Full wwPDB EM Validation Report ⓘ

Jun 5, 2023 – 06:39 PM EDT

PDB ID	:	8S9S
EMDB ID	:	EMD-40245
Title	:	Structure of the human ER membrane protein complex (EMC) in GDN
Authors	:	Tomaleri, G.P.; Nguyen, V.N.; Voorhees, R.M.
Deposited on	:	2023-03-30
Resolution	:	3.60 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:

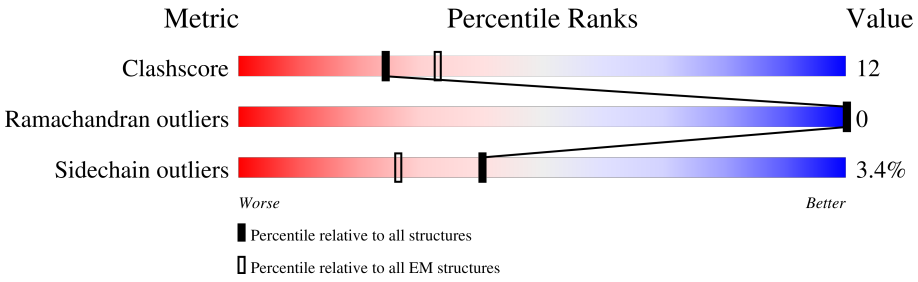
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.60 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 <=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	1	993	66% 26% • 6%
2	2	297	66% 28% • 5%
3	3	261	8% 59% 26% • 14%
4	4	183	34% 71% 7% • 21%
5	5	131	50% 24% • 23%
6	6	110	70% 20% 10%
7	7	242	41% 15% 44%
8	8	210	9% 53% 37% • 9%

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Mol	Chain	Length	Quality of chain
9	10	262	39% 19% 41%
10	A	2	50% 50%
10	B	2	50% 50%
10	C	2	50% 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18012 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	1	930	7367	4724	1262	1357	24	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	2	281	2306	1447	411	434	14	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	3	225	1833	1194	298	332	9	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	4	144	867	547	154	165	1	0	0

- Molecule 5 is a protein called Membrane magnesium transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	101	795	517	140	135	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	99	774	521	126	125	2	0	0

- Molecule 7 is a protein called ER membrane protein complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	136	Total	C	N	O	S	0	0
			1054	679	182	189	4		

- Molecule 8 is a protein called ER membrane protein complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	192	Total	C	N	O	S	0	0
			1533	968	266	287	12		

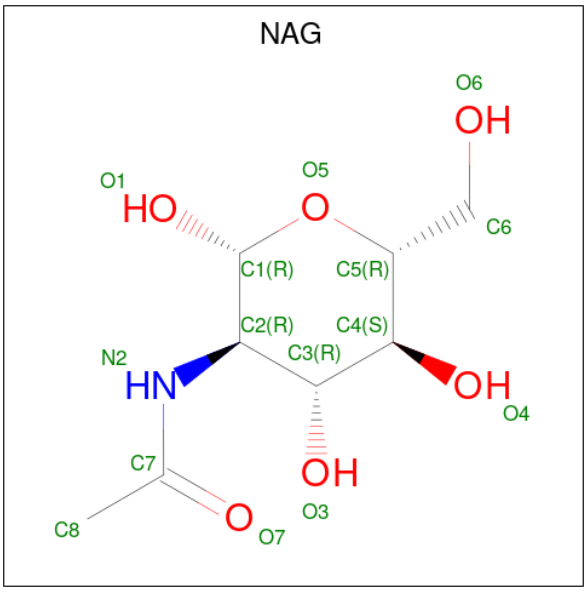
- Molecule 9 is a protein called ER membrane protein complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	10	154	Total	C	N	O	S	0	0
			1177	729	214	231	3		

