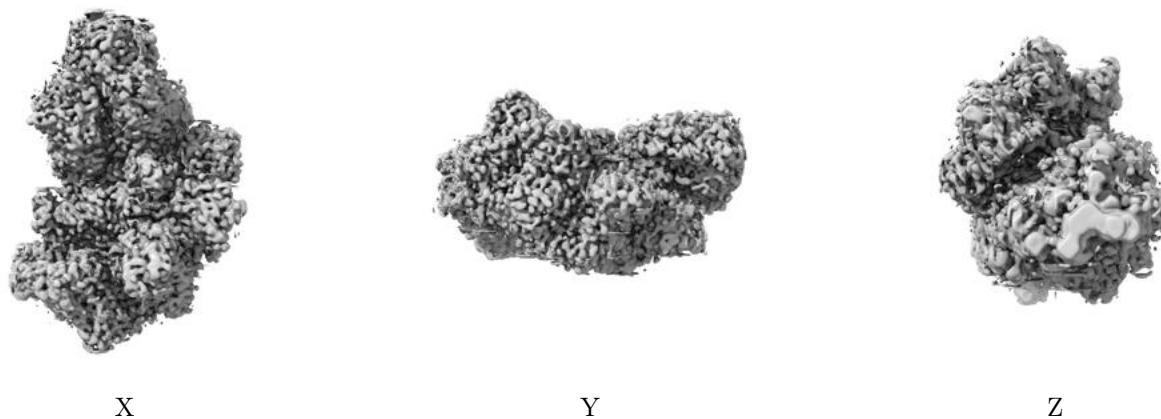


Z

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.

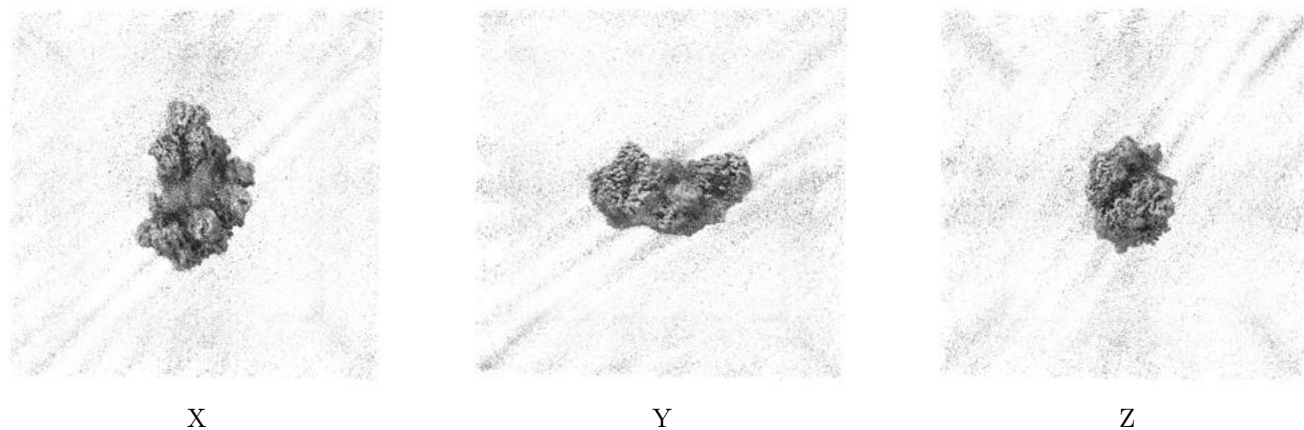
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00549. 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.

