



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 9CQL / pdb_00009cql
EMDB ID : EMD-45814
Title : Dimeric 9C2 gamma delta TCR bound by Fab 3
Authors : Hoque, M.; Saotome, K.; Franklin, M.C.
Deposited on : 2024-07-19
Resolution : 3.46 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:

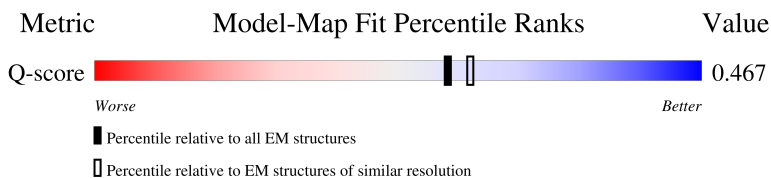
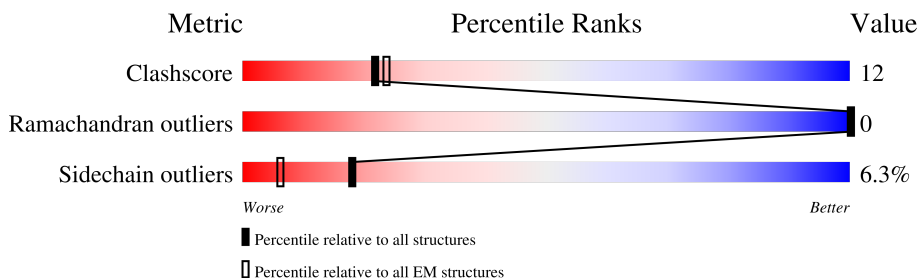
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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	280	
1	E	280	
2	B	294	
2	F	294	

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Mol	Chain	Length	Quality of chain
3	C	224	
3	J	224	
4	D	219	
4	K	219	
5	G	2	
5	H	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 9C2 TCR delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	202	Total	C	N	O	S	0	0
			1592	1015	269	301	7		
1	A	202	Total	C	N	O	S	0	0
			1592	1015	269	301	7		

- Molecule 2 is a protein called 9C2 TCR gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	222	Total	C	N	O	S	0	0
			1808	1159	307	336	6		
2	B	222	Total	C	N	O	S	0	0
			1808	1159	307	336	6		

- Molecule 3 is a protein called anti TCR variable delta 1 Fab heavy chain Fab 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	119	Total	C	N	O	S	0	0
			940	593	152	191	4		
3	C	119	Total	C	N	O	S	0	0
			940	593	152	191	4		

- Molecule 4 is a protein called anti TCR variable delta 1 Fab light chain Fab 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	112	Total	C	N	O	S	0	0
			854	546	141	164	3		
4	D	112	Total	C	N	O	S	0	0
			854	546	141	164	3		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



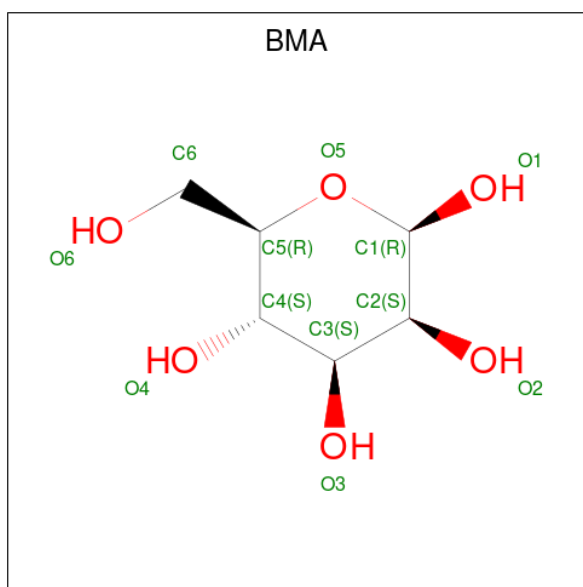
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

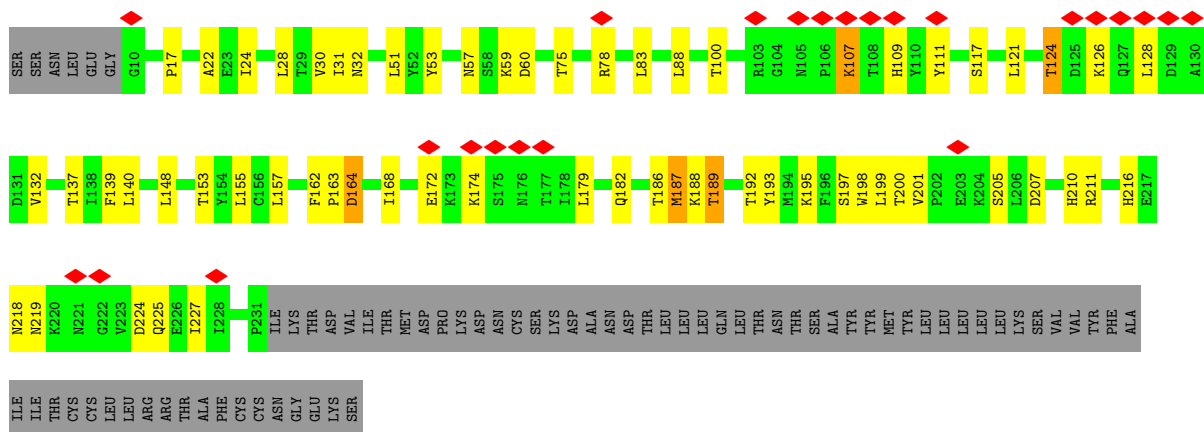


Mol	Chain	Residues	Atoms				AltConf
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

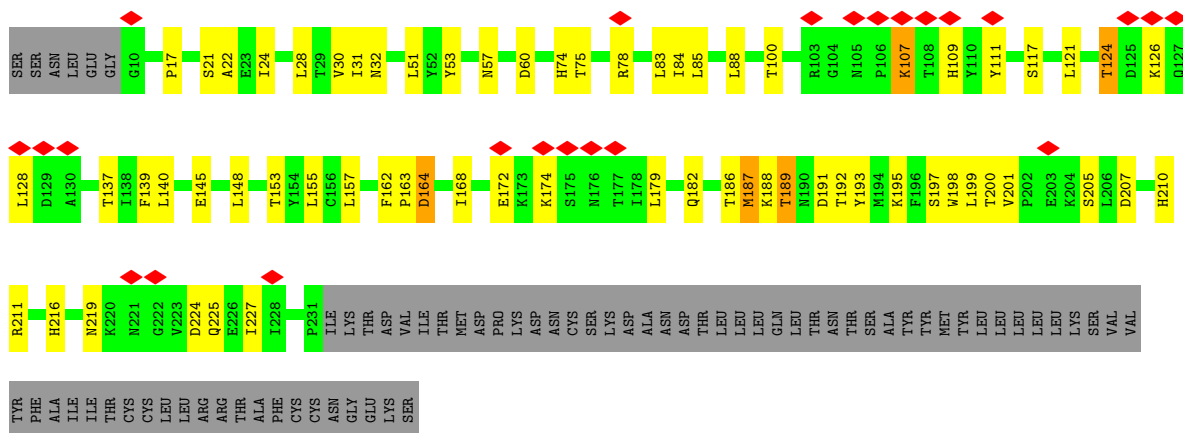
- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



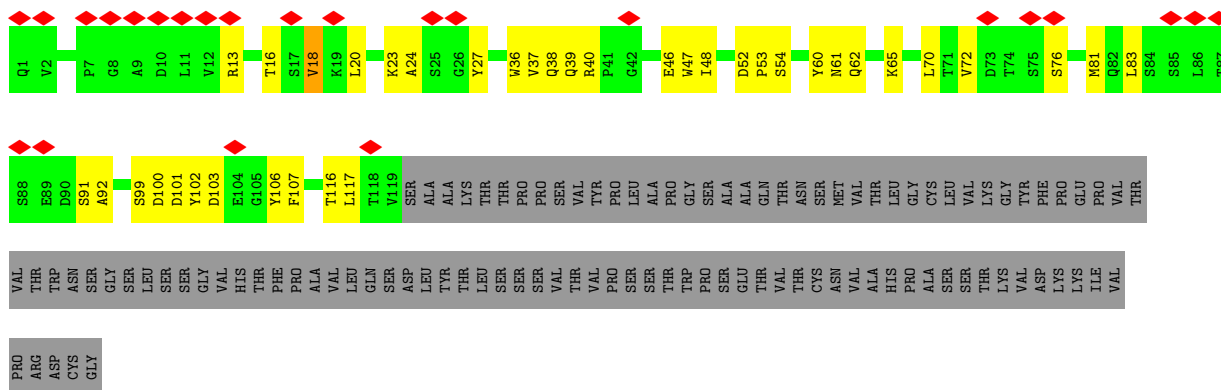
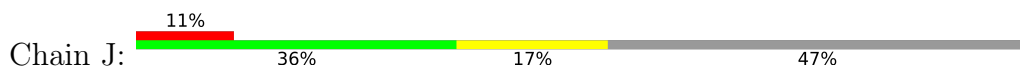
Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			11	6	5	
7	B	1	Total	C	O	0
			11	6	5	



