Full wwPDB EM Validation Report ⓘ

Oct 20, 2026 – 06:08 pm BST

PDB ID	:	34BQ / pdb_000034bq
EMDB ID	:	EMD-59745
Title	:	Cryo-EM structure of yeast EMC:Spf1 insertase:dislocase complex in digitonin
Authors	:	Klose, C.J.; Prabu, J.R.; Schulman, B.A.
Deposited on	:	2026-09-07
Resolution	:	4.20 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:

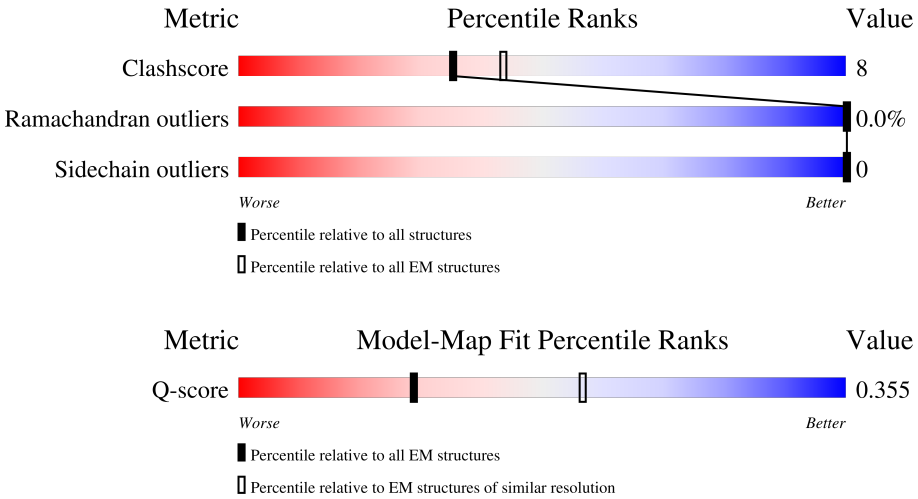
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 4.20 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	5410 (3.70 - 4.70)

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 <=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	760	77% 15% 8%
2	B	292	75% 25%
3	C	253	25% 68% 11% 21%
4	D	190	19% 62% 21% 18%

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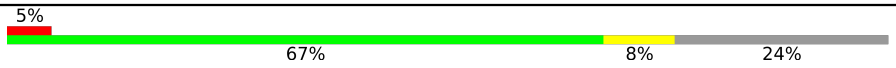
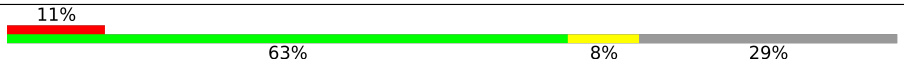
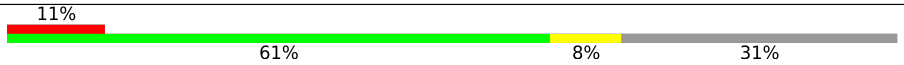
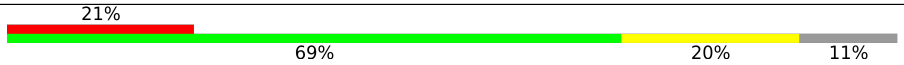
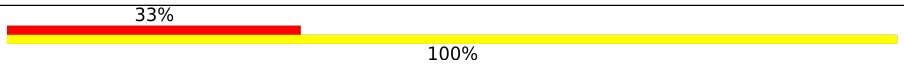
Mol	Chain	Length	Quality of chain
5	E	169	
6	F	108	
7	G	234	
8	H	205	
9	I	1227	
10	Z	3	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 23389 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 ER membrane protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	697	5432	3507	889	1023	13	0	0

- Molecule 2 is a protein called ER membrane protein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	292	2360	1516	379	453	12	0	0

- Molecule 3 is a protein called ER membrane protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	200	1534	1005	247	269	13	0	0

- Molecule 4 is a protein called ER membrane protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	156	1184	776	195	204	9	0	0

- Molecule 5 is a protein called ER membrane protein complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	128	1007	659	161	184	3	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	142	TRP	-	expression tag	UNP P40540
E	143	SER	-	expression tag	UNP P40540
E	144	HIS	-	expression tag	UNP P40540

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Chain	Residue	Modelled	Actual	Comment	Reference
E	145	PRO	-	expression tag	UNP P40540
E	146	GLN	-	expression tag	UNP P40540
E	147	PHE	-	expression tag	UNP P40540
E	148	GLU	-	expression tag	UNP P40540
E	149	LYS	-	expression tag	UNP P40540
E	150	GLY	-	expression tag	UNP P40540
E	151	GLY	-	expression tag	UNP P40540
E	152	GLY	-	expression tag	UNP P40540
E	153	SER	-	expression tag	UNP P40540
E	154	GLY	-	expression tag	UNP P40540
E	155	GLY	-	expression tag	UNP P40540
E	156	GLY	-	expression tag	UNP P40540
E	157	SER	-	expression tag	UNP P40540
E	158	GLY	-	expression tag	UNP P40540
E	159	GLY	-	expression tag	UNP P40540
E	160	SER	-	expression tag	UNP P40540
E	161	ALA	-	expression tag	UNP P40540
E	162	TRP	-	expression tag	UNP P40540
E	163	SER	-	expression tag	UNP P40540
E	164	HIS	-	expression tag	UNP P40540
E	165	PRO	-	expression tag	UNP P40540
E	166	GLN	-	expression tag	UNP P40540
E	167	PHE	-	expression tag	UNP P40540
E	168	GLU	-	expression tag	UNP P40540
E	169	LYS	-	expression tag	UNP P40540

- Molecule 6 is a protein called ER membrane protein complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			813	549	126	136	2		

- Molecule 7 is a protein called Protein SOP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	167	Total	C	N	O	S	0	0
			1329	852	223	250	4		

- Molecule 8 is a protein called Endoplasmic reticulum membrane protein complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	142	Total	C	N	O	S	0	0
			1052	656	167	225	4		

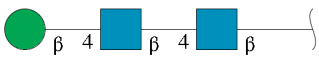
- Molecule 9 is a protein called Endoplasmic reticulum transmembrane helix translocase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1086	Total	C	N	O	S	0	0
			8484	5488	1386	1574	36		

There are 12 discrepancies between the modelled and reference sequences:

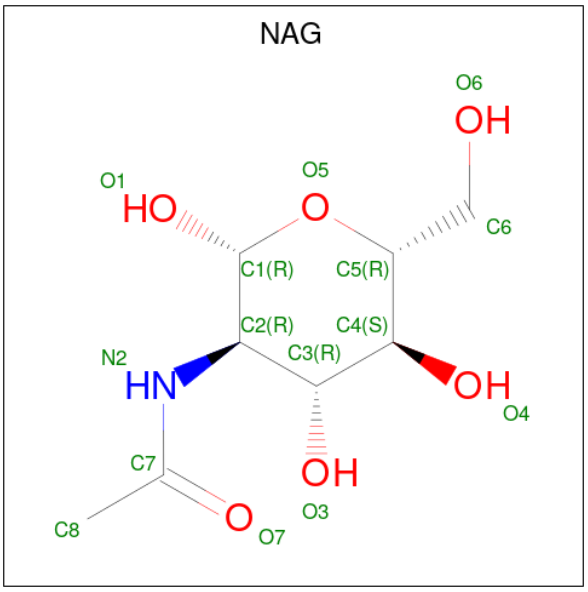
Chain	Residue	Modelled	Actual	Comment	Reference
I	1216	GLY	-	expression tag	UNP P39986
I	1217	SER	-	expression tag	UNP P39986
I	1218	SER	-	expression tag	UNP P39986
I	1219	GLY	-	expression tag	UNP P39986
I	1220	ASP	-	expression tag	UNP P39986
I	1221	TYR	-	expression tag	UNP P39986
I	1222	LYS	-	expression tag	UNP P39986
I	1223	ASP	-	expression tag	UNP P39986
I	1224	ASP	-	expression tag	UNP P39986
I	1225	ASP	-	expression tag	UNP P39986
I	1226	ASP	-	expression tag	UNP P39986
I	1227	LYS	-	expression tag	UNP P39986

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



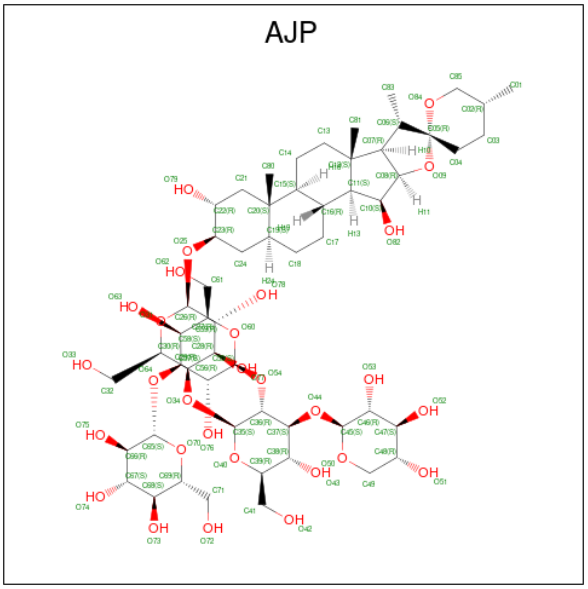
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O 14 8 1 5	0
11	A	1	Total C N O 14 8 1 5	0
11	A	1	Total C N O 14 8 1 5	0
11	G	1	Total C N O 14 8 1 5	0
11	G	1	Total C N O 14 8 1 5	0

- Molecule 12 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



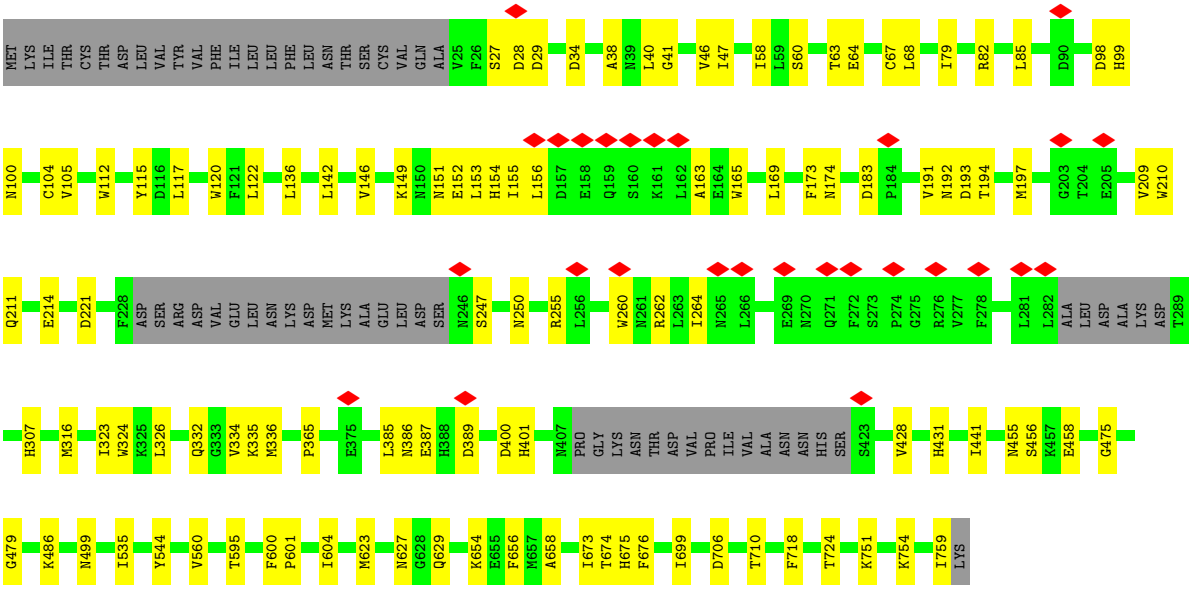
Mol	Chain	Residues	Atoms			AltConf
12	I	1	Total	C	O	0
			85	56	29	