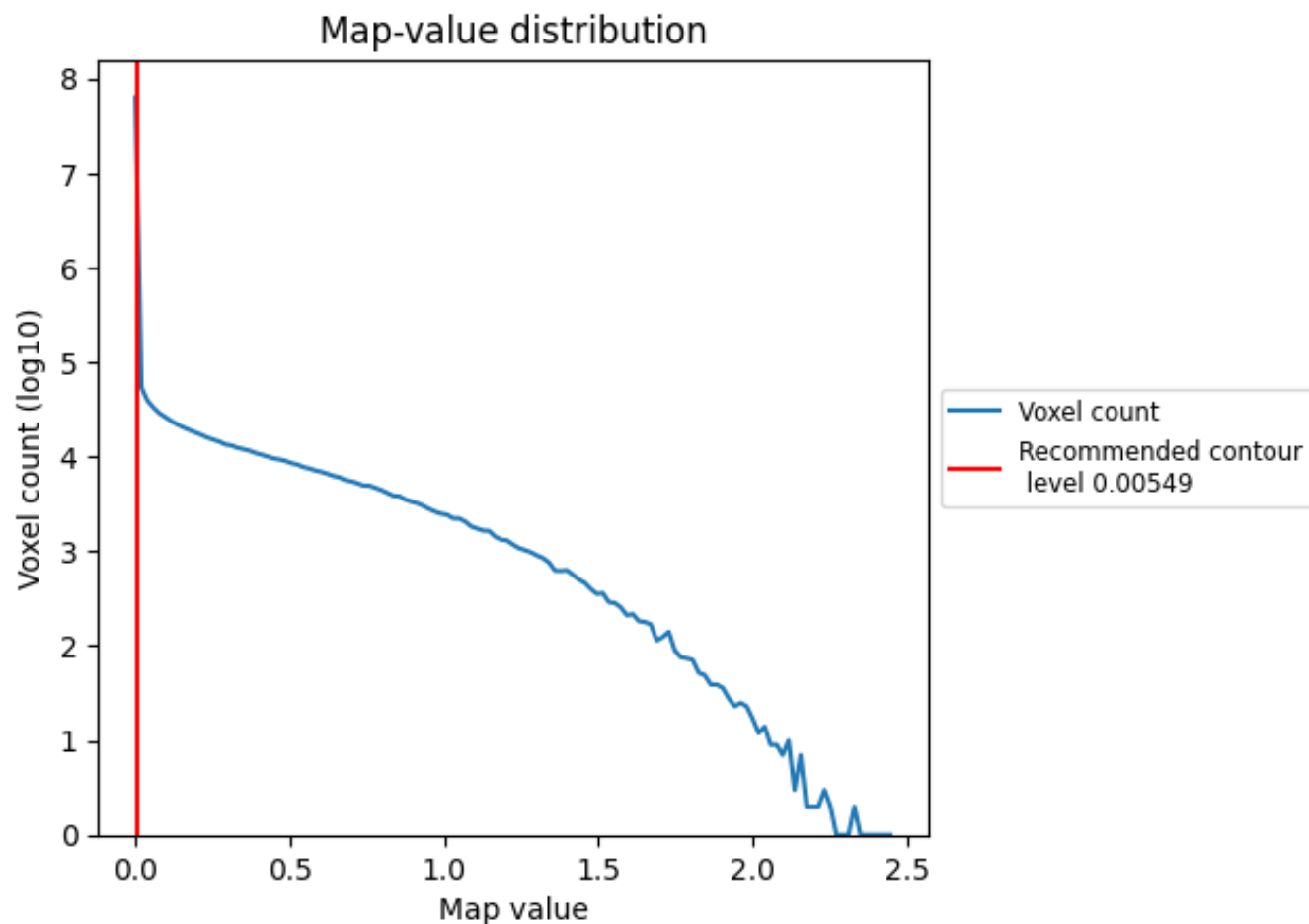
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