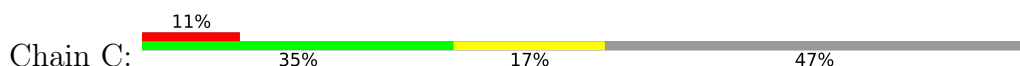
- Molecule 2: 9C2 TCR gamma chain

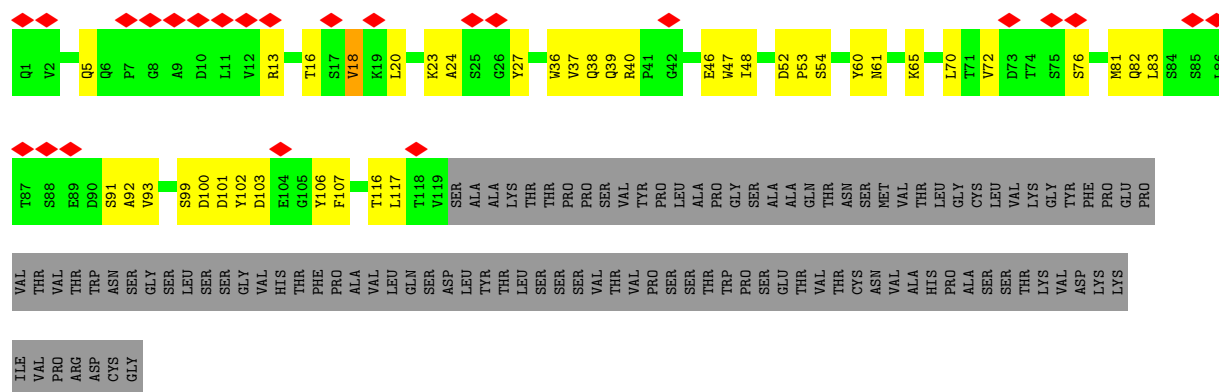


- Molecule 3: anti TCR variable delta 1 Fab heavy chain Fab 3

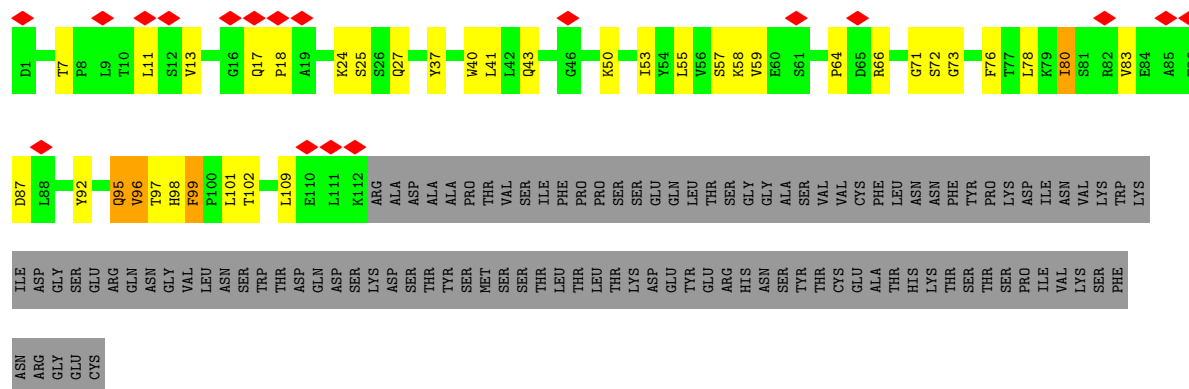
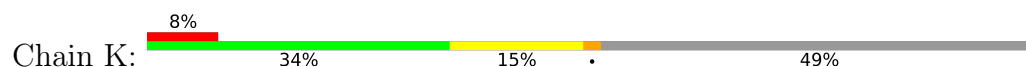


- Molecule 3: anti TCR variable delta 1 Fab heavy chain Fab 3

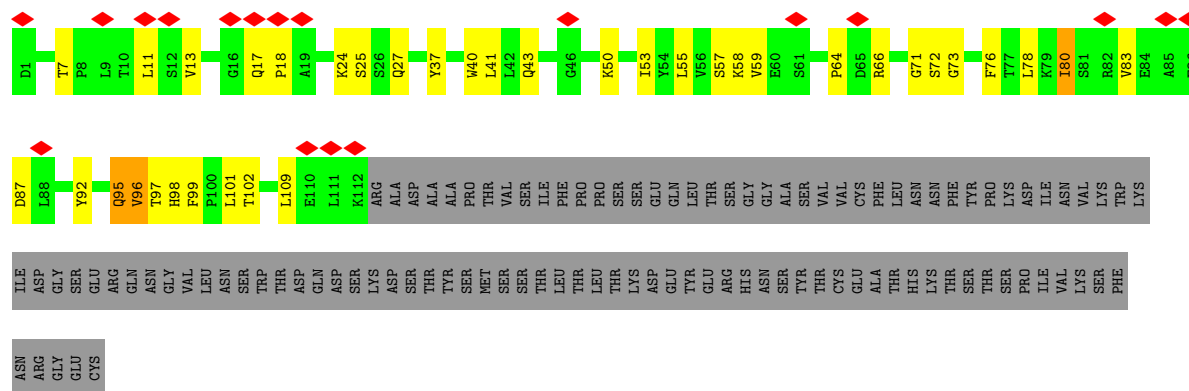
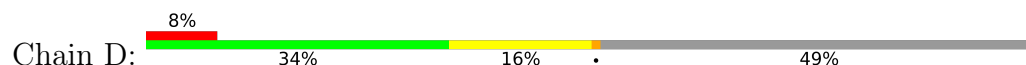




• Molecule 4: anti TCR variable delta 1 Fab light chain Fab 3



• Molecule 4: anti TCR variable delta 1 Fab light chain Fab 3



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	29351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.886	Depositor
Minimum map value	-0.573	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.151	Depositor
Map size ($\text{\AA}$)	402.72, 402.72, 402.72	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.839, 0.839, 0.839	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.14	0/1627	0.31	0/2200
1	E	0.14	0/1627	0.31	0/2200
2	B	0.15	0/1857	0.34	0/2522
2	F	0.15	0/1857	0.34	0/2522
3	C	0.12	0/965	0.28	0/1314
3	J	0.12	0/965	0.28	0/1314
4	D	0.13	0/871	0.33	0/1182
4	K	0.13	0/871	0.34	0/1182
All	All	0.14	0/10640	0.32	0/14436

There are no bond length outliers.

There are no bond angle outliers.

