



Full wwPDB EM Validation Report ⓘ

Jul 20, 2026 – 06:56 PM EDT

PDB ID : 13EU / pdb_000013eu
EMDB ID : EMD-77027
Title : Cryo-EM structure of HAdV-C6 hexon trimer in complex with human coagulation factor X (FX)
Authors : Ma, O.X.; Reddy, V.S.
Deposited on : 2026-05-03
Resolution : 3.26 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:

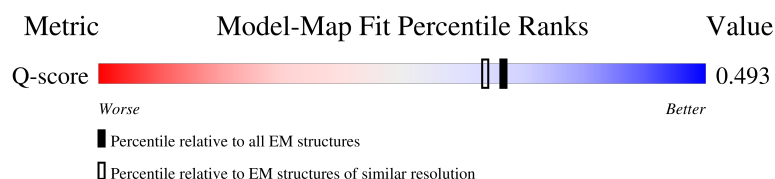
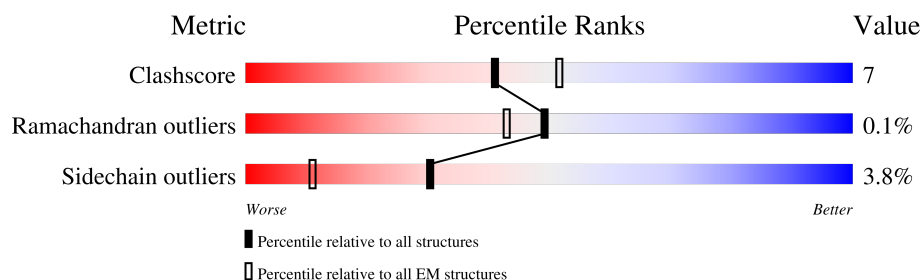
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.26 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	14557 (2.76 - 3.76)

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	963	
1	B	963	
1	C	963	
2	G	419	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22261 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	912	Total	C	N	O	S	0	0
			7286	4627	1236	1386	37		
1	B	911	Total	C	N	O	S	0	0
			7275	4620	1234	1385	36		
1	C	912	Total	C	N	O	S	0	0
			7285	4627	1235	1386	37		

- Molecule 2 is a protein called Coagulation factor X.

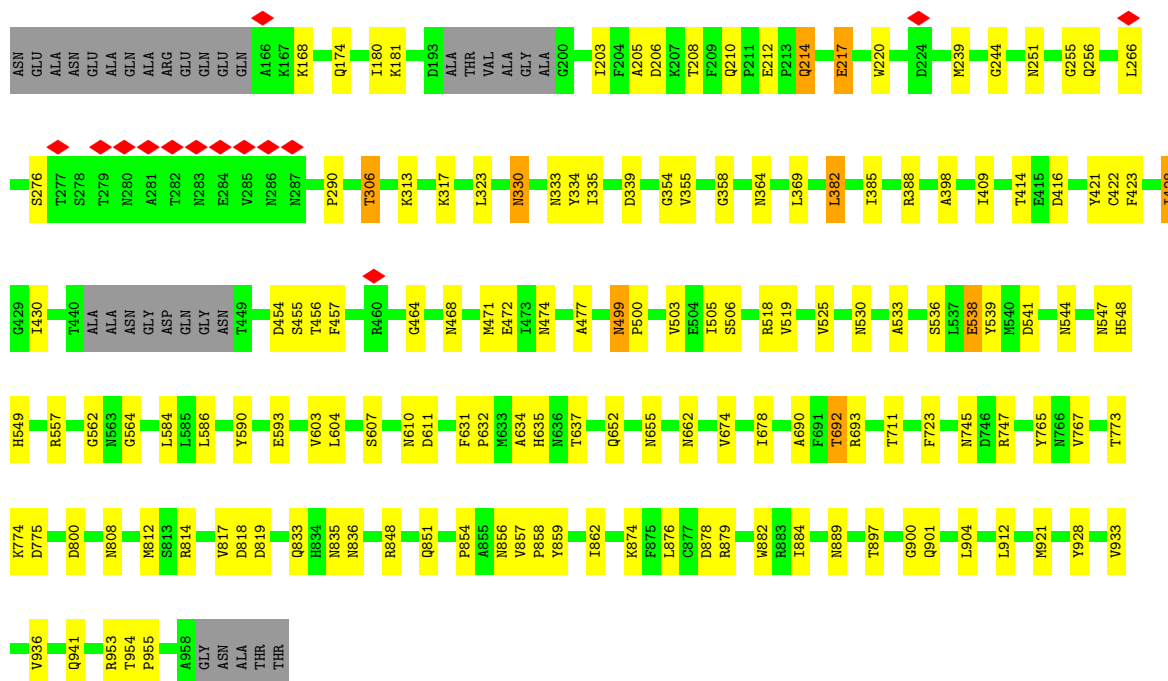
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	44	Total	C	N	O	S	0	0
			408	242	60	102	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	deletion	UNP P00742

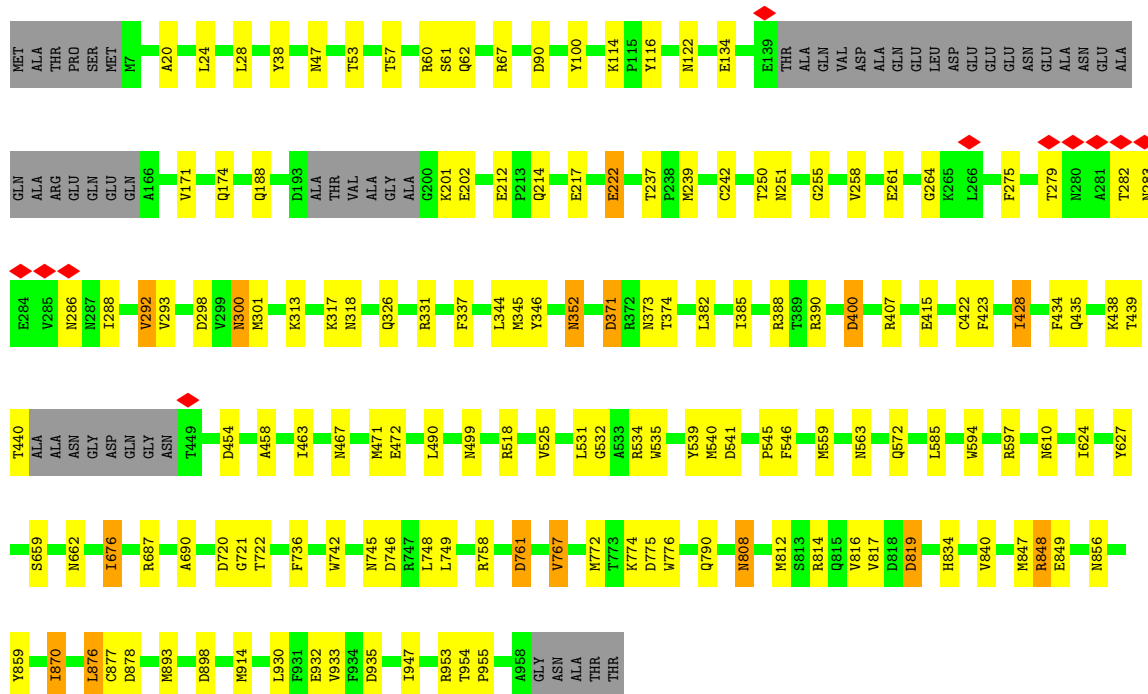
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	G	7	Total	Ca	0
			7	7	



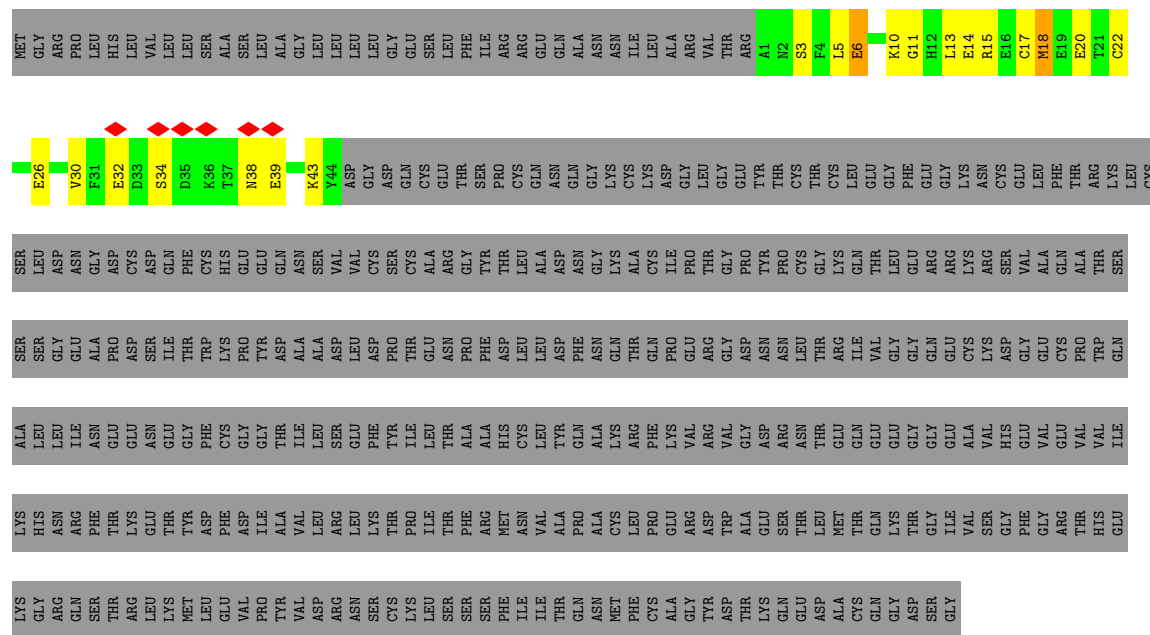
• Molecule 1: Hexon protein

Chain C: 79% 14% 5%



• Molecule 2: Coagulation factor X

Chain G: 6% 89%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68552	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.054	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	217.6, 217.6, 217.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	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: CGU, CA

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	0/7476	0.33	0/10165
1	B	0.14	0/7465	0.33	1/10150 (0.0%)
1	C	0.14	0/7475	0.33	1/10164 (0.0%)
2	G	0.09	0/275	0.26	0/353
All	All	0.14	0/22691	0.33	2/30832 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	539	TYR	N-CA-C	-6.70	103.97	111.28
1	B	538	GLU	CB-CA-C	5.50	119.51	110.88