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

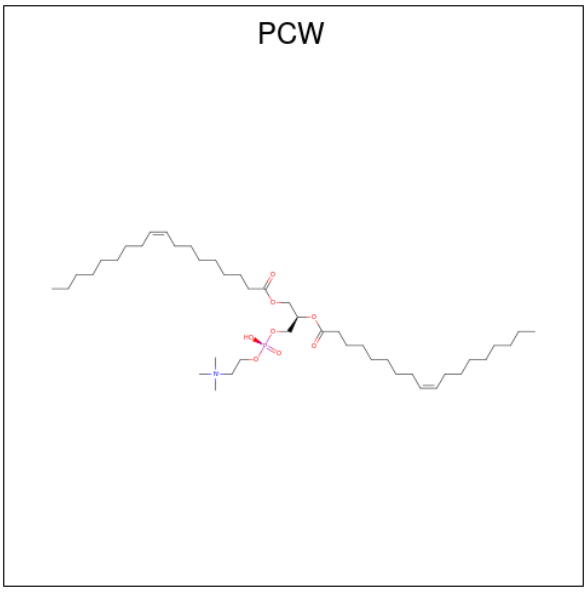
Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	2	Total	C	N	O	0	0
			28	16	2	10		
10	B	2	Total	C	N	O	0	0
			28	16	2	10		
10	C	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

- Molecule 12 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	1	1	Total	C	N	O	P	0
			30	20	1	8	1	
12	3	1	Total	C	N	O	P	0
			38	28	1	8	1	

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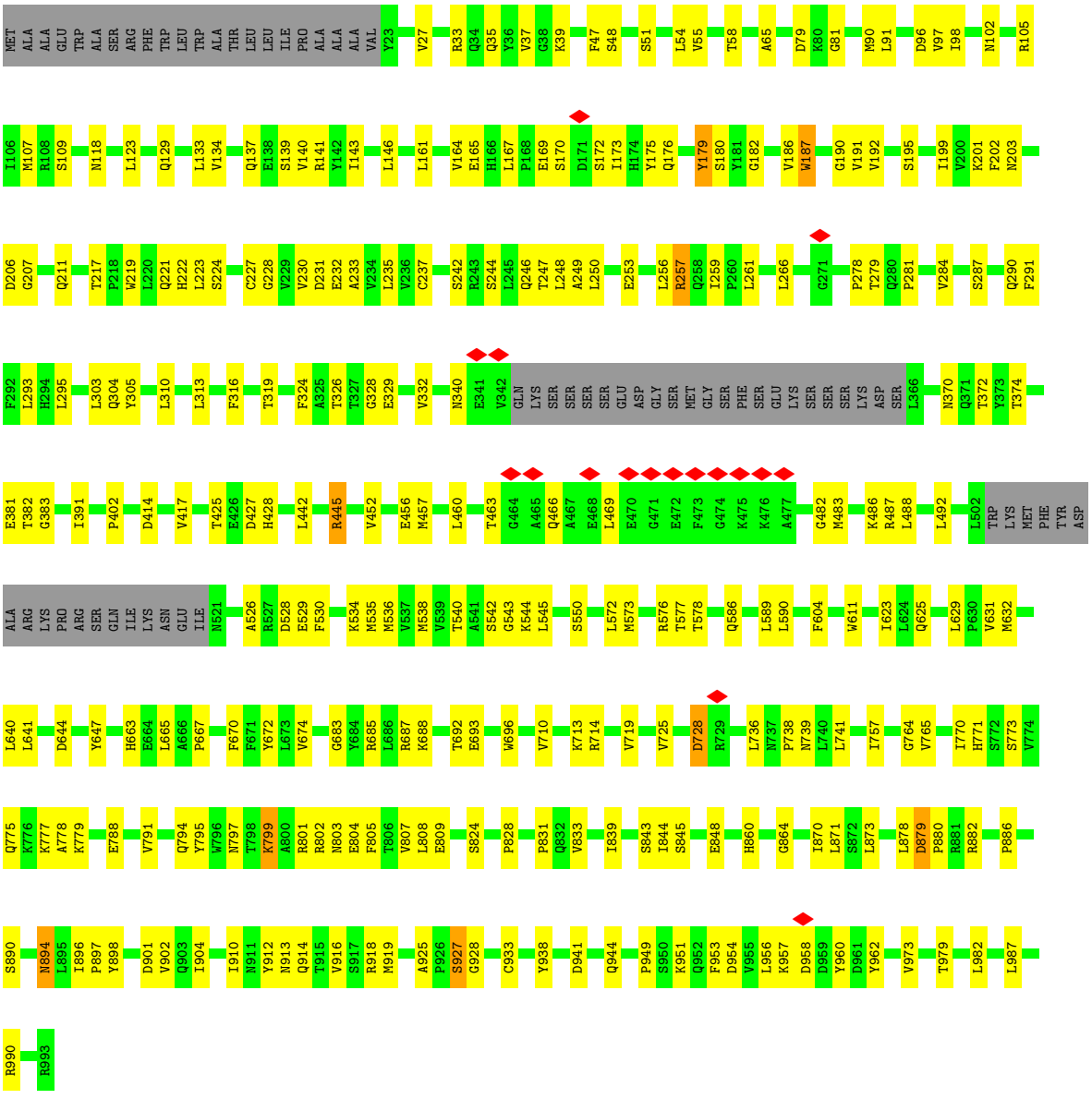
Mol	Chain	Residues	Atoms					AltConf
12	3	1	Total	C	N	O	P	0
			54	44	1	8	1	
12	3	1	Total	C	N	O	P	0
			34	24	1	8	1	
12	6	1	Total	C	N	O	P	0
			22	12	1	8	1	
12	6	1	Total	C	N	O	P	0
			30	20	1	8	1	