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	1592	0	1595	36	0
1	E	1592	0	1595	38	0
2	B	1808	0	1788	44	0
2	F	1808	0	1788	42	0
3	C	940	0	874	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	940	0	874	28	0
4	D	854	0	873	17	0
4	K	854	0	873	21	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	B	11	0	10	0	0
7	F	11	0	10	0	0
All	All	10522	0	10382	242	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 12.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ILE:HG12	2:F:32:ASN:HD22	1.51	0.76
2:B:31:ILE:HG12	2:B:32:ASN:HD22	1.51	0.74
2:B:17:PRO:HB3	2:B:126:LYS:HB3	1.70	0.74
4:K:40:TRP:HB2	4:K:53:ILE:HB	1.71	0.73
1:A:127:PRO:HB3	1:A:145:PHE:HB3	1.71	0.73
1:E:127:PRO:HB3	1:E:145:PHE:HB3	1.71	0.73
2:F:17:PRO:HB3	2:F:126:LYS:HB3	1.70	0.73
2:F:186:THR:OG1	2:F:195:LYS:NZ	2.23	0.71
4:D:40:TRP:HB2	4:D:53:ILE:HB	1.71	0.71
2:B:186:THR:OG1	2:B:195:LYS:NZ	2.23	0.71
1:E:124:HIS:ND1	1:E:196:ASP:OD2	2.25	0.69
3:C:20:LEU:HD12	3:C:83:LEU:HD11	1.75	0.69
1:A:124:HIS:ND1	1:A:196:ASP:OD2	2.25	0.68
1:E:65:ARG:NH2	1:E:88:ASP:OD2	2.27	0.68
4:K:64:PRO:HB2	4:K:66:ARG:HD3	1.76	0.67
3:J:20:LEU:HD12	3:J:83:LEU:HD11	1.75	0.67
1:A:65:ARG:NH2	1:A:88:ASP:OD2	2.27	0.67
1:E:185:ASP:HB2	1:E:188:SER:HB3	1.75	0.67
1:A:160:ILE:HD13	1:A:182:LYS:HG2	1.77	0.67
3:J:37:VAL:HG22	3:J:47:TRP:HA	1.76	0.67
1:A:185:ASP:HB2	1:A:188:SER:HB3	1.75	0.67
4:D:64:PRO:HB2	4:D:66:ARG:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:LYS:HE3	4:K:50:LYS:HA	1.77	0.66
2:B:139:PHE:HB2	2:B:155:LEU:HB3	1.78	0.66
2:F:139:PHE:HB2	2:F:155:LEU:HB3	1.77	0.66
3:C:37:VAL:HG22	3:C:47:TRP:HA	1.76	0.66
2:F:137:THR:HB	2:F:157:LEU:HD23	1.77	0.66
1:E:160:ILE:HD13	1:E:182:LYS:HG2	1.77	0.65
2:B:137:THR:HB	2:B:157:LEU:HD23	1.77	0.65
4:D:50:LYS:HE3	4:D:50:LYS:HA	1.77	0.65
3:J:99:SER:OG	3:J:100:ASP:N	2.31	0.64
3:C:99:SER:OG	3:C:100:ASP:N	2.31	0.64
4:K:17:GLN:NE2	4:K:18:PRO:O	2.31	0.63
4:D:17:GLN:NE2	4:D:18:PRO:O	2.31	0.63
1:E:168:VAL:HG21	2:F:182:GLN:HB3	1.83	0.61
1:A:168:VAL:HG21	2:B:182:GLN:HB3	1.83	0.61
1:A:138:VAL:HG11	1:A:189:VAL:HG21	1.84	0.59
2:B:51:LEU:HD21	2:B:83:LEU:HD11	1.85	0.59
2:F:172:GLU:HB2	2:F:179:LEU:HD11	1.85	0.58
2:B:164:ASP:N	2:B:164:ASP:OD1	2.33	0.58
2:B:172:GLU:HB2	2:B:179:LEU:HD11	1.85	0.58
3:J:18:VAL:HB	3:J:83:LEU:HD13	1.85	0.58
4:K:18:PRO:HA	4:K:80:ILE:O	2.04	0.58
3:C:18:VAL:HB	3:C:83:LEU:HD13	1.85	0.58
4:D:18:PRO:HA	4:D:80:ILE:O	2.04	0.58
1:E:138:VAL:HG11	1:E:189:VAL:HG21	1.84	0.58
3:J:60:TYR:HE1	3:J:70:LEU:HD13	1.69	0.58
3:C:53:PRO:HB3	3:C:72:VAL:HG21	1.86	0.58
2:F:51:LEU:HD21	2:F:83:LEU:HD11	1.85	0.57
1:E:89:SER:HA	1:E:115:VAL:O	2.05	0.57
3:C:60:TYR:HE1	3:C:70:LEU:HD13	1.69	0.57
4:D:7:THR:OG1	4:D:24:LYS:NZ	2.34	0.57
2:B:140:LEU:HD23	2:B:140:LEU:H	1.70	0.56
1:A:89:SER:HA	1:A:115:VAL:O	2.05	0.56
1:E:5:GLN:OE1	1:E:32:TRP:NE1	2.33	0.56
2:F:140:LEU:HD23	2:F:140:LEU:H	1.70	0.56
3:J:53:PRO:HB3	3:J:72:VAL:HG21	1.86	0.56
1:A:5:GLN:OE1	1:A:32:TRP:NE1	2.33	0.56
3:C:40:ARG:NH1	3:C:91:SER:O	2.40	0.55
3:J:40:ARG:NH1	3:J:91:SER:O	2.40	0.55
4:K:7:THR:OG1	4:K:24:LYS:NZ	2.34	0.55
2:B:182:GLN:OE1	2:B:198:TRP:NE1	2.39	0.55
2:F:182:GLN:OE1	2:F:198:TRP:NE1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:ASP:OD1	2:F:164:ASP:N	2.33	0.54
2:F:172:GLU:O	2:F:211:ARG:HG3	2.09	0.53
2:B:172:GLU:O	2:B:211:ARG:HG3	2.09	0.53
3:C:38:GLN:HG3	3:C:46:GLU:HB2	1.91	0.53
1:A:159:LYS:HG2	1:A:183:TYR:HE1	1.74	0.53
3:J:38:GLN:HG3	3:J:46:GLU:HB2	1.91	0.53
1:A:53:ARG:HH11	2:B:111:TYR:HD1	1.57	0.52
2:F:53:TYR:HD1	2:F:60:ASP:HB3	1.75	0.52
1:E:53:ARG:HH11	2:F:111:TYR:HD1	1.58	0.52
1:E:159:LYS:HG2	1:E:183:TYR:HE1	1.74	0.52
2:B:53:TYR:HD1	2:B:60:ASP:HB3	1.73	0.52
1:A:54:GLN:NE2	1:A:55:GLY:O	2.38	0.51
1:A:120:ARG:NH1	3:C:52:ASP:OD2	2.44	0.51
1:E:120:ARG:NH1	3:J:52:ASP:OD2	2.44	0.51
1:A:71:LYS:HB2	1:A:74:ALA:HB2	1.93	0.51
1:E:188:SER:O	1:E:188:SER:OG	2.29	0.51
2:F:219:ASN:HD21	2:F:225:GLN:HB2	1.76	0.50
2:F:162:PHE:HB3	2:F:163:PRO:HD3	1.93	0.50
2:F:224:ASP:OD1	2:F:224:ASP:N	2.45	0.50
3:J:102:TYR:HD1	3:J:102:TYR:O	1.95	0.50
3:C:13:ARG:O	3:C:16:THR:OG1	2.30	0.50
3:C:24:ALA:HB1	3:C:27:TYR:HE1	1.77	0.50
3:C:102:TYR:HD1	3:C:102:TYR:O	1.95	0.50
1:E:71:LYS:HB2	1:E:74:ALA:HB2	1.93	0.50
4:K:25:SER:OG	4:K:27:GLN:O	2.30	0.50
1:E:30:THR:OG1	1:E:31:SER:N	2.45	0.50
2:F:78:ARG:HH11	2:F:78:ARG:HG3	1.77	0.50
2:B:201:VAL:HG11	2:B:210:HIS:CE1	2.47	0.50
2:B:219:ASN:HD21	2:B:225:GLN:HB2	1.77	0.50
1:A:41:LYS:HE2	1:A:51:LEU:HD21	1.94	0.50
2:B:224:ASP:OD1	2:B:224:ASP:N	2.45	0.50
2:F:201:VAL:HG11	2:F:210:HIS:CE1	2.46	0.49
3:J:24:ALA:HB1	3:J:27:TYR:HE1	1.77	0.49
1:E:41:LYS:HE2	1:E:51:LEU:HD21	1.94	0.49
2:B:78:ARG:HG3	2:B:78:ARG:HH11	1.77	0.49
2:B:162:PHE:HB3	2:B:163:PRO:HD3	1.93	0.49
1:E:54:GLN:NE2	1:E:55:GLY:O	2.38	0.49
1:A:158:LYS:HA	1:A:158:LYS:HE2	1.95	0.48
1:E:57:ASP:OD1	1:E:57:ASP:N	2.32	0.48
3:J:13:ARG:O	3:J:16:THR:OG1	2.30	0.48
1:A:30:THR:OG1	1:A:31:SER:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:ASP:OD1	2:F:207:ASP:N	2.42	0.48
3:C:47:TRP:O	3:C:61:ASN:ND2	2.41	0.47
1:E:158:LYS:HE2	1:E:158:LYS:HA	1.95	0.47
1:A:191:CYS:HB2	1:A:202:SER:HB3	1.97	0.47
4:D:55:LEU:O	4:D:57:SER:N	2.43	0.47
2:B:163:PRO:HD2	2:B:216:HIS:CE1	2.50	0.47
2:B:199:LEU:HD22	2:B:201:VAL:HG13	1.96	0.47
4:D:72:SER:OG	4:D:73:GLY:N	2.47	0.47
1:A:127:PRO:HB2	1:A:142:VAL:HG13	1.97	0.47
1:E:127:PRO:HB2	1:E:142:VAL:HG13	1.97	0.47
2:F:163:PRO:HD2	2:F:216:HIS:CE1	2.50	0.47
2:F:201:VAL:HB	2:F:205:SER:HB2	1.98	0.46
4:K:55:LEU:O	4:K:57:SER:N	2.43	0.46
1:A:170:SER:OG	1:A:172:SER:OG	2.31	0.46
1:E:170:SER:OG	1:E:172:SER:OG	2.31	0.46
1:E:191:CYS:HB2	1:E:202:SER:HB3	1.97	0.46
2:B:201:VAL:HB	2:B:205:SER:HB2	1.98	0.46
2:F:199:LEU:HD22	2:F:201:VAL:HG13	1.96	0.46
2:B:207:ASP:OD1	2:B:207:ASP:N	2.42	0.46
2:F:174:LYS:HB2	2:F:174:LYS:NZ	2.30	0.46
1:E:43:LEU:HD11	1:E:49:ILE:HD11	1.98	0.46
2:F:124:THR:HG21	2:F:162:PHE:HE2	1.81	0.46
2:F:201:VAL:HG11	2:F:210:HIS:HE1	1.81	0.46
4:K:72:SER:OG	4:K:73:GLY:N	2.47	0.46
2:F:78:ARG:HG3	2:F:78:ARG:NH1	2.31	0.46
1:E:95:ALA:HB2	1:E:109:PHE:CE2	2.52	0.45
2:F:188:LYS:HA	2:F:193:TYR:HD1	1.82	0.45
1:A:95:ALA:HB2	1:A:109:PHE:CE2	2.52	0.45
4:D:13:VAL:HG11	4:D:83:VAL:HG21	1.98	0.45
2:F:168:ILE:HD12	2:F:195:LYS:HD3	1.99	0.45
3:J:47:TRP:O	3:J:61:ASN:ND2	2.41	0.45
2:B:201:VAL:HG11	2:B:210:HIS:HE1	1.81	0.45
4:D:25:SER:OG	4:D:27:GLN:O	2.30	0.45
2:B:78:ARG:HG3	2:B:78:ARG:NH1	2.31	0.45
4:K:13:VAL:HG11	4:K:83:VAL:HG21	1.98	0.45
2:F:211:ARG:HA	2:F:227:ILE:O	2.17	0.45
1:A:43:LEU:HD11	1:A:49:ILE:HD11	1.98	0.45
3:C:23:LYS:HA	3:C:23:LYS:HD2	1.81	0.45
1:E:93:PHE:HB3	1:E:109:PHE:HD2	1.82	0.45
1:E:71:LYS:HD2	1:E:74:ALA:HB2	1.98	0.45
1:A:162:GLU:OE2	1:A:162:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LYS:HA	2:B:193:TYR:HD1	1.82	0.44
3:C:106:TYR:CE1	4:D:96:VAL:HG11	2.52	0.44
1:A:71:LYS:HD2	1:A:74:ALA:HB2	1.98	0.44
2:B:211:ARG:HA	2:B:227:ILE:O	2.17	0.44
1:E:162:GLU:OE2	1:E:162:GLU:HA	2.17	0.44
3:J:106:TYR:CE1	4:K:96:VAL:HG11	2.52	0.44
2:B:124:THR:HG21	2:B:162:PHE:HE2	1.81	0.44
2:F:164:ASP:HB3	2:F:193:TYR:CD2	2.53	0.44
2:F:187:MET:HE3	2:F:187:MET:HB2	1.86	0.44
2:F:22:ALA:HB2	2:F:88:LEU:HD11	1.99	0.44
4:K:71:GLY:HA3	4:K:76:PHE:HA	2.00	0.44
1:A:93:PHE:HB3	1:A:109:PHE:HD2	1.82	0.44
3:C:40:ARG:HD2	3:C:92:ALA:HB2	2.00	0.44
2:B:191:ASP:OD1	2:B:191:ASP:N	2.49	0.44
4:D:87:ASP:OD1	4:D:87:ASP:N	2.51	0.44
2:F:153:THR:HG23	2:F:200:THR:HG22	2.00	0.43
2:F:189:THR:HG23	2:F:192:THR:HG23	2.00	0.43
3:J:23:LYS:HD2	3:J:23:LYS:HA	1.81	0.43
4:K:7:THR:HG1	4:K:24:LYS:HZ3	1.59	0.43
3:C:60:TYR:HB2	3:C:65:LYS:HE2	2.00	0.43
2:B:168:ILE:HD12	2:B:195:LYS:HD3	1.99	0.43
1:E:66:TYR:HB3	1:E:79:LEU:HD11	2.01	0.43
2:F:107:LYS:O	2:F:109:HIS:N	2.51	0.43
3:J:23:LYS:HE3	3:J:76:SER:O	2.18	0.43
2:B:153:THR:HG23	2:B:200:THR:HG22	2.01	0.43
1:A:5:GLN:HB3	1:A:96:LEU:HD23	2.01	0.43
1:A:201:HIS:HB2	1:A:204:ASP:OD1	2.19	0.43
2:B:107:LYS:O	2:B:109:HIS:N	2.51	0.43
1:A:66:TYR:HB3	1:A:79:LEU:HD11	2.01	0.43
2:B:164:ASP:HB3	2:B:193:TYR:CD2	2.53	0.43
3:C:101:ASP:OD2	3:C:101:ASP:C	2.62	0.43
3:J:60:TYR:HH	3:J:70:LEU:H	1.63	0.43
1:A:123:PRO:HD3	3:C:102:TYR:CE2	2.54	0.43
2:B:174:LYS:HZ3	2:B:174:LYS:HB2	1.83	0.43
1:E:5:GLN:HB3	1:E:96:LEU:HD23	2.01	0.43
3:J:60:TYR:HB2	3:J:65:LYS:HE2	2.00	0.43
1:A:30:THR:HG21	1:A:35:TYR:CE2	2.54	0.43
3:J:39:GLN:NE2	4:K:43:GLN:OE1	2.47	0.43
3:J:40:ARG:HD2	3:J:92:ALA:HB2	2.00	0.43
2:B:22:ALA:HB2	2:B:88:LEU:HD11	2.00	0.43
1:E:201:HIS:HB2	1:E:204:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HB3	3:C:102:TYR:OH	2.19	0.42
2:B:189:THR:HG23	2:B:192:THR:HG23	2.00	0.42
2:B:145:GLU:OE1	2:B:153:THR:OG1	2.32	0.42
4:D:71:GLY:HA3	4:D:76:PHE:HA	2.01	0.42
3:C:23:LYS:HE3	3:C:76:SER:O	2.18	0.42
3:C:40:ARG:HD2	3:C:40:ARG:HA	1.92	0.42
1:E:123:PRO:HB3	3:J:102:TYR:OH	2.19	0.42
1:E:123:PRO:HD3	3:J:102:TYR:CE2	2.54	0.42
2:F:107:LYS:O	2:F:107:LYS:NZ	2.53	0.42
2:B:28:LEU:HD13	2:B:100:THR:HG22	2.02	0.42
3:J:62:GLN:H	3:J:62:GLN:HG3	1.59	0.42
2:B:107:LYS:O	2:B:107:LYS:NZ	2.53	0.42
3:C:60:TYR:HH	3:C:70:LEU:H	1.63	0.42
3:J:24:ALA:HB1	3:J:27:TYR:CE1	2.55	0.42
4:K:87:ASP:OD1	4:K:87:ASP:N	2.51	0.42
4:D:43:GLN:NE2	4:D:92:TYR:OH	2.53	0.42
1:E:30:THR:HG21	1:E:35:TYR:CE2	2.54	0.41
2:F:24:ILE:HD11	2:F:121:LEU:HD13	2.02	0.41
3:J:101:ASP:OD2	3:J:101:ASP:C	2.62	0.41
4:K:43:GLN:NE2	4:K:92:TYR:OH	2.52	0.41
1:A:86:LEU:HD11	1:A:169:ILE:HG21	2.02	0.41
3:C:39:GLN:O	3:C:92:ALA:HB1	2.21	0.41
3:J:39:GLN:O	3:J:92:ALA:HB1	2.21	0.41
2:F:59:LYS:HE2	2:F:59:LYS:HB3	1.85	0.41
1:A:122:GLN:HB2	1:A:146:TYR:CD1	2.56	0.41
2:B:21:SER:HA	2:B:85:LEU:O	2.21	0.41
4:D:11:LEU:HB3	4:D:109:LEU:HD12	2.03	0.41
2:B:24:ILE:HD11	2:B:121:LEU:HD13	2.02	0.41
1:E:164:ASP:OD1	1:E:164:ASP:N	2.54	0.41
1:A:164:ASP:OD1	1:A:164:ASP:N	2.54	0.41
1:E:122:GLN:HB2	1:E:146:TYR:CD1	2.56	0.41
1:E:145:PHE:O	1:E:175:TYR:HB2	2.21	0.41
2:F:126:LYS:HA	2:F:126:LYS:HD2	1.81	0.41
4:K:95:GLN:HE21	4:K:95:GLN:HB3	1.56	0.41
1:A:145:PHE:O	1:A:175:TYR:HB2	2.21	0.41
3:C:36:TRP:O	3:C:48:ILE:HB	2.21	0.41
4:D:95:GLN:OE1	4:D:98:HIS:HB2	2.21	0.41
3:J:70:LEU:HD12	3:J:81:MET:HG3	2.03	0.41
4:K:95:GLN:OE1	4:K:98:HIS:HB2	2.21	0.41
1:A:160:ILE:HD12	1:A:182:LYS:O	2.20	0.41
2:B:187:MET:HE3	2:B:187:MET:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LEU:HD12	3:C:81:MET:HG3	2.03	0.41
4:K:37:TYR:HB2	4:K:97:THR:HG22	2.03	0.40
3:C:82:GLN:OE1	3:C:82:GLN:HA	2.21	0.40
1:E:123:PRO:HG2	4:K:99:PHE:CG	2.56	0.40
2:F:132:VAL:HG23	2:F:218:ASN:HD22	1.86	0.40
3:J:36:TRP:O	3:J:48:ILE:HB	2.21	0.40
2:F:28:LEU:HD13	2:F:100:THR:HG22	2.02	0.40
3:C:5:GLN:CD	3:C:23:LYS:HB3	2.47	0.40
4:K:11:LEU:HB3	4:K:109:LEU:HD12	2.03	0.40
2:B:174:LYS:HB2	2:B:174:LYS:NZ	2.36	0.40
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.55	0.40
1:E:160:ILE:HD12	1:E:182:LYS:O	2.21	0.40
2:B:74:HIS:HB2	2:B:84:ILE:HD11	2.04	0.40
3:C:5:GLN:OE1	3:C:23:LYS:HB3	2.22	0.40
4:D:37:TYR:HB2	4:D:97:THR:HG22	2.03	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	
1	A	200/280 (71%)	187 (94%)	13 (6%)	0	100	100
1	E	200/280 (71%)	187 (94%)	13 (6%)	0	100	100
2	B	220/294 (75%)	206 (94%)	14 (6%)	0	100	100
2	F	220/294 (75%)	206 (94%)	14 (6%)	0	100	100
3	C	117/224 (52%)	116 (99%)	1 (1%)	0	100	100
3	J	117/224 (52%)	116 (99%)	1 (1%)	0	100	100
4	D	110/219 (50%)	104 (94%)	6 (6%)	0	100	100
4	K	110/219 (50%)	104 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1294/2034 (64%)	1226 (95%)	68 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/248 (73%)	173 (96%)	7 (4%)	28	56
1	E	180/248 (73%)	170 (94%)	10 (6%)	19	47
2	B	203/269 (76%)	191 (94%)	12 (6%)	18	45
2	F	203/269 (76%)	191 (94%)	12 (6%)	18	45
3	C	103/194 (53%)	96 (93%)	7 (7%)	14	41
3	J	103/194 (53%)	97 (94%)	6 (6%)	18	45
4	D	99/196 (50%)	89 (90%)	10 (10%)	7	29
4	K	99/196 (50%)	89 (90%)	10 (10%)	7	29
All	All	1170/1814 (64%)	1096 (94%)	74 (6%)	18	44