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	7286	0	6995	121	0
1	B	7275	0	6980	114	0
1	C	7285	0	6996	112	0
2	G	408	0	313	7	0
3	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22261	0	21284	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (301) 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)
1:C:422:CYS:SG	1:C:471:MET:HB2	1.59	1.40
1:B:422:CYS:HB2	1:C:422:CYS:SG	1.71	1.31
1:A:422:CYS:SG	1:C:422:CYS:HB2	1.95	1.06
1:A:422:CYS:HB2	1:B:422:CYS:SG	1.97	1.04
1:A:422:CYS:SG	1:A:471:MET:HB2	2.08	0.94
1:C:422:CYS:SG	1:C:471:MET:CB	2.56	0.92
1:B:422:CYS:CB	1:C:422:CYS:SG	2.58	0.91
1:B:422:CYS:SG	1:B:471:MET:HB2	2.11	0.89
1:B:276:SER:HB3	1:B:290:PRO:HA	1.59	0.82
1:B:422:CYS:HB2	1:C:422:CYS:HG	1.42	0.81
1:A:919:ASP:N	1:A:919:ASP:OD1	2.15	0.78
1:B:422:CYS:CB	1:C:422:CYS:HG	1.94	0.77
1:B:500:PRO:HG2	1:B:503:VAL:HG21	1.69	0.75
1:A:422:CYS:HB2	1:B:422:CYS:HG	1.53	0.74
1:C:767:VAL:HG13	1:C:774:LYS:HG2	1.69	0.74
1:A:745:ASN:HB3	1:B:61:SER:HA	1.69	0.74
1:A:491:TYR:HH	1:A:549:HIS:HD1	1.34	0.74
1:B:584:LEU:HB3	1:B:652:GLN:HE22	1.56	0.71
1:C:283:ASN:O	1:C:286:ASN:ND2	2.26	0.69
1:B:174:GLN:HB2	1:C:428:ILE:HD12	1.75	0.69
1:C:239:MET:HG3	1:C:318:ASN:HD22	1.59	0.68
1:B:693:ARG:NH2	1:B:921:MET:SD	2.66	0.68
1:A:239:MET:HE2	1:A:318:ASN:HB2	1.76	0.68
1:A:233:LEU:HB3	1:A:237:THR:HG21	1.77	0.67
1:A:339:ASP:OD2	1:A:388:ARG:NH2	2.28	0.67
1:B:767:VAL:HG13	1:B:774:LYS:HG2	1.77	0.66
1:B:422:CYS:SG	1:B:471:MET:HE3	2.36	0.65
1:A:422:CYS:SG	1:C:422:CYS:CB	2.81	0.65
1:A:422:CYS:CB	1:B:422:CYS:HG	2.09	0.65
1:A:130:PRO:HG3	1:A:323:LEU:HG	1.79	0.64
1:B:499:ASN:OD1	1:B:518:ARG:NH1	2.31	0.64
1:B:897:THR:HG23	1:B:900:GLY:H	1.62	0.64
1:A:472:GLU:N	1:C:423:PHE:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:O	1:B:848:ARG:NH1	2.32	0.63
1:B:114:LYS:NZ	1:B:116:TYR:O	2.32	0.63
1:A:544:ASN:HB3	1:A:547:ASN:HD21	1.64	0.62
1:C:217:GLU:HB3	1:C:222:GLU:HG2	1.81	0.62
1:A:422:CYS:CB	1:B:422:CYS:SG	2.83	0.62
1:B:355:VAL:HB	1:B:593:GLU:HB3	1.80	0.62
1:C:834:HIS:ND1	1:C:834:HIS:O	2.32	0.61
1:B:313:LYS:NZ	1:B:317:LYS:O	2.28	0.61
1:C:808:ASN:ND2	1:C:878:ASP:O	2.30	0.61
2:G:34:SER:O	2:G:38:ASN:ND2	2.31	0.61
1:B:800:ASP:OD2	1:C:390:ARG:NH2	2.33	0.61
1:A:63:ARG:NH1	1:C:746:ASP:OD2	2.33	0.61
1:A:61:SER:HA	1:C:745:ASN:HB3	1.82	0.60
1:A:474:ASN:O	1:A:478:ASN:ND2	2.29	0.60
1:A:307:HIS:ND1	1:A:330:ASN:OD1	2.34	0.60
1:C:373:ASN:HB2	1:C:662:ASN:ND2	2.16	0.60
1:B:358:GLY:HA2	1:B:590:TYR:HA	1.84	0.60
1:B:40:SER:HB3	1:C:790:GLN:HE22	1.66	0.60
1:B:812:MET:HE1	1:B:876:LEU:HD13	1.83	0.60
1:A:559:MET:HE2	1:C:534:ARG:HB2	1.84	0.60
1:B:851:GLN:NE2	1:C:174:GLN:O	2.35	0.60
1:C:212:GLU:OE1	1:C:214:GLN:NE2	2.33	0.59
1:C:275:PHE:HB2	1:C:292:VAL:HG13	1.84	0.59
1:A:538:GLU:C	1:A:540:MET:H	2.10	0.59
1:C:662:ASN:OD1	1:C:930:LEU:CD1	2.51	0.59
1:A:499:ASN:OD1	1:A:518:ARG:NH1	2.35	0.59
1:C:772:MET:HE2	1:C:776:TRP:HD1	1.67	0.59
1:C:812:MET:HE1	1:C:876:LEU:HD13	1.85	0.59
1:B:536:SER:O	1:B:874:LYS:NZ	2.34	0.59
1:B:330:ASN:N	1:B:330:ASN:OD1	2.36	0.58
1:C:188:GLN:NE2	1:C:202:GLU:OE1	2.35	0.58
1:B:692:THR:HG21	1:B:723:PHE:HB3	1.85	0.58
1:B:422:CYS:HG	1:B:471:MET:HE3	1.68	0.58
2:G:17:CYS:HB3	2:G:22:CYS:SG	2.43	0.58
1:C:499:ASN:OD1	1:C:518:ARG:NH1	2.36	0.58
1:B:354:GLY:O	1:B:364:ASN:ND2	2.28	0.58
1:C:438:LYS:NZ	1:C:454:ASP:OD1	2.35	0.58
1:A:544:ASN:O	1:A:547:ASN:ND2	2.38	0.57
1:A:313:LYS:NZ	1:A:317:LYS:O	2.37	0.57
1:A:63:ARG:HH21	1:C:749:LEU:HD13	1.69	0.57
1:B:662:ASN:OD1	1:B:928:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD21	1:B:421:TYR:HE1	1.70	0.56
1:C:352:ASN:N	1:C:352:ASN:OD1	2.38	0.56
1:B:109:ARG:NH1	1:B:564:GLY:O	2.38	0.56
1:C:313:LYS:NZ	1:C:317:LYS:O	2.29	0.56
1:B:544:ASN:ND2	1:B:547:ASN:OD1	2.38	0.56
1:A:47:ASN:O	1:A:47:ASN:ND2	2.39	0.56
1:B:339:ASP:OD2	1:B:388:ARG:NH2	2.39	0.56
1:B:889:ASN:ND2	1:C:57:THR:OG1	2.39	0.55
1:C:933:VAL:HG21	1:C:953:ARG:HD2	1.88	0.55
1:B:382:LEU:HD23	1:B:385:ILE:HD11	1.88	0.55
1:B:398:ALA:O	1:B:557:ARG:NH1	2.39	0.55
1:A:815:GLN:HE22	1:B:562:GLY:HA3	1.71	0.55
1:B:745:ASN:HB2	1:C:61:SER:HA	1.87	0.55
1:B:541:ASP:OD2	1:B:874:LYS:NZ	2.39	0.55
1:A:927:LEU:HD23	1:A:928:TYR:H	1.71	0.55
1:A:55:ASP:OD1	1:A:637:THR:OG1	2.25	0.55
2:G:10:LYS:O	2:G:15:ARG:NH2	2.40	0.54
1:A:557:ARG:NH2	1:A:605:GLN:OE1	2.40	0.54
1:C:371:ASP:OD1	1:C:371:ASP:N	2.39	0.54
1:C:434:PHE:HB2	1:C:463:ILE:HD13	1.90	0.54
1:A:234:LYS:O	1:A:237:THR:HG22	2.08	0.54
1:A:659:SER:OG	1:A:933:VAL:O	2.26	0.54
1:A:802:MET:SD	1:A:879:ARG:NH1	2.81	0.54
1:A:114:LYS:NZ	1:A:116:TYR:O	2.34	0.54
1:A:526:ASP:OD1	1:A:527:CYS:N	2.38	0.54
1:A:901:GLN:NE2	1:B:51:ALA:O	2.42	0.53
1:A:422:CYS:HG	1:C:422:CYS:HB2	1.71	0.53
1:C:237:THR:OG1	1:C:298:ASP:OD1	2.26	0.53
1:A:132:SER:HB3	1:A:232:VAL:HG23	1.90	0.53
1:B:91:ASN:HD22	1:B:635:HIS:HB3	1.73	0.53
1:C:318:ASN:OD1	1:C:318:ASN:N	2.40	0.53
1:A:651:ASP:OD2	1:A:938:ARG:NH1	2.41	0.53
1:B:416:ASP:OD2	1:B:474:ASN:ND2	2.37	0.53
1:B:808:ASN:HD22	1:B:879:ARG:HB2	1.74	0.53
1:A:541:ASP:OD2	1:A:874:LYS:NZ	2.37	0.52
1:B:168:LYS:HE2	1:C:458:ALA:HA	1.91	0.52
1:A:767:VAL:HG13	1:A:774:LYS:HG2	1.91	0.52
1:A:575:GLN:NE2	1:A:592:TYR:OH	2.40	0.52
1:A:847:MET:HE1	1:B:220:TRP:HB3	1.91	0.52
1:B:112:THR:O	1:B:333:ASN:ND2	2.31	0.52
1:C:300:ASN:OD1	1:C:300:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:GLU:O	1:B:539:TYR:C	2.48	0.52
1:A:834:HIS:O	1:A:834:HIS:ND1	2.43	0.52
1:B:878:ASP:OD1	1:B:878:ASP:N	2.41	0.52
1:C:690:ALA:HB3	1:C:930:LEU:HB2	1.92	0.51
1:A:538:GLU:O	1:A:540:MET:N	2.43	0.51
1:B:205:ALA:HB1	1:B:210:GLN:HB3	1.90	0.51
1:A:91:ASN:HD22	1:A:635:HIS:HB3	1.76	0.51
1:B:414:THR:HG21	1:B:477:ALA:HA	1.92	0.51
1:A:600:VAL:HG11	1:A:617:ALA:HB3	1.93	0.51
1:C:720:ASP:OD1	1:C:721:GLY:N	2.43	0.51
1:C:114:LYS:NZ	1:C:116:TYR:O	2.37	0.51
1:A:256:GLN:HE21	1:C:856:ASN:HB3	1.76	0.51
1:A:275:PHE:HB2	1:A:292:VAL:HG13	1.93	0.51
1:B:610:ASN:N	1:B:610:ASN:OD1	2.43	0.51
1:B:423:PHE:O	1:C:472:GLU:N	2.43	0.51
1:A:241:PRO:HD3	1:A:325:GLN:HG3	1.94	0.50
2:G:3:SER:HB3	2:G:6:CGU:HB3	1.93	0.50
1:C:337:PHE:HE1	1:C:344:LEU:HD21	1.76	0.50
1:A:220:TRP:H	1:A:220:TRP:CD1	2.27	0.50
1:B:634:ALA:O	1:B:637:THR:OG1	2.29	0.50
1:A:689:TRP:NE1	1:A:914:MET:SD	2.85	0.50
1:C:24:LEU:HD22	1:C:28:LEU:HD23	1.94	0.49
1:A:387:ASP:OD1	1:A:388:ARG:N	2.45	0.49
1:A:89:GLY:HA3	1:A:92:ARG:HH11	1.76	0.49
1:B:455:SER:OG	1:B:456:THR:N	2.43	0.49
1:B:43:ASN:OD1	1:B:43:ASN:N	2.45	0.49
1:B:533:ALA:HB2	1:C:563:ASN:HB3	1.95	0.49
1:C:736:PHE:CE1	1:C:742:TRP:HB2	2.48	0.49
1:C:662:ASN:OD1	1:C:930:LEU:HD13	2.12	0.49
1:A:256:GLN:HE22	1:C:834:HIS:CE1	2.30	0.49
1:B:818:ASP:OD1	1:B:819:ASP:N	2.44	0.49
1:C:610:ASN:OD1	1:C:610:ASN:N	2.45	0.49
1:C:808:ASN:OD1	1:C:808:ASN:N	2.44	0.49
1:B:86:LEU:HB3	1:B:590:TYR:HB2	1.93	0.49
1:C:819:ASP:OD1	1:C:819:ASP:N	2.30	0.49
1:A:933:VAL:HB	1:A:955:PRO:HD2	1.94	0.48
1:B:217:GLU:OE2	1:C:467:ASN:N	2.46	0.48