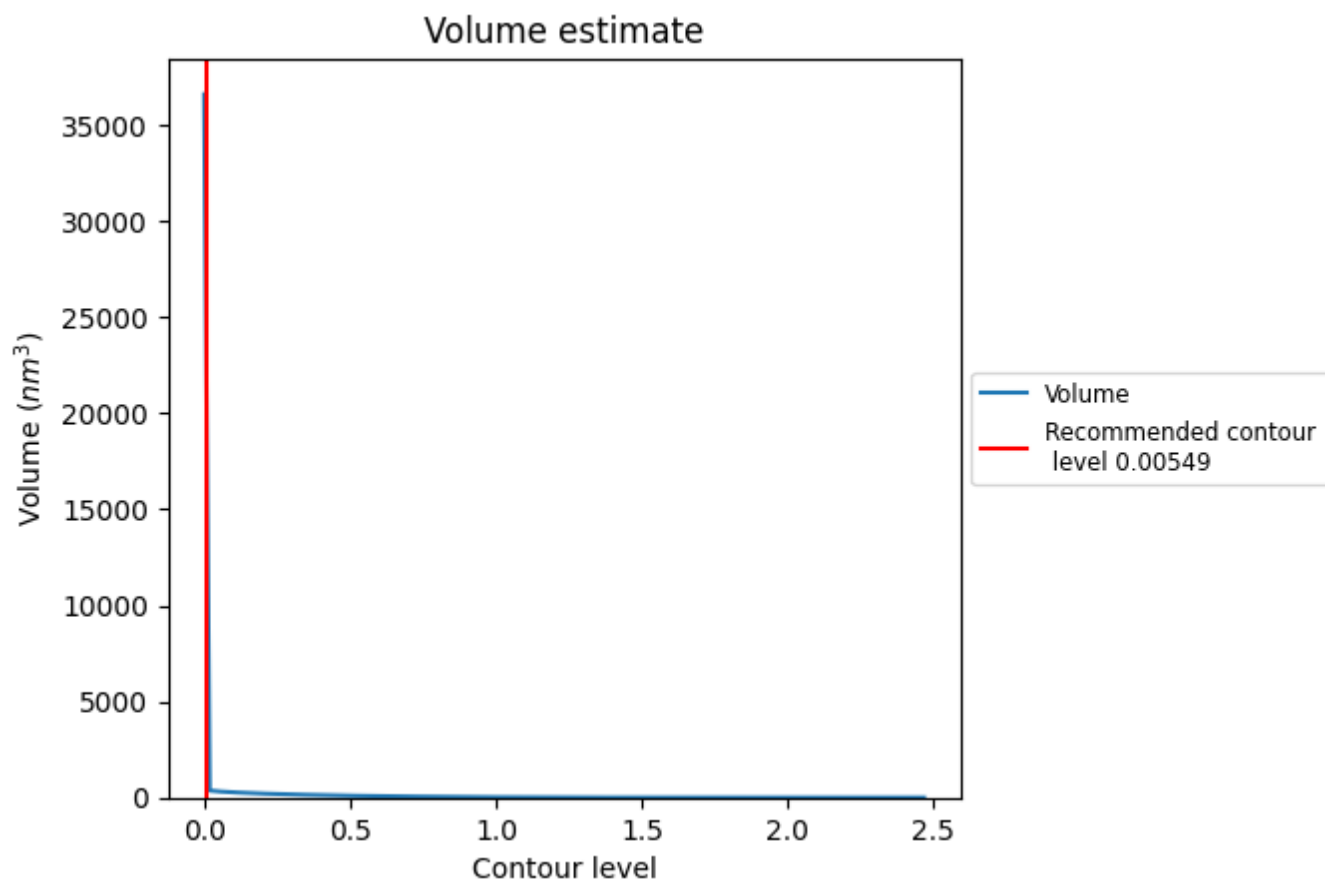
This section contains the results of statistical analysis of the map.

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.