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	THR
1	E	30	THR
1	E	57	ASP
1	E	68	VAL
1	E	86	LEU
1	E	102	LEU
1	E	104	THR
1	E	121	SER
1	E	126	LYS
1	E	153	ASN
2	F	30	VAL
2	F	57	ASN

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Mol	Chain	Res	Type
2	F	75	THR
2	F	107	LYS
2	F	117	SER
2	F	124	THR
2	F	128	LEU
2	F	148	LEU
2	F	164	ASP
2	F	187	MET
2	F	189	THR
2	F	197	SER
3	J	18	VAL
3	J	54	SER
3	J	103	ASP
3	J	107	PHE
3	J	116	THR
3	J	117	LEU
4	K	41	LEU
4	K	58	LYS
4	K	59	VAL
4	K	78	LEU
4	K	80	ILE
4	K	95	GLN
4	K	96	VAL
4	K	99	PHE
4	K	101	LEU
4	K	102	THR
1	A	30	THR
1	A	57	ASP
1	A	68	VAL
1	A	86	LEU
1	A	102	LEU
1	A	121	SER
1	A	153	ASN
2	B	30	VAL
2	B	57	ASN
2	B	75	THR
2	B	107	LYS
2	B	117	SER
2	B	124	THR
2	B	128	LEU
2	B	148	LEU
2	B	164	ASP

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Mol	Chain	Res	Type
2	B	187	MET
2	B	189	THR
2	B	197	SER
3	C	18	VAL
3	C	54	SER
3	C	93	VAL
3	C	103	ASP
3	C	107	PHE
3	C	116	THR
3	C	117	LEU
4	D	41	LEU
4	D	58	LYS
4	D	59	VAL
4	D	78	LEU
4	D	80	ILE
4	D	95	GLN
4	D	96	VAL
4	D	99	PHE
4	D	101	LEU
4	D	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	201	HIS
2	F	32	ASN
2	F	109	HIS
2	F	210	HIS
2	F	218	ASN
2	F	219	ASN
3	J	39	GLN
3	J	43	GLN
4	K	31	HIS
4	K	43	GLN
4	K	98	HIS
1	A	201	HIS
2	B	32	ASN
2	B	219	ASN
3	C	39	GLN
3	C	43	GLN
4	D	27	GLN
4	D	31	HIS

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Mol	Chain	Res	Type
4	D	43	GLN
4	D	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	1,5	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
5	NAG	G	2	5	14,14,15	0.72	0	17,19,21	0.84	0
5	NAG	H	1	1,5	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
5	NAG	H	2	5	14,14,15	0.72	0	17,19,21	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	G	1	NAG	C2-N2-C7	2.25	125.91	122.90
5	H	1	NAG	C2-N2-C7	2.25	125.91	122.90

There are no chirality outliers.

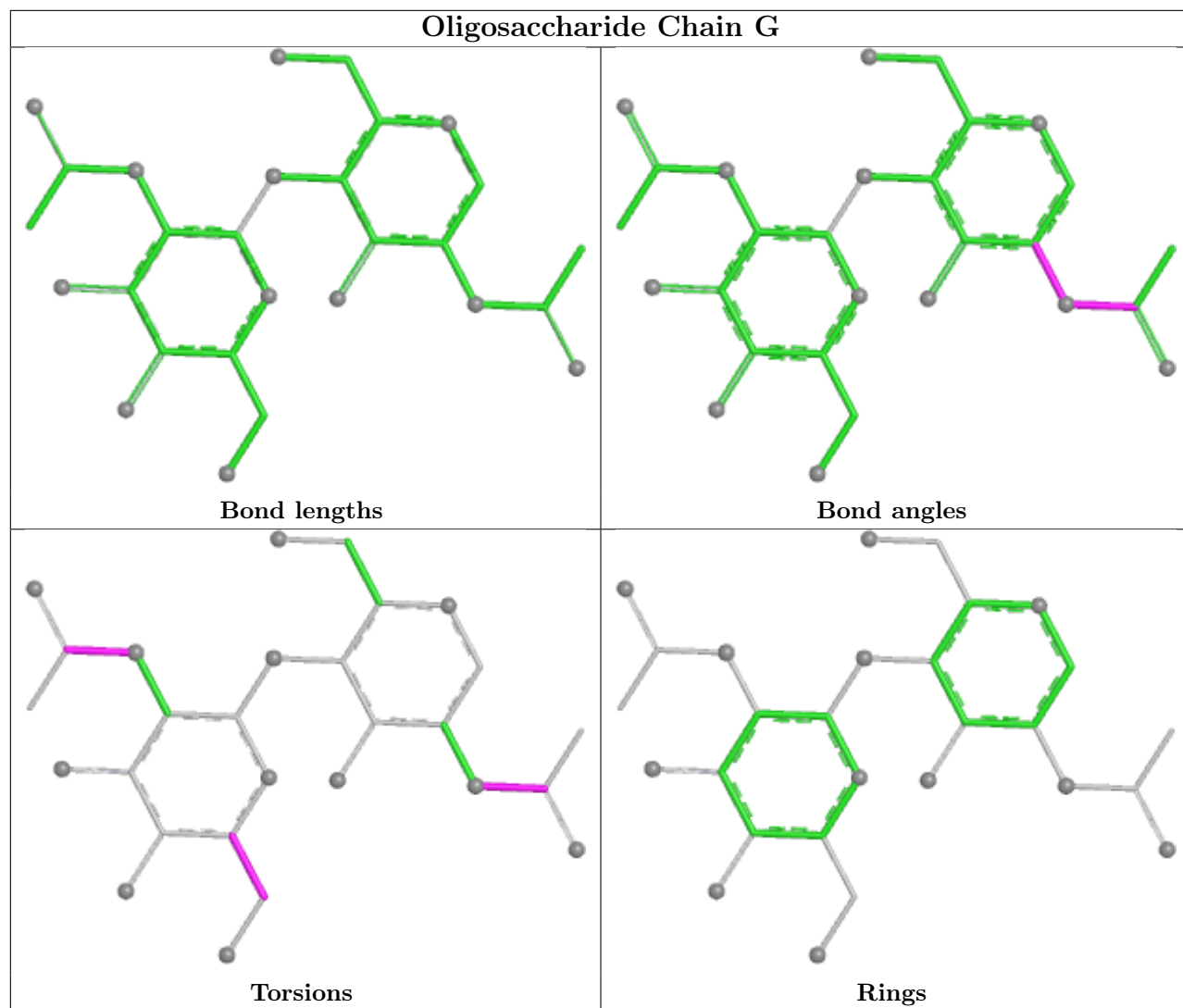
All (10) torsion outliers are listed below:

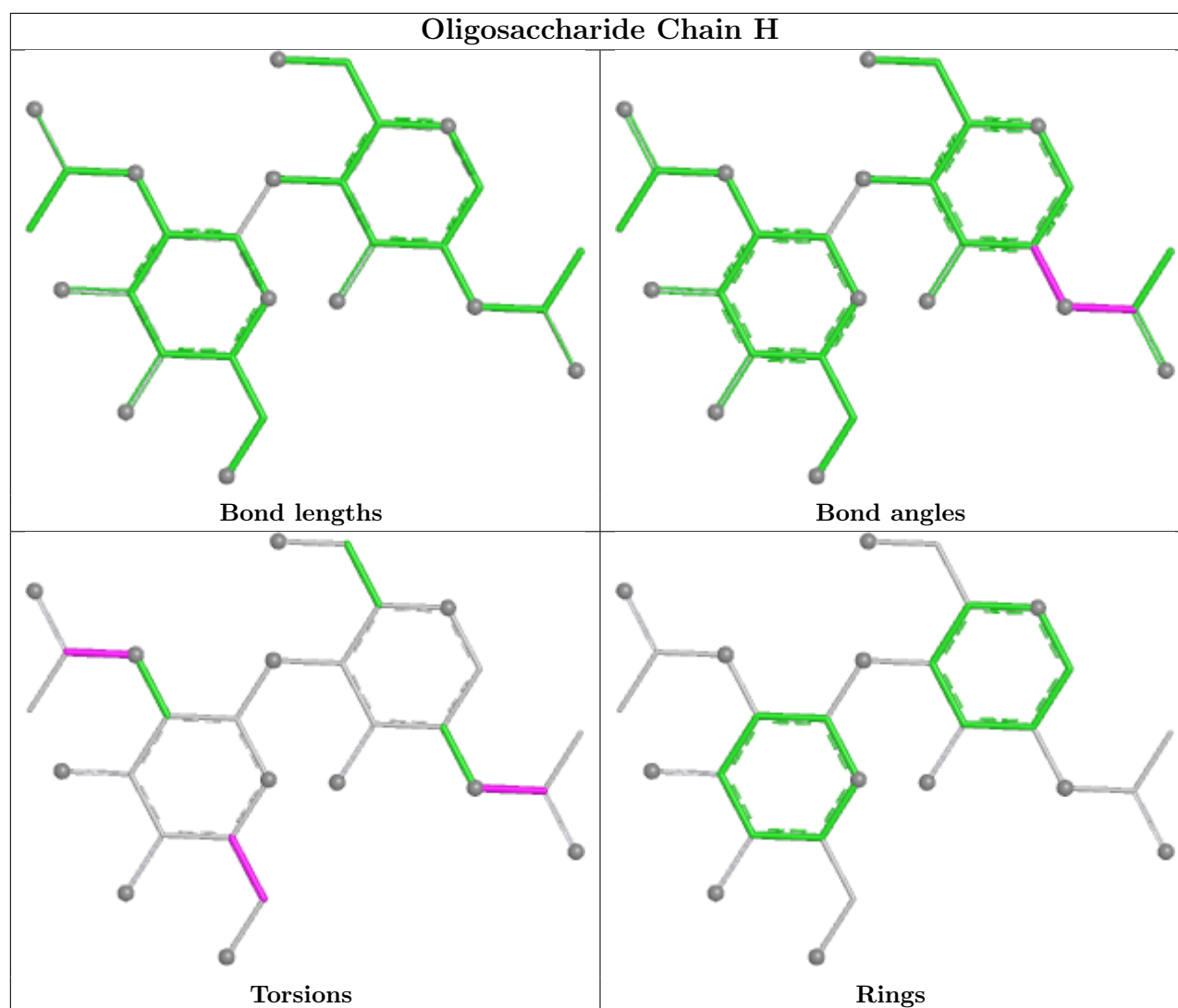
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	E	301	1	14,14,15	0.69	0	17,19,21	0.84	1 (5%)
7	BMA	F	301	-	11,11,12	0.87	0	15,15,17	2.09	4 (26%)
6	NAG	F	302	2	14,14,15	0.71	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	301	1	14,14,15	0.69	0	17,19,21	0.84	1 (5%)
7	BMA	B	301	-	11,11,12	0.88	0	15,15,17	2.09	4 (26%)
6	NAG	B	302	2	14,14,15	0.71	0	17,19,21	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	301	1	-	1/6/23/26	0/1/1/1
7	BMA	F	301	-	-	0/2/19/22	0/1/1/1
6	NAG	F	302	2	-	1/6/23/26	0/1/1/1
6	NAG	A	301	1	-	1/6/23/26	0/1/1/1
7	BMA	B	301	-	-	0/2/19/22	0/1/1/1
6	NAG	B	302	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	301	BMA	C1-O5-C5	6.03	120.26	112.19
7	F	301	BMA	C1-O5-C5	6.03	120.26	112.19
7	F	301	BMA	C3-C4-C5	2.74	115.20	110.23
7	B	301	BMA	C3-C4-C5	2.74	115.20	110.23
7	B	301	BMA	C2-C3-C4	2.41	115.09	110.86
7	F	301	BMA	C2-C3-C4	2.40	115.09	110.86
6	E	301	NAG	O5-C1-C2	-2.20	107.89	111.29
6	A	301	NAG	O5-C1-C2	-2.19	107.89	111.29
7	B	301	BMA	O4-C4-C3	-2.07	105.49	110.38
7	F	301	BMA	O4-C4-C3	-2.07	105.49	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	301	NAG	O5-C5-C6-O6
6	A	301	NAG	O5-C5-C6-O6
6	F	302	NAG	O5-C5-C6-O6
6	B	302	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

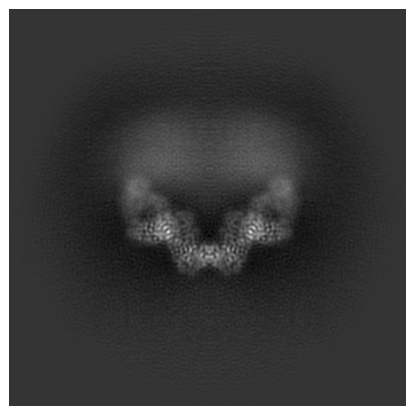
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45814. These allow visual inspection of the internal detail of the map and identification of artifacts.

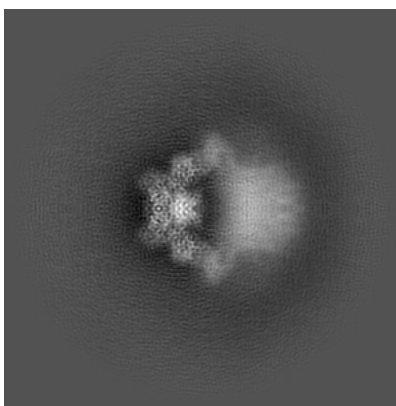
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

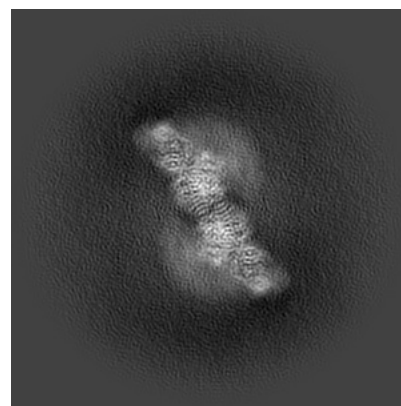
6.1.1 Primary map



X

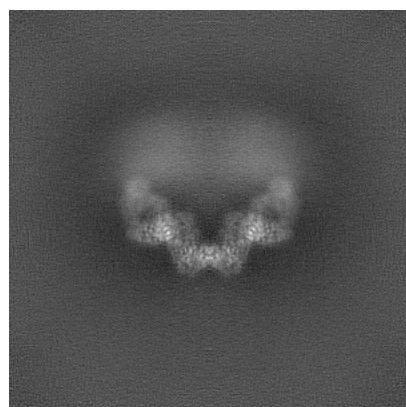


Y

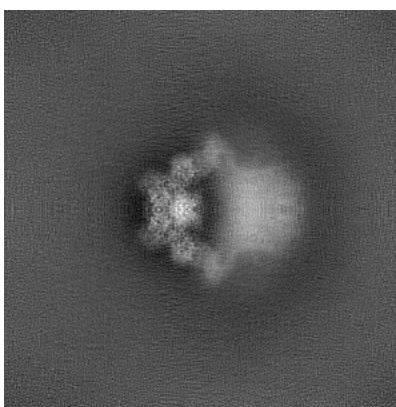


Z

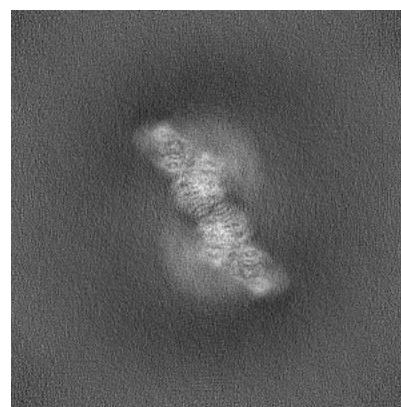
6.1.2 Raw map



X



Y

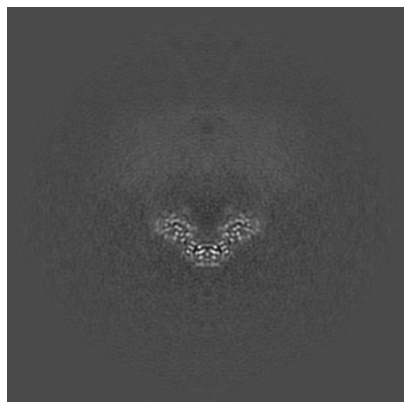


Z

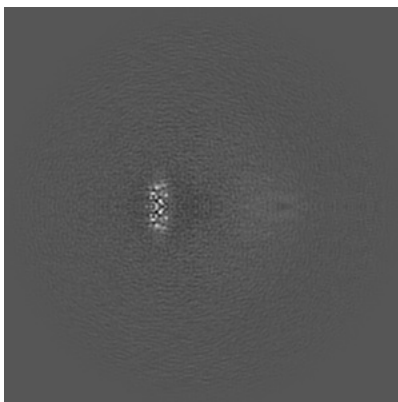
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

