



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 07:29 AM EST

PDB ID : 8CVZ
EMDB ID : EMD-27022
Title : Human glycogenin-1 and glycogen synthase-1 complex in the apo ordered state
Authors : Liu, Y.; Fastman, N.M.; Tzitzilonis, C.
Deposited on : 2022-05-18
Resolution : 3.52 Å (reported)
Based on initial models : 4QLB, 3Q4S

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:

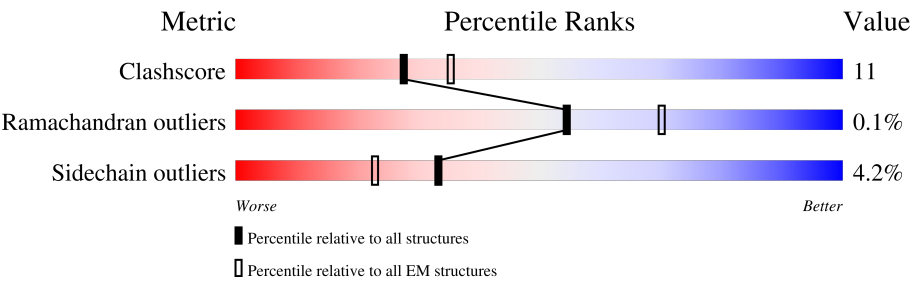
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	E	352	<div><div>9%</div><div>90%</div></div>
1	F	352	<div><div>9%</div><div>8%</div><div>90%</div></div>
1	G	352	<div><div>5%</div><div>8%</div><div>90%</div></div>
1	H	352	<div><div>8%</div><div>90%</div></div>
1	I	352	<div><div>21%</div><div>60%</div><div>15%</div><div>24%</div></div>
1	J	352	<div><div>21%</div><div>61%</div><div>13%</div><div>26%</div></div>
2	A	634	<div><div>69%</div><div>24%</div><div>5%</div></div>
2	B	634	<div><div>41%</div><div>70%</div><div>24%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	C	634	 67%27%• 5%
2	D	634	 72%22%• 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24517 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 Glycogenin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	261	Total	C	N	O	S	0	0
			2057	1334	333	381	9		
1	E	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	I	267	Total	C	N	O	S	0	0
			2100	1360	342	389	9		
1	F	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	G	34	Total	C	N	O	S	0	0
			285	175	50	59	1		
1	H	34	Total	C	N	O	S	0	0
			285	175	50	59	1		

There are 18 discrepancies between the modelled and reference sequences:

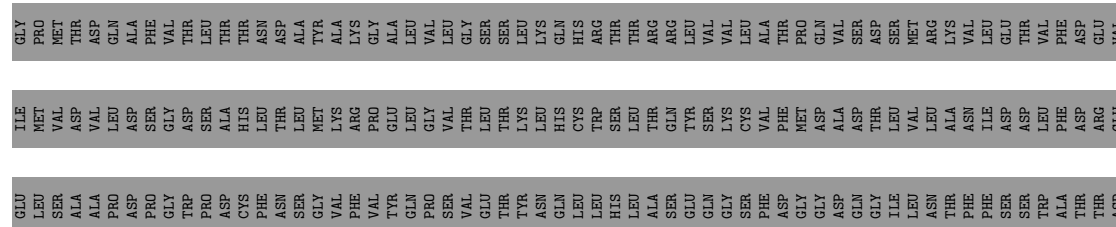
Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP P46976
J	0	PRO	-	expression tag	UNP P46976
J	195	PHE	TYR	engineered mutation	UNP P46976
E	-1	GLY	-	expression tag	UNP P46976
E	0	PRO	-	expression tag	UNP P46976
E	195	PHE	TYR	engineered mutation	UNP P46976
I	-1	GLY	-	expression tag	UNP P46976
I	0	PRO	-	expression tag	UNP P46976
I	195	PHE	TYR	engineered mutation	UNP P46976
F	-1	GLY	-	expression tag	UNP P46976
F	0	PRO	-	expression tag	UNP P46976
F	195	PHE	TYR	engineered mutation	UNP P46976
G	-1	GLY	-	expression tag	UNP P46976
G	0	PRO	-	expression tag	UNP P46976
G	195	PHE	TYR	engineered mutation	UNP P46976
H	-1	GLY	-	expression tag	UNP P46976
H	0	PRO	-	expression tag	UNP P46976
H	195	PHE	TYR	engineered mutation	UNP P46976

- Molecule 2 is a protein called Glycogen [starch] synthase, muscle.

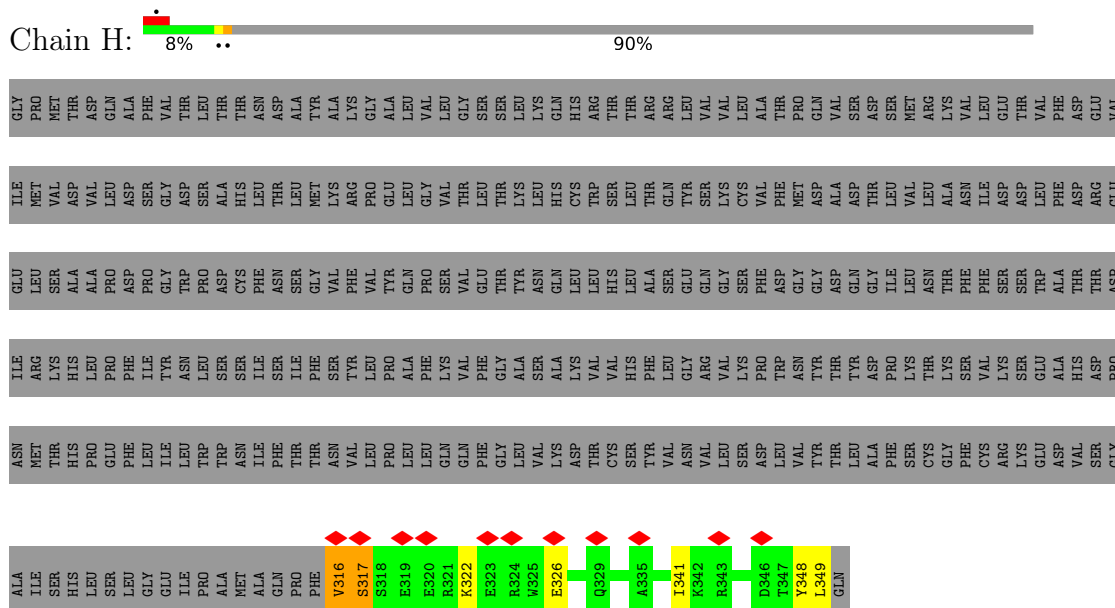
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	602	Total	C	N	O	S	0	0
			4808	3095	822	867	24		
2	C	600	Total	C	N	O	S	0	0
			4781	3075	824	857	25		
2	D	601	Total	C	N	O	S	0	0
			4777	3078	814	860	25		
2	A	601	Total	C	N	O	S	0	0
			4834	3108	834	869	23		

There are 8 discrepancies between the modelled and reference sequences:

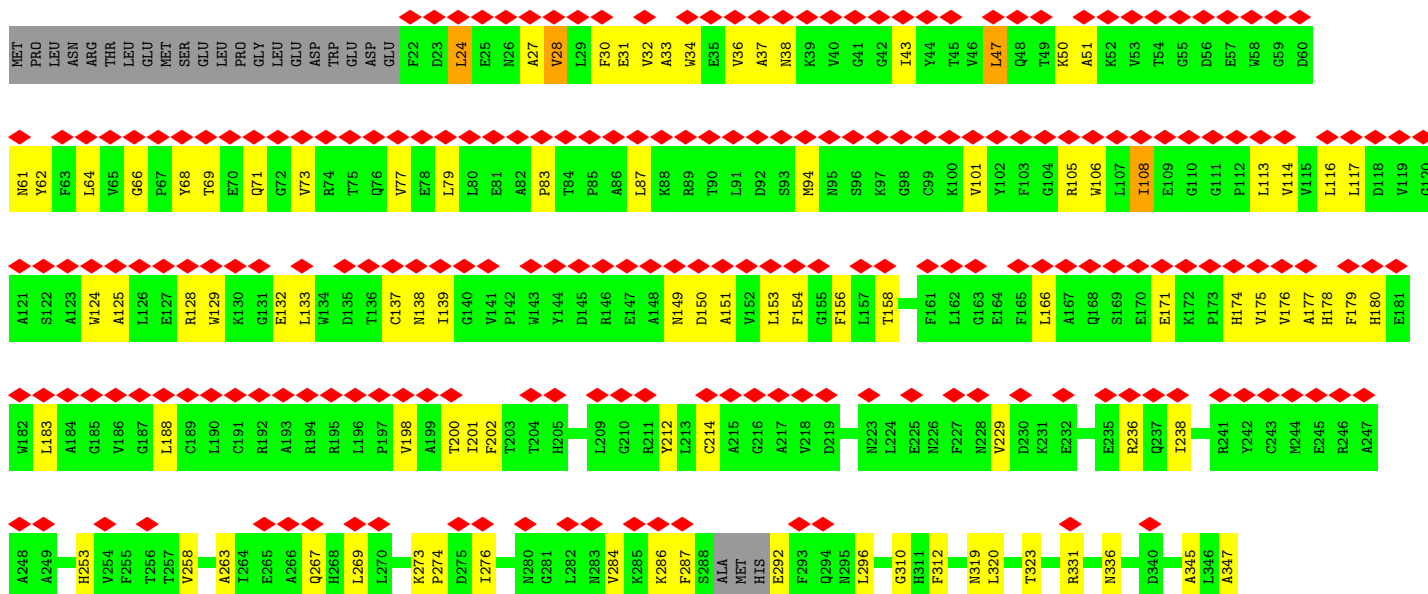
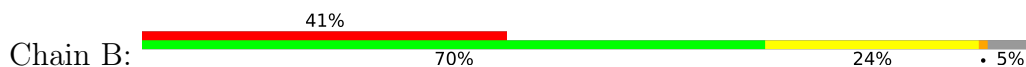
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLU	SER	engineered mutation	UNP P13807
B	11	GLU	SER	engineered mutation	UNP P13807
C	8	GLU	SER	engineered mutation	UNP P13807
C	11	GLU	SER	engineered mutation	UNP P13807
D	8	GLU	SER	engineered mutation	UNP P13807
D	11	GLU	SER	engineered mutation	UNP P13807
A	8	GLU	SER	engineered mutation	UNP P13807
A	11	GLU	SER	engineered mutation	UNP P13807

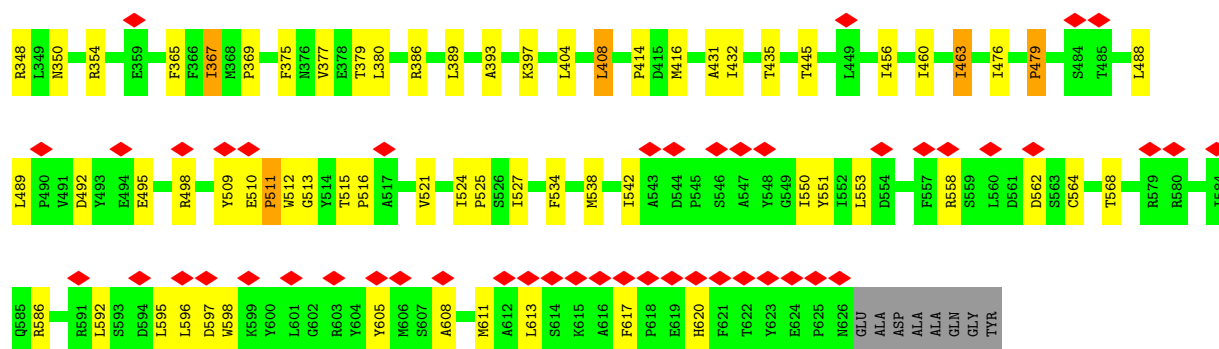


- Molecule 1: Glycogenin-1



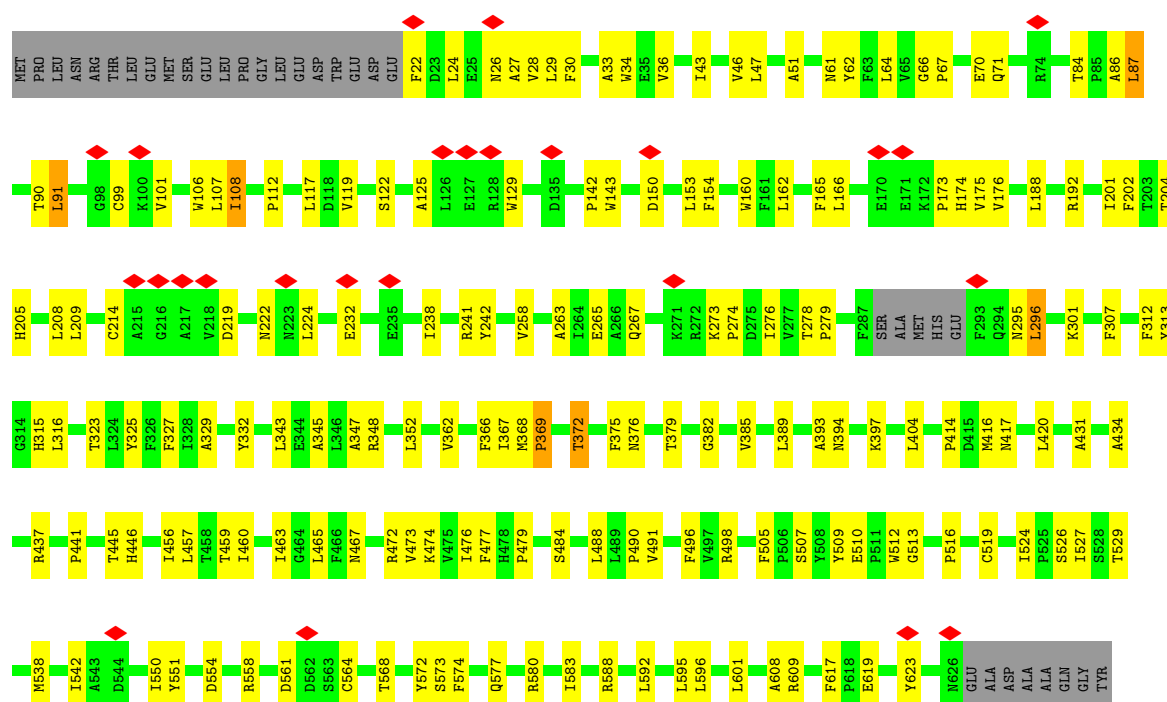
- Molecule 2: Glycogen [starch] synthase, muscle