1:B:239:MET:HE1	1:B:323:LEU:HD12	1.95	0.48
1:B:206:ASP:OD1	1:B:210:GLN:HB2	2.13	0.48
1:A:379:GLN:NE2	1:A:720:ASP:O	2.47	0.48
1:A:422:CYS:HG	1:C:422:CYS:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ILE:HG21	1:B:464:GLY:HA3	1.94	0.48
1:A:121:TYR:HB2	1:A:244:GLY:HA2	1.96	0.48
1:B:334:TYR:HB2	1:B:607:SER:HB3	1.96	0.48
1:A:63:ARG:HD3	1:A:66:LEU:HD23	1.96	0.48
1:A:928:TYR:CZ	1:A:930:LEU:HD11	2.49	0.48
1:C:382:LEU:HD23	1:C:385:ILE:HD11	1.96	0.48
2:G:17:CYS:CB	2:G:22:CYS:SG	3.02	0.47
1:A:728:THR:O	1:A:728:THR:OG1	2.31	0.47
1:A:812:MET:HE1	1:A:876:LEU:HD13	1.95	0.47
1:C:239:MET:HE2	1:C:318:ASN:HB2	1.96	0.47
1:B:655:ASN:HB3	1:B:936:VAL:HG12	1.95	0.47
1:A:782:LEU:HD22	1:A:891:MET:HG2	1.96	0.47
1:B:499:ASN:OD1	1:B:499:ASN:N	2.47	0.47
1:A:550:ARG:NH2	1:C:415:GLU:OE2	2.48	0.47
1:B:454:ASP:OD2	1:B:457:PHE:HB2	2.14	0.47
1:C:736:PHE:HE1	1:C:742:TRP:HB2	1.79	0.47
1:B:631:PHE:HD1	1:B:632:PRO:HD2	1.80	0.47
1:B:505:ILE:HG12	1:B:506:SER:H	1.80	0.47
1:C:20:ALA:H	1:C:47:ASN:HB3	1.80	0.47
1:A:277:THR:OG1	1:A:280:ASN:OD1	2.32	0.46
1:B:954:THR:HB	1:B:955:PRO:HD3	1.97	0.46
1:C:122:ASN:ND2	1:C:242:CYS:SG	2.84	0.46
1:C:535:TRP:CG	1:C:814:ARG:HD3	2.50	0.46
1:A:728:THR:OG1	1:A:919:ASP:OD1	2.29	0.46
1:A:933:VAL:HG12	1:A:955:PRO:HB2	1.97	0.46
1:A:952:LEU:HD22	1:B:13:MET:HE3	1.98	0.46
1:C:261:GLU:OE2	1:C:264:GLY:N	2.48	0.46
1:C:954:THR:HB	1:C:955:PRO:HD3	1.98	0.46
1:A:646:ARG:NH1	1:A:943:HIS:O	2.49	0.46
1:B:206:ASP:OD2	1:B:208:THR:OG1	2.34	0.46
1:A:375:GLU:OE1	1:A:576:LYS:NZ	2.36	0.46
1:B:586:LEU:HD12	1:B:941:GLN:HB2	1.98	0.46
1:A:439:THR:HB	1:A:451:TRP:HB3	1.98	0.46
1:B:611:ASP:HB2	1:B:711:THR:HB	1.98	0.45
1:B:692:THR:HG22	1:B:693:ARG:H	1.80	0.45
1:C:816:VAL:HG23	1:C:870:ILE:HG23	1.98	0.45
1:A:756:ILE:HG23	1:A:776:TRP:CD1	2.51	0.45
1:A:414:THR:HG21	1:A:477:ALA:HA	1.98	0.45
1:A:655:ASN:OD1	1:A:655:ASN:N	2.49	0.45
1:C:251:ASN:HD21	1:C:255:GLY:HA3	1.82	0.45
1:A:52:PRO:HD2	1:C:893:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ASP:OD1	1:A:868:ASP:N	2.45	0.45
1:B:745:ASN:ND2	1:C:60:ARG:O	2.47	0.45
1:B:530:ASN:OD1	1:B:814:ARG:NH2	2.49	0.45
1:B:833:GLN:HB3	1:B:857:VAL:HG22	1.98	0.45
1:A:237:THR:HG23	1:A:237:THR:O	2.17	0.45
1:A:217:GLU:HG2	1:A:222:GLU:HB2	1.98	0.45
1:A:693:ARG:NH1	1:A:728:THR:OG1	2.50	0.45
1:C:331:ARG:NH2	1:C:490:LEU:O	2.50	0.45
1:A:335:ILE:HA	1:A:605:GLN:O	2.17	0.45
1:A:538:GLU:C	1:A:540:MET:N	2.72	0.44
1:C:407:ARG:HE	1:C:545:PRO:HG3	1.81	0.44
1:A:256:GLN:NE2	1:C:856:ASN:HB3	2.31	0.44
1:A:451:TRP:CD1	1:A:451:TRP:H	2.35	0.44
1:B:96:MET:O	1:B:99:THR:OG1	2.30	0.44
1:B:369:LEU:HD13	1:B:953:ARG:HH21	1.81	0.44
1:B:468:ASN:O	1:C:848:ARG:NH1	2.51	0.44
1:C:134:GLU:HG2	1:C:171:VAL:HG22	2.00	0.44
1:A:666:PRO:HA	1:A:926:LEU:HD23	2.00	0.44
2:G:14:CGU:HA	2:G:18:MET:HB3	1.99	0.44
1:A:20:ALA:HB2	1:A:47:ASN:HB3	2.00	0.44
1:B:180:ILE:HG22	1:B:181:LYS:HG3	1.99	0.44
1:B:244:GLY:HA3	1:B:306:THR:HG21	1.98	0.44
1:A:39:PHE:HD1	1:A:39:PHE:HA	1.74	0.44
1:C:400:ASP:N	1:C:400:ASP:OD1	2.49	0.44
1:B:765:TYR:O	1:B:773:THR:HA	2.18	0.44
1:C:676:ILE:HG23	1:C:914:MET:HB2	1.99	0.44
1:B:678:ILE:HB	1:B:912:LEU:HB3	2.00	0.43
1:B:745:ASN:OD1	1:B:745:ASN:N	2.51	0.43
1:C:100:TYR:HD2	1:C:572:GLN:HB3	1.83	0.43
1:A:392:PHE:HB3	1:A:397:GLN:HB3	2.00	0.43
1:A:540:MET:HB3	1:A:540:MET:HE3	1.63	0.43
1:B:20:ALA:HA	1:B:23:TYR:CE2	2.53	0.43
1:B:212:GLU:OE1	1:B:214:GLN:NE2	2.33	0.43
1:C:439:THR:OG1	1:C:440:THR:N	2.52	0.43
1:C:758:ARG:NH2	1:C:761:ASP:OD1	2.51	0.43
1:C:817:VAL:HG21	1:C:859:TYR:CD2	2.54	0.43
1:C:898:ASP:N	1:C:898:ASP:OD1	2.51	0.43
1:A:931:PHE:O	1:A:933:VAL:HG13	2.19	0.43
1:A:364:ASN:OD1	1:A:365:ALA:N	2.52	0.42
1:C:546:PHE:CD1	1:C:722:THR:HB	2.54	0.42
1:C:585:LEU:HD11	1:C:947:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:LEU:HD22	1:C:775:ASP:HB3	2.01	0.42
1:A:216:GLY:HA3	1:C:849:GLU:HB2	2.01	0.42
1:A:939:VAL:HG22	1:A:949:THR:HG22	2.02	0.42
1:B:355:VAL:HA	1:B:364:ASN:ND2	2.34	0.42
1:C:47:ASN:O	1:C:47:ASN:ND2	2.53	0.42
1:B:210:GLN:O	1:B:212:GLU:N	2.53	0.42
1:A:544:ASN:HB3	1:A:547:ASN:ND2	2.33	0.42
1:B:812:MET:HE3	1:B:874:LYS:HG3	2.01	0.42
1:C:279:THR:O	1:C:282:THR:OG1	2.33	0.42
1:C:346:TYR:CE2	1:C:597:ARG:HG2	2.54	0.42
1:A:553:GLY:O	1:A:557:ARG:HG3	2.20	0.42
1:B:817:VAL:HG11	1:B:859:TYR:HD2	1.85	0.42
1:C:90:ASP:OD1	1:C:90:ASP:N	2.53	0.42
1:A:379:GLN:HE21	1:A:379:GLN:HB3	1.60	0.42
1:A:595:ASN:OD1	1:A:595:ASN:N	2.52	0.42
1:B:856:ASN:OD1	1:B:856:ASN:N	2.52	0.42
1:A:473:ILE:HB	1:C:422:CYS:HA	2.01	0.42
1:A:668:PRO:HG2	1:A:671:ALA:HB2	2.02	0.42
1:B:835:ASN:OD1	1:B:836:ASN:N	2.52	0.42
1:C:326:GLN:HE21	1:C:326:GLN:HB2	1.63	0.42
1:C:687:ARG:HB2	1:C:932:GLU:HB2	2.01	0.42
1:A:606:SER:OG	1:A:713:SER:OG	2.33	0.41
1:B:854:PRO:HG3	1:C:301:MET:HE1	2.00	0.41
1:A:816:VAL:HG23	1:A:870:ILE:HG23	2.02	0.41
1:B:471:MET:HE2	1:C:471:MET:HE2	2.02	0.41
1:B:690:ALA:HA	1:B:882:TRP:O	2.19	0.41
1:B:901:GLN:HE21	1:C:53:THR:HB	1.85	0.41
2:G:11:GLY:HA3	2:G:30:VAL:HG22	2.02	0.41
1:A:507:ASP:OD1	1:A:507:ASP:N	2.44	0.41
1:B:857:VAL:HB	1:B:858:PRO:HD3	2.02	0.41
1:A:115:PRO:HG2	1:C:532:GLY:HA3	2.01	0.41
1:A:423:PHE:O	1:B:472:GLU:N	2.53	0.41
1:B:113:PHE:HA	1:B:333:ASN:HB3	2.02	0.41
1:B:774:LYS:HE2	1:C:627:TYR:CE2	2.56	0.41
1:A:754:PHE:HE1	1:A:779:VAL:HG21	1.86	0.41
1:A:857:VAL:HB	1:A:858:PRO:HD3	2.02	0.41
1:A:800:ASP:OD2	1:A:807:ARG:HB2	2.21	0.41
1:B:113:PHE:HB2	1:B:335:ILE:HD12	2.03	0.41
1:C:239:MET:HG3	1:C:318:ASN:ND2	2.31	0.41
1:C:345:MET:HE2	1:C:594:TRP:NE1	2.36	0.41
1:A:222:GLU:H	1:A:222:GLU:HG2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:PHE:HB3	1:A:344:LEU:HD12	2.02	0.41
1:A:756:ILE:HG12	1:A:776:TRP:CE3	2.56	0.41
1:B:47:ASN:ND2	1:B:47:ASN:O	2.53	0.41
1:A:561:LEU:HD22	1:A:567:VAL:HG11	2.03	0.41
1:A:726:ASN:ND2	1:A:880:THR:O	2.38	0.41
1:B:276:SER:O	1:C:435:GLN:HG2	2.21	0.41
1:B:933:VAL:HG12	1:B:955:PRO:HG2	2.03	0.41
1:C:258:VAL:HG21	1:C:298:ASP:HB3	2.03	0.41
1:C:388:ARG:HA	1:C:388:ARG:HD2	1.81	0.41
1:C:659:SER:OG	1:C:935:ASP:N	2.49	0.41
1:A:116:TYR:CD2	1:C:531:LEU:HB3	2.56	0.41
1:B:251:ASN:OD1	1:B:255:GLY:N	2.48	0.41
1:B:603:VAL:HG23	1:B:604:LEU:HG	2.03	0.41
1:B:747:ARG:NH1	1:C:62:GLN:O	2.54	0.41
1:C:67:ARG:HB2	1:C:627:TYR:HE1	1.86	0.41
1:A:498:TYR:OH	1:A:843:LEU:O	2.33	0.40
1:A:954:THR:OG1	1:A:955:PRO:HD3	2.21	0.40
1:A:63:ARG:HA	1:C:746:ASP:O	2.21	0.40
1:A:736:PHE:CD1	1:A:912:LEU:HD13	2.57	0.40
1:C:540:MET:HE3	1:C:540:MET:HB3	2.00	0.40
1:A:337:PHE:CE2	1:A:571:ILE:HG21	2.57	0.40
1:B:19:ASP:OD1	1:B:20:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	904/963 (94%)	851 (94%)	51 (6%)	2 (0%)	43	70
1	B	903/963 (94%)	837 (93%)	66 (7%)	0	100	100
1	C	904/963 (94%)	844 (93%)	59 (6%)	1 (0%)	48	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	31/419 (7%)	23 (74%)	7 (23%)	1 (3%)	3	18
All	All	2742/3308 (83%)	2555 (93%)	183 (7%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	TYR
1	A	541	ASP
1	C	541	ASP
2	G	18	MET