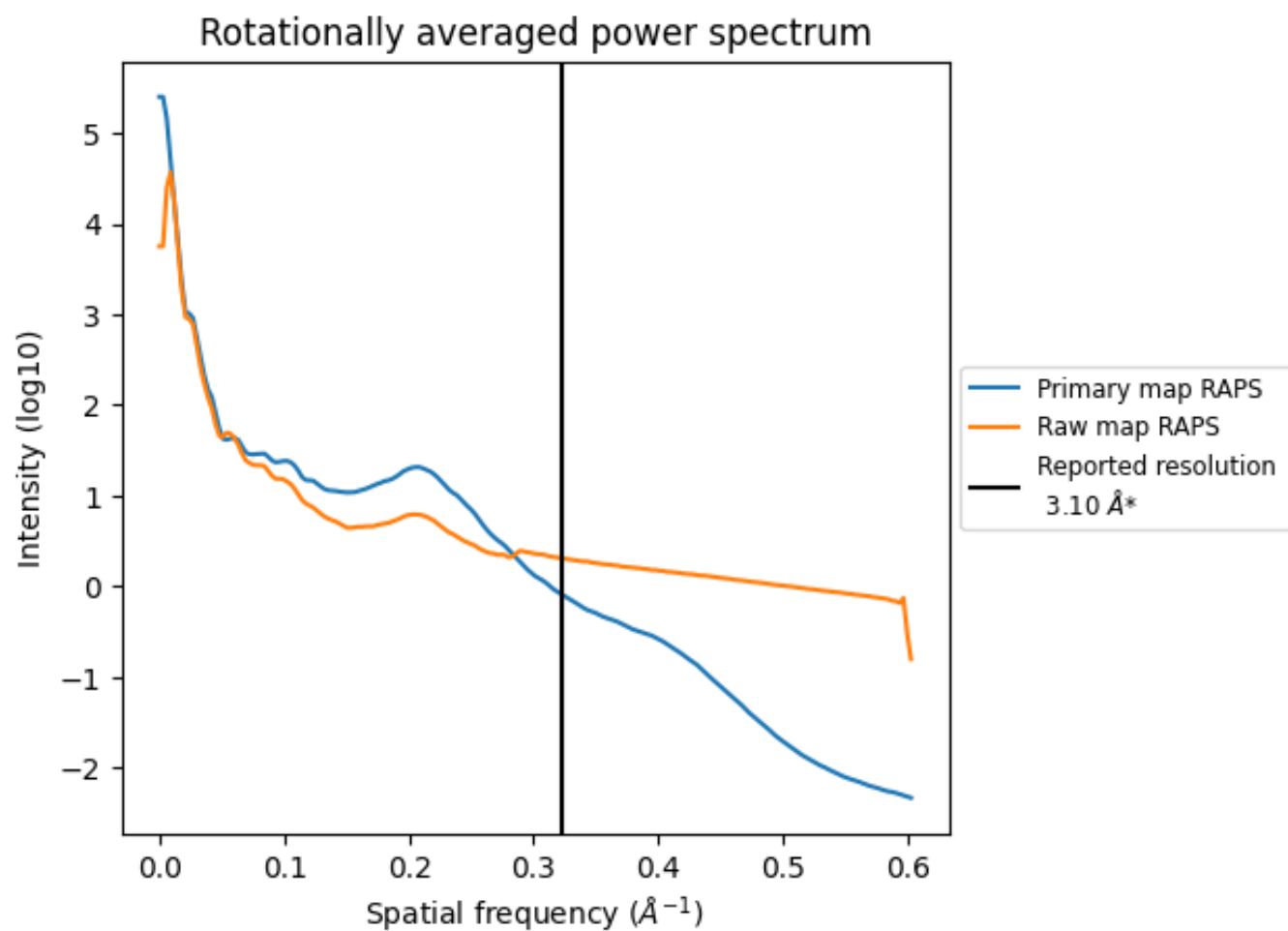
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 24533 nm³; this corresponds to an approximate mass of 22162 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 ⓘ