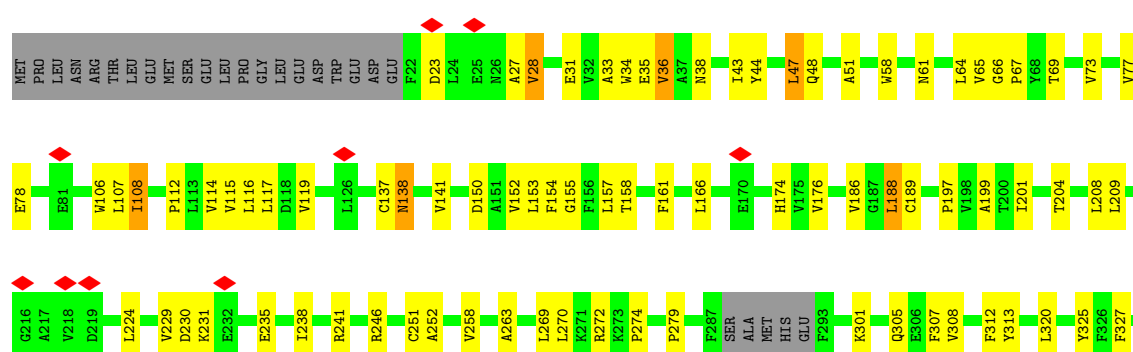
• Molecule 2: Glycogen [starch] synthase, muscle

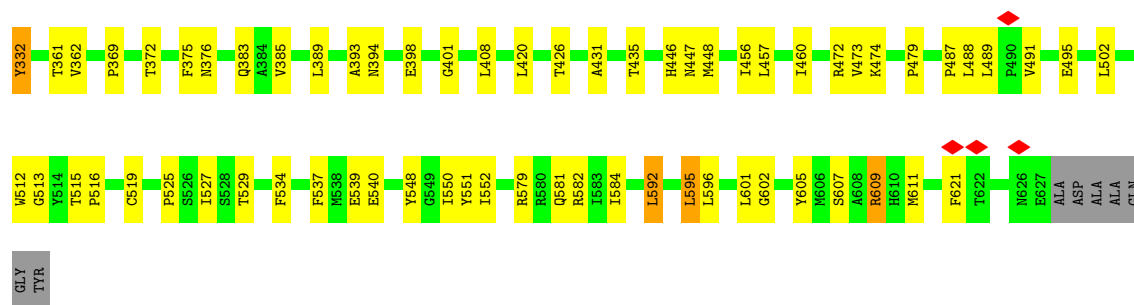
Chain C: 67% 27% • 5%



• Molecule 2: Glycogen [starch] synthase, muscle

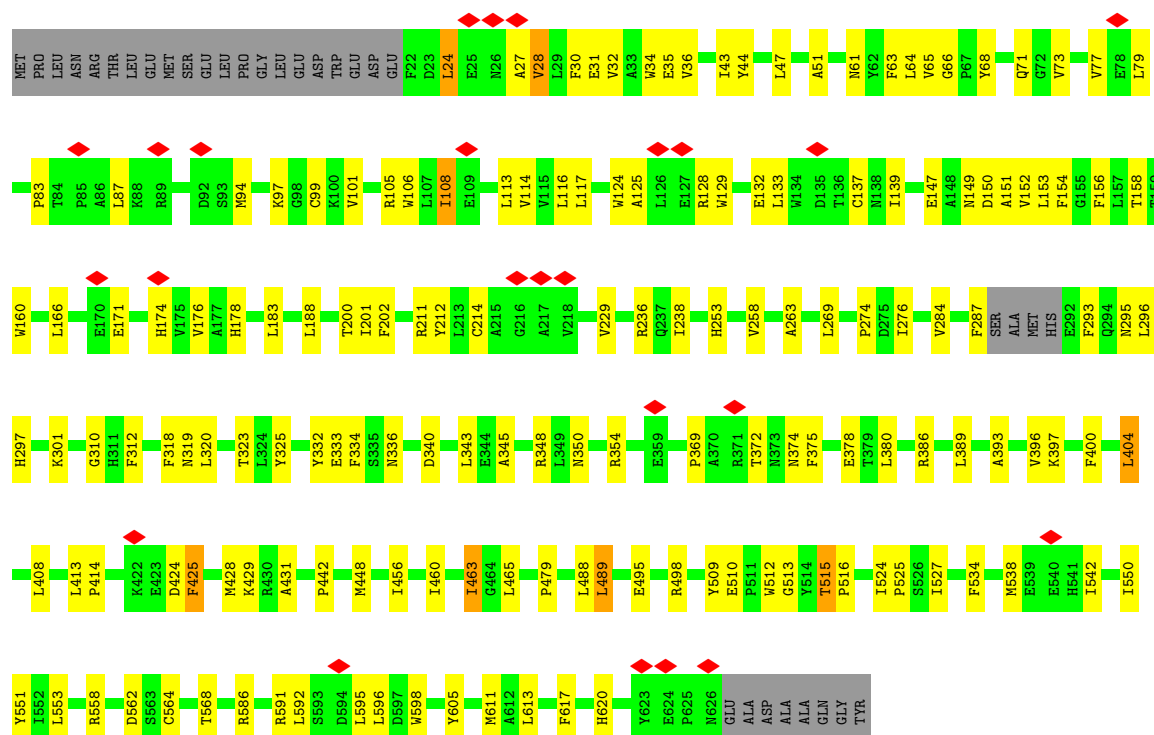
Chain D: 72% 22% • 5%





• Molecule 2: Glycogen [starch] synthase, muscle

Chain A: 69% 24% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	322214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed in batch in early steps. CTF correction was performed on per particle bases in the last iterations	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.469	Depositor
Minimum map value	-3.439	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	296.2008, 296.2008, 296.2008	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.9142, 0.9142, 0.9142	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	E	0.44	0/299	0.76	0/397
1	F	0.33	0/299	0.69	0/397
1	G	0.34	0/289	0.69	0/385
1	H	0.37	0/289	0.73	0/385
1	I	0.31	0/2158	0.68	0/2945
1	J	0.31	0/2112	0.67	0/2880
2	A	0.33	0/4963	0.71	0/6733
2	B	0.34	0/4937	0.73	0/6701
2	C	0.39	0/4907	0.78	0/6661
2	D	0.39	0/4905	0.76	0/6663
All	All	0.36	0/25158	0.73	0/34147

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	E	295	0	273	1	0
1	F	295	0	273	2	0
1	G	285	0	265	2	0
1	H	285	0	265	4	0
1	I	2100	0	2057	37	0
1	J	2057	0	2021	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4834	0	4705	118	0
2	B	4808	0	4653	120	0
2	C	4781	0	4641	124	0
2	D	4777	0	4611	106	0
All	All	24517	0	23764	517	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 11.