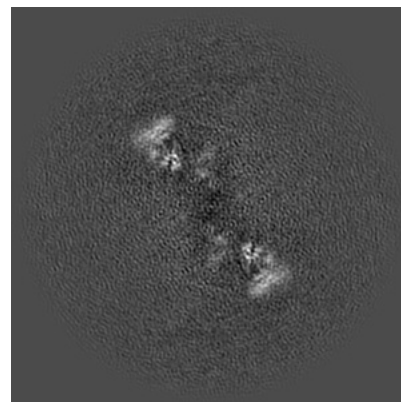
6.2.1 Primary map



X Index: 240

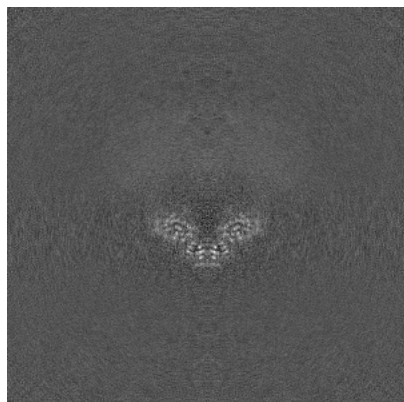


Y Index: 240

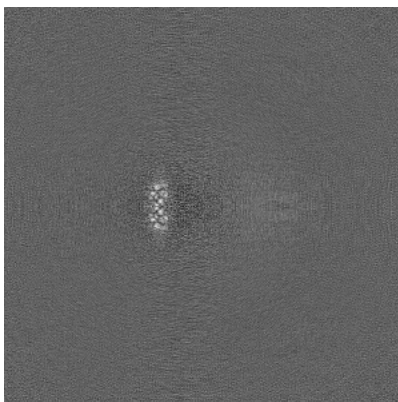


Z Index: 240

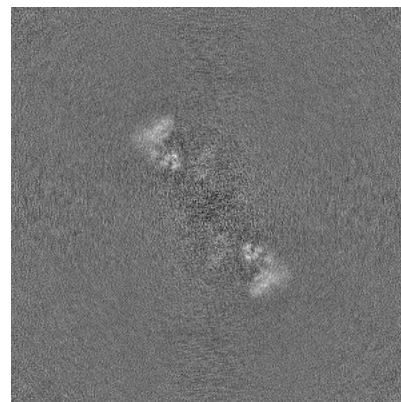
6.2.2 Raw map



X Index: 240



Y Index: 240

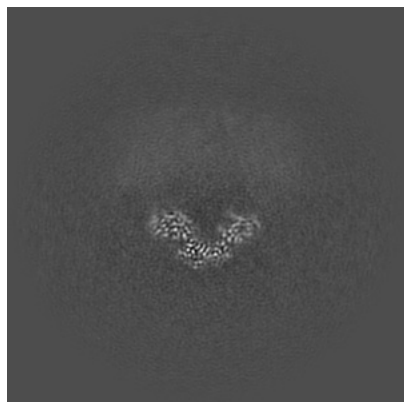


Z Index: 240

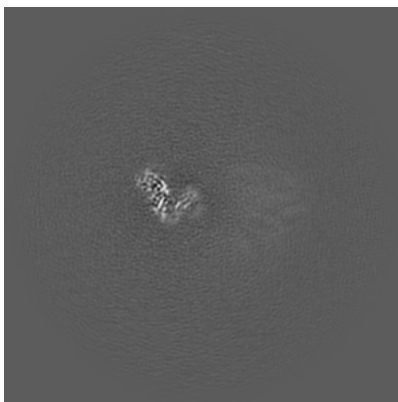
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

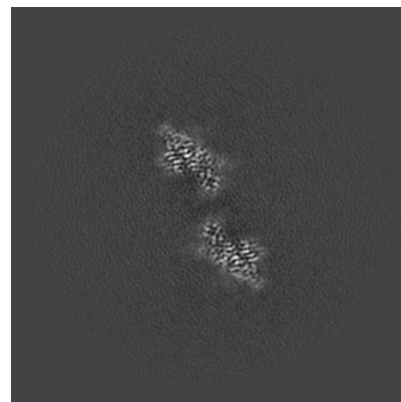
6.3.1 Primary map



X Index: 245

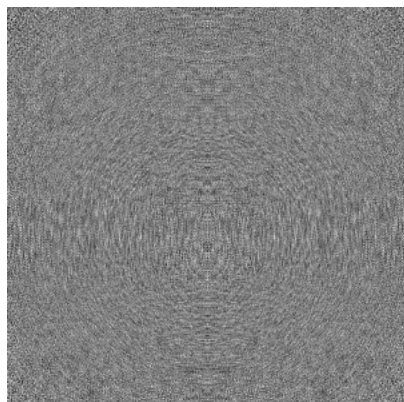


Y Index: 217

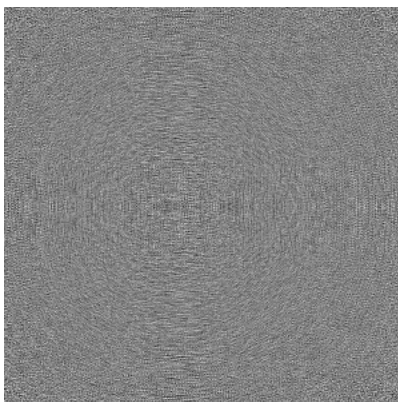


Z Index: 210

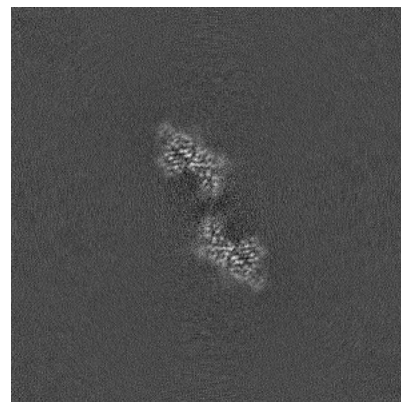
6.3.2 Raw map



X Index: 0



Y Index: 0

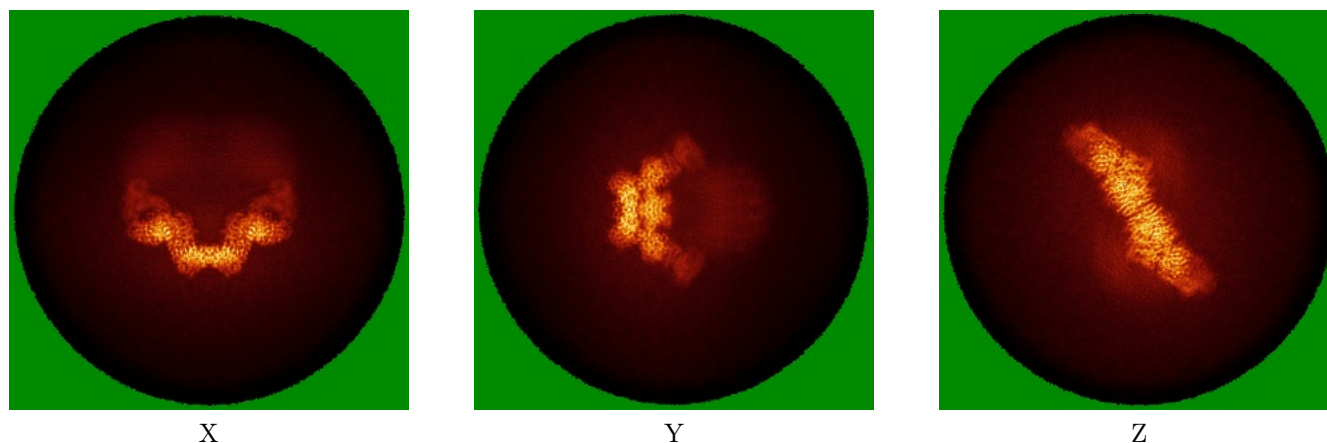


Z Index: 211

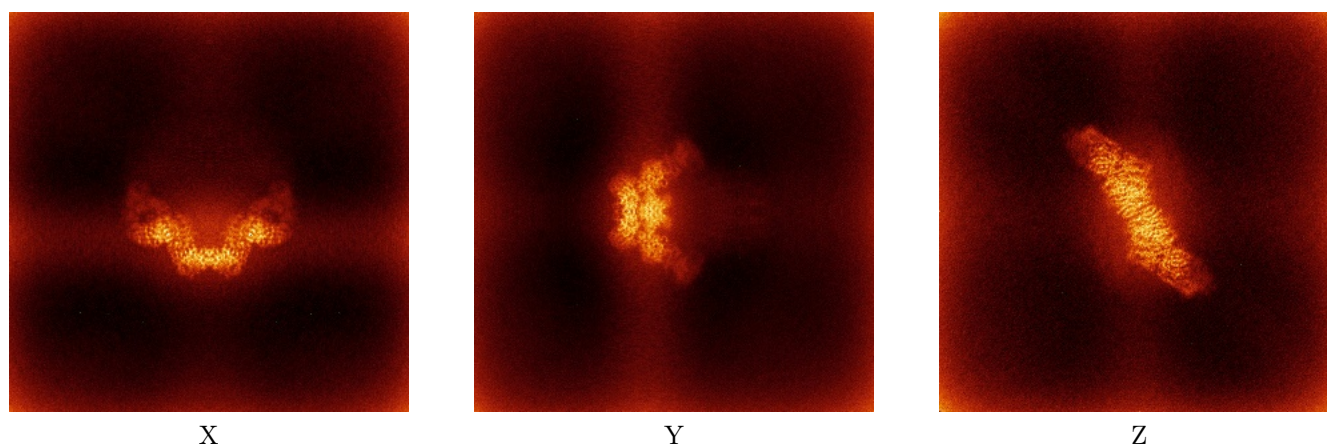
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