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	791/826 (96%)	756 (96%)	35 (4%)	25	52
1	B	789/826 (96%)	763 (97%)	26 (3%)	33	57
1	C	791/826 (96%)	764 (97%)	27 (3%)	32	57
2	G	30/350 (9%)	27 (90%)	3 (10%)	7	26
All	All	2401/2828 (85%)	2310 (96%)	91 (4%)	30	55

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	39	PHE
1	A	50	VAL
1	A	54	HIS
1	A	69	ILE
1	A	78	TYR
1	A	103	ILE
1	A	217	GLU
1	A	285	VAL
1	A	306	THR

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Mol	Chain	Res	Type
1	A	318	ASN
1	A	322	MET
1	A	368	ASP
1	A	400	ASP
1	A	412	HIS
1	A	430	ILE
1	A	451	TRP
1	A	540	MET
1	A	547	ASN
1	A	595	ASN
1	A	624	ILE
1	A	662	ASN
1	A	728	THR
1	A	736	PHE
1	A	767	VAL
1	A	840	VAL
1	A	848	ARG
1	A	853	TYR
1	A	868	ASP
1	A	870	ILE
1	A	881	LEU
1	A	919	ASP
1	A	927	LEU
1	A	950	VAL
1	A	954	THR
1	B	37	THR
1	B	43	ASN
1	B	54	HIS
1	B	109	ARG
1	B	203	ILE
1	B	214	GLN
1	B	217	GLU
1	B	256	GLN
1	B	266	LEU
1	B	306	THR
1	B	330	ASN
1	B	382	LEU
1	B	409	ILE
1	B	428	ILE
1	B	430	ILE
1	B	499	ASN
1	B	519	VAL

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Mol	Chain	Res	Type
1	B	525	VAL
1	B	548	HIS
1	B	549	HIS
1	B	674	VAL
1	B	692	THR
1	B	775	ASP
1	B	862	ILE
1	B	884	ILE
1	B	904	LEU
1	C	38	TYR
1	C	201	LYS
1	C	222	GLU
1	C	250	THR
1	C	288	ILE
1	C	292	VAL
1	C	293	VAL
1	C	300	ASN
1	C	352	ASN
1	C	371	ASP
1	C	374	THR
1	C	400	ASP
1	C	428	ILE
1	C	525	VAL
1	C	559	MET
1	C	624	ILE
1	C	676	ILE
1	C	761	ASP
1	C	767	VAL
1	C	808	ASN
1	C	819	ASP
1	C	840	VAL
1	C	847	MET
1	C	848	ARG
1	C	870	ILE
1	C	876	LEU
1	C	877	CYS
2	G	5	LEU
2	G	13	LEU
2	G	43	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	256	GLN
1	A	262	GLN
1	A	287	ASN
1	A	379	GLN
1	A	476	ASN
1	A	547	ASN
1	A	575	GLN
1	A	786	ASN
1	A	872	GLN
1	B	47	ASN
1	B	283	ASN
1	B	340	ASN
1	B	476	ASN
1	B	673	ASN
1	B	682	ASN
1	B	889	ASN
1	B	901	GLN
1	B	941	GLN
1	C	47	ASN
1	C	138	ASN
1	C	263	ASN
1	C	283	ASN
1	C	287	ASN
1	C	476	ASN
1	C	487	ASN
1	C	516	ASN
1	C	790	GLN
1	C	902	ASN
2	G	2	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CGU	G	14	2	9,11,12	1.36	0	10,14,16	0.87	0
2	CGU	G	19	2	9,11,12	1.40	0	10,14,16	0.88	0
2	CGU	G	26	3,2	9,11,12	1.40	1 (11%)	10,14,16	0.87	0
2	CGU	G	29	3,2	9,11,12	1.38	0	10,14,16	0.91	0
2	CGU	G	6	3,2	9,11,12	1.42	1 (11%)	10,14,16	0.88	0
2	CGU	G	20	3,2	9,11,12	1.34	1 (11%)	10,14,16	0.84	0
2	CGU	G	39	2	9,11,12	1.43	1 (11%)	10,14,16	0.88	0
2	CGU	G	7	3,2	9,11,12	1.29	0	10,14,16	0.87	0
2	CGU	G	25	3,2	9,11,12	1.39	0	10,14,16	0.88	0
2	CGU	G	16	3,2	9,11,12	1.36	0	10,14,16	0.87	0
2	CGU	G	32	2	9,11,12	1.48	1 (11%)	10,14,16	0.90	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
2	CGU	G	14	2	-	7/13/14/16	-
2	CGU	G	19	2	-	4/13/14/16	-
2	CGU	G	26	3,2	-	4/13/14/16	-
2	CGU	G	29	3,2	-	1/13/14/16	-
2	CGU	G	6	3,2	-	2/13/14/16	-
2	CGU	G	20	3,2	-	3/13/14/16	-
2	CGU	G	39	2	-	3/13/14/16	-
2	CGU	G	7	3,2	-	4/13/14/16	-
2	CGU	G	25	3,2	-	2/13/14/16	-
2	CGU	G	16	3,2	-	4/13/14/16	-
2	CGU	G	32	2	-	2/13/14/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	6	CGU	CG-CD2	2.25	1.55	1.52
2	G	32	CGU	CG-CD2	2.25	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	39	CGU	CG-CD2	2.14	1.54	1.52
2	G	20	CGU	CG-CD2	2.04	1.54	1.52
2	G	26	CGU	CG-CD2	2.02	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	6	CGU	C-CA-CB-CG
2	G	7	CGU	CA-CB-CG-CD1
2	G	14	CGU	O-C-CA-CB
2	G	14	CGU	C-CA-CB-CG
2	G	14	CGU	CA-CB-CG-CD1
2	G	14	CGU	CA-CB-CG-CD2
2	G	14	CGU	OE11-CD1-CG-CD2
2	G	14	CGU	OE12-CD1-CG-CD2
2	G	19	CGU	C-CA-CB-CG
2	G	19	CGU	CA-CB-CG-CD1
2	G	19	CGU	CA-CB-CG-CD2
2	G	20	CGU	O-C-CA-CB
2	G	32	CGU	C-CA-CB-CG
2	G	39	CGU	O-C-CA-CB
2	G	39	CGU	C-CA-CB-CG
2	G	16	CGU	CA-CB-CG-CD1
2	G	14	CGU	N-CA-CB-CG
2	G	19	CGU	N-CA-CB-CG
2	G	39	CGU	N-CA-CB-CG
2	G	16	CGU	OE11-CD1-CG-CB
2	G	16	CGU	OE12-CD1-CG-CB
2	G	20	CGU	OE11-CD1-CG-CB
2	G	26	CGU	OE11-CD1-CG-CB
2	G	26	CGU	OE12-CD1-CG-CB
2	G	16	CGU	CA-CB-CG-CD2
2	G	6	CGU	N-CA-CB-CG
2	G	7	CGU	N-CA-CB-CG
2	G	32	CGU	N-CA-CB-CG
2	G	20	CGU	OE12-CD1-CG-CB
2	G	7	CGU	OE21-CD2-CG-CD1
2	G	7	CGU	OE22-CD2-CG-CD1
2	G	25	CGU	OE11-CD1-CG-CD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	25	CGU	OE12-CD1-CG-CD2
2	G	26	CGU	OE11-CD1-CG-CD2
2	G	26	CGU	OE12-CD1-CG-CD2
2	G	29	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	14	CGU	1	0
2	G	6	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