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.

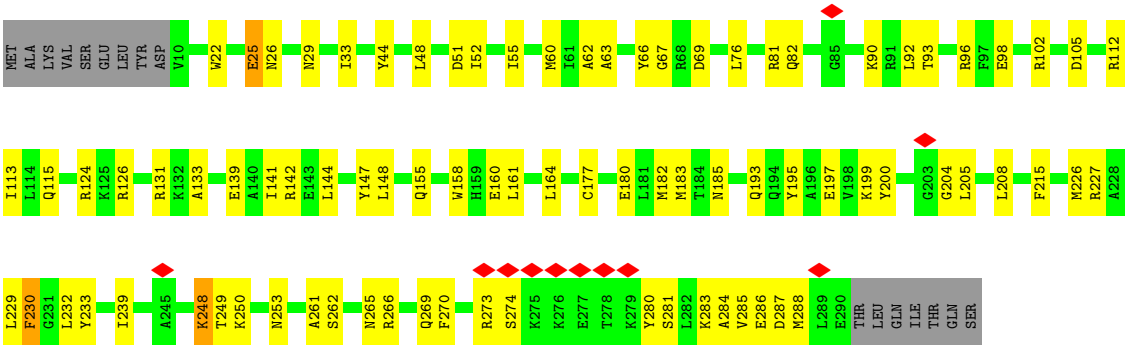
- Molecule 1: ER membrane protein complex subunit 1

Chain 1:



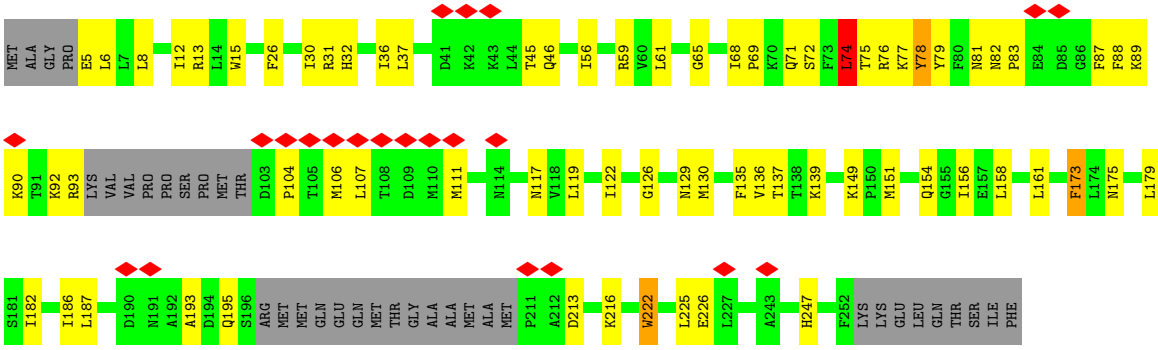
• Molecule 2: ER membrane protein complex subunit 2

Chain 2:



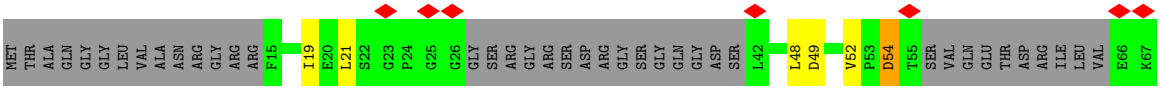
• Molecule 3: ER membrane protein complex subunit 3

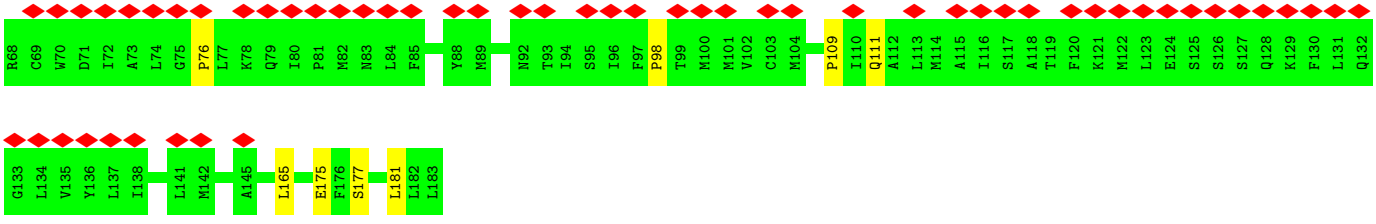
Chain 3:



• Molecule 4: ER membrane protein complex subunit 4

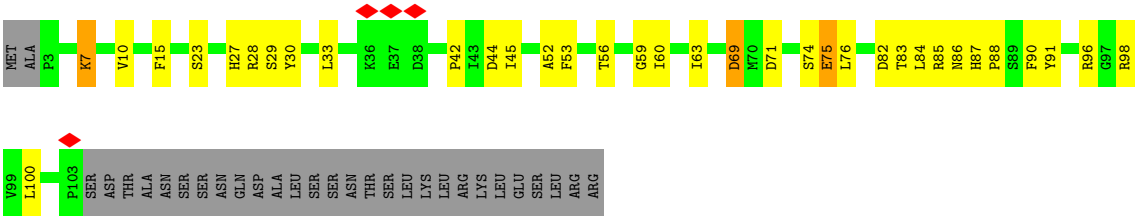
Chain 4:





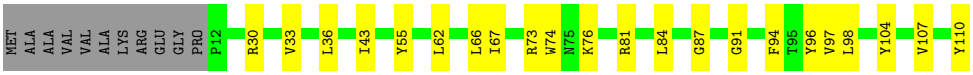
• Molecule 5: Membrane magnesium transporter 1

Chain 5:



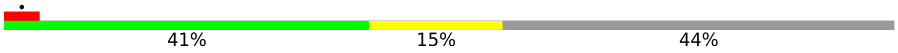
• Molecule 6: ER membrane protein complex subunit 6