All (517) 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:C:313:TYR:HD1	2:C:382:GLY:HA2	1.49	0.75
1:I:194:ILE:HG13	1:I:241:THR:HB	1.68	0.74
2:B:105:ARG:HD3	2:B:113:LEU:HD23	1.72	0.72
2:A:105:ARG:HD3	2:A:113:LEU:HD23	1.71	0.72
2:C:295:ASN:HD21	2:A:293:PHE:H	1.38	0.71
2:B:229:VAL:HG11	2:B:269:LEU:HA	1.73	0.71
2:A:229:VAL:HG11	2:A:269:LEU:HA	1.71	0.71
2:C:90:THR:HG21	2:C:165:PHE:HA	1.73	0.70
2:A:296:LEU:HD13	2:A:498:ARG:HH21	1.56	0.70
1:I:122:ALA:HB3	1:I:132:PHE:HB2	1.74	0.69
2:D:31:GLU:HB2	2:D:64:LEU:HD23	1.73	0.69
2:D:389:LEU:HD23	2:D:431:ALA:HB1	1.74	0.69
2:A:301:LYS:HG3	2:A:325:TYR:HE2	1.57	0.69
2:C:36:VAL:HB	2:C:66:GLY:HA3	1.74	0.68
2:B:397:LYS:HG3	2:C:397:LYS:HG3	1.74	0.68
2:C:107:LEU:O	2:D:426:THR:HB	1.93	0.68
2:A:389:LEU:HD23	2:A:431:ALA:HB1	1.76	0.67
2:D:389:LEU:HD22	2:A:408:LEU:HB3	1.77	0.67
2:D:446:HIS:HB2	2:D:479:PRO:HG2	1.77	0.67
2:A:65:VAL:HG11	2:A:158:THR:HG22	1.75	0.67
2:A:99:CYS:HG	2:A:160:TRP:HZ3	1.43	0.67
2:D:408:LEU:HB3	2:A:389:LEU:HD22	1.78	0.66
1:J:179:ILE:HB	1:I:179:ILE:HB	1.76	0.66
2:A:36:VAL:HB	2:A:66:GLY:HA3	1.77	0.66
2:D:36:VAL:HB	2:D:66:GLY:HA3	1.77	0.66
2:B:175:VAL:HB	2:B:198:VAL:CG1	2.27	0.65
2:B:312:PHE:HE1	2:B:476:ILE:HD11	1.61	0.64
2:D:229:VAL:HG11	2:D:269:LEU:HA	1.78	0.64
2:C:538:MET:HG3	2:C:550:ILE:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:LEU:HD13	2:C:101:VAL:HG13	1.80	0.64
2:A:151:ALA:HB2	2:A:183:LEU:HB2	1.79	0.64
2:B:151:ALA:HB2	2:B:183:LEU:HB2	1.79	0.63
2:D:305:GLN:HE21	2:D:320:LEU:HB3	1.62	0.63
2:B:331:ARG:HH21	2:B:336:ASN:HD22	1.47	0.63
2:A:524:ILE:HD12	2:A:586:ARG:HH22	1.63	0.63
1:I:61:VAL:HG12	1:I:85:THR:HG23	1.81	0.63
2:D:51:ALA:HB1	2:D:112:PRO:HG3	1.79	0.63
2:D:141:VAL:HG21	2:D:152:VAL:HG21	1.81	0.63
2:D:550:ILE:HD13	2:D:592:LEU:HD23	1.80	0.63
2:C:301:LYS:HG3	2:C:325:TYR:HE2	1.64	0.62
2:D:201:ILE:HD11	2:D:609:ARG:HA	1.81	0.62
2:C:125:ALA:HA	2:C:129:TRP:HB2	1.79	0.62
2:B:32:VAL:N	2:B:178:HIS:O	2.32	0.62
2:B:377:VAL:HG21	1:I:145:THR:OG1	1.99	0.61
2:B:524:ILE:HD12	2:B:586:ARG:HH22	1.65	0.61
2:C:208:LEU:HG	2:C:238:ILE:HD11	1.82	0.61
1:J:9:LEU:HD11	1:J:85:THR:HG22	1.83	0.61
2:C:596:LEU:HA	2:C:601:LEU:HD11	1.82	0.61
2:A:106:TRP:HB2	2:A:114:VAL:HG21	1.83	0.61
1:I:9:LEU:HD11	1:I:85:THR:HG22	1.83	0.60
2:C:379:THR:HG21	2:C:445:THR:HA	1.84	0.60
2:A:236:ARG:O	2:A:238:ILE:HG12	2.01	0.60
2:A:396:VAL:HG22	2:A:424:ASP:HB2	1.84	0.60
2:B:236:ARG:O	2:B:238:ILE:HG12	2.01	0.60
2:B:83:PRO:HD2	2:B:87:LEU:HD23	1.83	0.60
1:J:122:ALA:HB3	1:J:132:PHE:HB2	1.83	0.59
2:B:50:LYS:HE2	2:B:180:HIS:HE1	1.66	0.59
2:A:83:PRO:HD2	2:A:87:LEU:HD23	1.83	0.59
2:C:279:PRO:HG2	2:C:601:LEU:HD22	1.84	0.59
2:D:34:TRP:HH2	2:D:150:ASP:HB3	1.67	0.59
2:C:201:ILE:HD11	2:C:609:ARG:HA	1.85	0.59
2:B:175:VAL:HB	2:B:198:VAL:HG11	1.84	0.59
2:B:263:ALA:HB1	2:B:274:PRO:HG3	1.85	0.59
2:A:124:TRP:O	2:A:128:ARG:HB3	2.03	0.59
2:C:538:MET:HE1	2:C:592:LEU:HD13	1.85	0.58
2:B:558:ARG:HG2	2:B:562:ASP:HB2	1.86	0.58
2:A:263:ALA:HB1	2:A:274:PRO:HG3	1.85	0.58
2:A:558:ARG:HG2	2:A:562:ASP:HB2	1.86	0.58
2:C:347:ALA:HB2	2:C:463:ILE:HB	1.86	0.58
2:B:550:ILE:HD13	2:B:592:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:ILE:HD13	2:A:592:LEU:HD12	1.85	0.57
2:B:31:GLU:HB2	2:B:64:LEU:HD23	1.86	0.57
2:B:106:TRP:HB2	2:B:114:VAL:HG21	1.86	0.57
2:C:51:ALA:HB1	2:C:112:PRO:HG3	1.85	0.57
2:A:276:ILE:HD11	2:A:611:MET:HG3	1.86	0.57
2:D:166:LEU:HD13	2:D:197:PRO:HD2	1.87	0.57
1:I:40:THR:HB	1:I:41:PRO:HD2	1.85	0.57
2:C:208:LEU:HD21	2:C:241:ARG:HB3	1.86	0.57
2:B:564:CYS:O	2:B:568:THR:HG23	2.05	0.56
2:A:34:TRP:CH2	2:A:150:ASP:HB3	2.39	0.56
2:A:564:CYS:O	2:A:568:THR:HG23	2.05	0.56
2:B:117:LEU:HD11	2:B:154:PHE:HD1	1.70	0.56
2:A:372:THR:HG21	2:A:479:PRO:HG2	1.87	0.56
2:D:307:PHE:CD1	2:D:488:LEU:HD21	2.40	0.56
2:B:174:HIS:CE1	2:B:620:HIS:HB3	2.41	0.56
2:A:174:HIS:CE1	2:A:620:HIS:HB3	2.40	0.56
2:B:132:GLU:CD	2:B:156:PHE:HE1	2.09	0.56
2:B:188:LEU:HD13	2:B:202:PHE:HB2	1.87	0.56
2:C:34:TRP:HH2	2:C:150:ASP:HB3	1.71	0.56
2:A:132:GLU:CD	2:A:156:PHE:HE1	2.09	0.56
2:A:456:ILE:O	2:A:460:ILE:HG13	2.06	0.56
2:D:65:VAL:HG11	2:D:158:THR:HG22	1.87	0.56
2:D:312:PHE:HE1	2:D:474:LYS:HE3	1.71	0.56
2:C:263:ALA:HB1	2:C:274:PRO:HG3	1.88	0.56
2:C:46:VAL:HG11	2:C:205:HIS:HE1	1.69	0.55
2:A:174:HIS:CD2	2:A:617:PHE:HE2	2.24	0.55
2:C:204:THR:O	2:C:204:THR:OG1	2.12	0.55
2:C:527:ILE:HG23	2:C:551:TYR:HB2	1.87	0.55
2:A:188:LEU:HD13	2:A:202:PHE:HB2	1.89	0.55
1:J:159:PHE:HB2	1:I:203:VAL:HG21	1.88	0.55
2:C:564:CYS:O	2:C:568:THR:HG23	2.06	0.55
2:B:50:LYS:NZ	2:B:180:HIS:CE1	2.74	0.55
2:B:149:ASN:O	2:B:153:LEU:HG	2.07	0.55
2:B:212:TYR:HB3	2:B:236:ARG:HD3	1.89	0.55
2:B:534:PHE:CE1	2:B:596:LEU:HD11	2.42	0.55
2:C:28:VAL:HA	2:C:61:ASN:HB3	1.88	0.55
2:C:538:MET:O	2:C:542:ILE:HG22	2.07	0.55
2:B:174:HIS:CD2	2:B:617:PHE:HE2	2.25	0.55
2:D:539:GLU:HG3	2:D:552:ILE:HG13	1.88	0.55
2:A:460:ILE:HG22	2:A:465:LEU:O	2.07	0.55
2:A:534:PHE:CE1	2:A:596:LEU:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:TYR:CE2	2:C:64:LEU:HD11	2.42	0.54
2:C:367:ILE:HD11	2:C:496:PHE:CE1	2.43	0.54
1:J:40:THR:HB	1:J:41:PRO:HD2	1.89	0.54
2:B:37:ALA:HB2	2:B:116:LEU:HD23	1.88	0.54
2:D:27:ALA:HA	2:D:174:HIS:O	2.07	0.54
2:A:149:ASN:O	2:A:153:LEU:HG	2.08	0.54
2:C:26:ASN:HB3	2:C:173:PRO:HB3	1.90	0.54
2:C:295:ASN:ND2	2:A:293:PHE:H	2.03	0.54
2:C:238:ILE:HG13	2:C:241:ARG:HH11	1.72	0.54
2:C:376:ASN:HB3	2:C:379:THR:HG23	1.89	0.54
2:D:307:PHE:HA	2:D:383:GLN:HE21	1.71	0.54
2:B:258:VAL:HG21	2:B:512:TRP:HB2	1.90	0.54
2:D:251:CYS:HA	1:H:349:LEU:HD11	1.90	0.54
2:B:34:TRP:CH2	2:B:150:ASP:HB3	2.43	0.54
2:C:219:ASP:OD2	2:C:222:ASN:HB2	2.07	0.54
2:C:307:PHE:HE2	2:C:476:ILE:HG21	1.73	0.54
2:A:538:MET:O	2:A:542:ILE:HG22	2.07	0.54
2:C:463:ILE:HD11	2:C:465:LEU:HD12	1.88	0.54
1:E:322:LYS:O	1:E:326:GLU:HG2	2.07	0.54
1:I:36:VAL:HG21	1:I:95:TYR:CZ	2.42	0.54
2:B:538:MET:O	2:B:542:ILE:HG22	2.07	0.54
2:C:507:SER:H	2:C:529:THR:HG21	1.72	0.54
2:D:361:THR:HG1	2:D:472:ARG:HH11	1.55	0.54
2:D:33:ALA:HB3	2:D:36:VAL:HG23	1.91	0.53
2:D:141:VAL:HG21	2:D:152:VAL:CG2	2.39	0.53
2:D:64:LEU:HB2	2:D:114:VAL:HG22	1.90	0.53
1:I:212:HIS:CE1	1:I:214:LEU:HD21	2.43	0.53
2:D:420:LEU:HD11	2:A:400:PHE:HZ	1.74	0.53
2:C:62:TYR:CZ	2:C:64:LEU:HD11	2.44	0.53
1:I:117:ARG:HG3	1:I:183:LEU:HD21	1.91	0.53
2:D:376:ASN:HA	2:D:447:ASN:HD22	1.74	0.53
2:B:263:ALA:CB	2:B:274:PRO:HG3	2.39	0.53
2:D:34:TRP:CH2	2:D:150:ASP:HB3	2.44	0.53
2:D:389:LEU:HD11	2:D:435:THR:HG22	1.91	0.53
2:A:211:ARG:HG3	2:A:509:TYR:CE2	2.44	0.53
2:A:498:ARG:HA	2:A:524:ILE:HD11	1.91	0.53
2:A:65:VAL:CG1	2:A:158:THR:HG22	2.39	0.52
2:C:142:PRO:HA	1:G:326:GLU:HA	1.92	0.52
2:C:519:CYS:SG	2:C:526:SER:HB3	2.48	0.52
2:D:263:ALA:CB	2:D:274:PRO:HG2	2.39	0.52
2:A:31:GLU:HB2	2:A:64:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:PRO:HB2	1:I:124:PRO:HB2	1.91	0.52
2:B:331:ARG:NH2	2:B:336:ASN:HD22	2.07	0.52
2:A:524:ILE:HD12	2:A:586:ARG:NH2	2.24	0.52
1:H:322:LYS:O	1:H:326:GLU:HG2	2.10	0.52
2:C:22:PHE:HB2	2:C:623:TYR:HB3	1.90	0.52
2:A:350:ASN:O	2:A:354:ARG:HG2	2.10	0.52
2:D:114:VAL:HG12	2:D:116:LEU:HG	1.92	0.52
2:A:456:ILE:HG22	2:A:460:ILE:HD11	1.92	0.52
2:B:524:ILE:HD12	2:B:586:ARG:NH2	2.25	0.52
2:C:263:ALA:CB	2:C:274:PRO:HG3	2.40	0.52
2:A:35:GLU:HB3	2:A:44:TYR:HB2	1.90	0.52
2:A:99:CYS:SG	2:A:160:TRP:HZ3	2.32	0.52
2:A:332:TYR:HB2	2:A:369:PRO:O	2.10	0.52
1:F:322:LYS:O	1:F:326:GLU:HG2	2.10	0.52
2:B:138:ASN:HD21	1:F:321:ARG:HH22	1.56	0.52
2:B:284:VAL:HG23	2:B:597:ASP:OD1	2.09	0.52
2:C:312:PHE:HD1	2:C:441:PRO:HG2	1.75	0.52
1:G:322:LYS:O	1:G:326:GLU:HG2	2.10	0.52
2:D:106:TRP:HB2	2:D:114:VAL:HG21	1.92	0.52
2:D:456:ILE:O	2:D:460:ILE:HG13	2.09	0.51
2:C:33:ALA:HB3	2:C:36:VAL:HG23	1.93	0.51
2:C:267:GLN:HG2	2:C:273:LYS:HD2	1.91	0.51
2:D:362:VAL:HG12	2:D:473:VAL:HG13	1.92	0.51
2:A:425:PHE:HA	2:A:428:MET:HE2	1.91	0.51
2:B:350:ASN:O	2:B:354:ARG:HG2	2.10	0.51
2:C:484:SER:HA	2:C:490:PRO:O	2.10	0.51
2:C:404:LEU:HD12	2:C:414:PRO:HB3	1.91	0.51
2:C:456:ILE:O	2:C:460:ILE:HG13	2.10	0.51
2:B:183:LEU:HD23	2:B:183:LEU:H	1.75	0.51
2:A:94:MET:HB3	2:A:101:VAL:HG11	1.93	0.51
2:A:183:LEU:HD23	2:A:183:LEU:H	1.74	0.51
1:I:61:VAL:CG1	1:I:85:THR:HG23	2.40	0.51
2:B:498:ARG:HA	2:B:524:ILE:HD11	1.92	0.51
2:A:238:ILE:O	2:A:238:ILE:HG22	2.11	0.51
2:B:456:ILE:O	2:B:460:ILE:HG13	2.11	0.51
2:D:534:PHE:HE1	2:D:596:LEU:HD11	1.76	0.51
1:J:101:MET:HA	1:J:135:GLY:O	2.11	0.51
1:J:211:VAL:HG11	1:J:245:PHE:HB3	1.93	0.51
2:B:178:HIS:CD2	2:B:201:ILE:HB	2.46	0.51
2:C:507:SER:O	2:C:529:THR:HG21	2.11	0.51
2:D:534:PHE:CE1	2:D:596:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:ALA:CB	2:A:274:PRO:HG3	2.40	0.50
2:B:369:PRO:HA	2:B:479:PRO:O	2.12	0.50
2:A:97:LYS:HB3	2:A:160:TRP:HH2	1.76	0.50
2:A:117:LEU:HD11	2:A:154:PHE:HD1	1.76	0.50
2:A:133:LEU:HB2	2:A:156:PHE:HE2	1.76	0.50
2:B:94:MET:HB3	2:B:101:VAL:HG11	1.92	0.50
2:D:513:GLY:C	2:D:516:PRO:HD2	2.32	0.50
2:C:312:PHE:CE1	2:C:474:LYS:HD2	2.47	0.50
2:D:527:ILE:HG12	2:D:551:TYR:HB2	1.94	0.50
2:B:276:ILE:HD12	2:B:608:ALA:HA	1.94	0.50
2:C:34:TRP:CH2	2:C:150:ASP:HB3	2.46	0.50
2:D:313:TYR:CE1	2:D:385:VAL:HG11	2.46	0.50
2:C:389:LEU:HD22	2:C:431:ALA:HB1	1.94	0.49
2:D:602:GLY:HA2	2:D:605:TYR:CE2	2.48	0.49
1:I:222:TYR:HB2	1:I:250:TRP:HE1	1.77	0.49
2:B:389:LEU:HD11	2:B:435:THR:HG22	1.95	0.49
2:B:527:ILE:HG13	2:B:551:TYR:HB2	1.95	0.49
2:C:375:PHE:CD1	2:C:488:LEU:HD12	2.48	0.49
2:A:124:TRP:CB	2:A:128:ARG:HE	2.26	0.49
1:I:101:MET:HA	1:I:135:GLY:O	2.11	0.49
1:I:8:THR:HG23	1:I:37:VAL:HG23	1.94	0.49
2:B:238:ILE:HG22	2:B:238:ILE:O	2.12	0.49
2:A:106:TRP:HB2	2:A:114:VAL:CG2	2.41	0.49
2:B:389:LEU:HD23	2:B:431:ALA:HB1	1.94	0.49
1:J:36:VAL:HG13	1:J:57:GLU:HB2	1.95	0.49
2:A:200:THR:H	2:A:253:HIS:CD2	2.31	0.49
2:B:133:LEU:HB2	2:B:156:PHE:HE2	1.76	0.49
2:C:385:VAL:HG22	2:C:434:ALA:HB1	1.95	0.49
2:B:534:PHE:HE1	2:B:596:LEU:HD11	1.77	0.49
2:C:352:LEU:HD23	2:C:572:TYR:CG	2.48	0.49
2:A:527:ILE:HG13	2:A:551:TYR:HB2	1.95	0.49
2:B:50:LYS:HE2	2:B:180:HIS:CE1	2.47	0.49
2:D:73:VAL:HA	2:D:77:VAL:HB	1.95	0.49
2:A:258:VAL:HG21	2:A:512:TRP:HB2	1.95	0.49
2:A:345:ALA:HA	2:A:568:THR:HG22	1.95	0.48
2:D:48:GLN:HA	2:D:108:ILE:HD13	1.94	0.48
2:B:393:ALA:O	2:B:397:LYS:HB3	2.13	0.48
1:I:36:VAL:HG21	1:I:95:TYR:OH	2.12	0.48
1:J:153:ALA:HB2	1:J:166:ILE:CD1	2.43	0.48
2:B:106:TRP:HB2	2:B:114:VAL:CG2	2.42	0.48
2:B:345:ALA:HA	2:B:568:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:369:PRO:HA	2:D:479:PRO:O	2.13	0.48
2:B:175:VAL:HB	2:B:198:VAL:HG13	1.96	0.48
2:D:137:CYS:SG	2:D:189:CYS:HB3	2.53	0.48
2:A:297:HIS:HB2	2:A:586:ARG:NH1	2.28	0.48
2:B:38:ASN:HB3	2:B:69:THR:HG21	1.95	0.48
2:C:30:PHE:HE2	2:C:162:LEU:HB3	1.79	0.48
2:B:24:LEU:HB2	2:B:27:ALA:HB3	1.95	0.48
2:C:27:ALA:HA	2:C:174:HIS:O	2.12	0.48
2:D:601:LEU:HA	2:D:601:LEU:HD23	1.68	0.48
2:A:534:PHE:HE1	2:A:596:LEU:HD11	1.79	0.48
2:A:174:HIS:HD2	2:A:617:PHE:HE2	1.60	0.48
2:B:276:ILE:HD11	2:B:611:MET:HG3	1.95	0.48
2:D:258:VAL:HG21	2:D:512:TRP:HB2	1.96	0.48
2:D:375:PHE:CE1	2:D:487:PRO:HD2	2.49	0.47
2:A:413:LEU:HD23	2:A:414:PRO:HD2	1.94	0.47
2:A:598:TRP:CZ3	2:A:605:TYR:CE2	3.02	0.47
2:B:32:VAL:O	2:B:179:PHE:HA	2.14	0.47
2:B:598:TRP:CZ3	2:B:605:TYR:CE2	3.02	0.47
2:C:513:GLY:C	2:C:516:PRO:HD2	2.35	0.47
2:D:65:VAL:CG1	2:D:158:THR:HG22	2.44	0.47
2:D:209:LEU:HD23	2:D:229:VAL:HG12	1.96	0.47
2:D:307:PHE:HD1	2:D:488:LEU:HD21	1.77	0.47
2:A:513:GLY:C	2:A:516:PRO:HD2	2.34	0.47
1:I:50:VAL:HG21	1:I:261:LEU:HD23	1.95	0.47
2:B:28:VAL:HA	2:B:61:ASN:HB3	1.97	0.47
2:C:313:TYR:HD2	2:C:437:ARG:HB3	1.78	0.47
2:D:188:LEU:HD11	2:D:252:ALA:HA	1.96	0.47
2:D:332:TYR:HB2	2:D:369:PRO:O	2.13	0.47
2:A:211:ARG:HG3	2:A:509:TYR:HE2	1.78	0.47
2:C:258:VAL:HG21	2:C:512:TRP:HB2	1.96	0.47