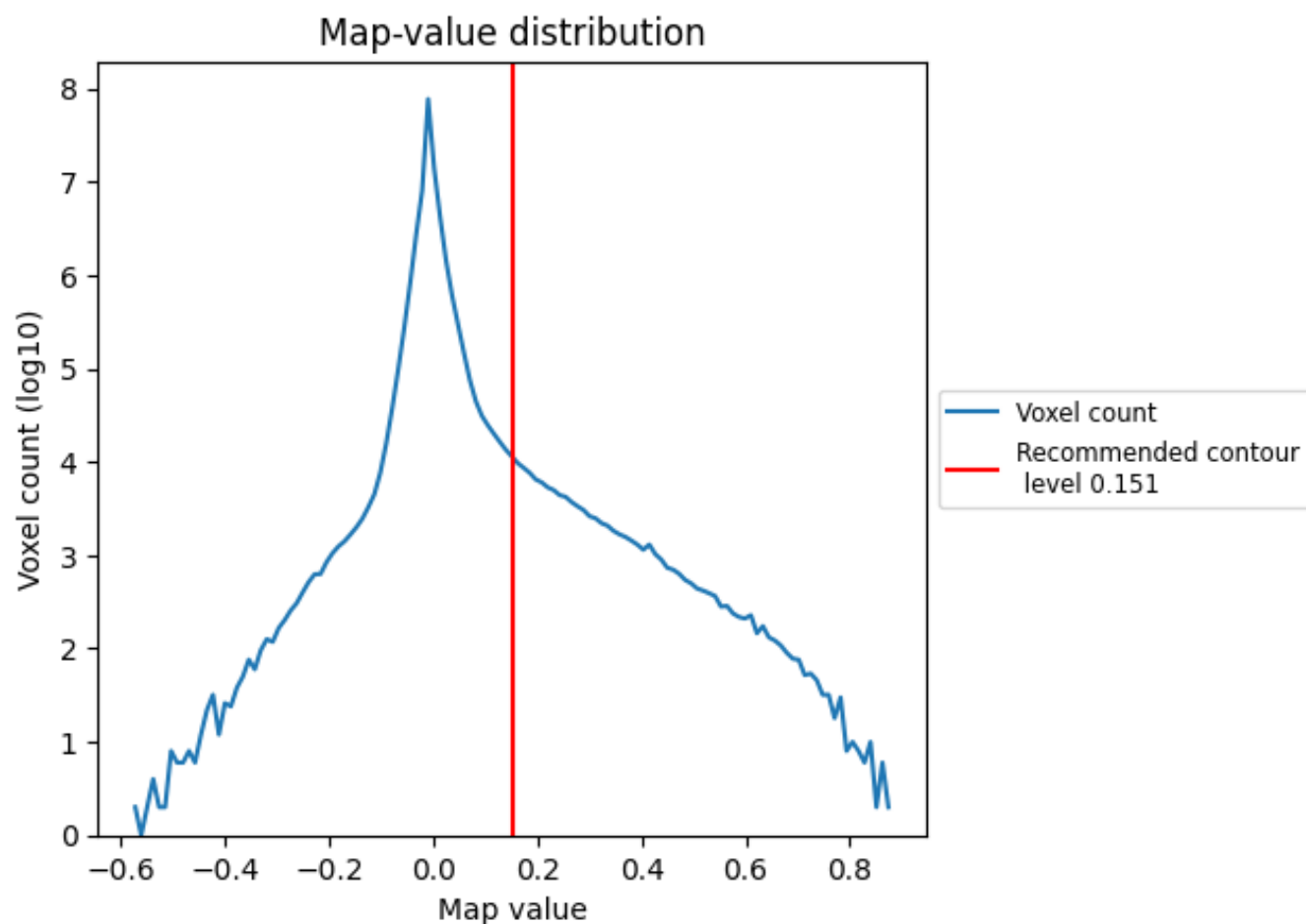
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

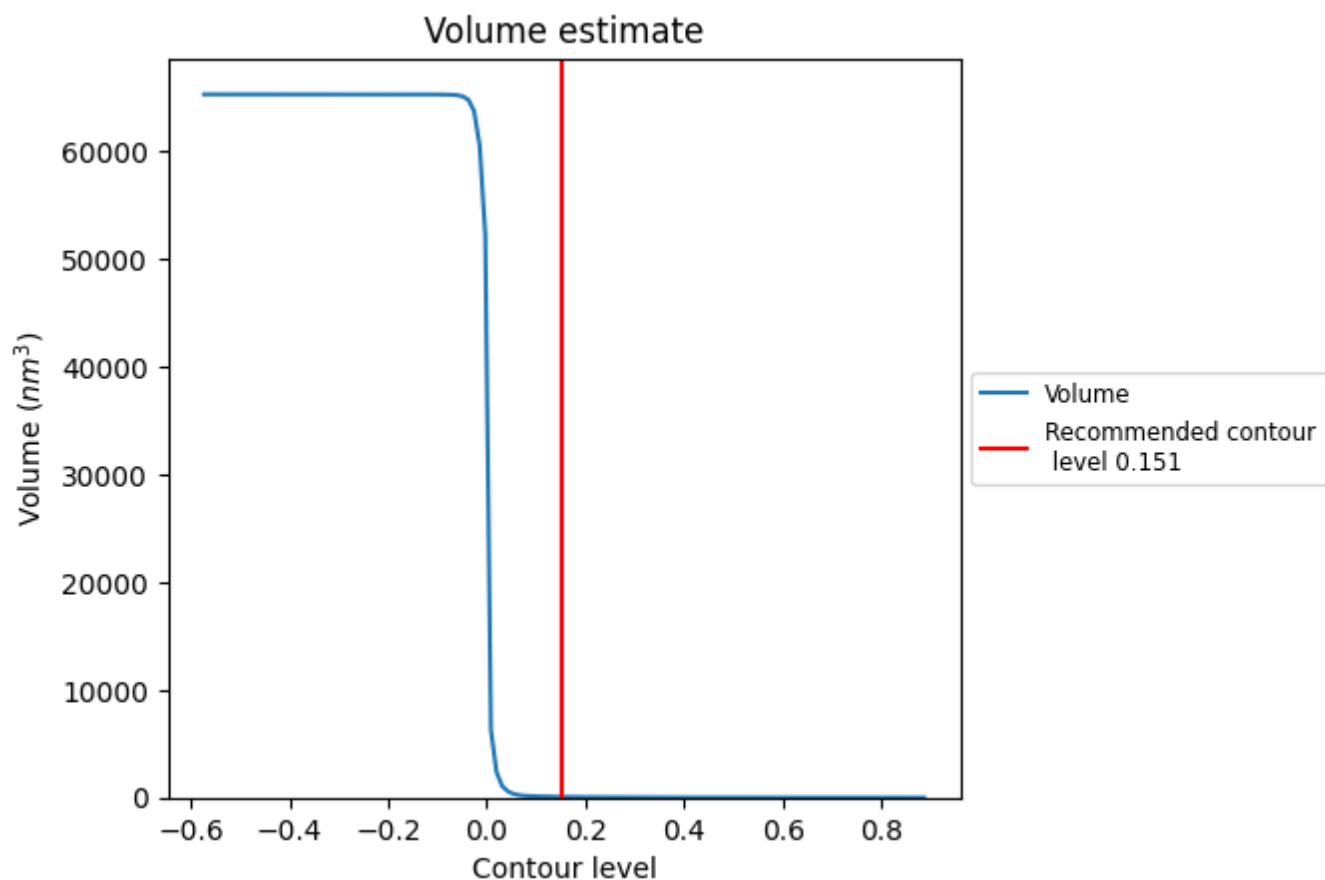
This section contains the results of statistical analysis of the map.

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.

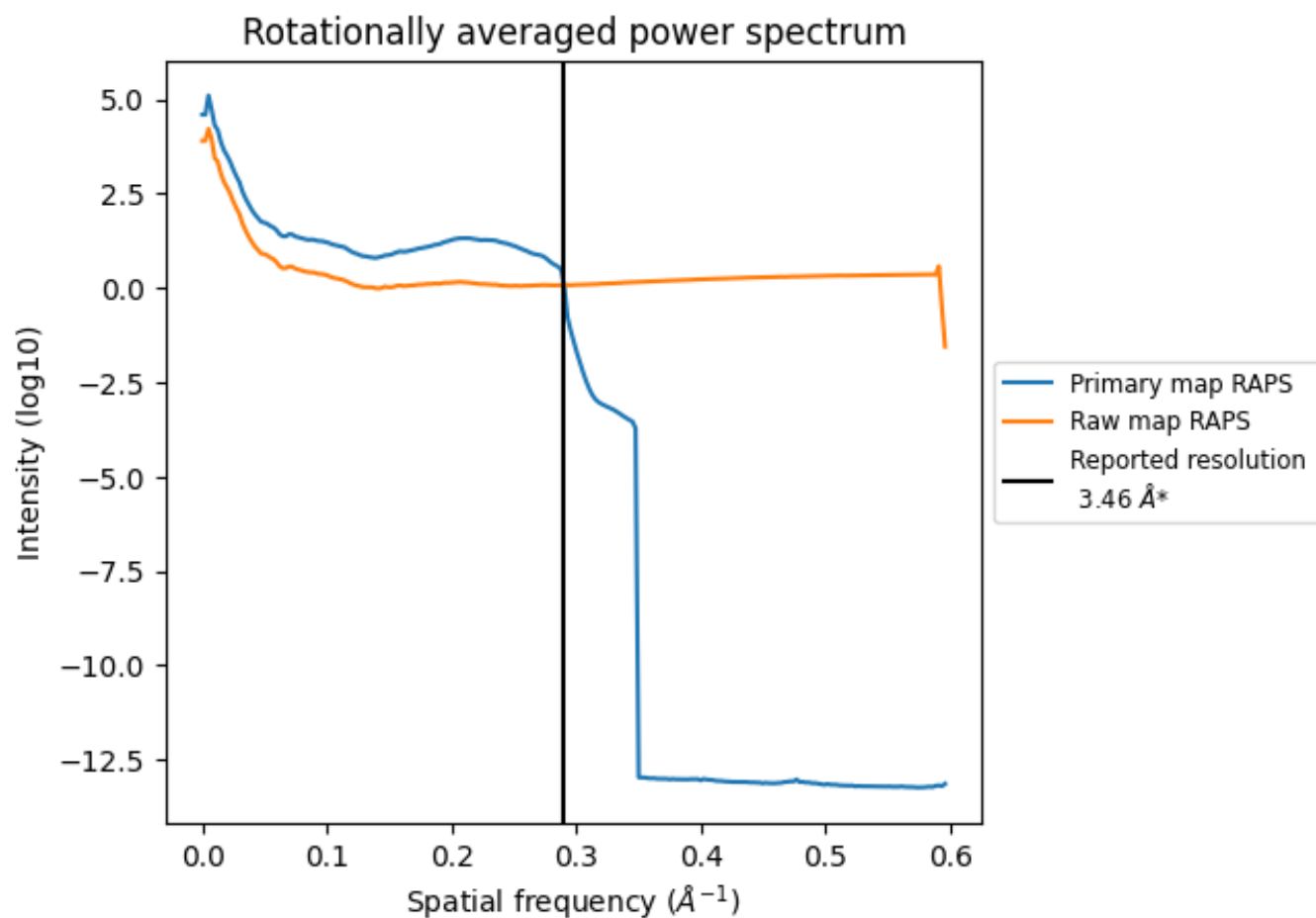
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 57 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 ⓘ