3 Residue-property plots (i)

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

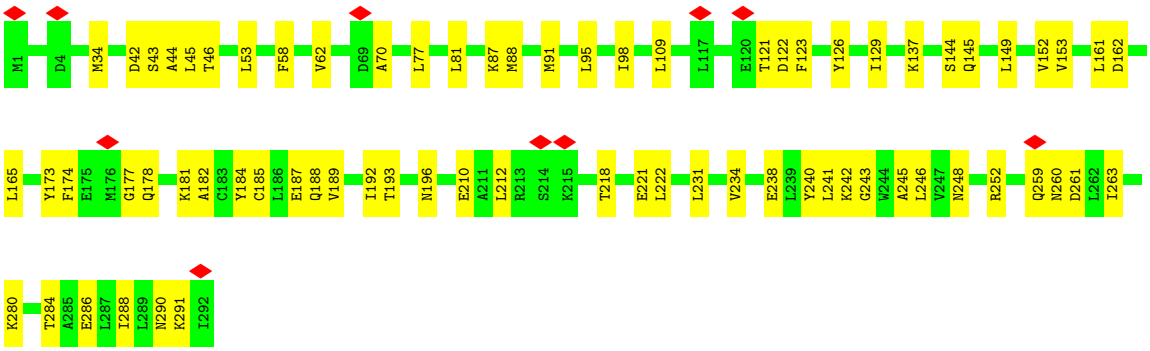
• Molecule 1: ER membrane protein complex subunit 1

Chain A:



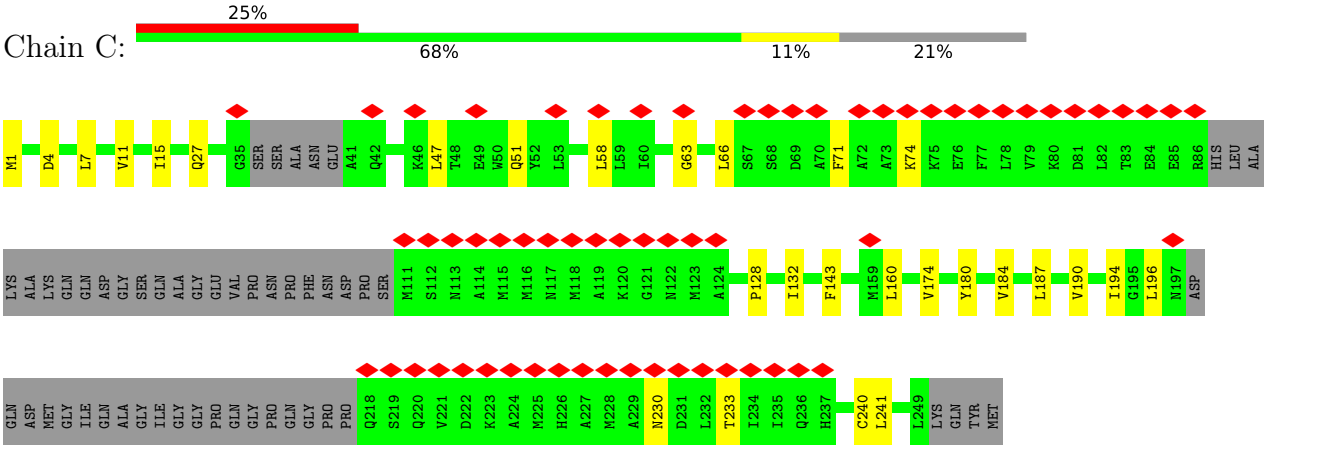
• Molecule 2: ER membrane protein complex subunit 2

Chain B:



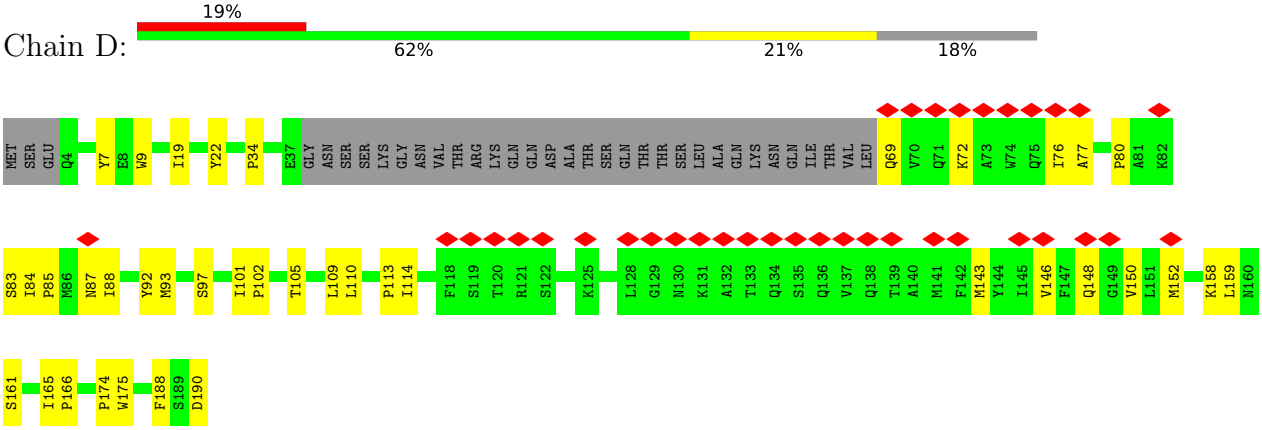
• Molecule 3: ER membrane protein complex subunit 3

Chain C:



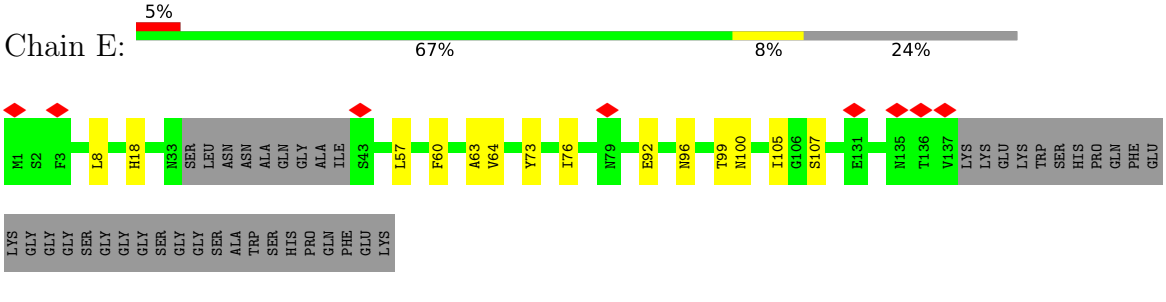
• Molecule 4: ER membrane protein complex subunit 4

Chain D:



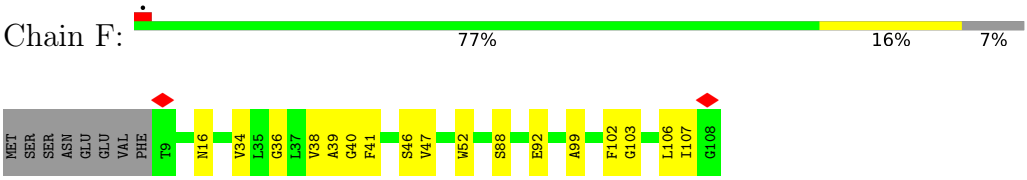
• Molecule 5: ER membrane protein complex subunit 5

Chain E:



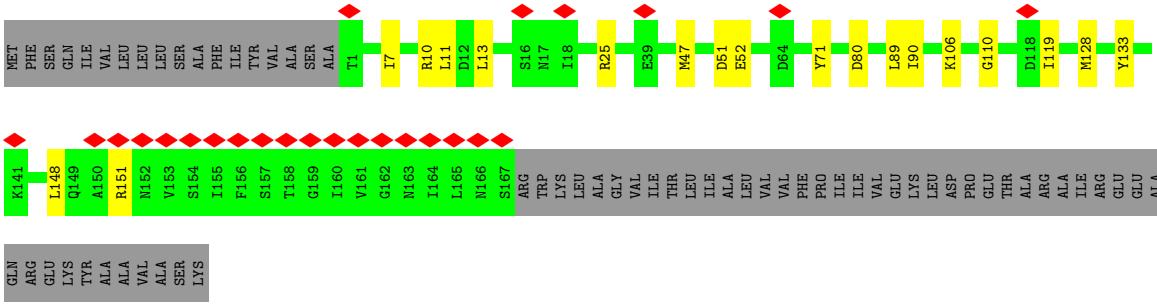
• Molecule 6: ER membrane protein complex subunit 6

Chain F:



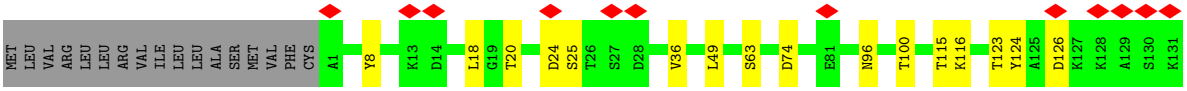
• Molecule 7: Protein SOP4

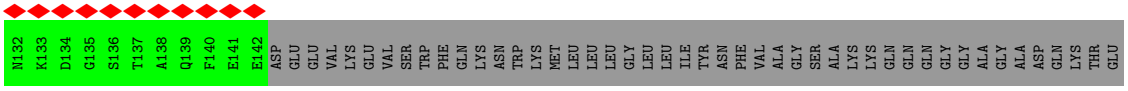
Chain G:



• Molecule 8: Endoplasmic reticulum membrane protein complex subunit 10

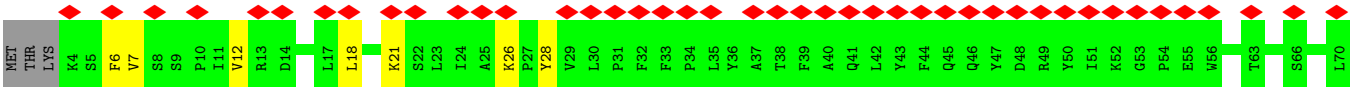
Chain H:

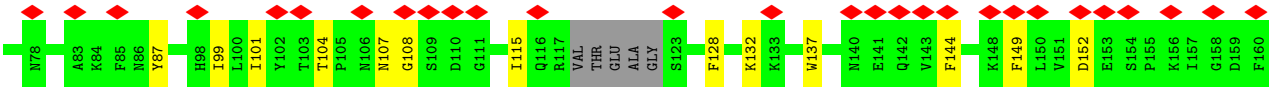


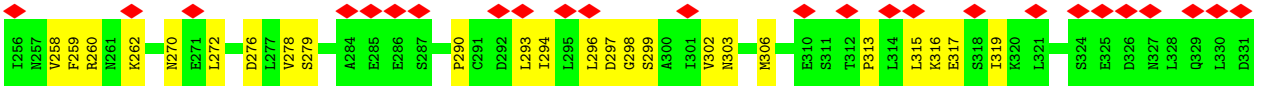


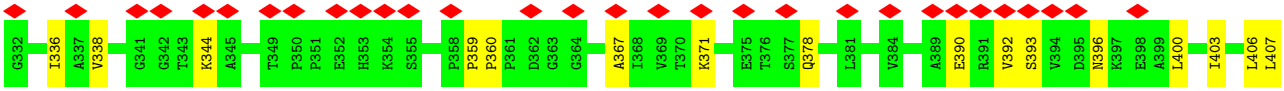
• Molecule 9: Endoplasmic reticulum transmembrane helix translocase

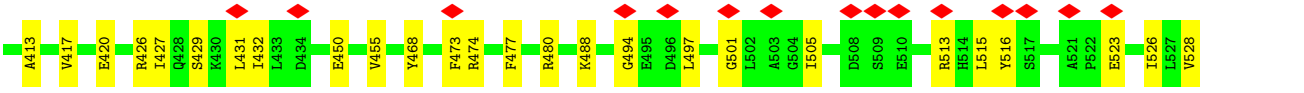
Chain I:

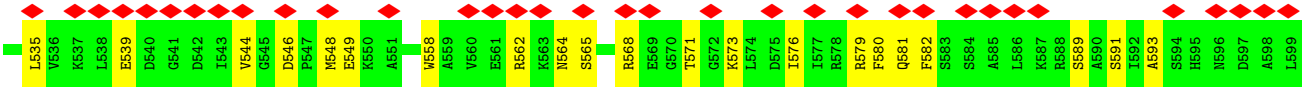


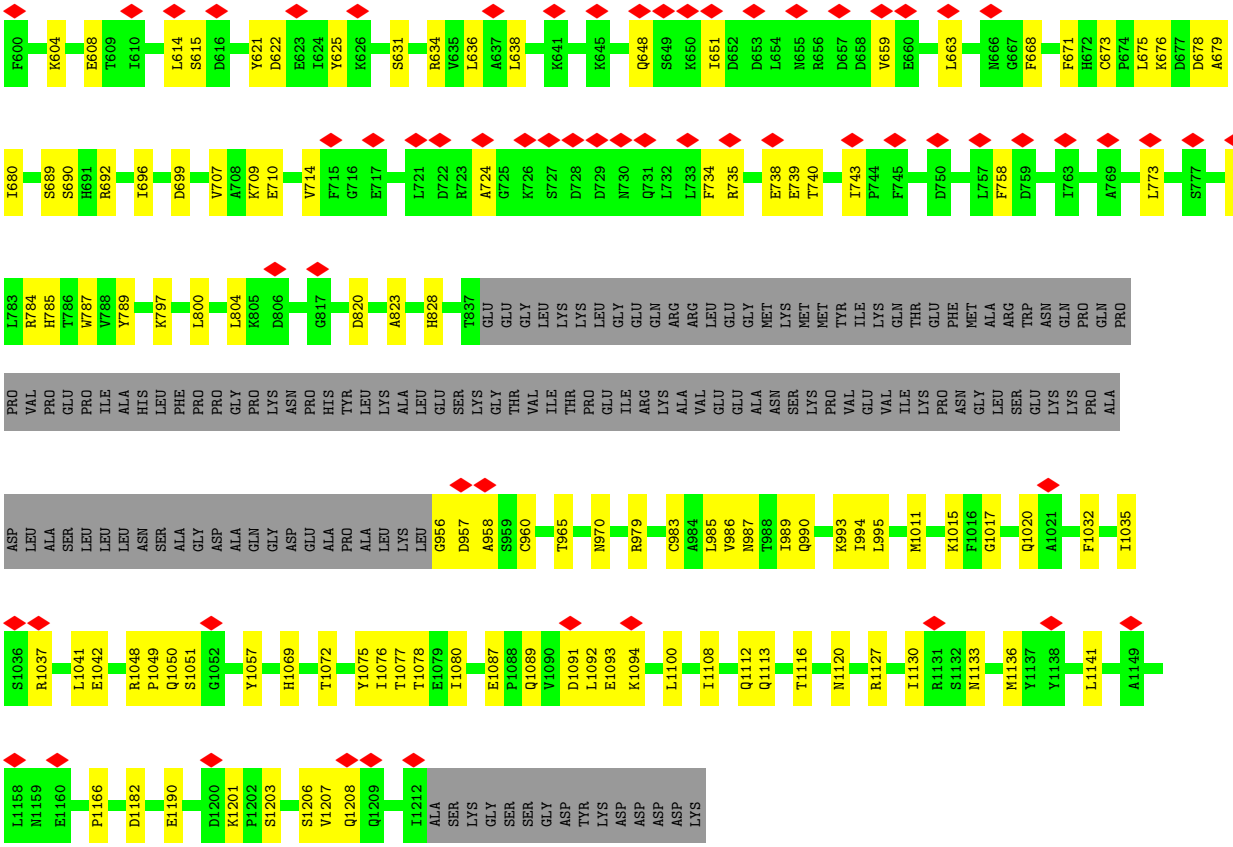






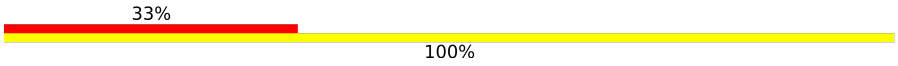






• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	645091	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	118.892	Depositor
Minimum map value	-2.651	Depositor
Average map value	-0.066	Depositor
Map value standard deviation	1.293	Depositor
Recommended contour level	6.15	Depositor
Map size (Å)	342.0352, 342.0352, 342.0352	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82219994, 0.82219994, 0.82219994	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/5560	0.34	0/7599
2	B	0.14	0/2395	0.36	0/3229
3	C	0.12	0/1565	0.30	0/2128
4	D	0.15	0/1218	0.38	0/1660
5	E	0.12	0/1030	0.27	0/1395
6	F	0.15	0/837	0.36	0/1138
7	G	0.12	0/1360	0.29	0/1842
8	H	0.11	0/1066	0.28	0/1454
9	I	0.16	0/8671	0.35	0/11765
All	All	0.14	0/23702	0.34	0/32210

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	474	ARG	Sidechain

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	5432	0	5194	80	0
2	B	2360	0	2394	54	0
3	C	1534	0	1509	21	0
4	D	1184	0	1143	33	0
5	E	1007	0	995	11	0
6	F	813	0	811	10	0
7	G	1329	0	1286	14	0
8	H	1052	0	995	10	0
9	I	8484	0	8519	157	0
10	Z	39	0	34	0	0
11	A	42	0	39	0	0
11	G	28	0	26	0	0
12	I	85	0	0	1	0
All	All	23389	0	22945	368	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 8.