2:D:375:PHE:CE2	2:D:488:LEU:HB2	2.50	0.47
1:J:10:THR:HG22	1:J:15:TYR:O	2.14	0.47
2:C:313:TYR:CD1	2:C:382:GLY:HA2	2.40	0.47
2:C:345:ALA:HA	2:C:568:THR:HG22	1.96	0.47
2:D:238:ILE:HG13	2:D:241:ARG:HD2	1.96	0.47
2:C:86:ALA:O	2:C:90:THR:HG23	2.13	0.47
2:B:24:LEU:CB	2:B:27:ALA:HB3	2.45	0.47
2:B:36:VAL:HB	2:B:66:GLY:HA3	1.96	0.47
2:B:114:VAL:HG12	2:B:116:LEU:HG	1.97	0.47
2:B:124:TRP:CB	2:B:128:ARG:HE	2.27	0.47
2:B:365:PHE:HB3	2:B:367:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:HIS:CD2	2:A:201:ILE:HB	2.50	0.47
2:A:509:TYR:O	2:A:510:GLU:C	2.53	0.47
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.79	0.47
2:A:369:PRO:HA	2:A:479:PRO:O	2.14	0.47
2:B:30:PHE:N	2:B:176:VAL:O	2.41	0.47
2:B:495:GLU:HA	2:B:495:GLU:OE1	2.15	0.47
2:B:513:GLY:C	2:B:516:PRO:HD2	2.36	0.47
1:J:9:LEU:HD22	1:J:86:LYS:HB2	1.97	0.47
2:C:394:ASN:HA	2:C:397:LYS:HE2	1.96	0.47
1:I:31:THR:HG21	1:I:35:LEU:HD21	1.97	0.47
2:C:30:PHE:CE2	2:C:162:LEU:HB3	2.50	0.46
2:C:332:TYR:HE1	2:C:477:PHE:CZ	2.34	0.46
2:A:114:VAL:HG12	2:A:116:LEU:HG	1.97	0.46
1:I:36:VAL:HG13	1:I:57:GLU:HB2	1.97	0.46
2:A:27:ALA:HA	2:A:174:HIS:O	2.14	0.46
1:I:117:ARG:HG3	1:I:183:LEU:CD2	2.45	0.46
2:A:378:GLU:HG2	2:A:442:PRO:HD3	1.98	0.46
2:B:174:HIS:HD2	2:B:617:PHE:HE2	1.62	0.46
2:C:202:PHE:O	2:C:202:PHE:CG	2.68	0.46
2:D:106:TRP:HB2	2:D:114:VAL:CG2	2.45	0.46
2:A:495:GLU:OE1	2:A:495:GLU:HA	2.16	0.46
2:B:36:VAL:HG11	2:B:64:LEU:HB3	1.97	0.46
2:D:28:VAL:HA	2:D:61:ASN:HB3	1.97	0.46
2:D:152:VAL:HA	2:D:186:VAL:HG21	1.98	0.46
2:D:548:TYR:HB3	2:D:592:LEU:HD22	1.98	0.46
1:I:10:THR:HG22	1:I:15:TYR:O	2.16	0.46
2:B:125:ALA:HA	2:B:129:TRP:HB2	1.96	0.46
2:B:177:ALA:HB3	2:B:200:THR:HG22	1.98	0.46
1:I:63:VAL:HG12	1:I:70:ALA:HB3	1.97	0.46
2:B:200:THR:H	2:B:253:HIS:HD2	1.62	0.46
2:B:310:GLY:HA2	2:B:386:ARG:HB2	1.98	0.46
2:C:188:LEU:CD1	2:C:202:PHE:HB2	2.46	0.46
2:D:38:ASN:HB3	2:D:69:THR:HG21	1.98	0.46
2:B:416:MET:HG2	2:C:417:ASN:H	1.81	0.45
2:C:307:PHE:CE2	2:C:476:ILE:HG21	2.51	0.45
2:D:51:ALA:HB1	2:D:112:PRO:CG	2.46	0.45
2:A:68:TYR:HD1	2:A:73:VAL:HG21	1.82	0.45
2:B:124:TRP:HB3	2:B:128:ARG:HE	1.81	0.45
2:A:125:ALA:HA	2:A:129:TRP:HB2	1.97	0.45
2:A:343:LEU:HD11	2:A:456:ILE:HG23	1.98	0.45
2:A:372:THR:HG22	2:A:448:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:VAL:HA	2:C:278:THR:O	2.16	0.45
2:C:327:PHE:CZ	2:C:505:PHE:HZ	2.34	0.45
2:D:308:VAL:O	2:D:312:PHE:HD2	2.00	0.45
2:A:28:VAL:HA	2:A:61:ASN:HB3	1.97	0.45
2:A:212:TYR:HB3	2:A:236:ARG:HD3	1.98	0.45
2:A:348:ARG:HD2	2:A:568:THR:HG21	1.98	0.45
2:B:27:ALA:HA	2:B:174:HIS:O	2.16	0.45
2:B:77:VAL:HG11	2:B:116:LEU:HD11	1.98	0.45
2:C:313:TYR:CD2	2:C:437:ARG:HB3	2.51	0.45
2:C:368:MET:HB2	2:C:477:PHE:HE1	1.82	0.45
2:D:115:VAL:HG21	2:D:161:PHE:CE2	2.51	0.45
2:D:231:LYS:O	2:D:235:GLU:HG2	2.17	0.45
2:B:50:LYS:HZ1	2:B:180:HIS:CE1	2.35	0.45
2:C:519:CYS:SG	2:C:524:ILE:HB	2.56	0.45
2:D:607:SER:O	2:D:611:MET:HG2	2.17	0.45
2:B:286:LYS:HG3	2:B:521:VAL:HG12	1.99	0.45
2:C:117:LEU:HD11	2:C:154:PHE:CD1	2.51	0.45
2:B:68:TYR:HD1	2:B:73:VAL:HG21	1.82	0.45
2:C:119:VAL:HG12	2:C:119:VAL:O	2.16	0.45
2:A:312:PHE:HD2	2:A:318:PHE:CZ	2.34	0.45
2:D:401:GLY:HA3	2:A:397:LYS:HD2	1.99	0.45
2:D:489:LEU:HD12	2:D:489:LEU:HA	1.88	0.45
2:B:117:LEU:HD11	2:B:154:PHE:CD1	2.51	0.45
2:C:467:ASN:HB3	2:C:474:LYS:HD3	1.99	0.45
2:A:310:GLY:HA2	2:A:386:ARG:HB2	1.99	0.45
2:C:446:HIS:HB2	2:C:479:PRO:HD2	1.99	0.45
2:A:525:PRO:HD3	2:A:586:ARG:HD2	1.99	0.45
1:I:9:LEU:HD22	1:I:86:LYS:HB2	1.98	0.45
2:D:327:PHE:HZ	2:D:519:CYS:HG	1.65	0.44
2:C:574:PHE:O	2:C:577:GLN:HB2	2.17	0.44
2:A:147:GLU:HG3	2:A:183:LEU:HD13	1.98	0.44
1:J:159:PHE:CB	1:I:203:VAL:HG21	2.48	0.44
2:C:416:MET:O	2:C:417:ASN:HB2	2.18	0.44
2:A:132:GLU:CD	2:A:156:PHE:CE1	2.91	0.44
2:D:23:ASP:OD2	2:D:621:PHE:HB3	2.18	0.44
2:B:68:TYR:CD1	2:B:73:VAL:HG21	2.52	0.44
2:C:509:TYR:O	2:C:510:GLU:C	2.56	0.44
1:I:151:HIS:CE1	1:I:155:GLU:HG3	2.52	0.44
1:J:8:THR:HG23	1:J:37:VAL:HG23	1.98	0.44
2:D:33:ALA:O	2:D:67:PRO:HD3	2.18	0.44
2:D:332:TYR:CE2	2:D:456:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:489:LEU:HD23	2:A:489:LEU:HA	1.87	0.44
1:J:117:ARG:HG3	1:J:183:LEU:CD2	2.48	0.44
2:D:502:LEU:HD12	2:D:525:PRO:HB2	2.00	0.44
2:A:393:ALA:O	2:A:397:LYS:HB3	2.17	0.44
1:J:194:ILE:HB	1:J:201:PHE:HB2	2.00	0.44
2:C:296:LEU:HD13	2:C:296:LEU:HA	1.81	0.44
2:D:258:VAL:O	2:D:279:PRO:HA	2.17	0.44
2:B:348:ARG:HD2	2:B:568:THR:HG21	2.00	0.43
2:C:273:LYS:HE3	2:C:273:LYS:HB3	1.75	0.43
2:D:138:ASN:HB3	1:H:341:ILE:HD12	2.00	0.43
2:D:488:LEU:HD22	2:D:489:LEU:HB2	2.00	0.43
2:A:68:TYR:CD1	2:A:73:VAL:HG21	2.53	0.43
2:A:77:VAL:HG11	2:A:116:LEU:HD11	2.00	0.43
2:D:47:LEU:HD23	2:D:64:LEU:HD22	2.00	0.43
2:D:176:VAL:HA	2:D:199:ALA:O	2.19	0.43
2:A:334:PHE:CE2	2:A:340:ASP:HB3	2.53	0.43
2:C:224:LEU:HD21	2:C:265:GLU:HA	2.00	0.43
2:C:343:LEU:HG	2:C:366:PHE:CZ	2.54	0.43
1:J:120:LEU:HD23	1:J:171:PHE:CZ	2.53	0.43
2:B:200:THR:H	2:B:253:HIS:CD2	2.35	0.43
2:A:400:PHE:CE2	2:A:404:LEU:HD13	2.53	0.43
2:A:515:THR:HG23	2:A:516:PRO:HD3	1.99	0.43
2:B:404:LEU:HD12	2:B:408:LEU:HD13	2.00	0.43
2:D:43:ILE:HD12	2:D:43:ILE:H	1.83	0.43
2:A:375:PHE:CE2	2:A:488:LEU:HB2	2.53	0.43
2:B:509:TYR:O	2:B:510:GLU:C	2.57	0.43
2:C:84:THR:HB	2:C:87:LEU:HB3	2.00	0.43
2:D:117:LEU:HG	2:D:157:LEU:HB3	2.01	0.43
2:D:119:VAL:O	2:D:153:LEU:HD13	2.19	0.43
2:C:573:SER:O	2:C:577:GLN:HG3	2.19	0.43
1:I:37:VAL:HG13	1:I:58:VAL:HG13	2.00	0.43
2:B:151:ALA:HB1	2:B:183:LEU:O	2.19	0.42
2:B:404:LEU:HD13	2:B:414:PRO:HG3	2.01	0.42
2:C:28:VAL:O	2:C:175:VAL:HG13	2.19	0.42
2:C:366:PHE:HD1	2:C:366:PHE:H	1.67	0.42
2:D:394:ASN:O	2:D:398:GLU:HG3	2.19	0.42
1:H:316:VAL:HB	1:H:317:SER:H	1.71	0.42
2:B:258:VAL:CG2	2:B:512:TRP:HB2	2.49	0.42
2:B:525:PRO:HD3	2:B:586:ARG:HD2	2.01	0.42
2:D:581:GLN:HA	2:D:584:ILE:HD12	2.01	0.42
1:J:90:TRP:CZ2	1:J:120:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ALA:HA	2:C:404:LEU:HD23	2.02	0.42
2:C:209:LEU:HD21	2:C:232:GLU:HB2	2.01	0.42
2:C:301:LYS:HG3	2:C:325:TYR:CE2	2.51	0.42
2:C:329:ALA:HA	2:C:367:ILE:O	2.19	0.42
2:C:348:ARG:HD2	2:C:568:THR:HG21	2.01	0.42
2:C:393:ALA:O	2:C:397:LYS:HB3	2.18	0.42
2:C:554:ASP:O	2:C:558:ARG:HD2	2.19	0.42
1:I:185:PHE:HZ	1:I:193:SER:HB3	1.84	0.42
2:B:296:LEU:HD22	2:B:498:ARG:NH2	2.34	0.42
2:C:29:LEU:HD12	2:C:176:VAL:O	2.19	0.42
2:C:498:ARG:HA	2:C:524:ILE:HD11	2.01	0.42
2:C:595:LEU:HD13	2:C:595:LEU:HA	1.93	0.42
2:A:132:GLU:OE2	2:A:156:PHE:HE1	2.03	0.42
2:A:174:HIS:CD2	2:A:613:LEU:HG	2.55	0.42
1:J:128:TRP:CH2	1:I:189:LEU:HD11	2.54	0.42
1:J:40:THR:HA	1:J:61:VAL:O	2.20	0.42
1:J:218:LYS:HD3	1:J:218:LYS:HA	1.78	0.42
2:B:511:PRO:HB2	2:B:512:TRP:H	1.58	0.42
2:C:372:THR:OG1	2:C:446:HIS:HB3	2.20	0.42
2:D:263:ALA:HB1	2:D:274:PRO:HG2	2.00	0.42
1:I:21:VAL:HG11	1:I:249:TRP:CD1	2.55	0.42
1:J:21:VAL:HG11	1:J:249:TRP:CD1	2.55	0.42
2:D:224:LEU:HD12	2:D:224:LEU:HA	1.79	0.42
2:D:246:ARG:HG3	2:D:270:LEU:O	2.19	0.42
2:D:301:LYS:HG3	2:D:325:TYR:HE2	1.84	0.42
2:A:24:LEU:H	2:A:24:LEU:HG	1.69	0.42
2:A:137:CYS:HB2	2:A:139:ILE:HG22	2.02	0.42
2:B:43:ILE:HD12	2:B:43:ILE:H	1.85	0.42
2:C:343:LEU:HD23	2:C:343:LEU:HA	1.96	0.42
2:D:279:PRO:HD2	2:D:601:LEU:HD22	2.02	0.42
2:B:33:ALA:HB2	2:B:180:HIS:HB2	2.01	0.42
2:C:362:VAL:HB	2:C:473:VAL:HG22	2.02	0.42
2:C:580:ARG:HA	2:C:583:ILE:HD12	2.01	0.42
1:I:34:ARG:HE	1:I:34:ARG:HB3	1.65	0.42
1:J:120:LEU:N	1:J:138:VAL:O	2.52	0.41
2:B:375:PHE:HB3	2:B:380:LEU:HG	2.02	0.41
2:C:368:MET:O	2:C:369:PRO:C	2.59	0.41
2:A:154:PHE:O	2:A:158:THR:HG23	2.20	0.41
2:A:258:VAL:CG2	2:A:512:TRP:HB2	2.49	0.41
2:A:598:TRP:HZ3	2:A:605:TYR:CE2	2.38	0.41
1:I:50:VAL:HG22	1:I:264:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:H	2:B:24:LEU:HG	1.72	0.41
2:B:31:GLU:HG3	2:B:62:TYR:HE1	1.85	0.41
2:B:132:GLU:OE2	2:B:156:PHE:HE1	2.02	0.41
2:B:137:CYS:HB2	2:B:139:ILE:HG22	2.02	0.41
2:B:151:ALA:CB	2:B:183:LEU:HB2	2.47	0.41
2:C:166:LEU:HD21	2:C:175:VAL:HG23	2.02	0.41
2:C:507:SER:H	2:C:529:THR:CG2	2.32	0.41
1:I:133:ASN:HB3	1:I:188:ASN:ND2	2.35	0.41
2:C:332:TYR:CE1	2:C:456:ILE:HD13	2.55	0.41
2:C:472:ARG:HE	2:C:472:ARG:HA	1.85	0.41
2:C:538:MET:HE1	2:C:592:LEU:CD1	2.49	0.41
2:C:588:ARG:HH21	2:A:591:ARG:NH2	2.18	0.41
2:D:579:ARG:HD2	2:D:582:ARG:HH21	1.85	0.41
2:B:347:ALA:HB2	2:B:463:ILE:HG13	2.02	0.41
2:B:379:THR:HG22	2:B:488:LEU:HD22	2.01	0.41
2:C:106:TRP:CD2	2:C:108:ILE:HG12	2.55	0.41
2:A:43:ILE:HD12	2:A:43:ILE:H	1.85	0.41
2:A:51:ALA:HB3	2:A:108:ILE:CD1	2.51	0.41
2:A:595:LEU:HD13	2:A:595:LEU:HA	1.92	0.41
1:I:218:LYS:HB3	1:I:219:PRO:HD2	2.02	0.41
1:J:194:ILE:HG12	1:J:195:PHE:N	2.35	0.41
2:B:51:ALA:HB3	2:B:108:ILE:CD1	2.50	0.41
2:B:284:VAL:HG12	2:B:287:PHE:CD2	2.56	0.41
2:C:258:VAL:CG2	2:C:512:TRP:HB2	2.50	0.41
2:C:276:ILE:HD13	2:C:608:ALA:HA	2.02	0.41
2:D:258:VAL:CG2	2:D:512:TRP:HB2	2.51	0.41
2:B:36:VAL:HG22	2:B:47:LEU:HD22	2.03	0.41
2:B:132:GLU:CD	2:B:156:PHE:CE1	2.91	0.41
2:D:375:PHE:CE2	2:D:488:LEU:CB	3.04	0.41
2:D:537:PHE:CE2	2:D:595:LEU:HD23	2.56	0.41
2:A:200:THR:H	2:A:253:HIS:HD2	1.68	0.41
1:I:257:VAL:O	1:I:260:LEU:N	2.54	0.41
2:D:313:TYR:CD1	2:D:385:VAL:HG21	2.55	0.41
2:B:489:LEU:HD12	2:B:489:LEU:HA	1.94	0.41
2:C:122:SER:HA	2:C:153:LEU:HD11	2.03	0.41
2:C:343:LEU:HD13	2:C:459:THR:HB	2.02	0.41
2:D:36:VAL:HG11	2:D:64:LEU:O	2.21	0.41
2:D:448:MET:HB3	2:D:448:MET:HE3	1.88	0.41
2:D:592:LEU:HD12	2:D:592:LEU:HA	1.69	0.41
2:B:30:PHE:O	2:B:178:HIS:N	2.37	0.41
2:B:106:TRP:CD2	2:B:108:ILE:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LEU:HD23	2:B:323:THR:HG21	2.02	0.41
2:C:34:TRP:CD2	2:C:67:PRO:HG3	2.55	0.41
2:C:70:GLU:HG3	2:C:71:GLN:N	2.35	0.41
2:D:78:GLU:HB2	2:D:107:LEU:HD21	2.02	0.41
2:D:515:THR:OG1	2:D:516:PRO:HD3	2.20	0.41
2:A:31:GLU:HG2	2:A:178:HIS:HB3	2.03	0.41
2:A:117:LEU:HD11	2:A:154:PHE:CD1	2.54	0.41
2:B:174:HIS:CD2	2:B:613:LEU:HG	2.56	0.41
2:C:99:CYS:SG	2:C:160:TRP:HZ3	2.44	0.41
2:D:361:THR:HG23	2:D:472:ARG:O	2.21	0.41
2:D:488:LEU:C	2:D:488:LEU:HD23	2.41	0.41
2:A:106:TRP:CD2	2:A:108:ILE:HG12	2.56	0.41
2:D:313:TYR:HD1	2:D:385:VAL:HG21	1.86	0.40
1:I:194:ILE:HD12	1:I:242:HIS:HB2	2.02	0.40
1:J:224:TYR:CE1	1:J:254:THR:HG21	2.56	0.40
2:B:267:GLN:HG2	2:B:273:LYS:HG2	2.03	0.40
2:C:580:ARG:HH22	2:A:284:VAL:HG21	1.86	0.40
2:A:32:VAL:N	2:A:178:HIS:O	2.50	0.40
2:A:149:ASN:O	2:A:152:VAL:HG22	2.21	0.40
2:A:333:GLU:HG2	2:A:336:ASN:HB2	2.02	0.40
2:C:64:LEU:HD12	2:C:64:LEU:N	2.36	0.40
2:C:258:VAL:O	2:C:279:PRO:HA	2.21	0.40
2:D:35:GLU:HB3	2:D:44:TYR:HB2	2.04	0.40
2:A:30:PHE:HA	2:A:63:PHE:O	2.22	0.40
2:A:463:ILE:CG2	2:A:465:LEU:HG	2.51	0.40
1:J:201:PHE:O	1:J:205:GLY:N	2.54	0.40
1:J:203:VAL:HG21	1:I:159:PHE:HB3	2.03	0.40
2:B:154:PHE:O	2:B:158:THR:HG23	2.22	0.40
2:B:595:LEU:HD13	2:B:595:LEU:HA	1.93	0.40
2:D:106:TRP:CD2	2:D:108:ILE:HG12	2.56	0.40
2:D:155:GLY:HA3	2:D:186:VAL:HB	2.03	0.40
2:D:393:ALA:HA	2:A:404:LEU:HD23	2.03	0.40
2:A:320:LEU:HD23	2:A:323:THR:HG21	2.03	0.40
2:B:296:LEU:HD22	2:B:498:ARG:HH21	1.85	0.40
2:C:43:ILE:HD12	2:C:43:ILE:H	1.86	0.40
2:C:192:ARG:HD2	2:C:192:ARG:HA	1.77	0.40
2:D:154:PHE:O	2:D:158:THR:HG23	2.21	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	E	33/352 (9%)	31 (94%)	2 (6%)	0	100	100
1	F	33/352 (9%)	30 (91%)	3 (9%)	0	100	100
1	G	32/352 (9%)	29 (91%)	3 (9%)	0	100	100
1	H	32/352 (9%)	28 (88%)	4 (12%)	0	100	100
1	I	265/352 (75%)	253 (96%)	12 (4%)	0	100	100
1	J	257/352 (73%)	247 (96%)	10 (4%)	0	100	100
2	A	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
2	B	598/634 (94%)	583 (98%)	14 (2%)	1 (0%)	47	80
2	C	596/634 (94%)	572 (96%)	23 (4%)	1 (0%)	47	80
2	D	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
All	All	3040/4648 (65%)	2947 (97%)	91 (3%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	511	PRO
2	C	369	PRO