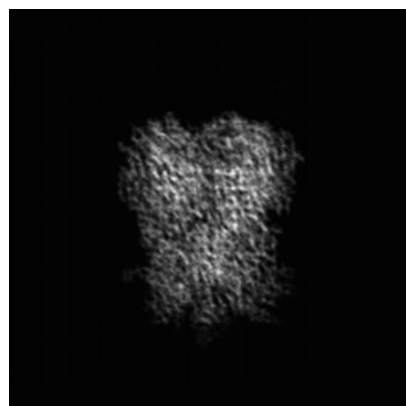
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77027. These allow visual inspection of the internal detail of the map and identification of artifacts.

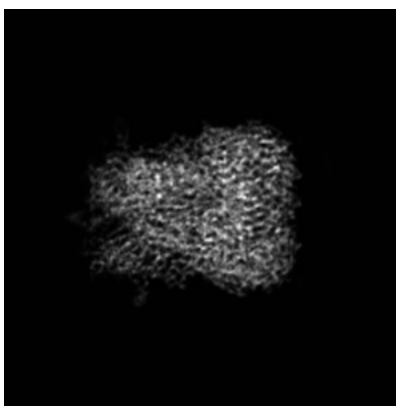
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

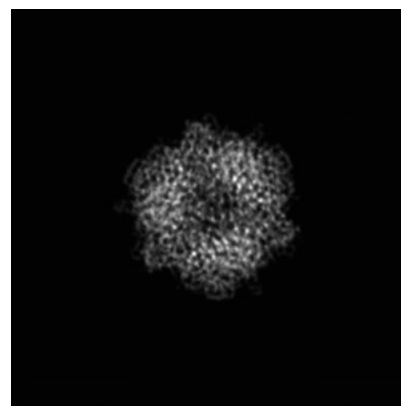
6.1.1 Primary map



X

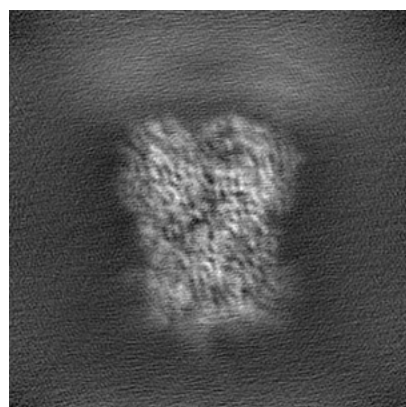


Y

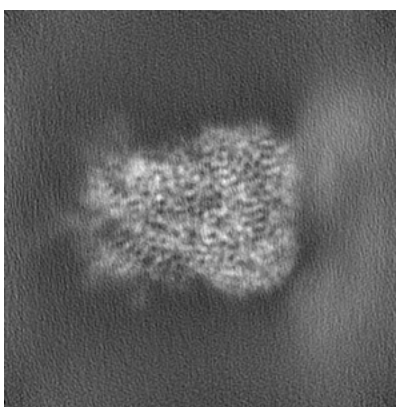


Z

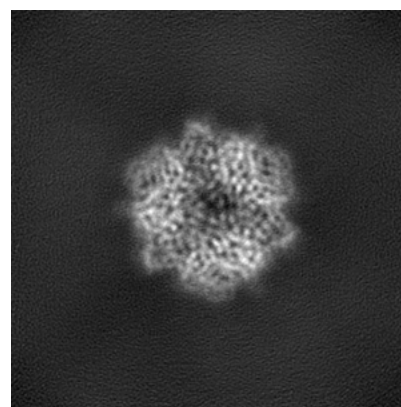
6.1.2 Raw map



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: 128

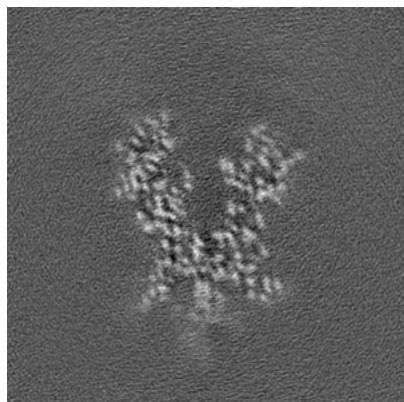


Y Index: 128

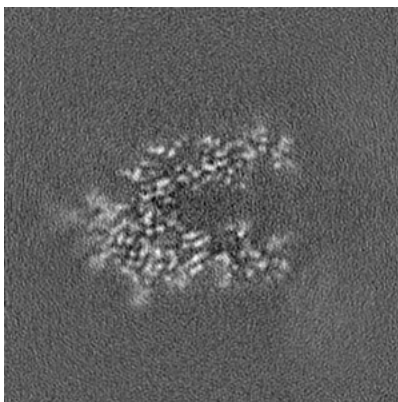


Z Index: 128

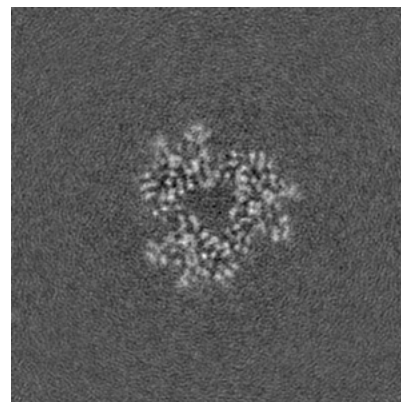
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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: 145

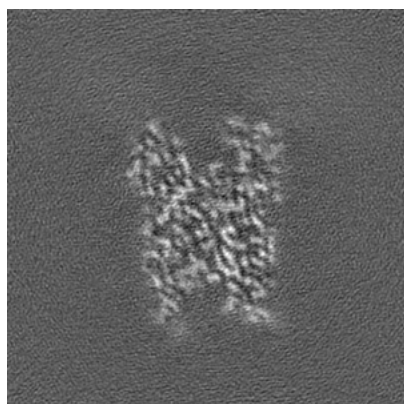


Y Index: 144

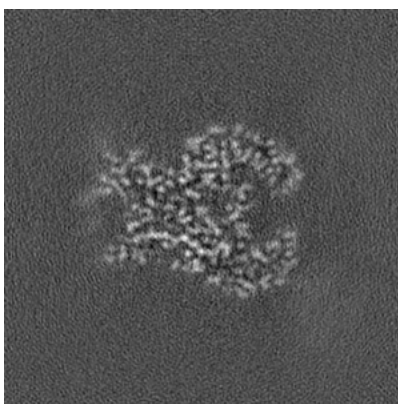


Z Index: 141

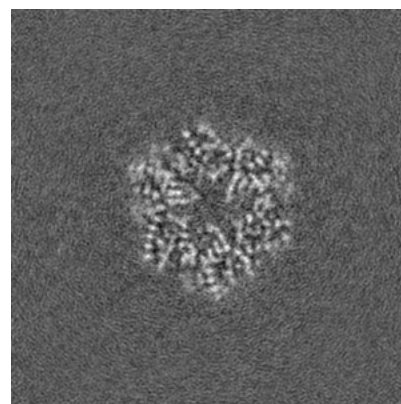
6.3.2 Raw map



X Index: 145



Y Index: 144

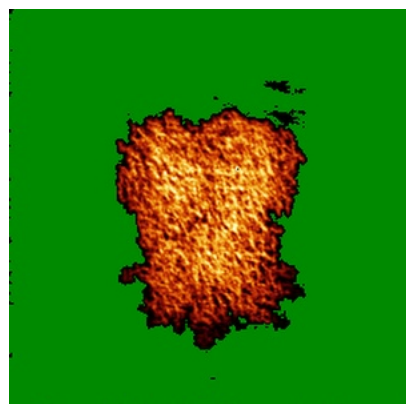


Z Index: 141

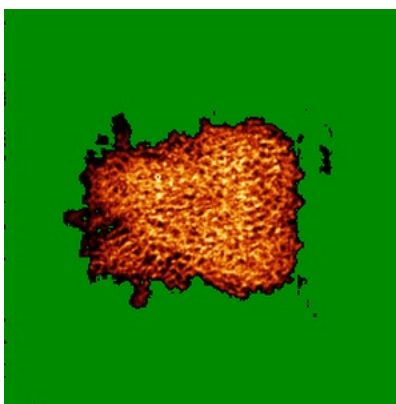
The images above show the largest variance slices of the map in three orthogonal directions.