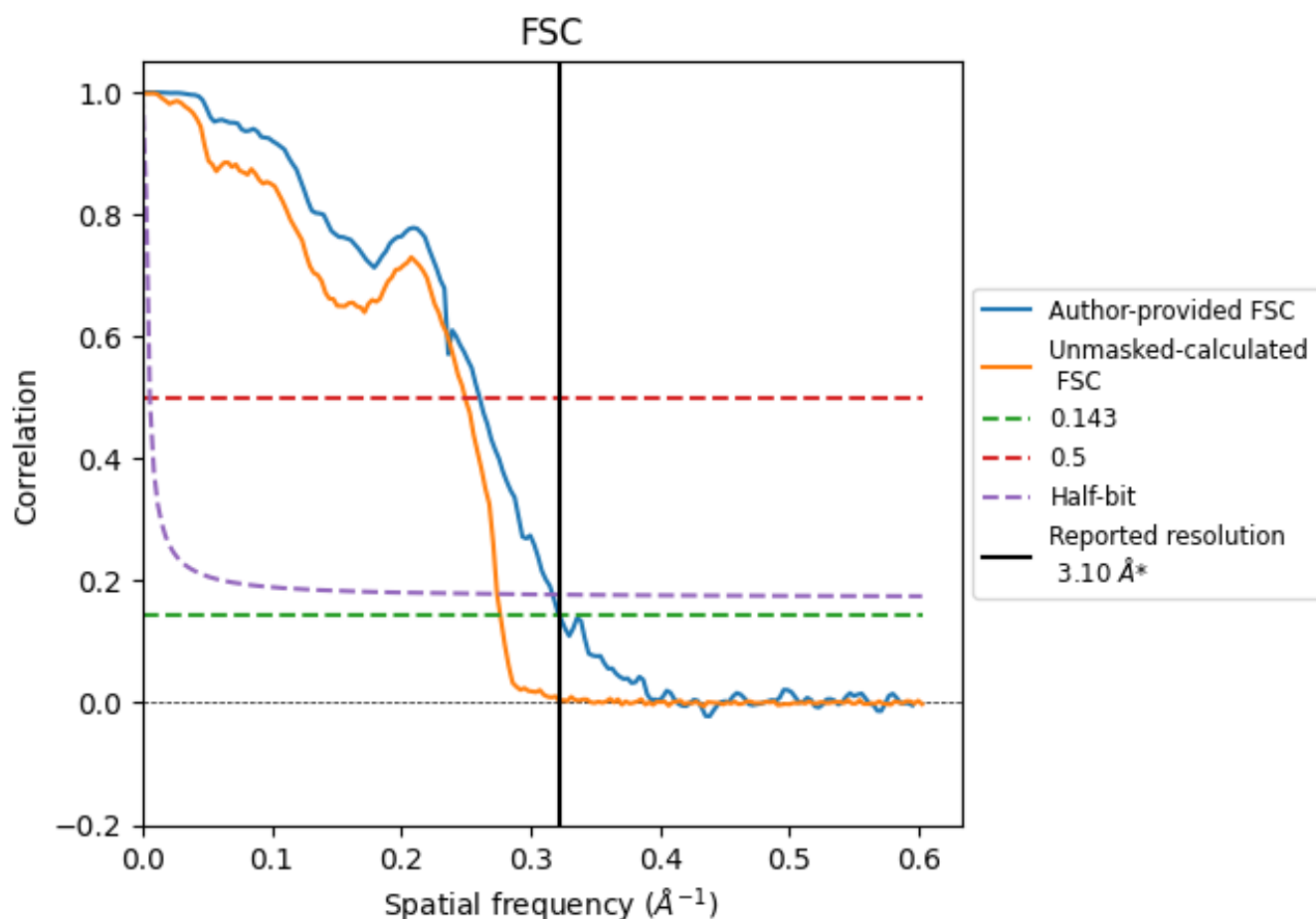


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

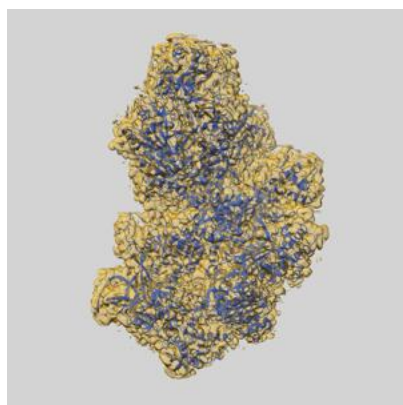
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.84	3.15
Unmasked-calculated*	3.61	4.01	3.65