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	E	31/311 (10%)	28 (90%)	3 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	31/311 (10%)	28 (90%)	3 (10%)	8	34
1	G	30/311 (10%)	27 (90%)	3 (10%)	7	33
1	H	30/311 (10%)	27 (90%)	3 (10%)	7	33
1	I	233/311 (75%)	227 (97%)	6 (3%)	46	74
1	J	229/311 (74%)	219 (96%)	10 (4%)	28	62
2	A	511/545 (94%)	489 (96%)	22 (4%)	29	62
2	B	505/545 (93%)	485 (96%)	20 (4%)	31	64
2	C	501/545 (92%)	482 (96%)	19 (4%)	33	65
2	D	499/545 (92%)	478 (96%)	21 (4%)	30	63
All	All	2600/4046 (64%)	2490 (96%)	110 (4%)	33	63

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	90	TRP
1	J	120	LEU
1	J	163	ASP
1	J	189	LEU
1	J	194	ILE
1	J	198	LEU
1	J	232	LYS
1	J	241	THR
1	J	242	HIS
1	J	261	LEU
2	B	24	LEU
2	B	28	VAL
2	B	47	LEU
2	B	71	GLN
2	B	79	LEU
2	B	108	ILE
2	B	166	LEU
2	B	171	GLU
2	B	214	CYS
2	B	292	GLU
2	B	319	ASN
2	B	367	ILE
2	B	408	LEU
2	B	432	ILE
2	B	445	THR