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

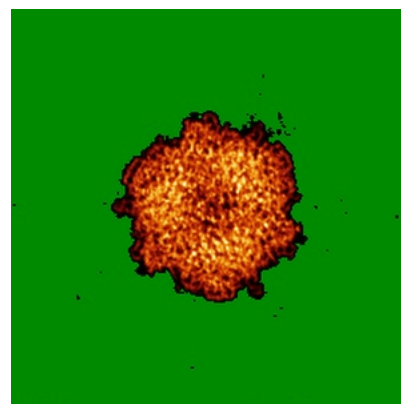
6.4.1 Primary map



X

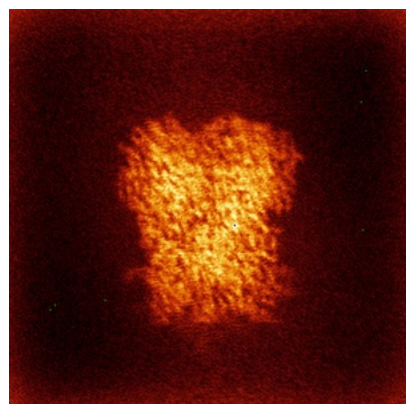


Y

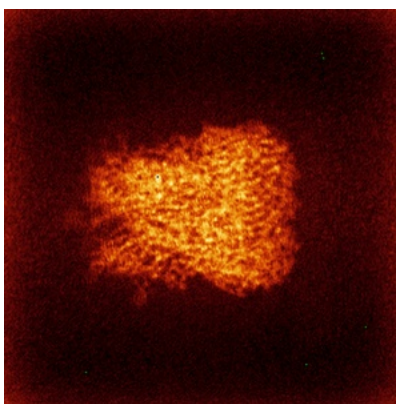


Z

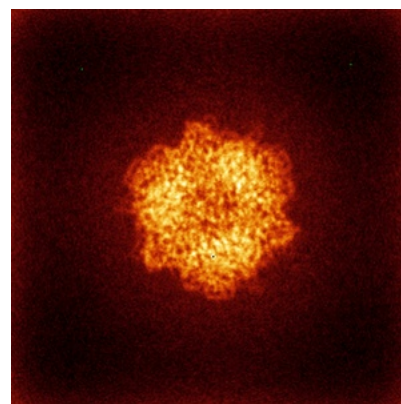
6.4.2 Raw map



X



Y

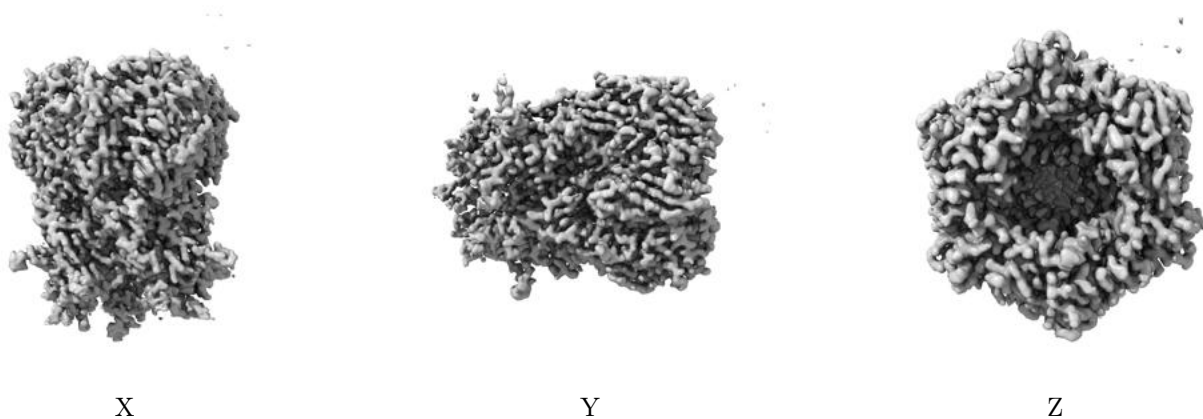


Z

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

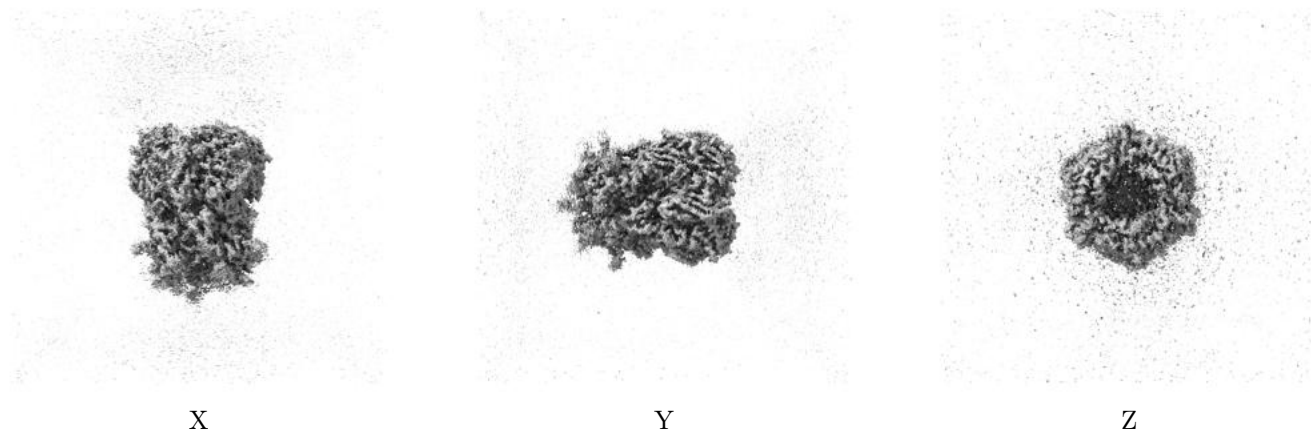
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

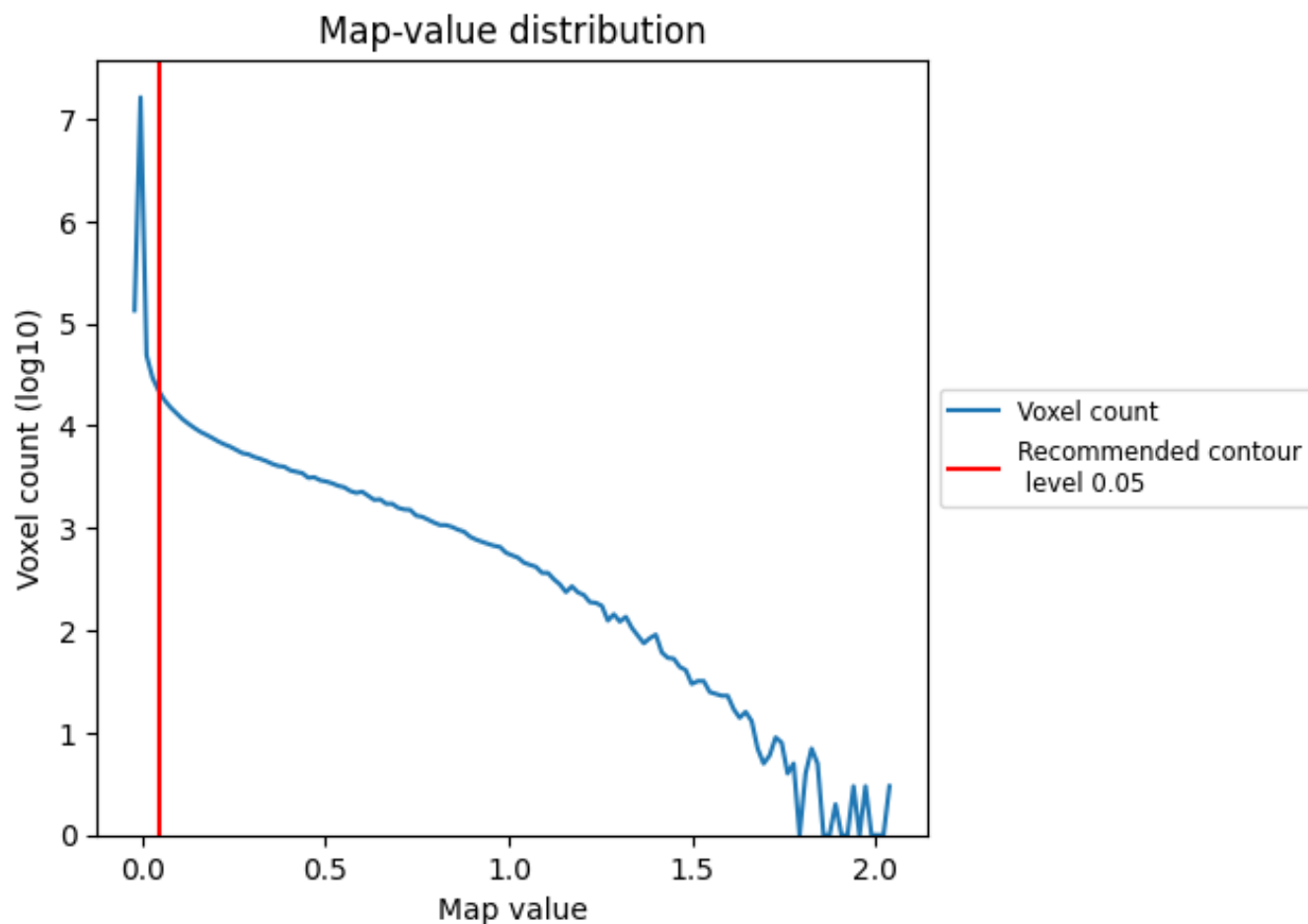
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