All (368) 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)
9:I:477:PHE:HE2	9:I:828:HIS:HB3	1.29	0.94
9:I:956:GLY:N	9:I:960:CYS:HG	1.70	0.90
1:A:323:ILE:HG13	1:A:324:TRP:HD1	1.40	0.83
1:A:191:VAL:HG11	1:A:197:MET:HE3	1.60	0.83
9:I:987:ASN:HB2	9:I:1127:ARG:HH22	1.43	0.82
1:A:724:THR:HG21	7:G:151:ARG:HD3	1.62	0.80
9:I:427:ILE:H	9:I:1092:LEU:HD22	1.47	0.78
1:A:142:LEU:H	1:A:146:VAL:HB	1.51	0.76
9:I:477:PHE:CE2	9:I:828:HIS:HB3	2.18	0.74
3:C:66:LEU:CD1	3:C:74:LYS:HZ2	2.00	0.74
2:B:173:TYR:HB3	2:B:178:GLN:HE21	1.52	0.74
2:B:286:GLU:O	2:B:290:ASN:ND2	2.21	0.74
2:B:184:TYR:HE1	2:B:188:GLN:HE21	1.37	0.71
9:I:1015:LYS:HG3	9:I:1094:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HE1	2:B:53:LEU:O	1.92	0.70
3:C:66:LEU:CD1	3:C:74:LYS:NZ	2.54	0.69
9:I:104:THR:OG1	9:I:107:ASN:ND2	2.26	0.68
9:I:488:LYS:NZ	9:I:673:CYS:SG	2.67	0.68
1:A:174:ASN:ND2	1:A:193:ASP:OD1	2.28	0.67
9:I:568:ARG:HB3	9:I:571:THR:HB	1.76	0.66
1:A:307:HIS:NE2	1:A:332:GLN:OE1	2.29	0.66
4:D:174:PRO:HG2	4:D:175:TRP:CZ3	2.31	0.66
5:E:60:PHE:CE1	6:F:34:VAL:HG21	2.32	0.65
9:I:246:PHE:HE1	9:I:249:MET:HE2	1.61	0.65
1:A:676:PHE:O	7:G:25:ARG:NH2	2.29	0.65
3:C:66:LEU:HD13	3:C:74:LYS:NZ	2.11	0.65
9:I:548:MET:HE2	9:I:636:LEU:HD12	1.79	0.65
9:I:696:ILE:HG12	9:I:789:TYR:HD2	1.61	0.65
9:I:191:GLU:OE1	9:I:191:GLU:N	2.30	0.64
9:I:392:VAL:HG22	9:I:393:SER:H	1.62	0.64
1:A:209:VAL:HG23	1:A:210:TRP:CD1	2.32	0.64
2:B:77:LEU:HB3	2:B:88:MET:HE1	1.79	0.64
9:I:993:LYS:HD2	9:I:1120:ASN:HD21	1.62	0.64
9:I:634:ARG:N	9:I:671:PHE:O	2.31	0.64
9:I:1076:ILE:HG21	9:I:1108:ILE:HD11	1.80	0.63
2:B:184:TYR:HE1	2:B:188:GLN:NE2	1.96	0.63
1:A:458:GLU:OE2	1:A:499:ASN:ND2	2.32	0.63
3:C:4:ASP:HB3	3:C:7:LEU:HD23	1.79	0.63
9:I:1077:THR:HA	9:I:1080:ILE:HG22	1.79	0.63
9:I:488:LYS:HE2	9:I:707:VAL:HG21	1.80	0.63
9:I:1130:ILE:HG23	9:I:1136:MET:HB3	1.80	0.62
4:D:76:ILE:O	4:D:80:PRO:HD2	1.99	0.62
9:I:420:GLU:HG2	9:I:1011:MET:HE3	1.82	0.62
3:C:27:GLN:HG2	3:C:196:LEU:HD12	1.81	0.62
3:C:47:LEU:O	3:C:51:GLN:HG2	2.00	0.61
1:A:191:VAL:HG23	1:A:192:ASN:H	1.65	0.61
9:I:983:CYS:SG	9:I:1127:ARG:NH2	2.73	0.61
5:E:8:LEU:HB3	5:E:63:ALA:HB2	1.82	0.61
2:B:121:THR:HG21	2:B:126:TYR:HB2	1.82	0.61
9:I:302:VAL:O	9:I:316:LYS:NZ	2.33	0.61
1:A:316:MET:HE1	1:A:699:ILE:HD13	1.83	0.61
4:D:7:TYR:HD2	4:D:9:TRP:HE1	1.48	0.61
9:I:608:GLU:OE1	9:I:608:GLU:N	2.34	0.61
1:A:151:ASN:HA	1:A:169:LEU:HD12	1.83	0.60
9:I:987:ASN:HB2	9:I:1127:ARG:NH2	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ASP:OD1	2:B:43:SER:N	2.35	0.59
8:H:74:ASP:OD1	8:H:96:ASN:ND2	2.35	0.59
4:D:92:TYR:HD1	4:D:93:MET:HE2	1.66	0.59
9:I:820:ASP:HB2	9:I:823:ALA:HB3	1.85	0.59
9:I:7:VAL:HA	9:I:144:PHE:HB2	1.85	0.59
9:I:576:ILE:HG13	9:I:593:ALA:HB2	1.84	0.58
2:B:240:TYR:HD1	2:B:243:GLY:H	1.50	0.58
1:A:173:PHE:H	1:A:191:VAL:HA	1.69	0.58
2:B:174:PHE:O	4:D:22:TYR:OH	2.21	0.58
3:C:230:ASN:O	3:C:233:THR:OG1	2.21	0.58
9:I:758:PHE:HZ	9:I:782:LEU:HA	1.69	0.58
5:E:57:LEU:HD13	6:F:38:VAL:HG21	1.85	0.58
5:E:76:ILE:HD12	5:E:105:ILE:HG12	1.85	0.58
2:B:152:VAL:HG13	2:B:165:LEU:HD12	1.84	0.58
9:I:494:GLY:HA2	9:I:676:LYS:HE2	1.85	0.57
9:I:188:THR:OG1	9:I:191:GLU:OE1	2.22	0.57
2:B:240:TYR:CE1	2:B:242:LYS:HB3	2.39	0.57
7:G:71:TYR:HD2	7:G:89:LEU:HD11	1.69	0.57
9:I:546:ASP:HB3	9:I:549:GLU:HG3	1.86	0.57
1:A:673:ILE:HG21	1:A:710:THR:HG21	1.87	0.57
7:G:106:LYS:HG2	7:G:128:MET:HE3	1.86	0.57
1:A:455:ASN:OD1	1:A:456:SER:N	2.30	0.56
9:I:426:ARG:HG2	9:I:431:LEU:HD13	1.87	0.56
9:I:1017:GLY:N	9:I:1020:GLN:OE1	2.35	0.56
7:G:25:ARG:NH1	7:G:80:ASP:OD1	2.38	0.56
8:H:49:LEU:HD12	8:H:63:SER:HB2	1.88	0.56
1:A:100:ASN:HA	1:A:117:LEU:HD12	1.87	0.56
1:A:560:VAL:HG22	1:A:595:THR:HG22	1.87	0.56
3:C:66:LEU:HD13	3:C:74:LYS:HZ1	1.70	0.56
9:I:278:VAL:HG22	9:I:279:SER:H	1.70	0.56
9:I:956:GLY:N	9:I:960:CYS:SG	2.78	0.56
9:I:468:TYR:HB2	9:I:965:THR:CG2	2.35	0.56
1:A:209:VAL:HG23	1:A:210:TRP:HD1	1.69	0.56
3:C:160:LEU:HB3	3:C:174:VAL:HG12	1.88	0.56
1:A:260:TRP:O	1:A:264:ILE:HD12	2.06	0.55
9:I:564:ASN:HB3	9:I:576:ILE:HG22	1.87	0.55
9:I:258:VAL:HG22	9:I:278:VAL:HG23	1.86	0.55
9:I:1080:ILE:HD11	9:I:1100:LEU:HB3	1.87	0.55
4:D:158:LYS:O	4:D:161:SER:OG	2.22	0.55
3:C:190:VAL:O	3:C:194:ILE:HG12	2.07	0.55
4:D:102:PRO:HA	4:D:105:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1050:GLN:HE21	9:I:1051:SER:H	1.53	0.55
1:A:120:TRP:HE1	7:G:47:MET:HE1	1.71	0.55
1:A:152:GLU:OE1	1:A:154:HIS:NE2	2.40	0.55
1:A:27:SER:HA	7:G:148:LEU:HD23	1.89	0.55
9:I:315:LEU:HD23	9:I:581:GLN:HE22	1.72	0.55
2:B:260:ASN:OD1	2:B:261:ASP:N	2.40	0.54
9:I:149:PHE:HZ	9:I:371:LYS:HG2	1.71	0.54
9:I:206:VAL:HA	9:I:209:VAL:HG12	1.89	0.54
2:B:178:GLN:HE22	2:B:182:ALA:H	1.54	0.54
9:I:709:LYS:HD3	9:I:714:VAL:HG23	1.90	0.54
2:B:238:GLU:HB2	5:E:100:ASN:HD21	1.71	0.54
9:I:480:ARG:HB2	9:I:1048:ARG:NH2	2.22	0.54
9:I:614:LEU:HD23	9:I:663:LEU:HB2	1.90	0.54
9:I:513:ARG:NH2	9:I:631:SER:OG	2.41	0.54
9:I:205:GLN:NE2	9:I:228:ILE:HG12	2.23	0.54
9:I:1069:HIS:ND1	9:I:1112:GLN:OE1	2.26	0.54
2:B:177:GLY:HA2	4:D:22:TYR:CE2	2.42	0.53
9:I:735:ARG:HB3	9:I:739:GLU:HG2	1.89	0.53
1:A:98:ASP:OD1	1:A:99:HIS:N	2.41	0.53
1:A:326:LEU:HD22	1:A:365:PRO:HG2	1.89	0.53
2:B:252:ARG:HH11	2:B:291:LYS:HE3	1.73	0.53
9:I:724:ALA:O	9:I:735:ARG:NH2	2.42	0.53
1:A:323:ILE:HG13	1:A:324:TRP:CD1	2.32	0.52
3:C:240:CYS:SG	3:C:241:LEU:N	2.82	0.52
9:I:315:LEU:HD23	9:I:581:GLN:NE2	2.24	0.52
1:A:40:LEU:HD11	1:A:79:ILE:HD11	1.91	0.52
2:B:58:PHE:CE1	2:B:70:ALA:HB1	2.44	0.52
1:A:604:ILE:HD12	1:A:623:MET:HE2	1.89	0.52
1:A:718:PHE:HE1	3:C:1:MET:HE1	1.74	0.52
9:I:6:PHE:O	9:I:144:PHE:N	2.27	0.52
7:G:11:LEU:HG	7:G:13:LEU:HD23	1.91	0.52
4:D:83:SER:O	4:D:87:ASN:ND2	2.42	0.52
1:A:156:LEU:HG	1:A:163:ALA:HB2	1.93	0.51
9:I:1089:GLN:HG2	9:I:1091:ASP:H	1.75	0.51
2:B:45:LEU:O	2:B:46:THR:OG1	2.27	0.51
9:I:137:TRP:HB2	9:I:144:PHE:CE1	2.46	0.51
1:A:41:GLY:N	1:A:214:GLU:OE2	2.43	0.51
9:I:468:TYR:HB2	9:I:965:THR:HG23	1.92	0.51
9:I:692:ARG:NE	9:I:1208:GLN:OE1	2.43	0.51
9:I:528:VAL:HG12	9:I:638:LEU:HD12	1.92	0.51
1:A:82:ARG:NH2	1:A:706:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:258:VAL:HG21	9:I:272:LEU:HD13	1.92	0.51
2:B:58:PHE:HE1	2:B:70:ALA:HB1	1.76	0.51
6:F:40:GLY:HA3	6:F:103:GLY:HA3	1.93	0.51
9:I:505:ILE:HB	9:I:516:TYR:CD2	2.45	0.51
1:A:262:ARG:HG2	1:A:262:ARG:HH11	1.75	0.50
9:I:260:ARG:NH2	9:I:276:ASP:OD2	2.39	0.50
4:D:77:ALA:HA	4:D:143:MET:SD	2.51	0.50
1:A:535:ILE:HG13	1:A:544:TYR:HB3	1.93	0.50
9:I:313:PRO:HG2	9:I:544:VAL:HG13	1.92	0.50
9:I:734:PHE:HB2	9:I:743:ILE:HB	1.92	0.50
9:I:317:GLU:H	9:I:336:ILE:HG22	1.76	0.50
9:I:172:HIS:O	9:I:176:LEU:HG	2.12	0.50
6:F:46:SER:OG	6:F:47:VAL:N	2.44	0.49
9:I:293:LEU:HB3	9:I:367:ALA:HB1	1.93	0.49
8:H:74:ASP:OD1	8:H:100:THR:OG1	2.30	0.49
9:I:789:TYR:CE2	9:I:800:LEU:HD21	2.47	0.49
1:A:115:TYR:CE1	1:A:122:LEU:HD13	2.47	0.49
9:I:1113:GLN:O	9:I:1116:THR:OG1	2.28	0.49
5:E:60:PHE:O	5:E:64:VAL:HG23	2.13	0.49
9:I:539:GLU:O	9:I:562:ARG:NH2	2.46	0.49
9:I:675:LEU:HD11	9:I:710:GLU:HB3	1.95	0.49
2:B:210:GLU:HG2	2:B:222:LEU:HD13	1.94	0.49
9:I:621:TYR:CE1	9:I:668:PHE:HZ	2.31	0.49
2:B:184:TYR:O	2:B:187:GLU:HG2	2.13	0.49
3:C:187:LEU:HD22	3:C:190:VAL:HG11	1.95	0.49
9:I:413:ALA:O	9:I:417:VAL:HG23	2.13	0.49
9:I:648:GLN:HA	9:I:651:ILE:HD12	1.95	0.49
1:A:60:SER:OG	1:A:68:LEU:HB3	2.13	0.48
2:B:240:TYR:HE1	2:B:242:LYS:HB3	1.78	0.48
9:I:18:LEU:HB3	9:I:87:TYR:HB3	1.95	0.48
2:B:231:LEU:HA	2:B:234:VAL:HG22	1.94	0.48
9:I:979:ARG:NH2	9:I:1042:GLU:O	2.43	0.48
2:B:187:GLU:HG3	3:C:74:LYS:NZ	2.27	0.48
9:I:251:ILE:HD11	9:I:290:PRO:HA	1.95	0.48
9:I:426:ARG:HE	9:I:1092:LEU:HD21	1.78	0.48
9:I:615:SER:N	9:I:663:LEU:O	2.27	0.48
6:F:41:PHE:HD1	6:F:107:ILE:HG13	1.78	0.48
2:B:260:ASN:HB3	2:B:263:ILE:HG22	1.95	0.48
9:I:1087:GLU:HA	9:I:1087:GLU:OE1	2.14	0.48
1:A:155:ILE:HB	1:A:165:TRP:HB2	1.95	0.48
9:I:576:ILE:HD13	9:I:579:ARG:HE	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ILE:HG22	1:A:674:THR:H	1.79	0.48
4:D:85:PRO:HA	4:D:88:ILE:HG22	1.95	0.48
9:I:497:LEU:HB3	9:I:671:PHE:HD2	1.79	0.48
1:A:38:ALA:HB1	1:A:82:ARG:HH12	1.78	0.47
1:A:46:VAL:HG22	1:A:58:ILE:HG12	1.95	0.47
1:A:431:HIS:HE1	4:D:190:ASP:O	1.97	0.47
4:D:72:LYS:O	4:D:76:ILE:HG13	2.14	0.47
9:I:589:SER:HB3	9:I:604:LYS:HE3	1.96	0.47
9:I:758:PHE:CZ	9:I:782:LEU:HA	2.49	0.47
9:I:523:GLU:HA	9:I:526:ILE:HB	1.96	0.47
5:E:73:TYR:HB3	5:E:105:ILE:HD12	1.97	0.47
6:F:39:ALA:HB2	6:F:52:TRP:CZ3	2.50	0.47