*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 3.61 differs from the reported value 3.1 by more than 10 %

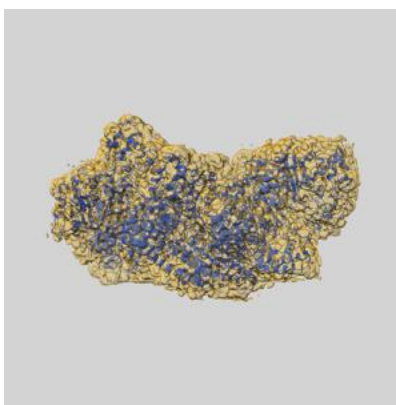
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60235 and PDB model 8ZM3. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

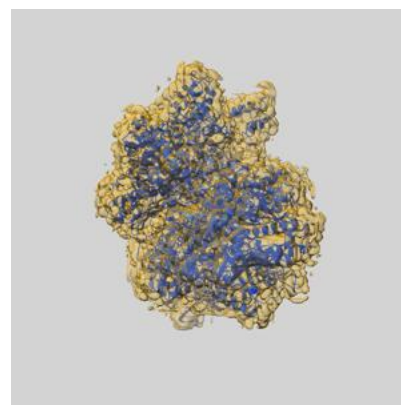
9.1 Map-model overlay [i](#)



X



Y



Z

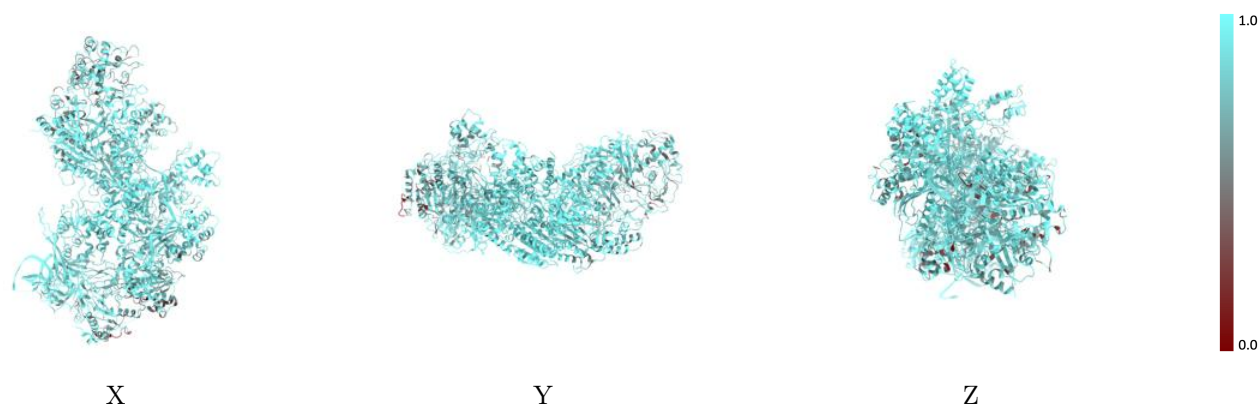
The images above show the 3D surface view of the map at the recommended contour level 0.00549 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