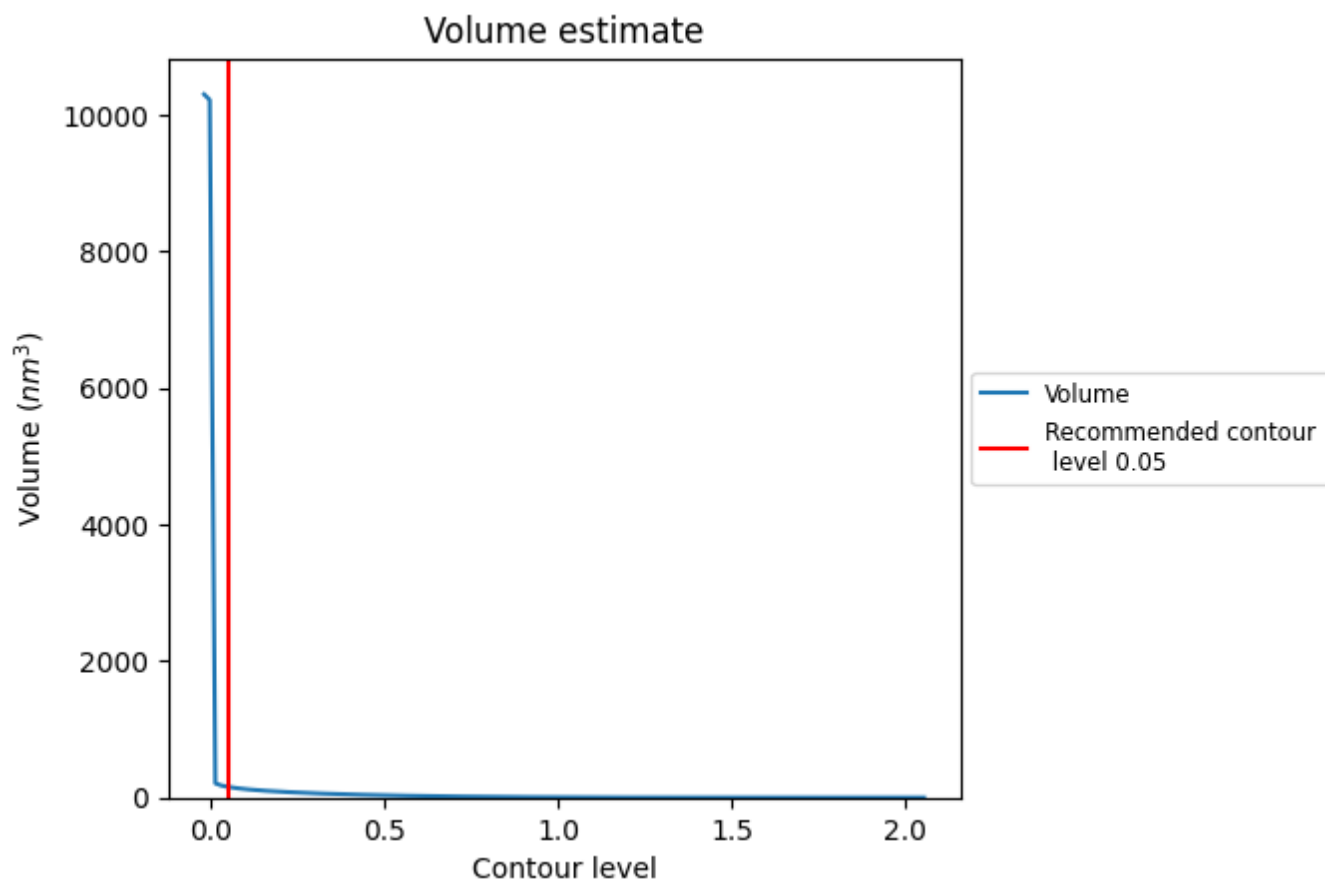
This section contains the results of statistical analysis of the map.

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.

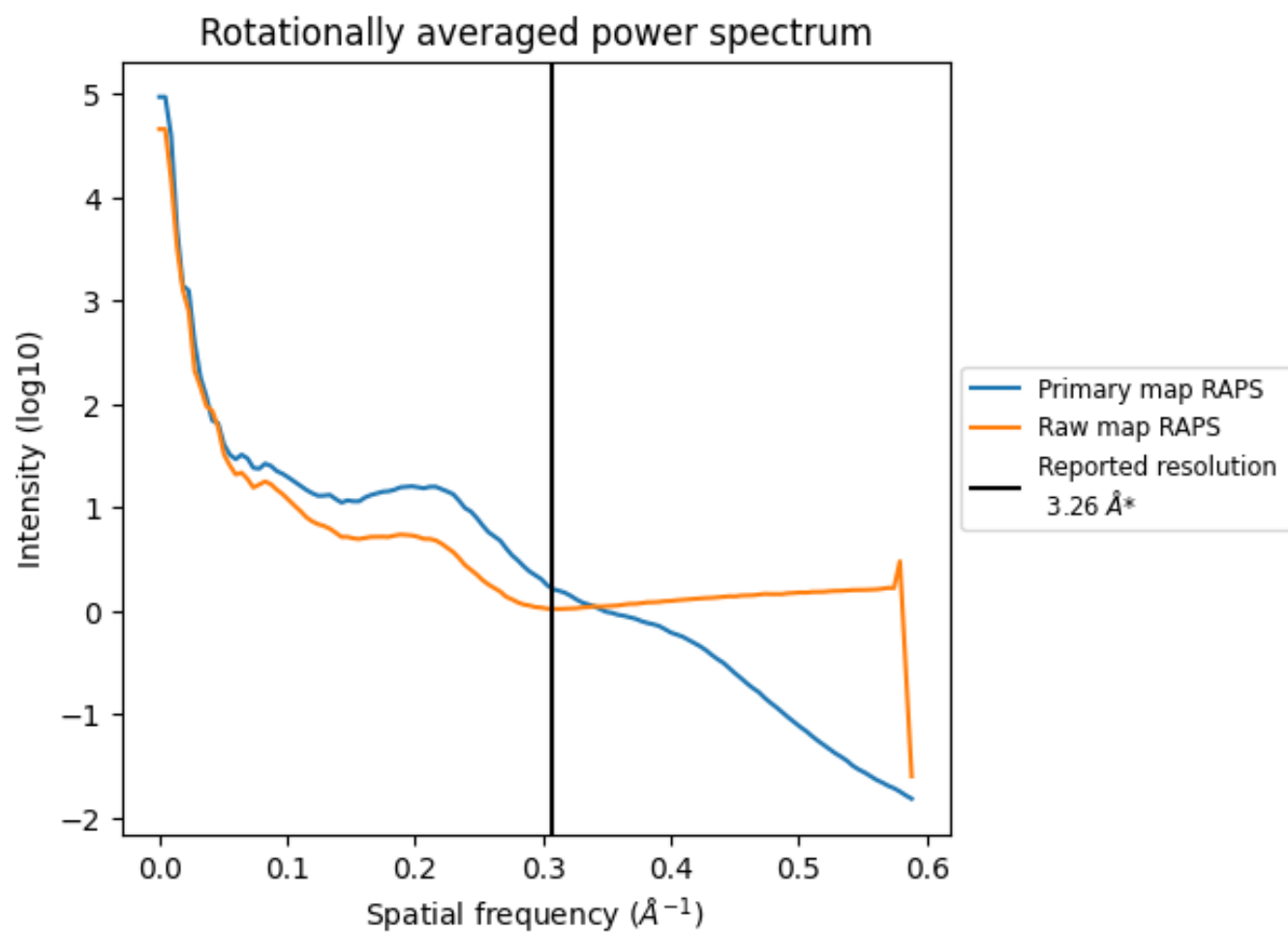
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 141 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 ⓘ

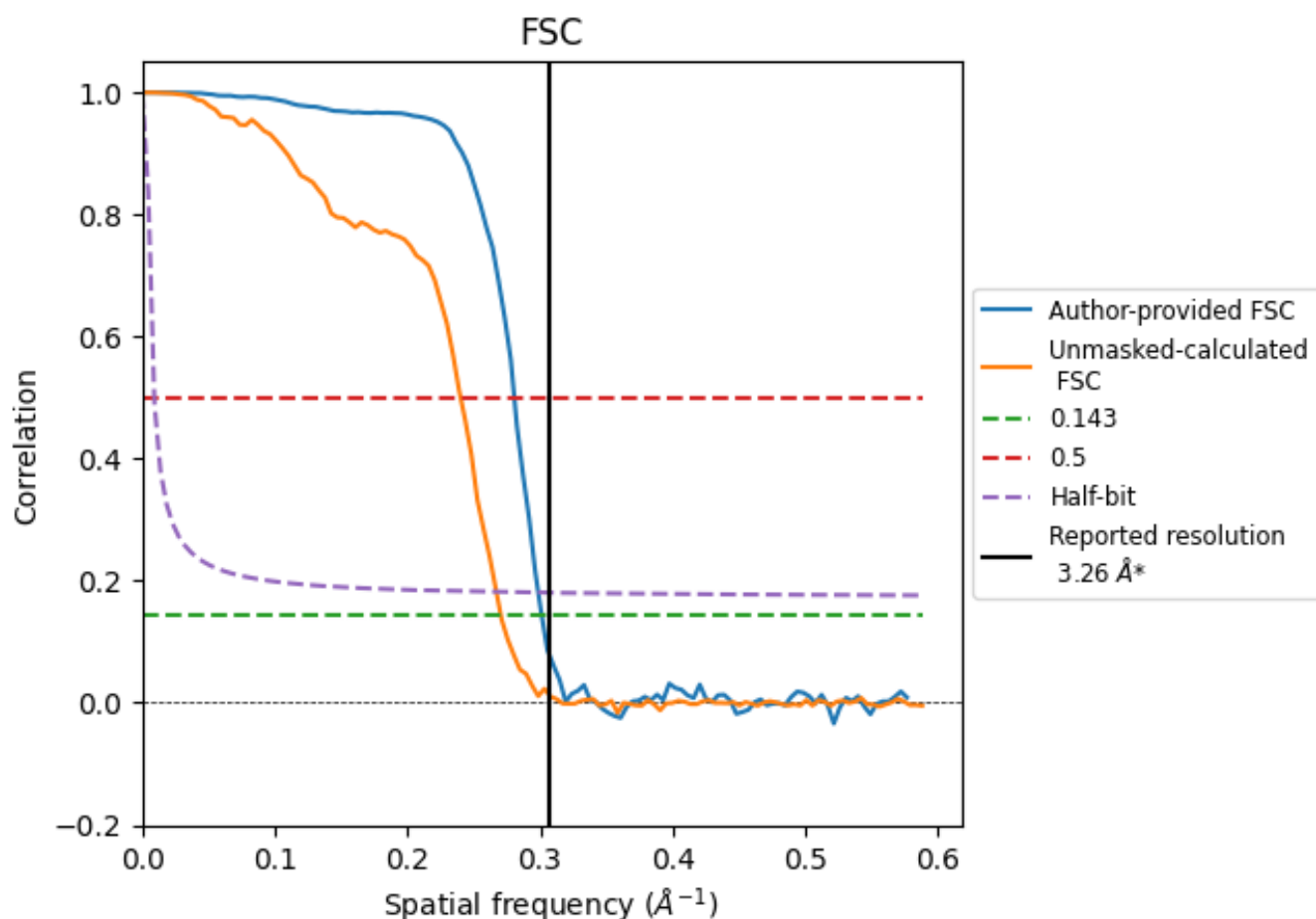


*Reported resolution corresponds to spatial frequency of $0.307 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.307 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