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Mol	Chain	Res	Type
2	B	463	ILE
2	B	479	PRO
2	B	492	ASP
2	B	515	THR
2	B	553	LEU
2	C	24	LEU
2	C	47	LEU
2	C	87	LEU
2	C	91	LEU
2	C	108	ILE
2	C	143	TRP
2	C	214	CYS
2	C	242	TYR
2	C	296	LEU
2	C	315	HIS
2	C	316	LEU
2	C	323	THR
2	C	372	THR
2	C	420	LEU
2	C	457	LEU
2	C	491	VAL
2	C	561	ASP
2	C	617	PHE
2	C	619	GLU
2	D	28	VAL
2	D	36	VAL
2	D	47	LEU
2	D	58	TRP
2	D	108	ILE
2	D	138	ASN
2	D	188	LEU
2	D	204	THR
2	D	208	LEU
2	D	230	ASP
2	D	272	ARG
2	D	332	TYR
2	D	372	THR
2	D	457	LEU
2	D	491	VAL
2	D	495	GLU
2	D	529	THR
2	D	540	GLU

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Mol	Chain	Res	Type
2	D	592	LEU
2	D	595	LEU
2	D	609	ARG
2	A	24	LEU
2	A	28	VAL
2	A	47	LEU
2	A	71	GLN
2	A	79	LEU
2	A	108	ILE
2	A	166	LEU
2	A	171	GLU
2	A	176	VAL
2	A	214	CYS
2	A	287	PHE
2	A	295	ASN
2	A	319	ASN
2	A	374	ASN
2	A	380	LEU
2	A	404	LEU
2	A	425	PHE
2	A	429	LYS
2	A	463	ILE
2	A	489	LEU
2	A	515	THR
2	A	553	LEU
1	E	316	VAL
1	E	317	SER
1	E	348	TYR
1	I	90	TRP
1	I	120	LEU
1	I	189	LEU
1	I	193	SER
1	I	194	ILE
1	I	233	SER
1	F	316	VAL
1	F	317	SER
1	F	348	TYR
1	G	316	VAL
1	G	317	SER
1	G	348	TYR
1	H	316	VAL
1	H	317	SER

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Mol	Chain	Res	Type
1	H	348	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	140	GLN
2	B	95	ASN
2	B	138	ASN
2	B	174	HIS
2	B	180	HIS
2	B	205	HIS
2	B	253	HIS
2	B	260	GLN
2	B	336	ASN
2	B	388	GLN
2	B	438	GLN
2	B	530	ASN
2	B	576	GLN
2	B	587	ASN
2	C	95	ASN
2	C	138	ASN
2	C	205	HIS
2	C	240	HIS
2	C	280	ASN
2	C	283	ASN
2	C	295	ASN
2	C	299	GLN
2	C	388	GLN
2	C	436	GLN
2	D	138	ASN
2	D	280	ASN
2	D	305	GLN
2	D	336	ASN
2	D	360	GLN
2	D	436	GLN
2	D	447	ASN
2	D	581	GLN
2	D	620	HIS
2	A	174	HIS
2	A	178	HIS
2	A	205	HIS
2	A	253	HIS

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Mol	Chain	Res	Type
2	A	260	GLN
2	A	299	GLN
2	A	388	GLN
2	A	417	ASN
2	A	530	ASN
2	A	576	GLN
2	A	587	ASN
2	A	620	HIS
1	E	350	GLN
1	I	140	GLN
1	I	164	GLN
1	F	350	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

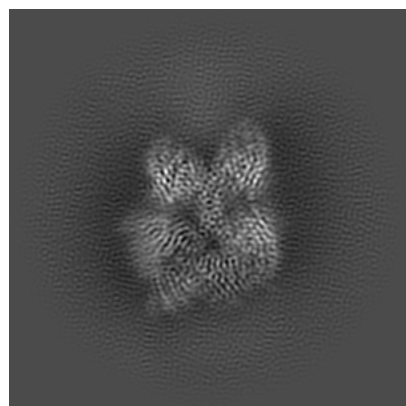
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27022. These allow visual inspection of the internal detail of the map and identification of artifacts.

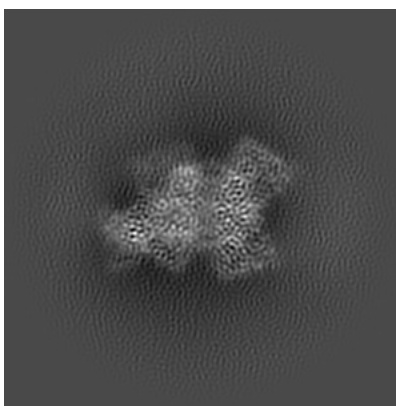
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

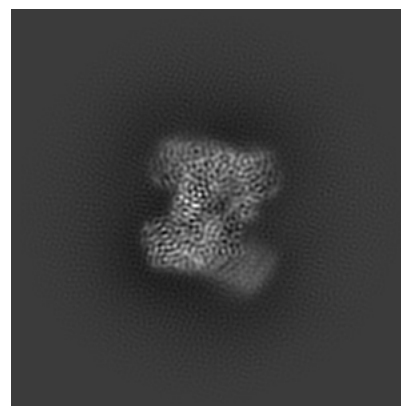
6.1.1 Primary map



X

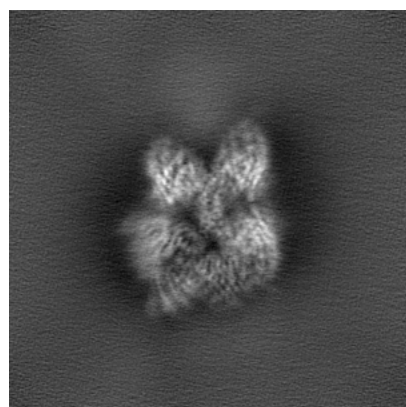


Y

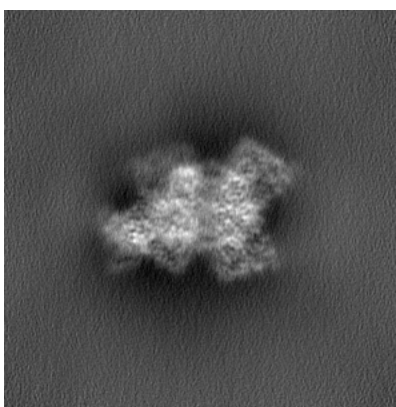


Z

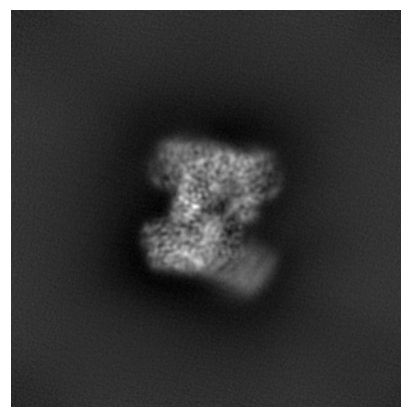
6.1.2 Raw map



X



Y

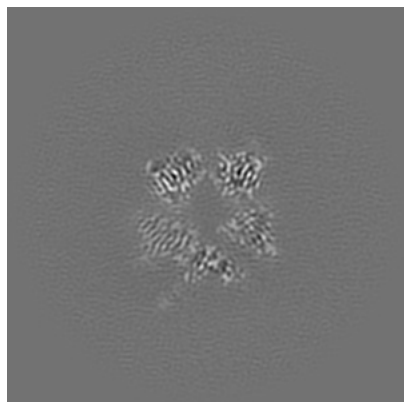


Z

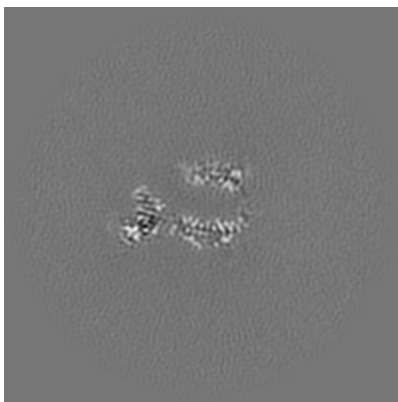
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

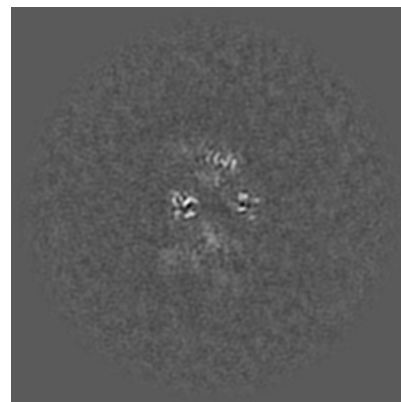
6.2.1 Primary map



X Index: 162

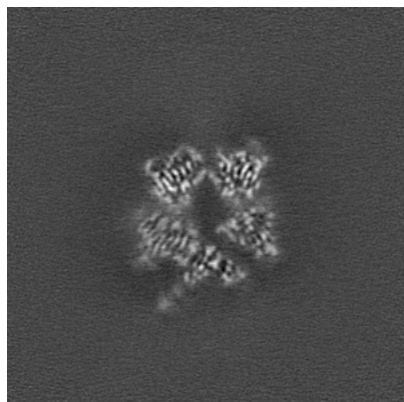


Y Index: 162

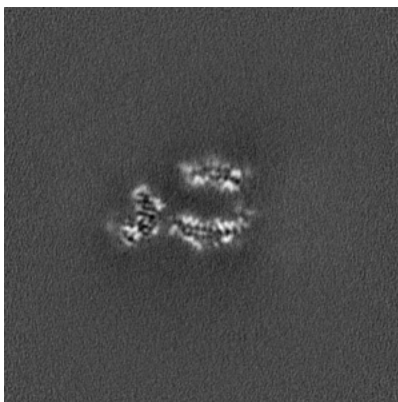


Z Index: 162

6.2.2 Raw map



X Index: 162



Y Index: 162

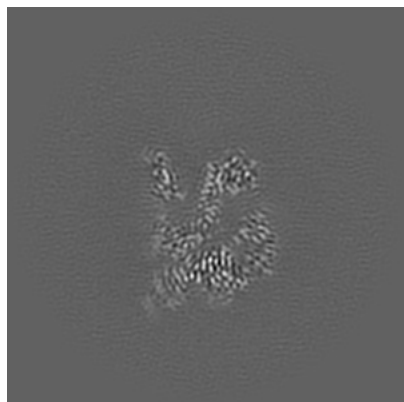


Z Index: 162

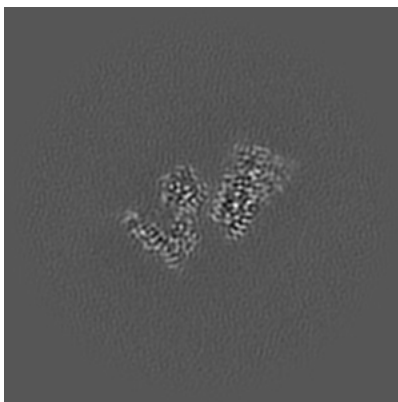
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

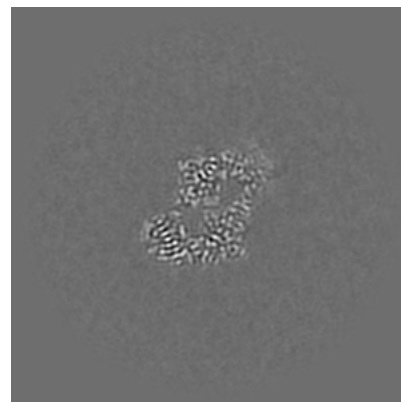
6.3.1 Primary map



X Index: 147

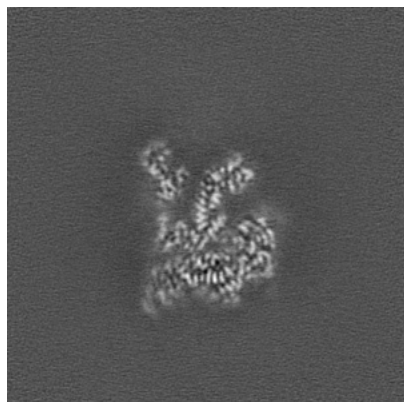


Y Index: 195

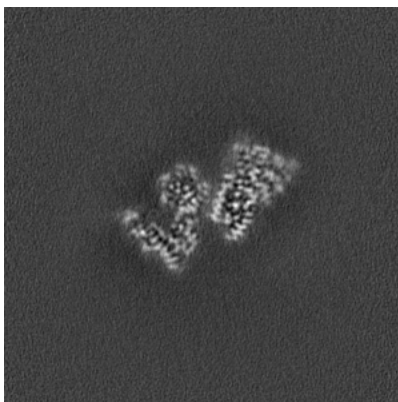


Z Index: 186

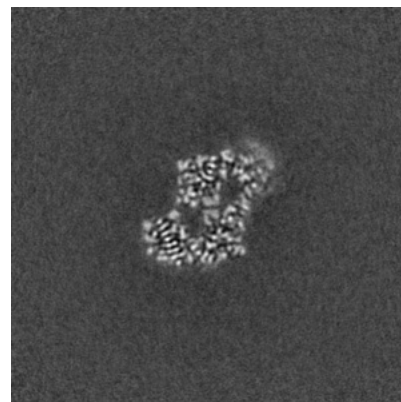
6.3.2 Raw map



X Index: 142



Y Index: 195

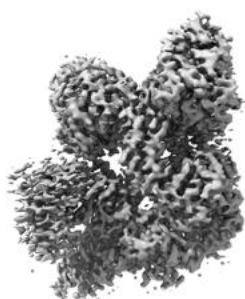


Z Index: 187

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

6.4 Orthogonal surface views [i](#)

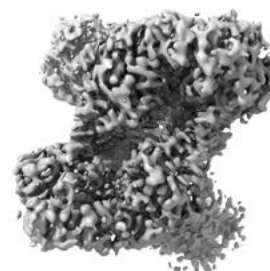
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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.