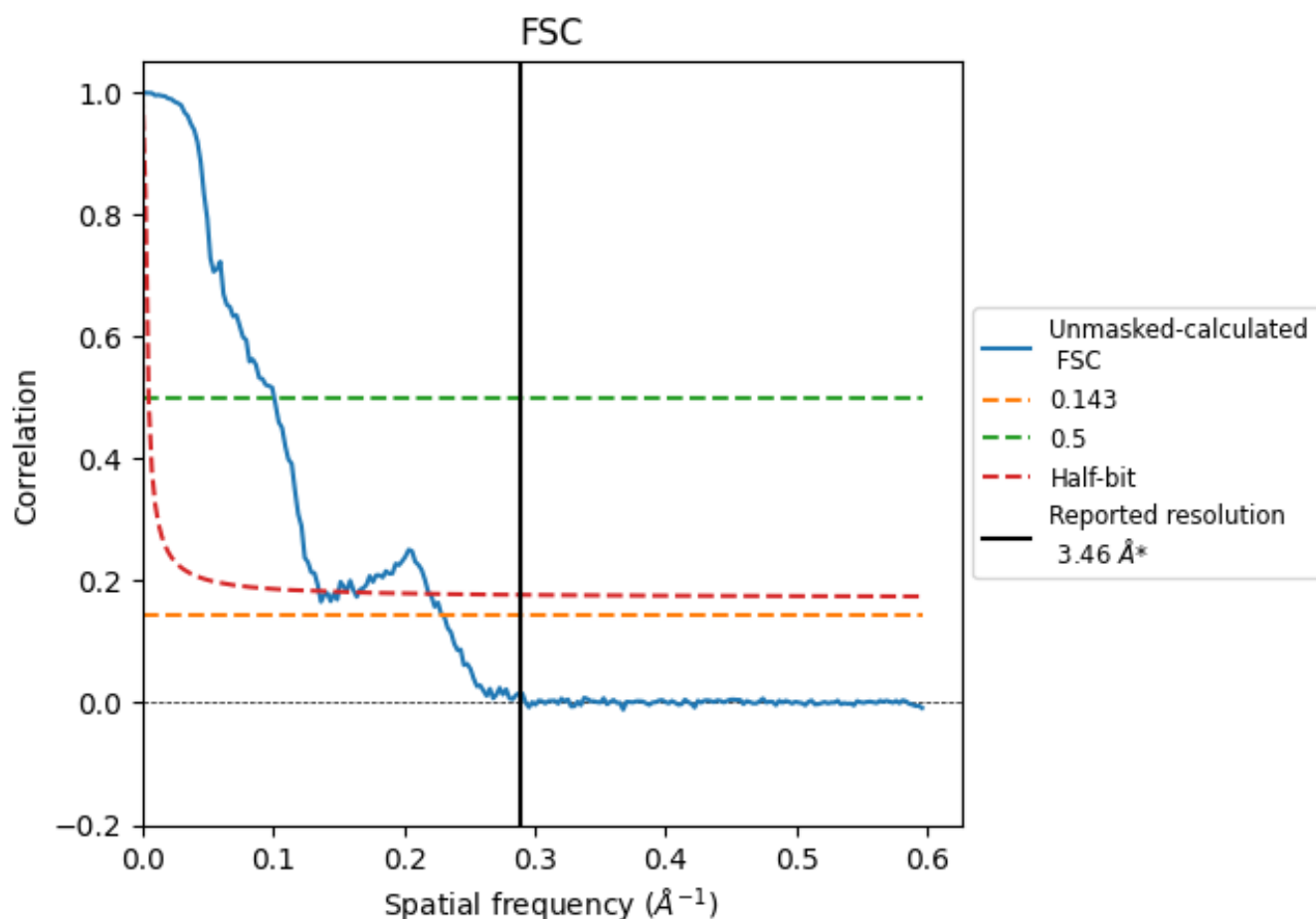


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

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 0.289 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	9.92	7.41

*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 4.36 differs from the reported value 3.46 by more than 10 %

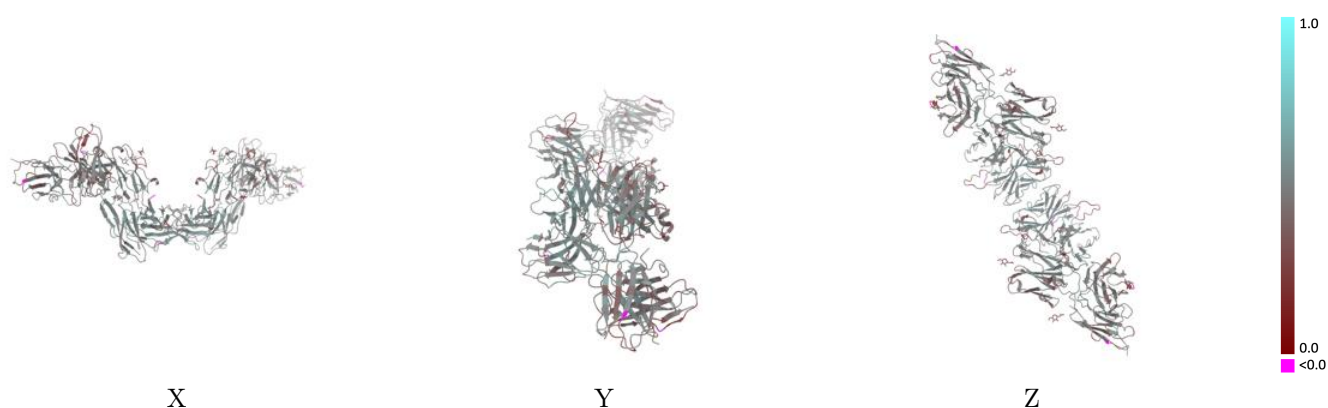
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45814 and PDB model 9CQL. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

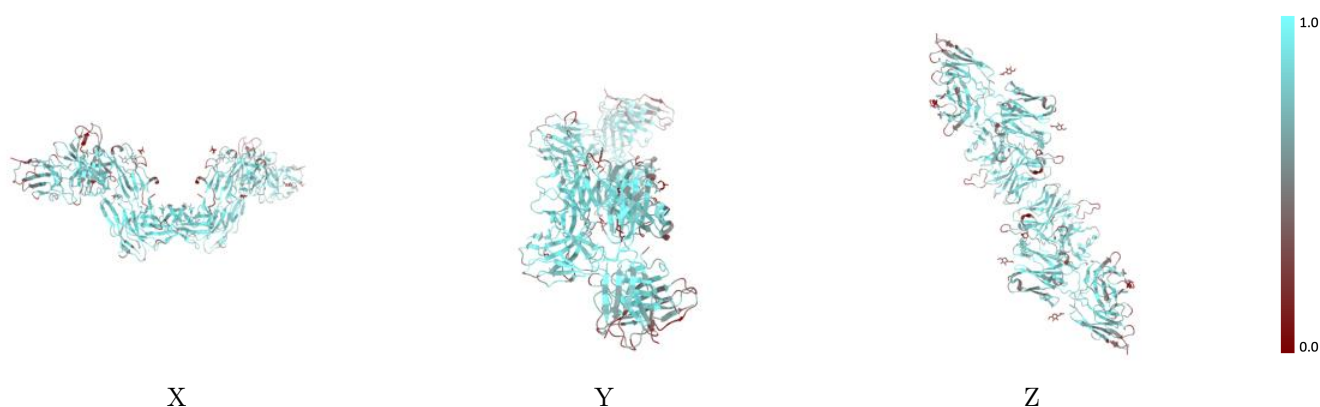
This section was not generated.

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



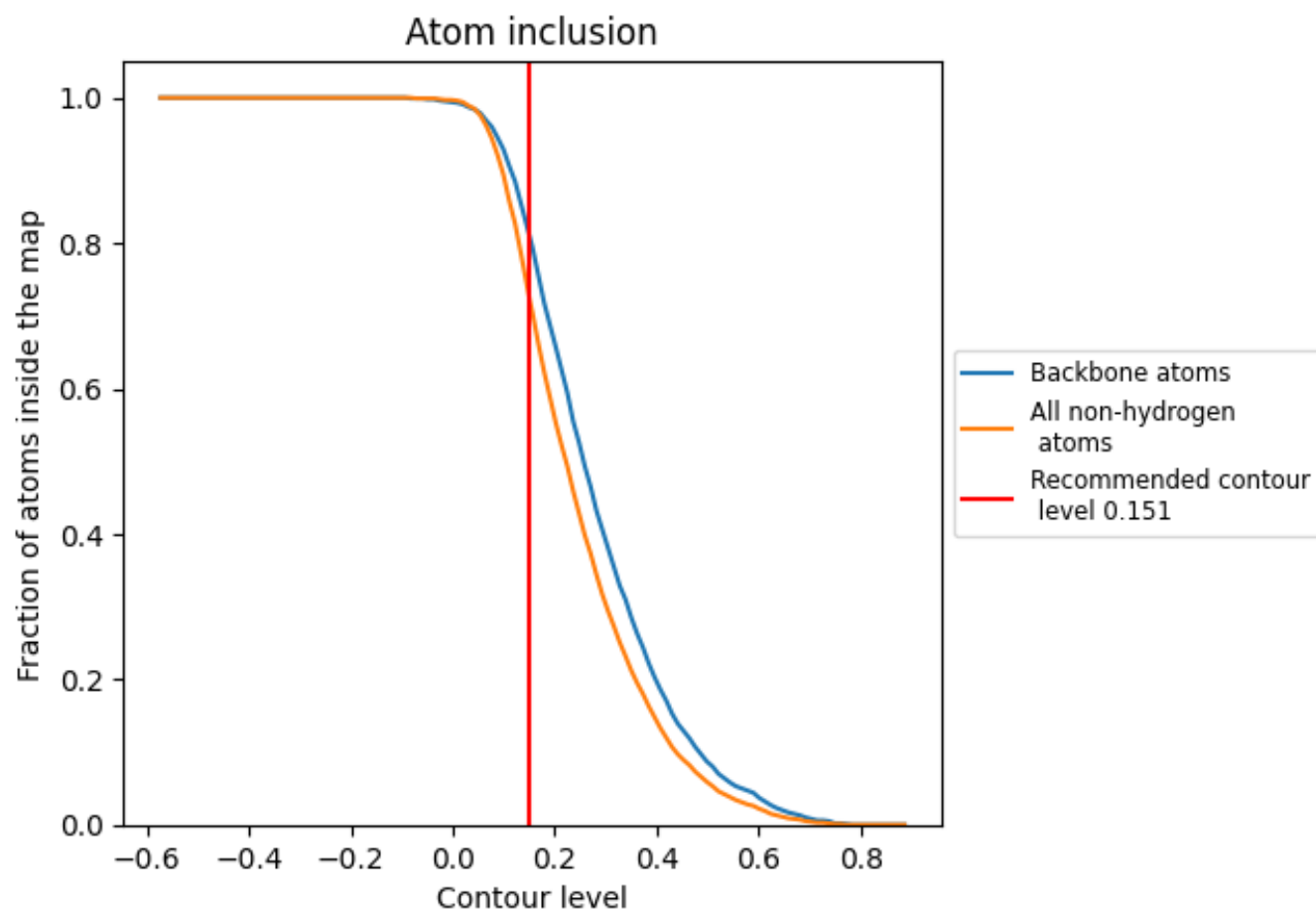
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.151).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4670
A	0.7790	0.4880
B	0.7270	0.4670
C	0.6590	0.4360
D	0.6700	0.4570
E	0.7790	0.4900
F	0.7260	0.4670
G	0.6070	0.5120
H	0.6070	0.5000
J	0.6590	0.4370
K	0.6700	0.4550