2:B:252:ARG:NH1	2:B:291:LYS:HE3	2.30	0.47
1:A:724:THR:HG23	1:A:724:THR:O	2.15	0.47
2:B:121:THR:HG22	2:B:122:ASP:O	2.15	0.47
9:I:172:HIS:CE1	9:I:176:LEU:HD11	2.50	0.47
9:I:582:PHE:HA	9:I:589:SER:HB2	1.97	0.47
4:D:113:PRO:HB2	4:D:152:MET:CE	2.44	0.47
9:I:132:LYS:HE2	9:I:184:ILE:HD13	1.97	0.47
2:B:185:CYS:O	2:B:189:VAL:HG23	2.15	0.47
2:B:193:THR:HB	2:B:196:ASN:ND2	2.30	0.47
9:I:1203:SER:HB2	9:I:1206:SER:HB2	1.97	0.47
1:A:627:ASN:ND2	1:A:629:GLN:OE1	2.48	0.46
2:B:122:ASP:OD1	2:B:123:PHE:N	2.41	0.46
9:I:1136:MET:HE2	9:I:1136:MET:HA	1.97	0.46
12:I:1301:AJP:O63	12:I:1301:AJP:O75	2.33	0.46
1:A:455:ASN:HB3	1:A:458:GLU:OE1	2.15	0.46
2:B:149:LEU:HD21	2:B:173:TYR:CE1	2.50	0.46
2:B:161:LEU:HD11	3:C:58:LEU:HD12	1.97	0.46
4:D:110:LEU:O	4:D:114:ILE:HG12	2.16	0.46
9:I:1050:GLN:HG3	9:I:1051:SER:N	2.31	0.46
9:I:1075:TYR:O	9:I:1078:THR:HG22	2.15	0.46
2:B:109:LEU:HD22	2:B:129:ILE:HG23	1.98	0.46
7:G:119:ILE:HD11	8:H:116:LYS:HB3	1.98	0.46
9:I:12:VAL:HG13	9:I:101:ILE:HG23	1.96	0.46
9:I:501:GLY:HA3	9:I:515:LEU:HB3	1.97	0.46
9:I:1037:ARG:HG3	9:I:1133:ASN:HD21	1.81	0.46
4:D:84:ILE:HB	4:D:85:PRO:HD3	1.98	0.46
9:I:152:ASP:N	9:I:152:ASP:OD1	2.49	0.46
4:D:110:LEU:HD11	4:D:159:LEU:HD21	1.96	0.46
3:C:66:LEU:HD11	3:C:74:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:784:ARG:HG2	9:I:785:HIS:CD2	2.50	0.46
2:B:178:GLN:OE1	2:B:181:LYS:HG3	2.16	0.46
9:I:259:PHE:CE2	9:I:262:LYS:HA	2.51	0.45
9:I:580:PHE:HE2	9:I:659:VAL:HG21	1.81	0.45
1:A:221:ASP:OD2	1:A:336:MET:N	2.44	0.45
9:I:278:VAL:HG22	9:I:279:SER:N	2.30	0.45
4:D:87:ASN:HB3	4:D:109:LEU:HD11	1.98	0.45
1:A:153:LEU:HD11	1:A:169:LEU:HD23	1.99	0.45
1:A:255:ARG:HH21	5:E:18:HIS:CD2	2.34	0.45
4:D:105:THR:O	4:D:109:LEU:HD23	2.16	0.45
4:D:146:VAL:O	4:D:150:VAL:HG23	2.17	0.45
6:F:36:GLY:HA3	6:F:99:ALA:HB3	1.98	0.45
9:I:299:SER:OG	9:I:316:LYS:O	2.23	0.45
9:I:128:PHE:HE1	9:I:144:PHE:CD1	2.35	0.45
9:I:580:PHE:O	9:I:589:SER:OG	2.35	0.45
1:A:262:ARG:HG2	1:A:262:ARG:NH1	2.31	0.45
8:H:123:THR:HG23	8:H:126:ASP:H	1.82	0.45
3:C:180:TYR:O	3:C:184:VAL:HG23	2.17	0.45
9:I:108:GLY:N	9:I:390:GLU:OE2	2.50	0.45
9:I:576:ILE:HD11	9:I:591:SER:HB2	1.99	0.45
4:D:110:LEU:HD11	4:D:159:LEU:HD11	1.99	0.45
5:E:96:ASN:O	5:E:99:THR:OG1	2.35	0.45
9:I:196:HIS:CE1	9:I:239:ARG:HH11	2.35	0.45
9:I:403:ILE:O	9:I:407:LEU:HD23	2.17	0.45
9:I:692:ARG:CZ	9:I:787:TRP:HE1	2.31	0.45
1:A:34:ASP:OD2	1:A:675:HIS:NE2	2.49	0.44
1:A:751:LYS:HD2	1:A:751:LYS:O	2.16	0.44
2:B:95:LEU:HD12	2:B:98:ILE:HD11	1.98	0.44
2:B:252:ARG:HE	2:B:252:ARG:HB2	1.54	0.44
9:I:297:ASP:OD1	9:I:298:GLY:N	2.51	0.44
1:A:105:VAL:HG23	1:A:105:VAL:O	2.18	0.44
6:F:102:PHE:CE1	6:F:106:LEU:HD22	2.53	0.44
1:A:34:ASP:OD1	1:A:34:ASP:N	2.49	0.44
1:A:400:ASP:OD1	1:A:401:HIS:N	2.43	0.44
9:I:378:GLN:O	9:I:378:GLN:NE2	2.49	0.44
9:I:1112:GLN:NE2	9:I:1182:ASP:OD2	2.49	0.44
1:A:28:ASP:OD1	1:A:29:ASP:N	2.50	0.44
1:A:67:CYS:SG	1:A:68:LEU:N	2.91	0.44
3:C:7:LEU:HD12	3:C:143:PHE:CE2	2.52	0.44
4:D:174:PRO:HG2	4:D:175:TRP:CE3	2.53	0.44
9:I:576:ILE:HG21	9:I:579:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLY:HA2	1:A:486:LYS:HG3	2.00	0.44
4:D:92:TYR:CD1	4:D:93:MET:HE2	2.50	0.44
5:E:92:GLU:O	6:F:16:ASN:ND2	2.34	0.44
9:I:558:TRP:CE3	9:I:568:ARG:HB2	2.53	0.44
1:A:197:MET:HG2	1:A:211:GLN:OE1	2.18	0.44
2:B:87:LYS:O	2:B:91:MET:HG3	2.18	0.44
9:I:26:LYS:HD3	9:I:28:TYR:HE1	1.82	0.44
9:I:303:ASN:N	9:I:344:LYS:O	2.50	0.43
9:I:296:LEU:HA	9:I:319:ILE:HG12	2.00	0.43
1:A:334:VAL:HG12	1:A:335:LYS:HG2	2.00	0.43
1:A:479:GLY:N	1:A:654:LYS:O	2.52	0.43
2:B:42:ASP:OD1	2:B:44:ALA:N	2.26	0.43
5:E:76:ILE:HD13	5:E:107:SER:HB3	2.00	0.43
9:I:426:ARG:HB3	9:I:431:LEU:HD22	2.00	0.43
9:I:1041:LEU:HG	9:I:1042:GLU:H	1.82	0.43
1:A:656:PHE:O	1:A:658:ALA:N	2.48	0.43
7:G:51:ASP:OD1	7:G:51:ASP:N	2.50	0.43
9:I:1201:LYS:HA	9:I:1201:LYS:HD2	1.81	0.43
1:A:428:VAL:HA	4:D:188:PHE:O	2.18	0.43
8:H:20:THR:HG23	8:H:36:VAL:HB	2.01	0.43
9:I:174:LYS:HE3	9:I:179:GLU:HG2	2.01	0.43
9:I:149:PHE:CZ	9:I:371:LYS:HG2	2.51	0.43
1:A:759:ILE:HD11	2:B:81:LEU:HD12	2.01	0.43
4:D:7:TYR:HD2	4:D:9:TRP:NE1	2.14	0.43
4:D:165:ILE:HA	4:D:166:PRO:HD3	1.89	0.43
9:I:535:LEU:HD21	9:I:549:GLU:HB2	2.00	0.43
9:I:1072:THR:HG21	9:I:1182:ASP:HB2	2.01	0.43
1:A:115:TYR:HE1	1:A:122:LEU:HD13	1.83	0.43
1:A:316:MET:HE1	1:A:699:ILE:HG21	2.01	0.43
2:B:218:THR:HA	2:B:221:GLU:CD	2.44	0.43
2:B:241:LEU:HD21	2:B:284:THR:HG23	2.00	0.43
9:I:99:ILE:HB	9:I:115:ILE:HD11	2.01	0.43
9:I:227:MET:HE2	9:I:227:MET:HA	2.01	0.43
9:I:986:VAL:HA	9:I:989:ILE:HG22	2.01	0.43
2:B:245:ALA:HB1	2:B:288:ILE:HD13	2.01	0.42
2:B:248:ASN:OD1	2:B:252:ARG:NH2	2.52	0.42
1:A:191:VAL:HG23	1:A:192:ASN:N	2.32	0.42
1:A:387:GLU:H	1:A:387:GLU:CD	2.27	0.42
6:F:88:SER:O	6:F:92:GLU:HG2	2.18	0.42
9:I:1057:TYR:OH	9:I:1190:GLU:OE2	2.29	0.42
1:A:247:SER:HB3	1:A:250:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ILE:O	1:A:674:THR:OG1	2.31	0.42
4:D:101:ILE:HB	4:D:102:PRO:HD3	2.01	0.42
9:I:359:PRO:HA	9:I:360:PRO:HD2	1.96	0.42
9:I:990:GLN:O	9:I:994:ILE:HG12	2.19	0.42
1:A:324:TRP:HE3	1:A:365:PRO:HD3	1.85	0.42
1:A:386:ASN:HB3	1:A:389:ASP:HB2	2.01	0.42
9:I:306:MET:HA	9:I:958:ALA:HA	2.02	0.42
1:A:194:THR:OG1	1:A:214:GLU:O	2.38	0.42
9:I:429:SER:O	9:I:432:ILE:HG22	2.20	0.42
1:A:47:ILE:HG21	1:A:136:LEU:HD22	2.02	0.42
1:A:85:LEU:HD21	1:A:120:TRP:CZ2	2.55	0.42
2:B:212:LEU:HD23	4:D:19:ILE:HG21	2.01	0.42
9:I:689:SER:OG	9:I:690:SER:N	2.53	0.42
9:I:957:ASP:OD1	9:I:957:ASP:N	2.51	0.42
1:A:63:THR:HG22	1:A:64:GLU:N	2.35	0.41
9:I:294:ILE:HG12	9:I:338:VAL:HG22	2.01	0.41
9:I:679:ALA:HB3	9:I:680:ILE:HD12	2.00	0.41
9:I:696:ILE:HG21	9:I:797:LYS:HG3	2.02	0.41
2:B:162:ASP:OD2	2:B:165:LEU:HD23	2.20	0.41
3:C:63:GLY:HA3	3:C:71:PHE:CE1	2.55	0.41
4:D:69:GLN:OE1	4:D:69:GLN:N	2.54	0.41
7:G:7:ILE:HD13	7:G:90:ILE:HD13	2.02	0.41
7:G:10:ARG:HD2	7:G:133:TYR:CE1	2.55	0.41
9:I:488:LYS:HD3	9:I:699:ASP:OD2	2.21	0.41
9:I:1032:PHE:HA	9:I:1035:ILE:HG22	2.03	0.41
1:A:754:LYS:HG2	1:A:759:ILE:HD12	2.03	0.41
4:D:97:SER:O	4:D:102:PRO:HG2	2.21	0.41
9:I:450:GLU:OE2	9:I:995:LEU:HD12	2.21	0.41
1:A:79:ILE:HD13	1:A:79:ILE:HA	1.90	0.41
1:A:149:LYS:HB2	1:A:149:LYS:HE2	1.81	0.41
9:I:565:SER:HB2	9:I:573:LYS:HE2	2.03	0.41
9:I:696:ILE:HG12	9:I:789:TYR:CD2	2.50	0.41
1:A:104:CYS:O	1:A:112:TRP:HA	2.21	0.41
2:B:188:GLN:O	2:B:192:ILE:HG12	2.21	0.41
3:C:128:PRO:O	3:C:132:ILE:HG12	2.20	0.41
8:H:124:TYR:CD1	9:I:1166:PRO:HG3	2.55	0.41
9:I:622:ASP:HA	9:I:625:TYR:CE2	2.56	0.41
9:I:773:LEU:HD23	9:I:773:LEU:HA	1.94	0.41
9:I:1092:LEU:HG	9:I:1093:GLU:N	2.36	0.41
1:A:385:LEU:HD11	1:A:441:ILE:HD13	2.03	0.41
2:B:280:LYS:HE3	4:D:7:TYR:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:8:TYR:CD1	8:H:18:LEU:HD13	2.56	0.41
9:I:201:LEU:HD12	9:I:201:LEU:HA	1.93	0.41
9:I:396:ASN:O	9:I:400:LEU:HD23	2.21	0.41
2:B:144:SER:OG	2:B:145:GLN:N	2.54	0.40
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.78	0.40
2:B:259:GLN:HG2	2:B:259:GLN:O	2.21	0.40
8:H:24:ASP:OD1	8:H:25:SER:N	2.52	0.40
9:I:253:PRO:HG3	9:I:270:ASN:HB3	2.04	0.40
9:I:804:LEU:HD12	9:I:804:LEU:HA	1.95	0.40
4:D:148:GLN:O	4:D:152:MET:HG2	2.21	0.40
9:I:738:GLU:HB3	9:I:740:THR:HG23	2.02	0.40
9:I:1141:LEU:HD23	9:I:1141:LEU:HA	1.96	0.40
9:I:1207:VAL:O	9:I:1207:VAL:HG13	2.21	0.40
7:G:10:ARG:NH2	7:G:52:GLU:OE1	2.54	0.40
7:G:110:GLY:O	8:H:115:THR:HG22	2.21	0.40
9:I:406:LEU:HD23	9:I:406:LEU:HA	1.90	0.40
9:I:455:VAL:HG21	9:I:473:PHE:CD1	2.56	0.40
1:A:600:PHE:CG	1:A:601:PRO:HD2	2.57	0.40
1:A:604:ILE:CD1	1:A:623:MET:HE2	2.51	0.40
2:B:58:PHE:O	2:B:62:VAL:HG23	2.21	0.40
2:B:137:LYS:HD2	2:B:137:LYS:HA	1.90	0.40
2:B:153:VAL:HG23	4:D:34:PRO:HD3	2.03	0.40
3:C:11:VAL:O	3:C:15:ILE:HG22	2.21	0.40
9:I:21:LYS:HE3	9:I:87:TYR:C	2.47	0.40
9:I:678:ASP:OD2	9:I:970:ASN:HB3	2.21	0.40
9:I:985:LEU:HD23	9:I:1049:PRO:HB2	2.02	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	689/760 (91%)	636 (92%)	52 (8%)	1 (0%)	48	82
2	B	290/292 (99%)	276 (95%)	14 (5%)	0	100	100
3	C	192/253 (76%)	186 (97%)	6 (3%)	0	100	100
4	D	152/190 (80%)	147 (97%)	5 (3%)	0	100	100
5	E	124/169 (73%)	119 (96%)	5 (4%)	0	100	100
6	F	98/108 (91%)	94 (96%)	4 (4%)	0	100	100
7	G	165/234 (70%)	157 (95%)	8 (5%)	0	100	100
8	H	140/205 (68%)	138 (99%)	2 (1%)	0	100	100
9	I	1080/1227 (88%)	1020 (94%)	60 (6%)	0	100	100
All	All	2930/3438 (85%)	2773 (95%)	156 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASP