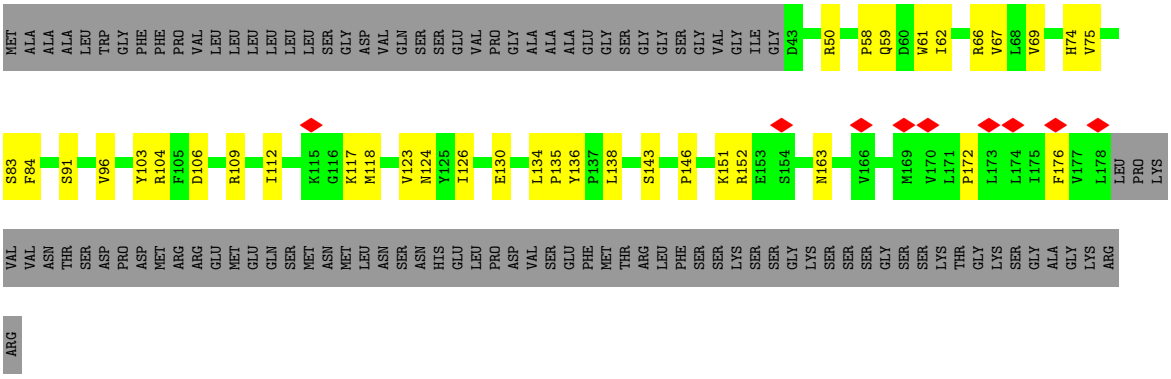
Chain 6:



• Molecule 7: ER membrane protein complex subunit 7

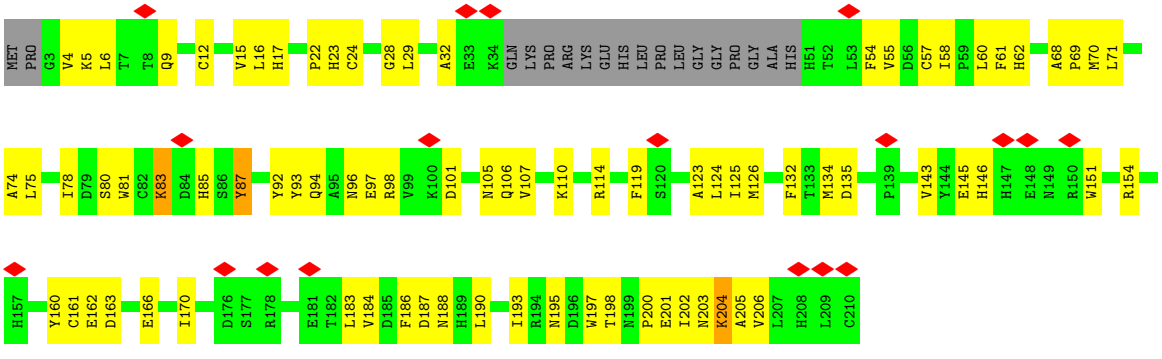
Chain 7:





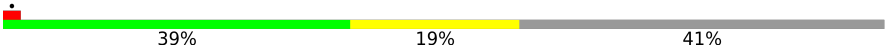
• Molecule 8: ER membrane protein complex subunit 8

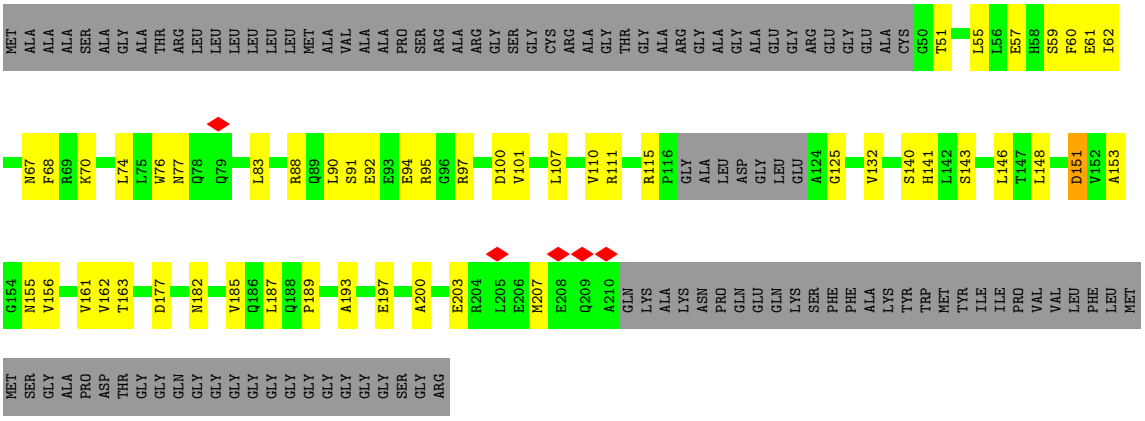
Chain 8:



• Molecule 9: ER membrane protein complex subunit 10

Chain 10:





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

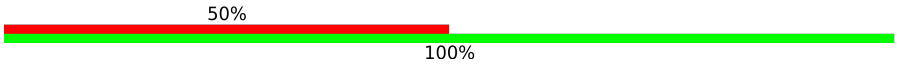
Chain A:

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

Chain B:

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

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.436	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.101	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.27	0/7533	0.52	1/10238 (0.0%)
2	2	0.25	0/2349	0.49	0/3158
3	3	0.27	0/1875	0.57	2/2537 (0.1%)
4	4	0.25	0/884	0.45	0/1219
5	5	0.27	0/816	0.50	0/1104
6	6	0.27	0/795	0.48	0/1077
7	7	0.27	0/1084	0.59	0/1475
8	8	0.25	0/1572	0.51	0/2141
9	10	0.27	0/1197	0.60	0/1625
All	All	0.26	0/18105	0.53	3/24574 (0.0%)

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
4	4	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	83	PRO	CA-N-CD	-9.84	97.73	111.50
1	1	728	ASP	CB-CG-OD1	7.36	124.92	118.30
3	3	74	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	76	PRO	Mainchain
4	4	98	PRO	Mainchain

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	1	7367	0	7409	182	0
2	2	2306	0	2241	63	0
3	3	1833	0	1842	54	0
4	4	867	0	623	12	0
5	5	795	0	793	29	0
6	6	774	0	803	19	0
7	7	1054	0	1014	23	0
8	8	1533	0	1470	59	0
9	10	1177	0	1146	33	0
10	A	28	0	25	1	0
10	B	28	0	25	0	0
10	C	28	0	25	0	0
11	1	14	0	13	0	0
12	1	30	0	32	1	0
12	3	126	0	173	5	0
12	6	52	0	54	1	0
All	All	18012	0	17688	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (426) 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)
7:7:134:LEU:HD12	7:7:135:PRO:HD2	1.46	0.97
3:3:75:THR:HB	4:4:48:LEU:HD21	1.58	0.85
1:1:98:ILE:HD13	1:1:143:ILE:HD11	1.57	0.84
2:2:285:VAL:HA	2:2:288:MET:HG2	1.61	0.83
3:3:180:ARG:HH22	6:6:91:GLY:HA2	1.45	0.80
3:3:180:ARG:HD3	3:3:195:GLN:HE22	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:10:74:LEU:HB3	9:10:83:LEU:HD11	1.65	0.79
1:1:161:LEU:HD21	1:1:164:VAL:HG23	1.65	0.76
5:5:27:HIS:O	5:5:30:TYR:HB2	1.87	0.75