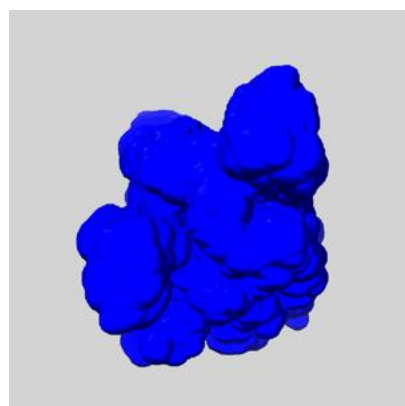
6.5 Mask visualisation [i](#)

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

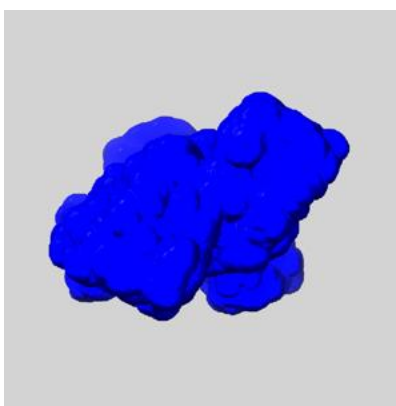
A mask typically either:

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

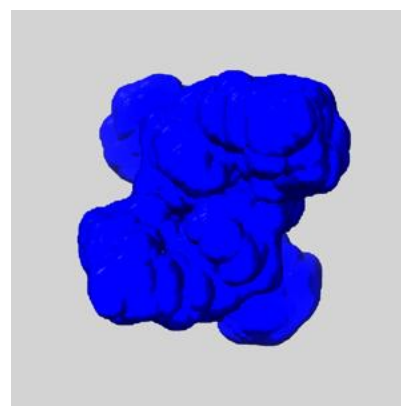
6.5.1 emd_27022_msk_1.map [i](#)



X



Y

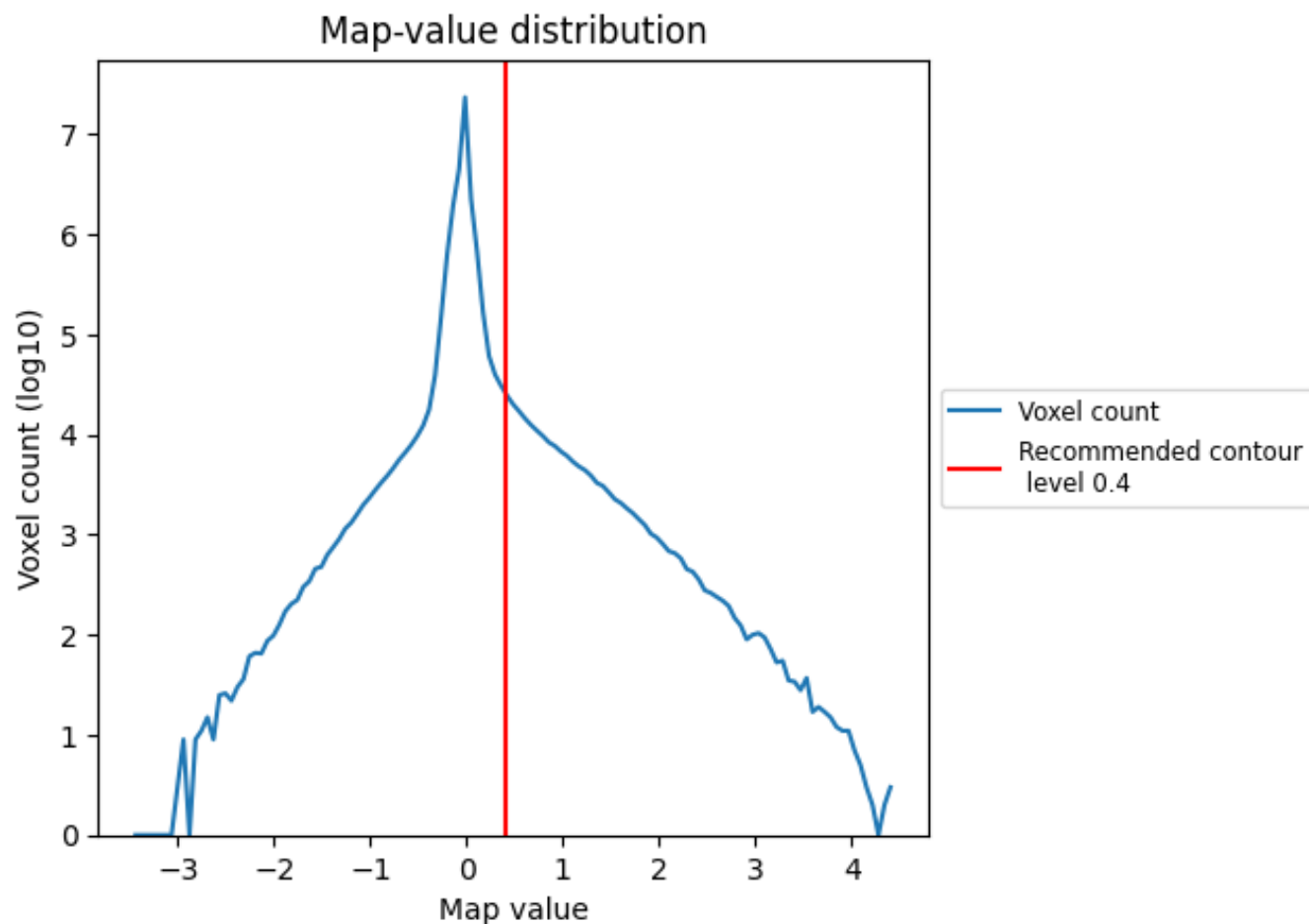


Z

7 Map analysis [i](#)

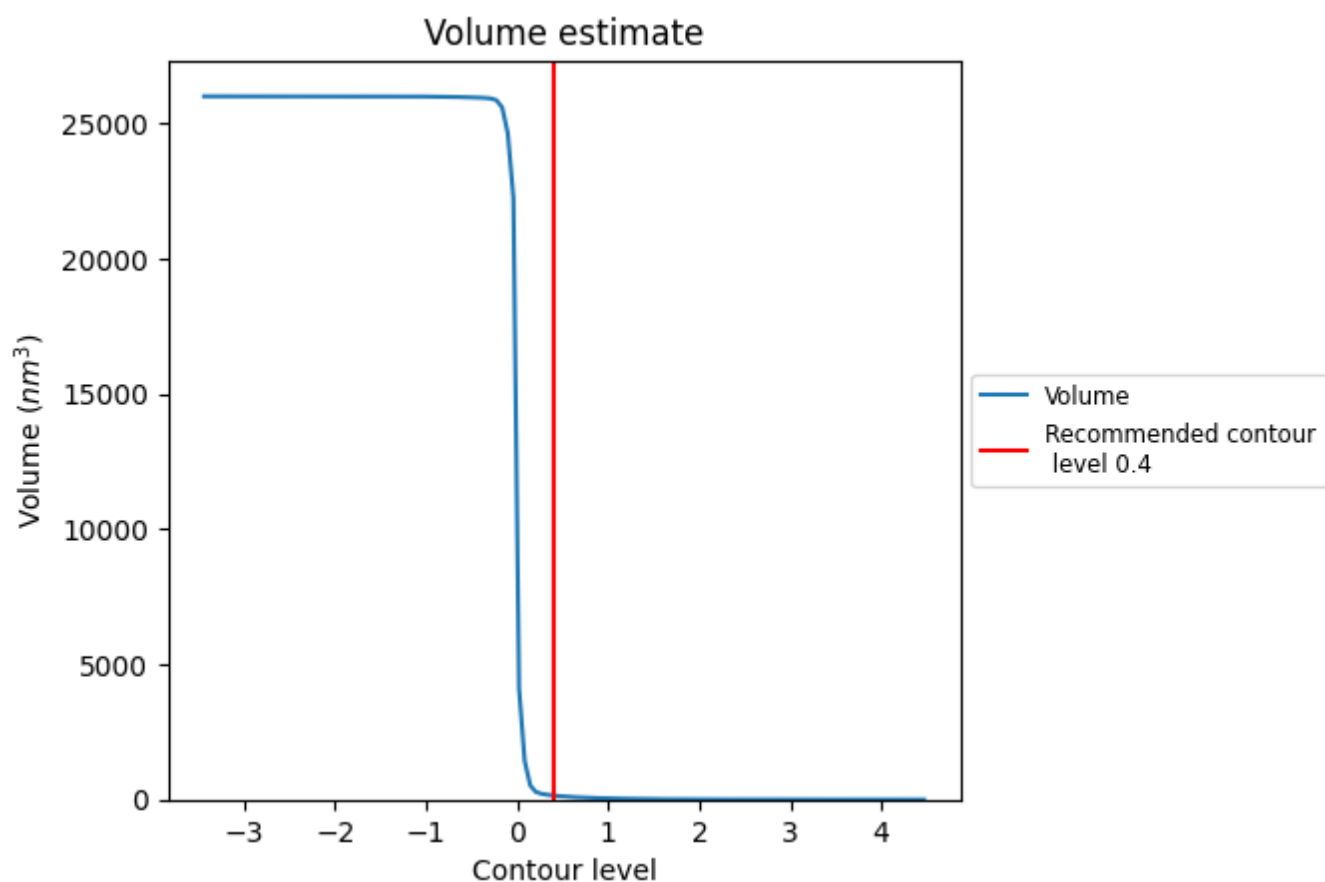
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

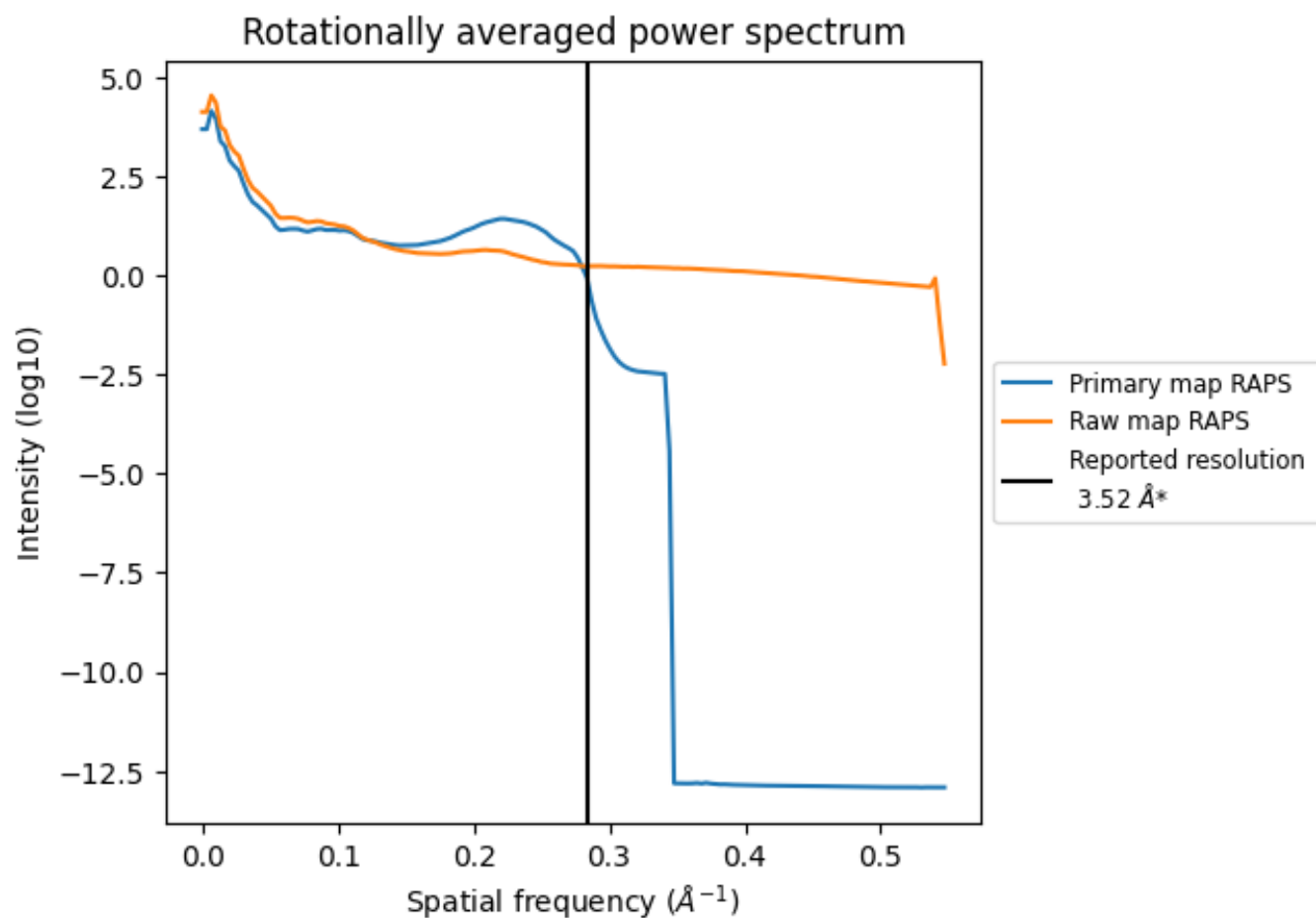
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