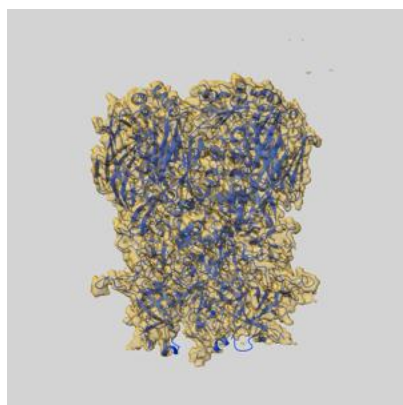
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.32	3.56	3.35
Unmasked-calculated*	3.70	4.16	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.26 by more than 10 %

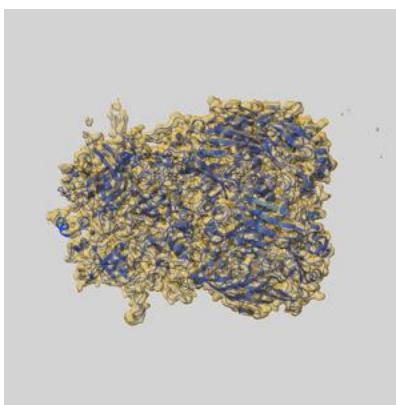
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77027 and PDB model 13EU. Per-residue inclusion information can be found in section [3](#) on page [4](#).

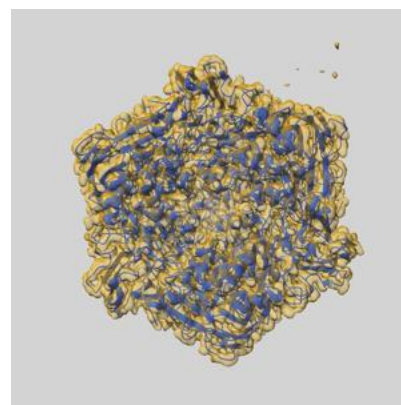
9.1 Map-model overlay [i](#)



X



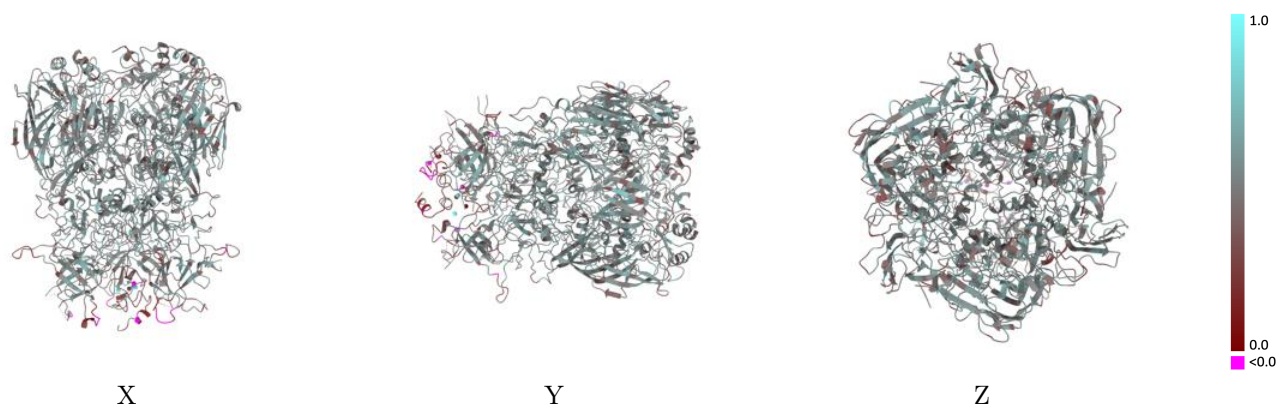
Y



Z

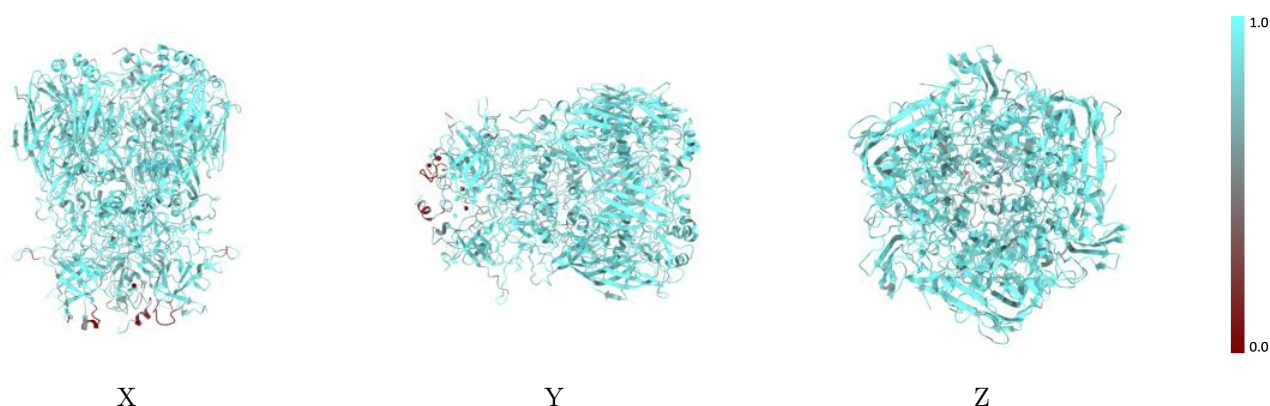
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



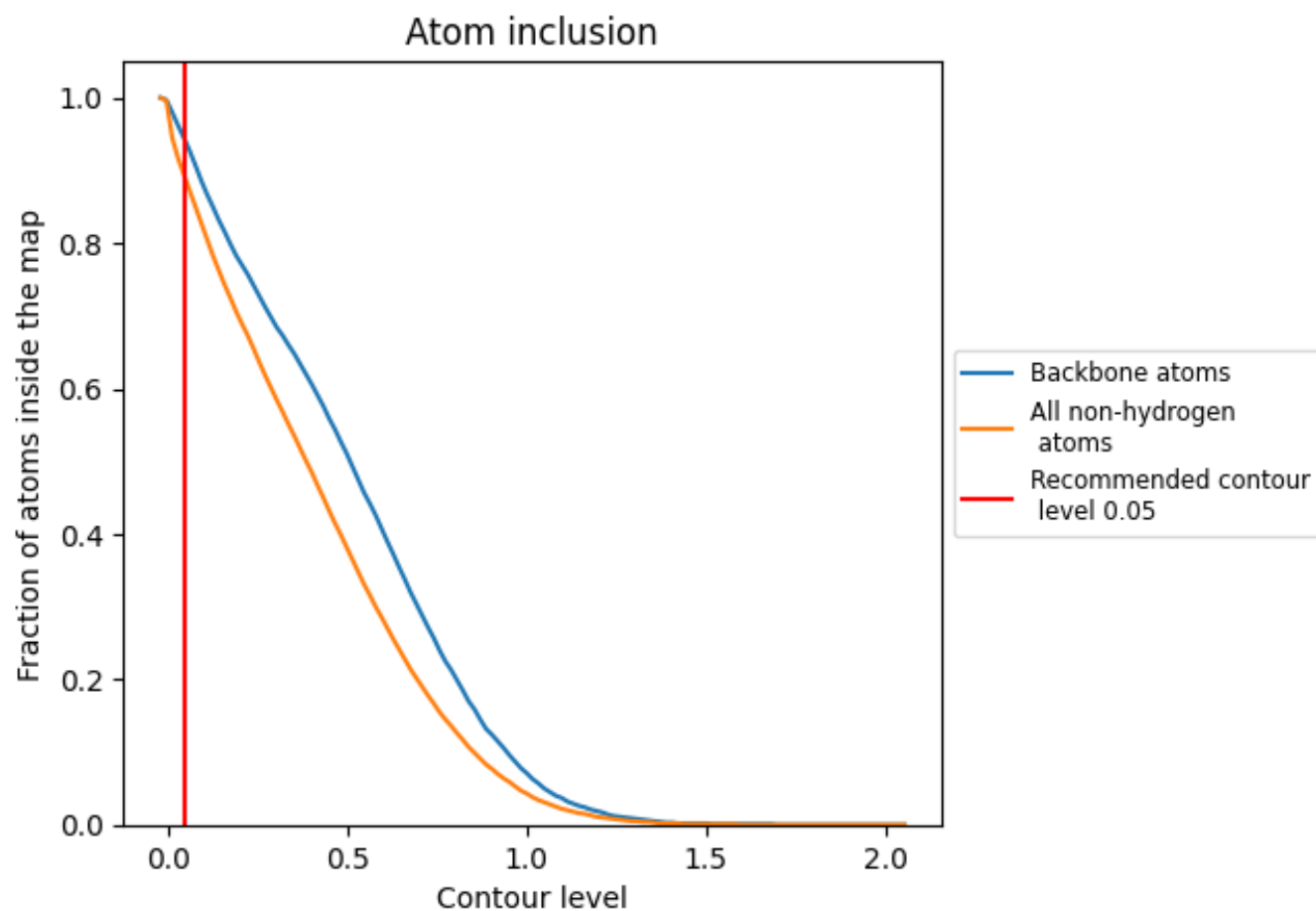
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.4930
A	0.8940	0.4990
B	0.8930	0.4920
C	0.8890	0.4980
G	0.6590	0.3290