6:6:33:VAL:HG21	6:6:62:LEU:HD13	1.68	0.74
7:7:69:VAL:HB	7:7:74:HIS:HB2	1.69	0.73
1:1:230:VAL:HG12	1:1:278:PRO:HB3	1.70	0.73
4:4:19:ILE:HG22	8:8:114:ARG:HG3	1.69	0.73
5:5:82:ASP:OD1	8:8:62:HIS:NE2	2.21	0.73
1:1:794:GLN:HE21	1:1:803:ASN:HB3	1.54	0.73
9:10:61:GLU:OE2	9:10:67:ASN:ND2	2.22	0.73
4:4:19:ILE:HD11	8:8:71:LEU:HB3	1.72	0.72
1:1:281:PRO:HB3	1:1:326:THR:HG21	1.73	0.71
3:3:89:LYS:O	3:3:92:LYS:NZ	2.23	0.71
1:1:173:ILE:HD12	1:1:192:VAL:HG23	1.73	0.70
8:8:29:LEU:HD11	8:8:75:LEU:HD23	1.73	0.69
1:1:901:ASP:HB2	7:7:126:ILE:HD11	1.74	0.69
8:8:57:CYS:SG	8:8:58:ILE:N	2.65	0.68
8:8:28:GLY:HA2	8:8:60:LEU:HG	1.74	0.68
1:1:625:GLN:NE2	4:4:181:LEU:O	2.27	0.67
1:1:279:THR:HB	1:1:324:PHE:HD2	1.59	0.67
2:2:283:LYS:O	2:2:286:GLU:HB3	1.95	0.67
2:2:270:PHE:HD2	2:2:273:ARG:HH21	1.42	0.67
8:8:32:ALA:HA	8:8:55:VAL:HG12	1.76	0.66
1:1:79:ASP:O	1:1:918:ARG:NH2	2.29	0.66
2:2:215:PHE:HB3	2:2:232:LEU:HB2	1.77	0.66
1:1:807:VAL:HG21	1:1:878:LEU:HB3	1.76	0.66
8:8:184:VAL:HG13	8:8:188:ASN:HB2	1.78	0.66
3:3:87:PHE:O	3:3:89:LYS:NZ	2.24	0.66
2:2:62:ALA:O	2:2:66:TYR:N	2.28	0.65
7:7:109:ARG:HB2	7:7:123:VAL:HG12	1.79	0.64
9:10:55:LEU:HD21	9:10:57:GLU:HG3	1.78	0.64
1:1:257:ARG:HH22	1:1:259:ILE:HB	1.63	0.64
1:1:187:TRP:CH2	1:1:201:LYS:HD2	2.33	0.63
2:2:26:ASN:O	5:5:86:ASN:ND2	2.31	0.63
1:1:316:PHE:HB3	1:1:319:THR:HG21	1.80	0.62
1:1:326:THR:HG22	1:1:328:GLY:H	1.63	0.62
2:2:22:TRP:CE3	2:2:33:ILE:HG22	2.36	0.61
2:2:60:MET:SD	2:2:92:LEU:HD12	2.40	0.61
6:6:73:ARG:HH12	6:6:76:LYS:HE2	1.65	0.61
1:1:427:ASP:OD2	1:1:544:LYS:NZ	2.26	0.61
8:8:98:ARG:HB2	8:8:101:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:719:VAL:HG21	1:1:736:LEU:HD11	1.83	0.61
1:1:775:GLN:HG2	9:10:193:ALA:HB3	1.83	0.61
9:10:51:THR:HG22	9:10:77:ASN:HB2	1.83	0.60
1:1:248:LEU:HB2	1:1:256:LEU:HD23	1.83	0.60
7:7:69:VAL:HG22	7:7:96:VAL:HG22	1.82	0.60
7:7:59:GLN:OE1	7:7:59:GLN:N	2.30	0.60
2:2:205:LEU:HD11	2:2:239:ILE:HG23	1.83	0.60
8:8:125:ILE:HG22	8:8:143:VAL:HG22	1.84	0.60
2:2:273:ARG:HD2	2:2:274:SER:N	2.17	0.60
3:3:137:THR:O	6:6:110:TYR:OH	2.20	0.60