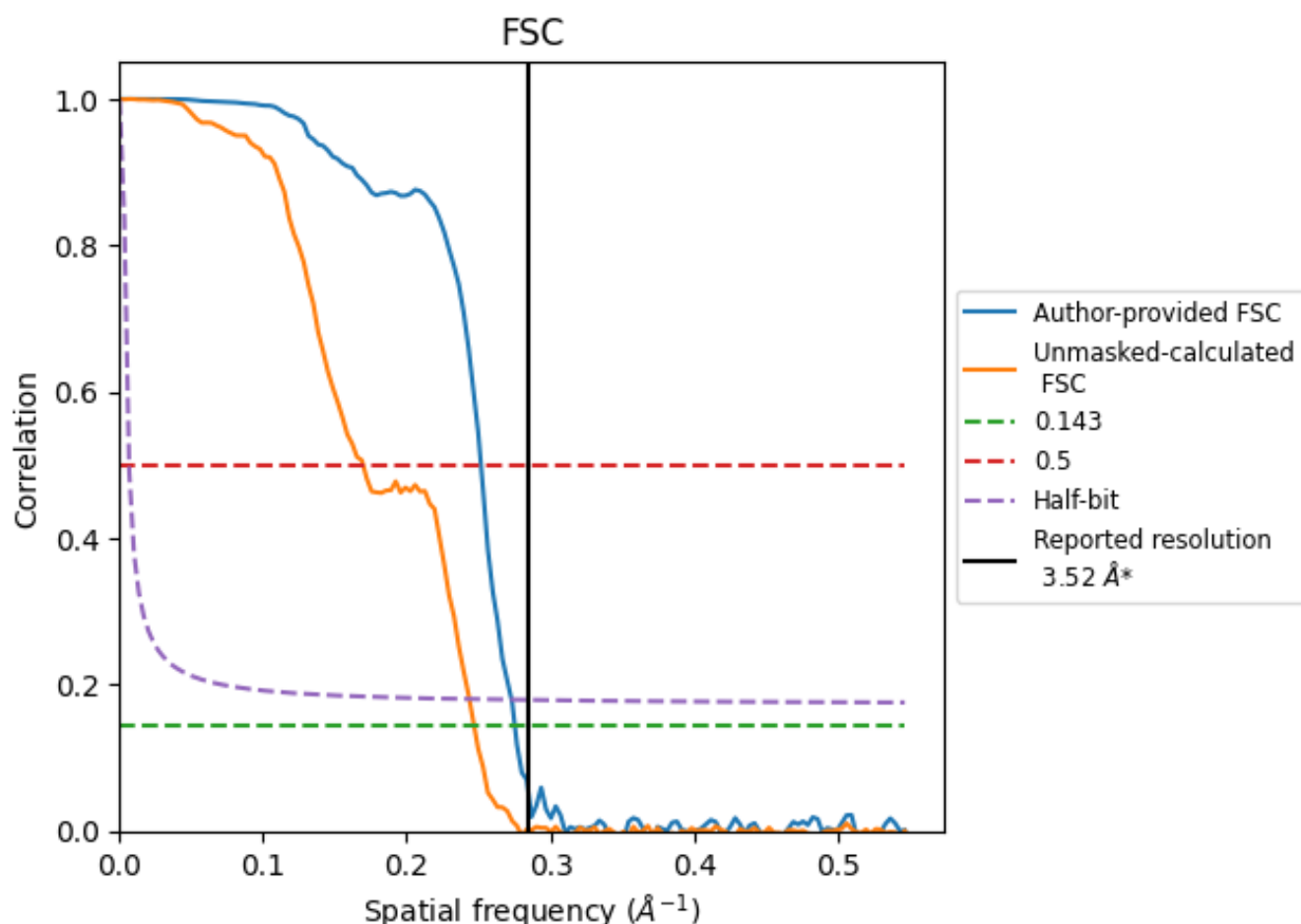


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

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 0.284 \AA^{-1}

8.2 Resolution estimates [i](#)

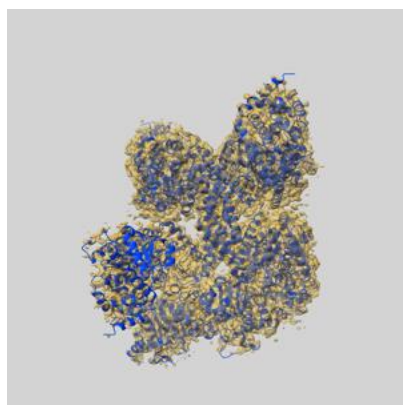
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.63	3.97	3.66
Unmasked-calculated*	4.05	5.89	4.11

*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 4.05 differs from the reported value 3.52 by more than 10 %

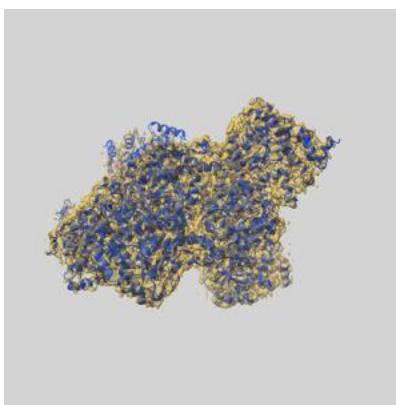
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27022 and PDB model 8CVZ. Per-residue inclusion information can be found in section 3 on page 6.

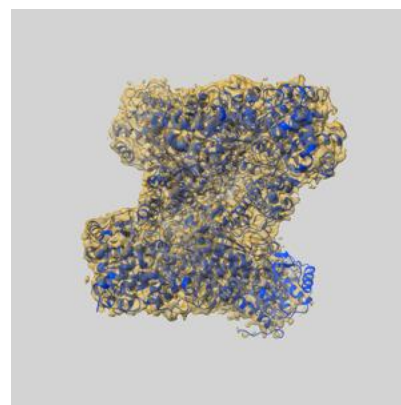
9.1 Map-model overlay [i](#)



X



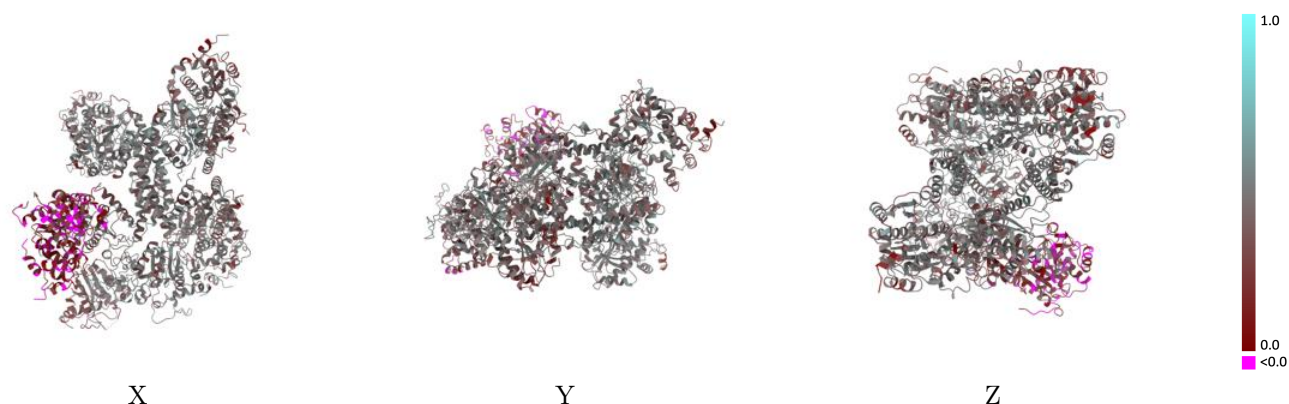
Y



Z

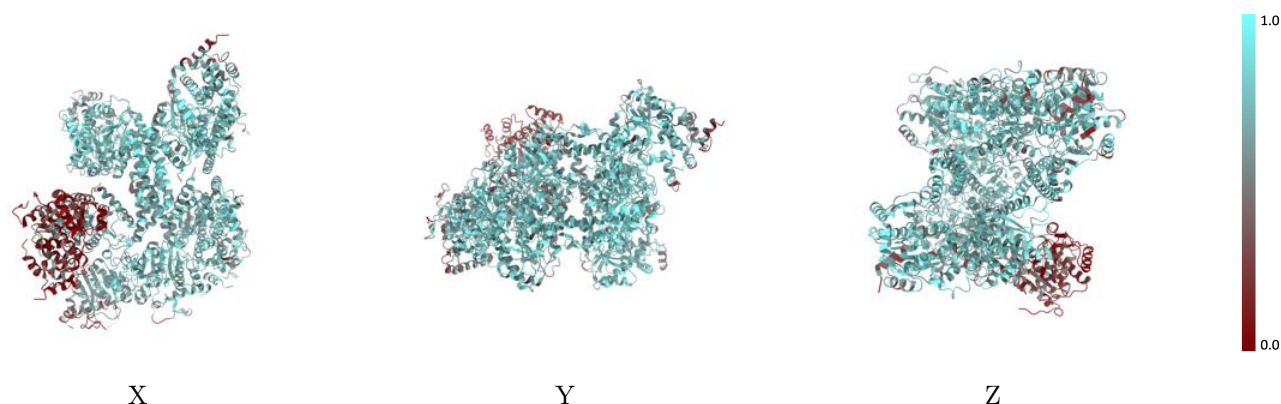
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



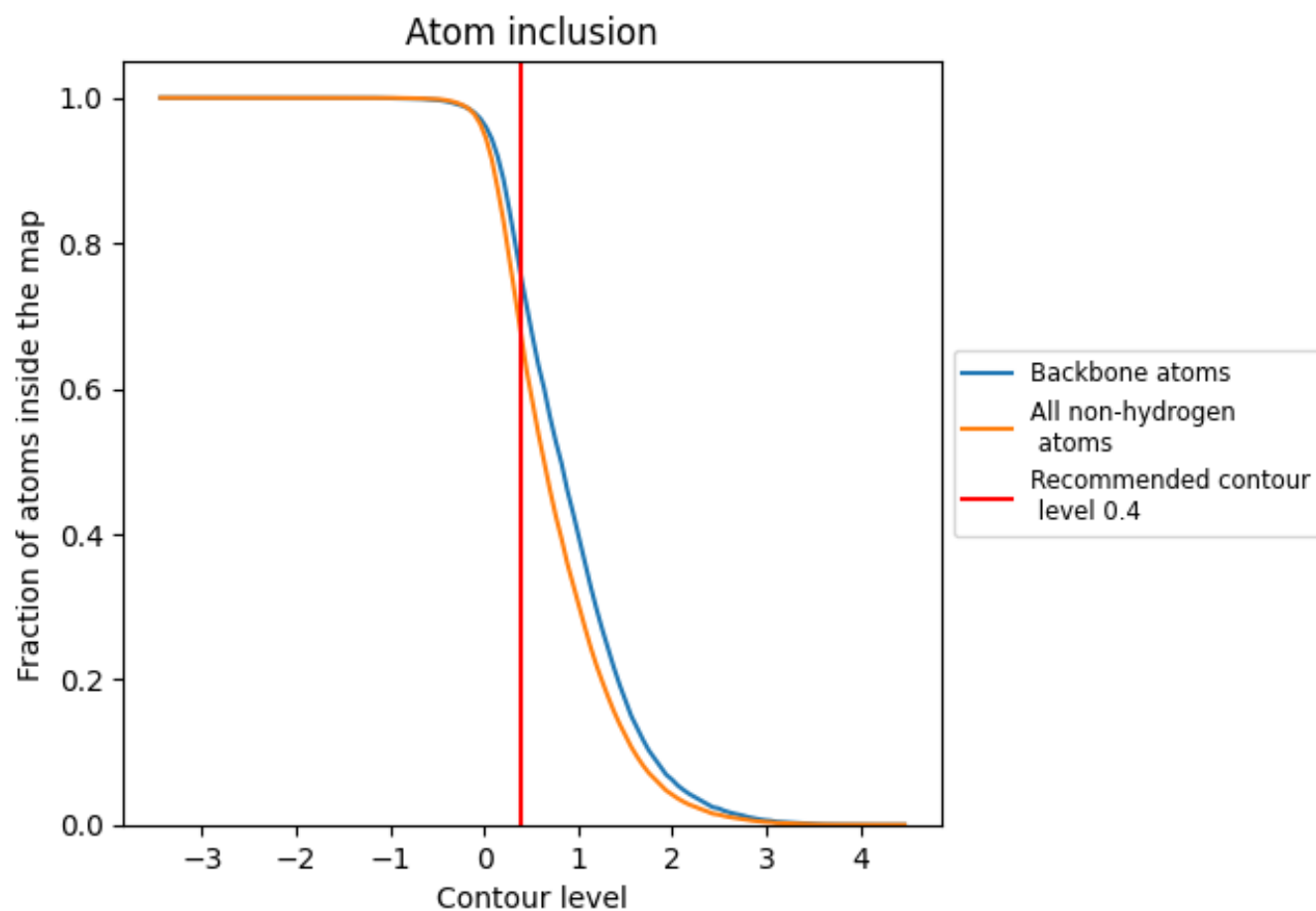
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6671	<div></div> 0.3830
A	<div></div> 0.7327	<div></div> 0.4090
B	<div></div> 0.4567	<div></div> 0.2430
C	<div></div> 0.7592	<div></div> 0.4390
D	<div></div> 0.7821	<div></div> 0.4470
E	<div></div> 0.6853	<div></div> 0.4090
F	<div></div> 0.1503	<div></div> 0.0810
G	<div></div> 0.4312	<div></div> 0.2730
H	<div></div> 0.5435	<div></div> 0.3190
I	<div></div> 0.7514	<div></div> 0.4560
J	<div></div> 0.5579	<div></div> 0.3550

1.0

0.0

<0.0