5.3.2 Protein sidechains (i)

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	585/707 (83%)	585 (100%)	0	100	100
2	B	259/264 (98%)	259 (100%)	0	100	100
3	C	157/217 (72%)	157 (100%)	0	100	100
4	D	118/166 (71%)	118 (100%)	0	100	100
5	E	110/145 (76%)	110 (100%)	0	100	100
6	F	86/95 (90%)	86 (100%)	0	100	100
7	G	142/204 (70%)	142 (100%)	0	100	100
8	H	112/178 (63%)	112 (100%)	0	100	100
9	I	928/1060 (88%)	928 (100%)	0	100	100
All	All	2497/3036 (82%)	2497 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	HIS
2	B	188	GLN
4	D	12	HIS
5	E	110	ASN
9	I	205	GLN
9	I	378	GLN
9	I	581	GLN
9	I	706	HIS
9	I	976	ASN
9	I	1050	GLN

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

3 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	$\#\|Z\| > 2$
10	NAG	Z	1	10,1	14,14,15	0.75	0	17,19,21	1.00	2 (11%)
10	NAG	Z	2	10	14,14,15	0.75	0	17,19,21	0.91	1 (5%)
10	BMA	Z	3	10	11,11,12	0.86	0	15,15,17	2.24	3 (20%)

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
10	NAG	Z	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	3	BMA	C1-O5-C5	6.97	121.63	112.19
10	Z	1	NAG	O5-C1-C2	-2.86	106.77	111.29
10	Z	3	BMA	C2-C3-C4	2.30	114.88	110.89
10	Z	2	NAG	O5-C1-C2	-2.28	107.69	111.29
10	Z	3	BMA	C3-C4-C5	2.18	114.14	110.24
10	Z	1	NAG	O4-C4-C3	-2.05	105.62	110.35

There are no chirality outliers.

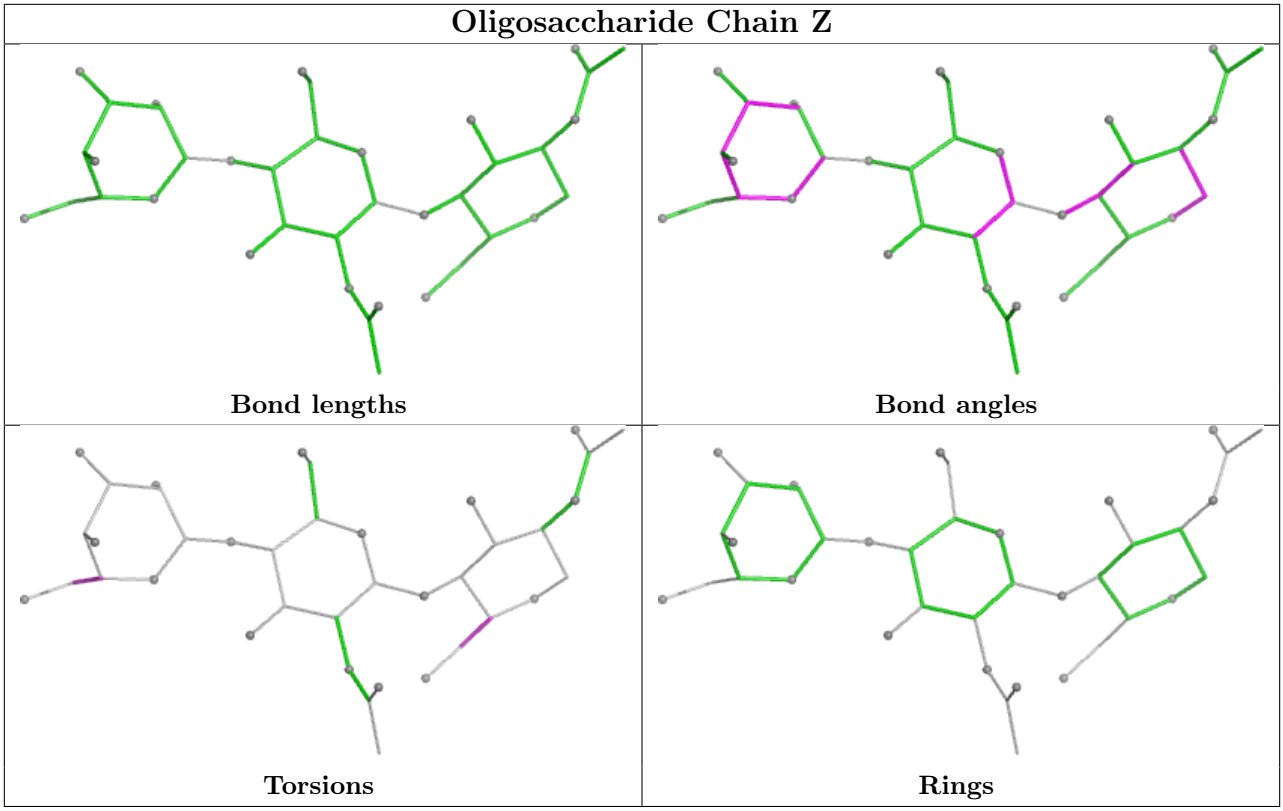
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Z	3	BMA	O5-C5-C6-O6
10	Z	1	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	$\#\|Z\|>2$
11	NAG	G	302	7	14,14,15	0.76	0	17,19,21	0.79	0
11	NAG	A	802	1	14,14,15	0.90	0	17,19,21	1.09	0
12	AJP	I	1301	-	95,95,95	0.14	0	143,149,149	0.53	2 (1%)
11	NAG	A	803	1	14,14,15	0.67	0	17,19,21	1.31	2 (11%)
11	NAG	A	801	1	14,14,15	0.72	0	17,19,21	0.88	0
11	NAG	G	301	7	14,14,15	0.75	0	17,19,21	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
11	NAG	G	302	7	-	0/6/23/26	0/1/1/1
11	NAG	A	802	1	-	3/6/23/26	0/1/1/1
12	AJP	I	1301	-	-	11/28/220/220	0/11/11/11
11	NAG	A	803	1	-	2/6/23/26	0/1/1/1
11	NAG	A	801	1	-	0/6/23/26	0/1/1/1
11	NAG	G	301	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	803	NAG	C1-O5-C5	3.15	116.45	112.19
11	A	803	NAG	O5-C1-C2	-2.84	106.80	111.29
12	I	1301	AJP	O44-C37-C36	-2.40	101.39	107.48
12	I	1301	AJP	C12-C11-C16	-2.12	110.77	113.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	1301	AJP	C56-C57-O64-C65
12	I	1301	AJP	C37-C36-O54-C55
11	A	802	NAG	O5-C5-C6-O6
12	I	1301	AJP	C36-C37-O44-C45
11	A	803	NAG	C4-C5-C6-O6
11	A	802	NAG	C4-C5-C6-O6
12	I	1301	AJP	C38-C37-O44-C45
11	A	803	NAG	O5-C5-C6-O6
12	I	1301	AJP	O60-C55-O54-C36
12	I	1301	AJP	O31-C30-C32-O33
11	A	802	NAG	C1-C2-N2-C7
12	I	1301	AJP	C56-C55-O54-C36
12	I	1301	AJP	O31-C26-O25-C23
12	I	1301	AJP	C27-C26-O25-C23
12	I	1301	AJP	O70-C65-O64-C57
12	I	1301	AJP	C66-C65-O64-C57

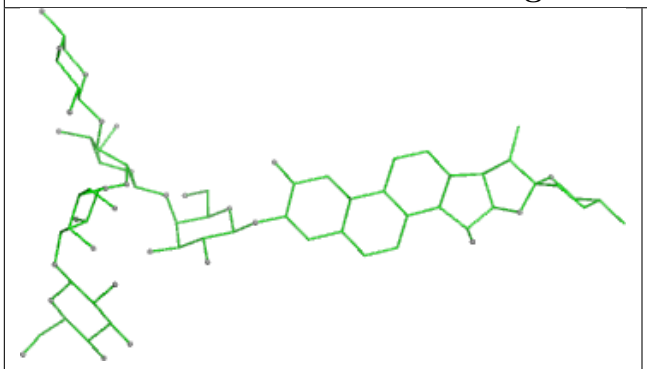
There are no ring outliers.

1 monomer is involved in 1 short contact:

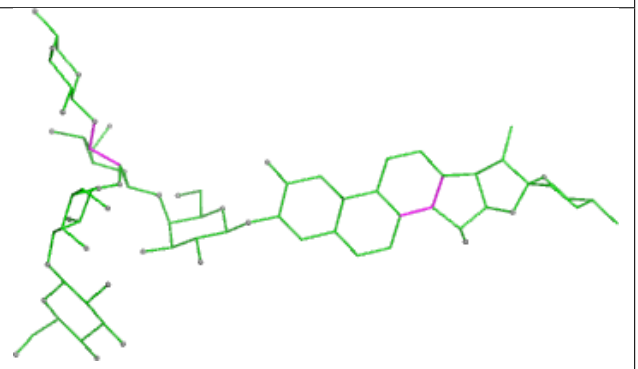
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	1301	AJP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

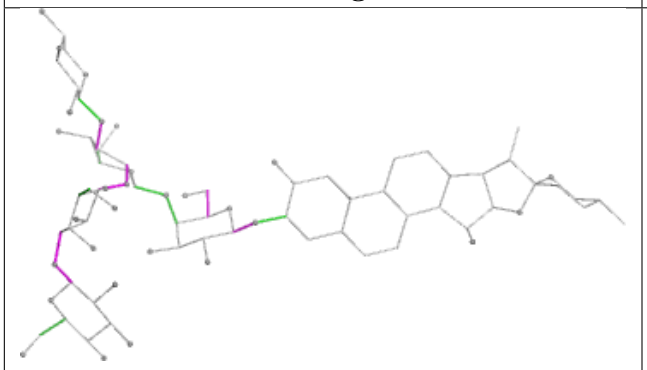
Ligand AJP I 1301



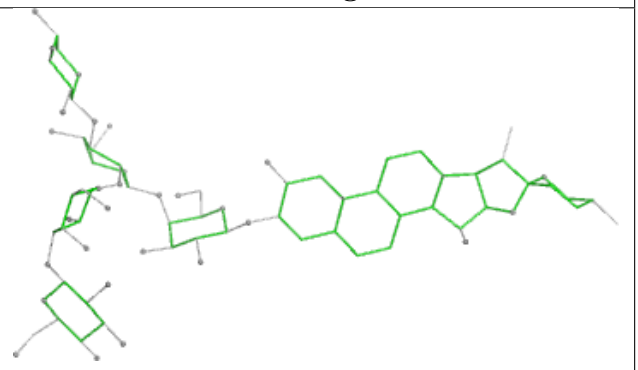
Bond lengths



Bond angles



Torsions



Rings

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.

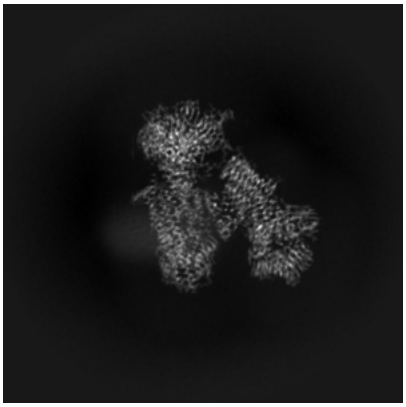
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-59745. These allow visual inspection of the internal detail of the map and identification of artifacts.