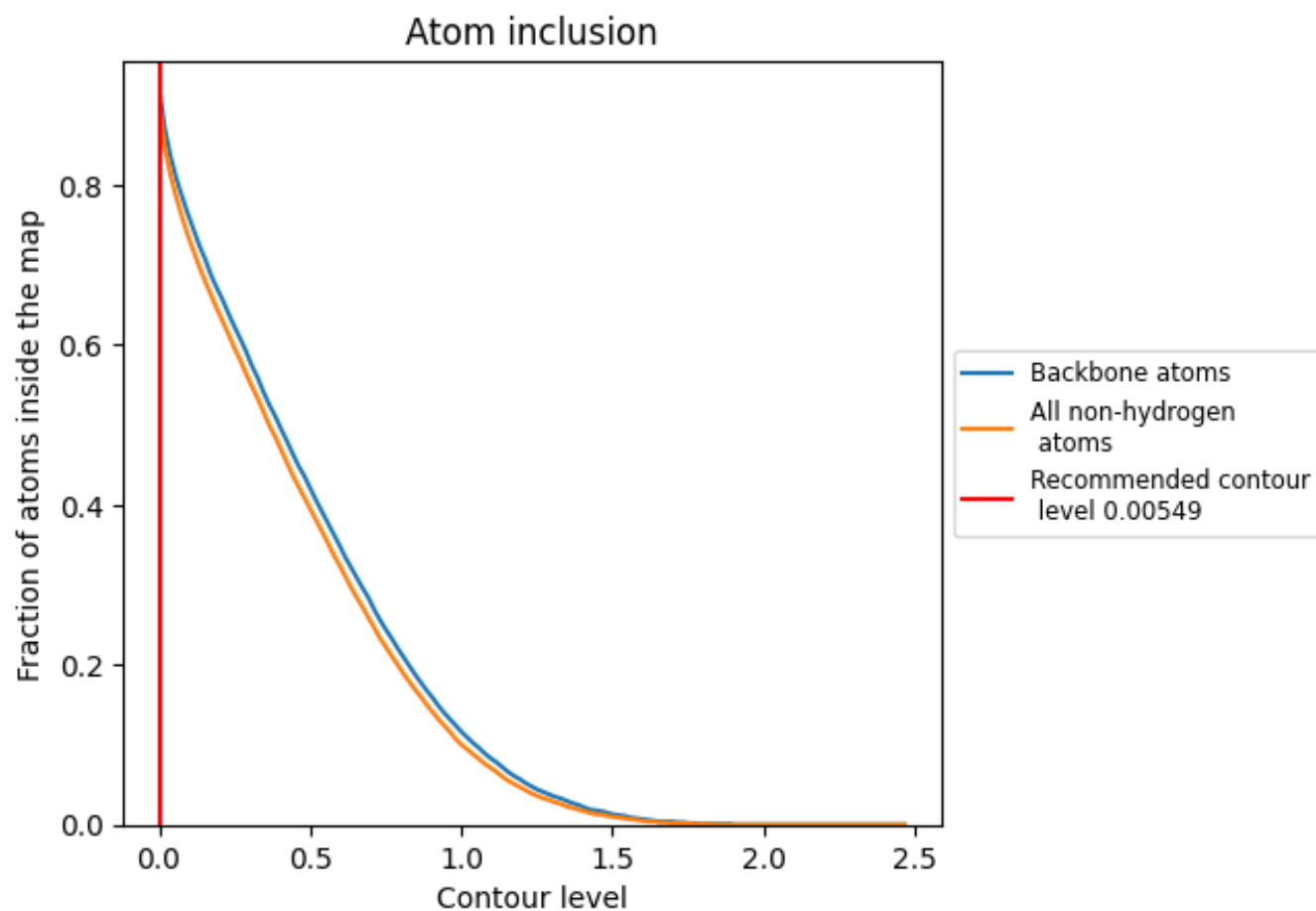
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00549).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00549) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.2200
A	 0.8960	 0.2010
B	 0.8900	 0.2430
C	 0.8260	 0.1030
D	 0.9260	 0.2400
E	 0.9730	 0.3790
F	 0.9030	 0.2570
G	 0.9010	 0.2380
H	 0.9700	 0.3680
I	 0.9150	 0.2530
J	 0.7950	 0.0540
K	 0.8310	 0.1890