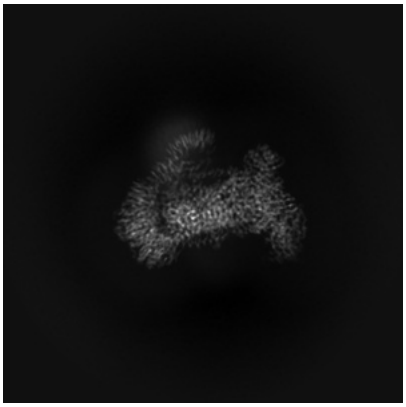
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

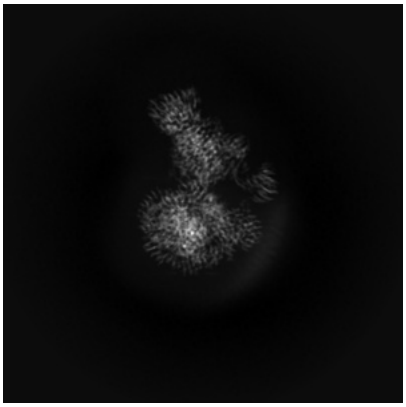
6.1.1 Primary map



X



Y



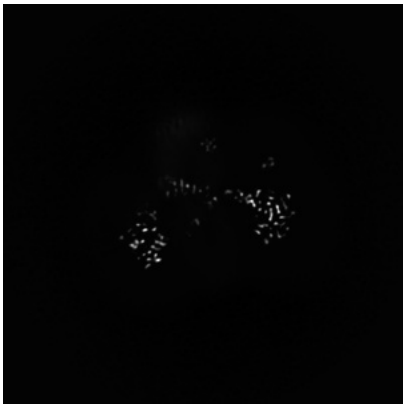
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 208



Y Index: 208

Z Index: 208

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 197

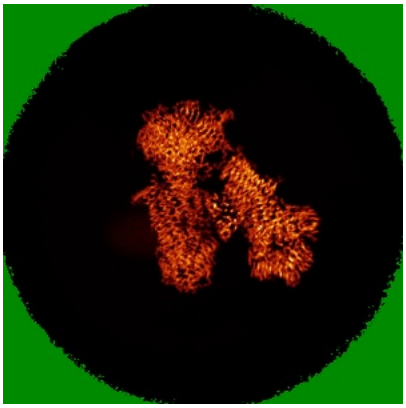
Y Index: 181

Z Index: 181

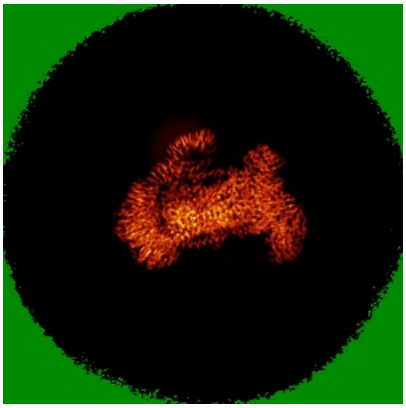
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

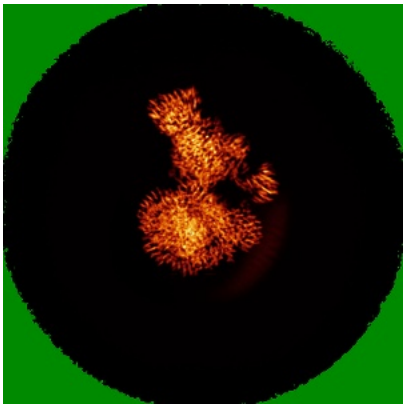
6.4.1 Primary map



X



Y



Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

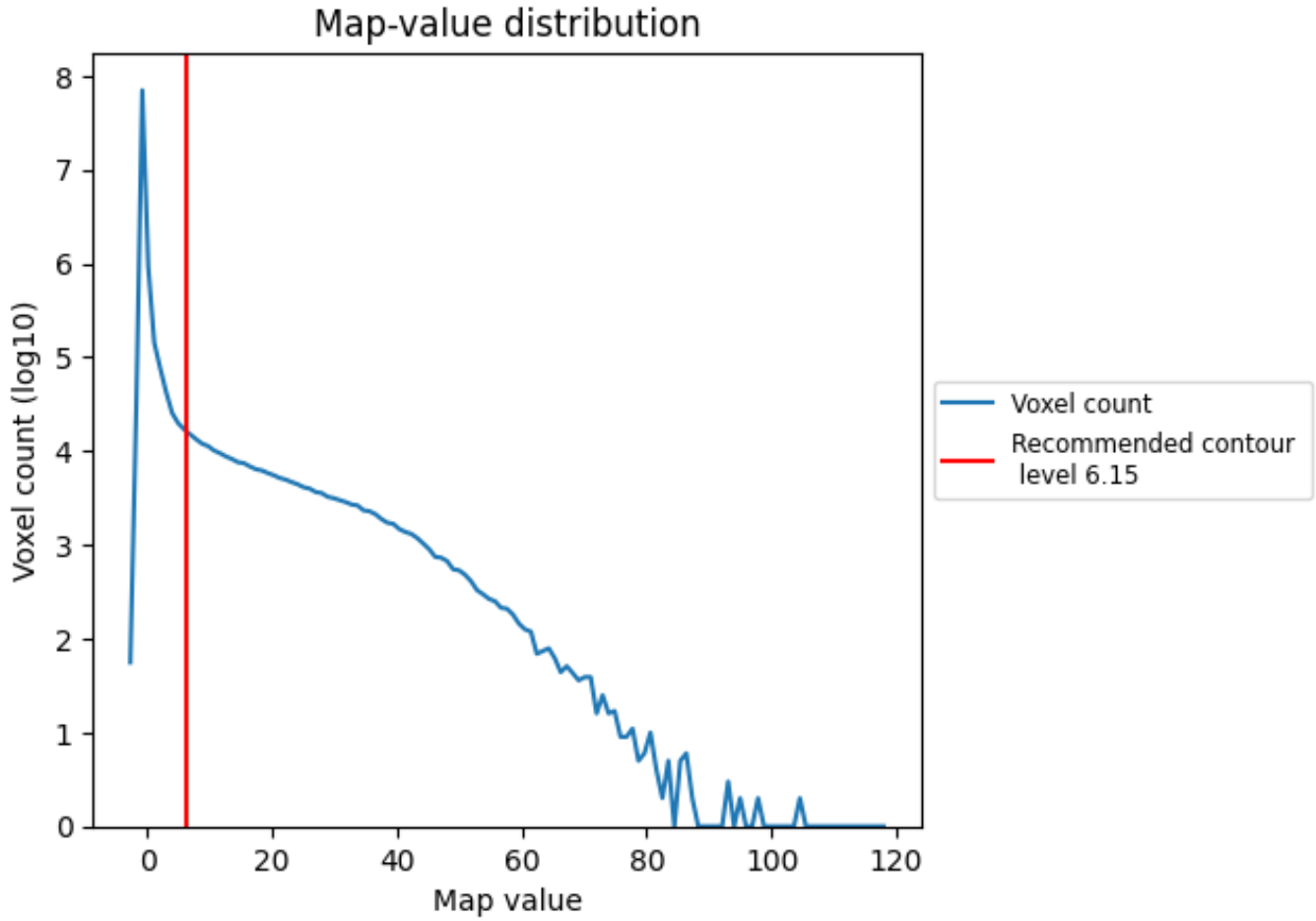
6.6 Mask visualisation (i)

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

7 Map analysis

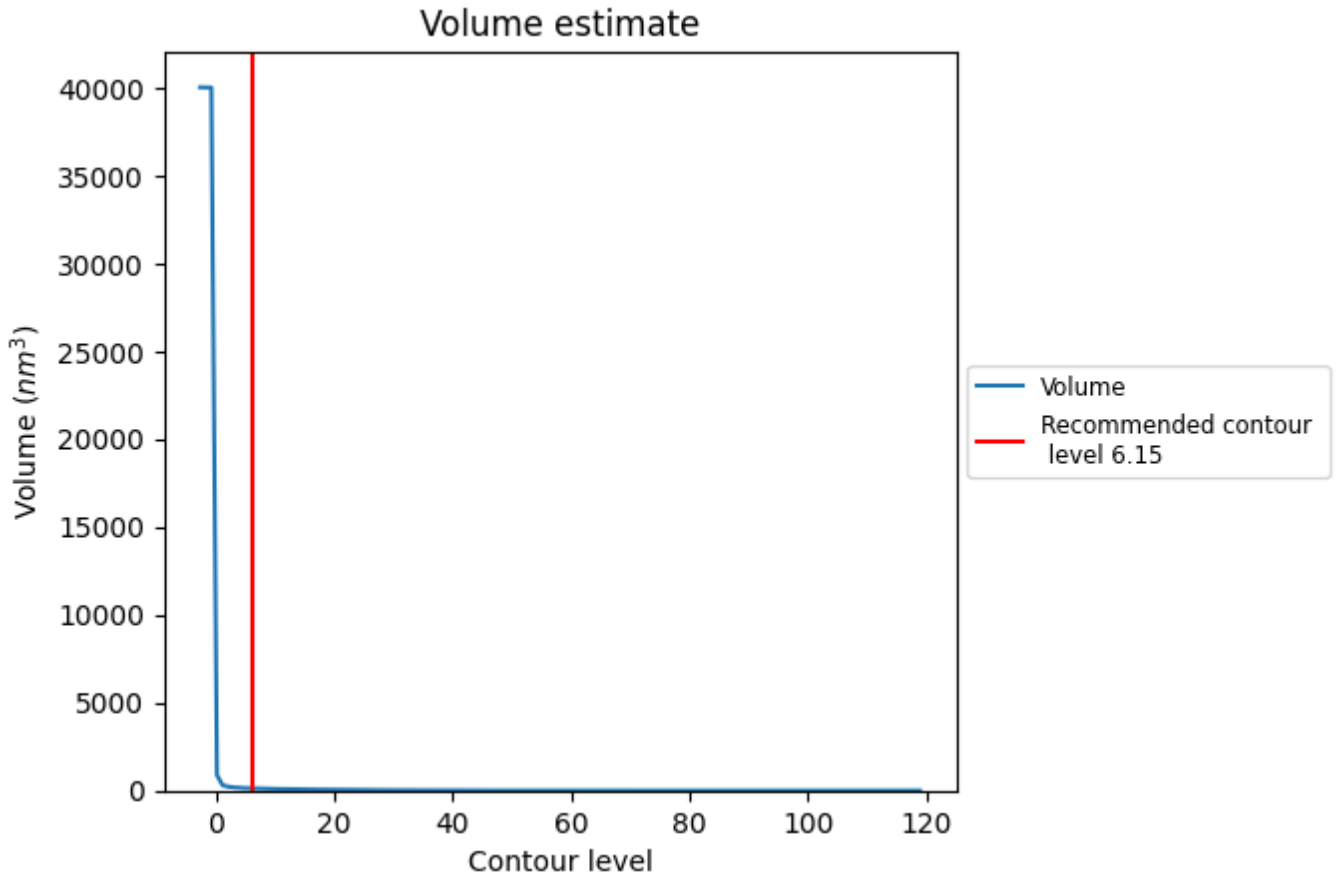
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

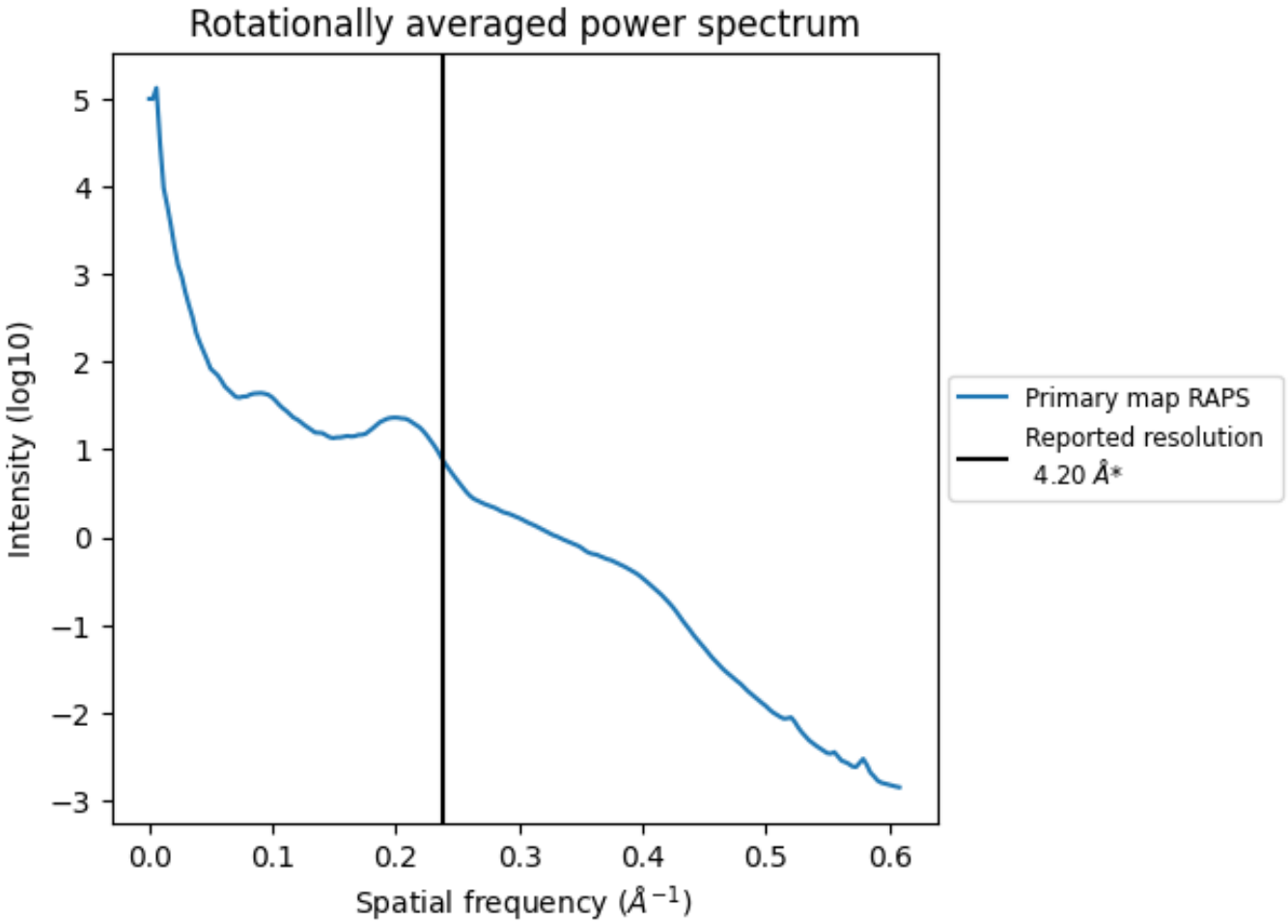
7.2 Volume estimate



The volume at the recommended contour level is 126 nm^3; this corresponds to an approximate mass of 114 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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

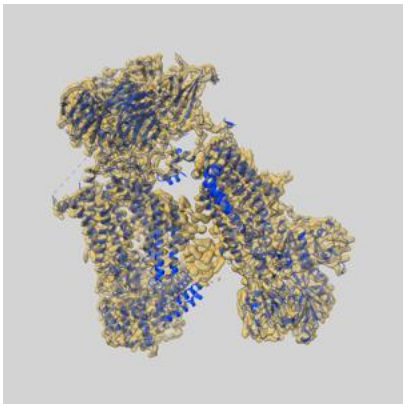
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

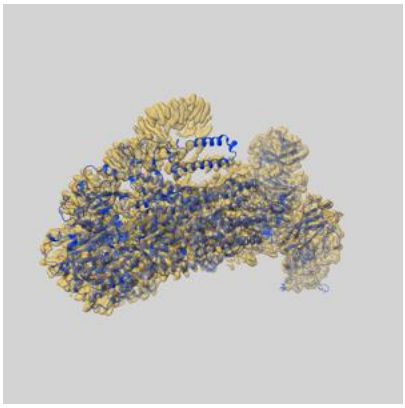
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-59745 and PDB model 34BQ. Per-residue inclusion information can be found in section 3 on page 9.

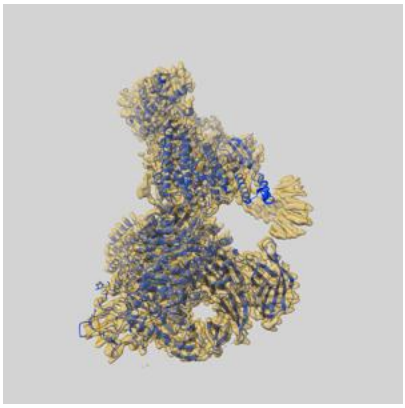
9.1 Map-model overlay



X



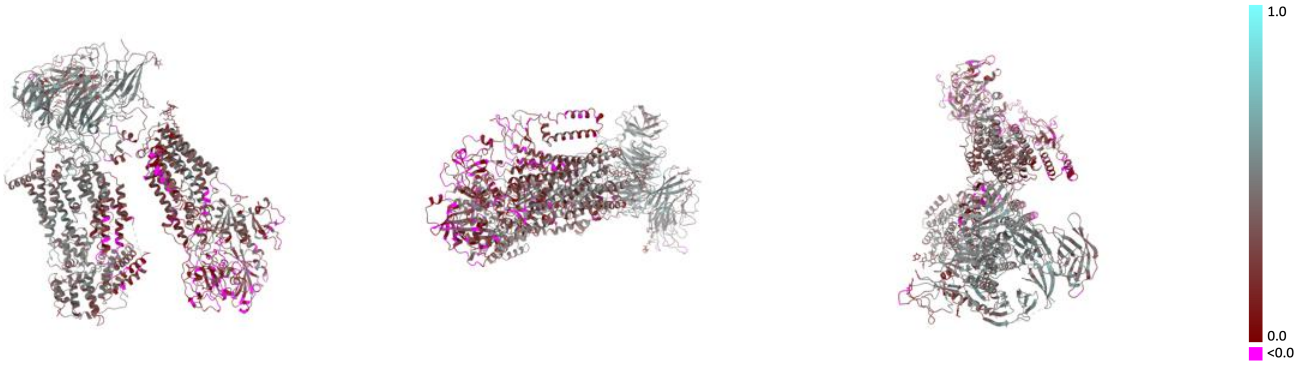
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.15 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.

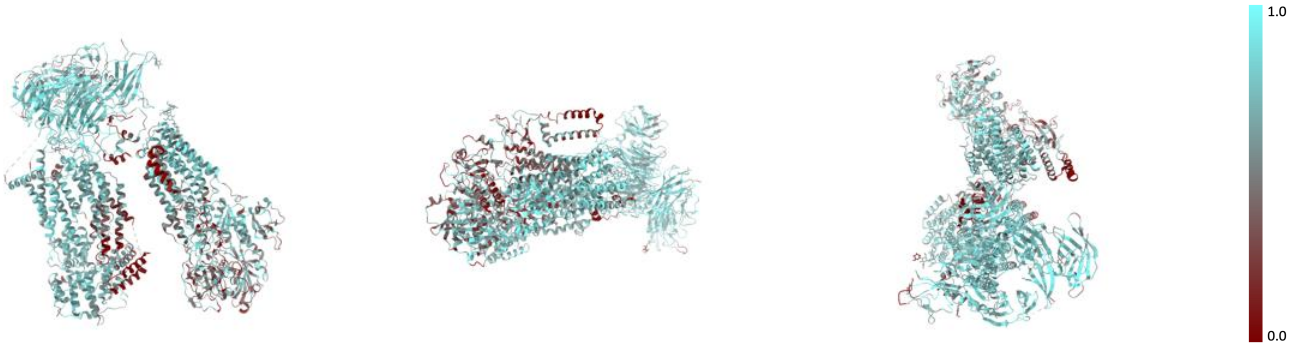
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

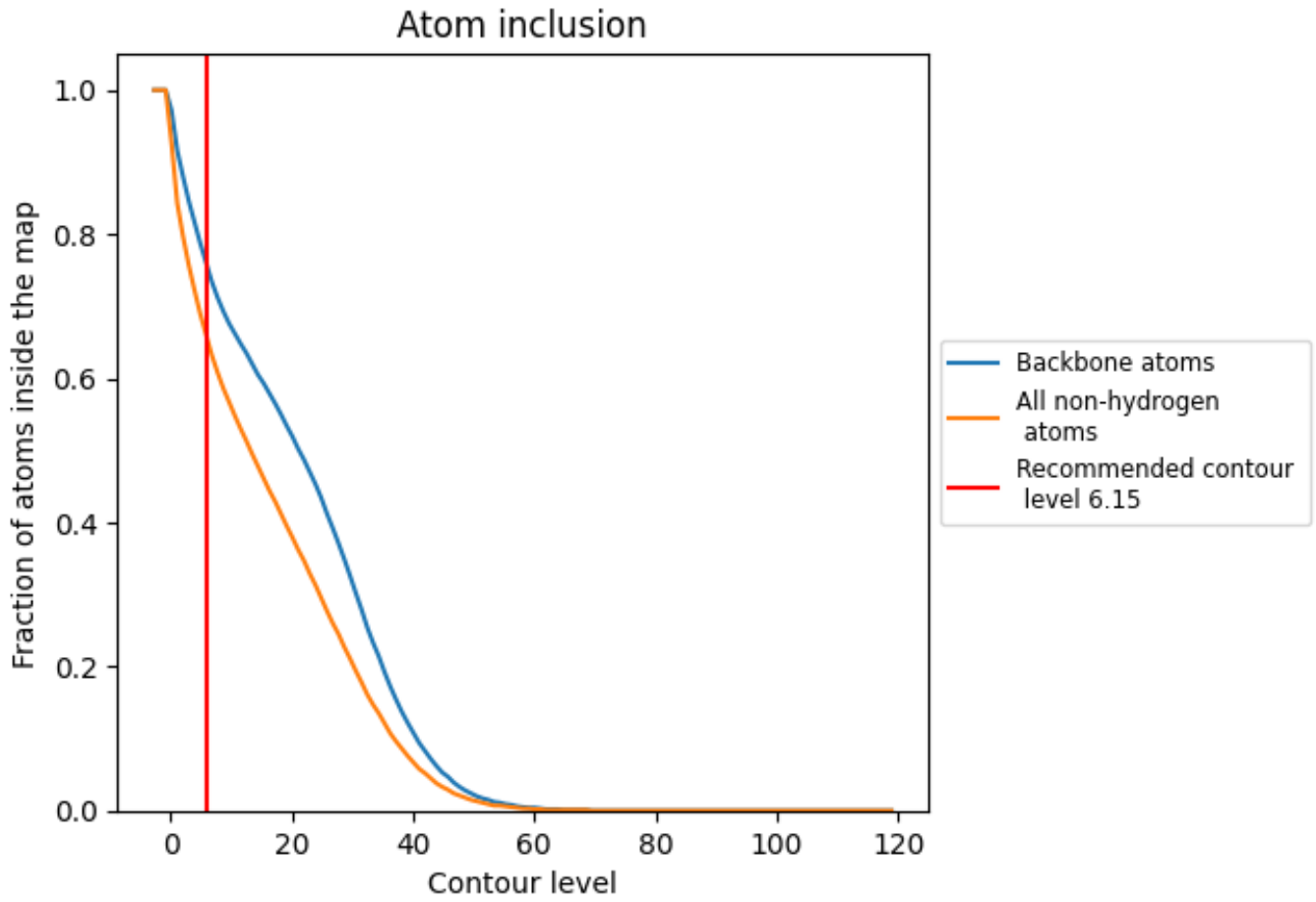
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (6.15).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 65% 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 (6.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.3550
A	0.7460	0.4600
B	0.7240	0.4060
C	0.5490	0.3480
D	0.5690	0.3180
E	0.7040	0.4160
F	0.7630	0.4540
G	0.6880	0.4320
H	0.6620	0.4000
I	0.5810	0.2480
Z	0.4620	0.2630