9:10:140:SER:OG	9:10:143:SER:OG	2.18	0.60
2:2:52:ILE:O	2:2:55:ILE:HB	2.02	0.60
1:1:293:LEU:HD22	1:1:295:LEU:HD23	1.84	0.59
1:1:487:ARG:NH2	5:5:44:ASP:OD2	2.35	0.59
2:2:76:LEU:HD21	2:2:93:THR:HG22	1.84	0.59
1:1:170:SER:HA	1:1:173:ILE:HG22	1.85	0.59
1:1:221:GLN:OE1	1:1:222:HIS:ND1	2.29	0.59
1:1:487:ARG:NH1	5:5:23:SER:OG	2.35	0.59
1:1:667:PRO:O	1:1:685:ARG:NH2	2.36	0.59
2:2:102:ARG:NH1	2:2:105:ASP:OD2	2.36	0.59
8:8:110:LYS:HA	8:8:110:LYS:HE3	1.84	0.59
2:2:25:GLU:HB2	5:5:83:THR:HG21	1.85	0.58
1:1:313:LEU:HD12	1:1:383:GLY:H	1.69	0.58
8:8:74:ALA:O	8:8:78:ILE:HG12	2.02	0.58
9:10:88:ARG:NH2	9:10:94:GLU:OE2	2.37	0.58
6:6:74:TRP:HE1	6:6:81:ARG:HH21	1.52	0.58
1:1:674:VAL:HG21	1:1:710:VAL:HG11	1.85	0.58
3:3:32:HIS:HB2	3:3:193:ALA:HB2	1.86	0.57
8:8:193:ILE:HD12	8:8:193:ILE:H	1.69	0.57
1:1:91:LEU:HD13	1:1:133:LEU:HD11	1.86	0.57
3:3:82:ASN:H	3:3:89:LYS:HZ1	1.52	0.57
1:1:713:LYS:NZ	1:1:788:GLU:O	2.35	0.57
7:7:104:ARG:NH1	7:7:143:SER:OG	2.37	0.57
2:2:160:GLU:OE1	5:5:87:HIS:ND1	2.34	0.57
1:1:179:TYR:HD2	1:1:180:SER:N	2.03	0.56
1:1:233:ALA:HB1	1:1:250:LEU:HD23	1.86	0.56
1:1:540:THR:HG22	1:1:542:SER:H	1.70	0.56
2:2:261:ALA:O	2:2:265:ASN:ND2	2.38	0.56
4:4:21:LEU:HD11	8:8:107:VAL:HG13	1.87	0.56
1:1:488:LEU:O	1:1:492:LEU:HG	2.06	0.56
1:1:802:ARG:HD2	1:1:839:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:93:ARG:NH2	3:3:213:ASP:OD1	2.38	0.56
5:5:85:ARG:NH2	8:8:24:CYS:SG	2.79	0.56
1:1:457:MET:SD	1:1:536:MET:HG2	2.45	0.56
2:2:98:GLU:OE1	2:2:126:ARG:NH2	2.29	0.56
5:5:59:GLY:O	5:5:63:ILE:HG12	2.04	0.56
1:1:456:GLU:HB2	1:1:572:LEU:HD23	1.88	0.55
3:3:104:PRO:HG2	3:3:107:LEU:HB2	1.88	0.55
7:7:58:PRO:O	7:7:62:ILE:HG23	2.06	0.55
2:2:69:ASP:OD1	2:2:96:ARG:NH1	2.38	0.55
2:2:76:LEU:HD11	2:2:93:THR:HG23	1.87	0.55
1:1:402:PRO:HA	1:1:425:THR:HA	1.89	0.55
1:1:896:ILE:H	1:1:896:ILE:HD12	1.72	0.55
2:2:249:THR:O	2:2:253:ASN:ND2	2.40	0.55
3:3:32:HIS:CG	3:3:187:LEU:HD21	2.42	0.55
12:3:303:PCW:H381	12:3:303:PCW:H161	1.88	0.55
5:5:71:ASP:OD1	5:5:71:ASP:N	2.39	0.55
3:3:81:ASN:HD22	3:3:226:GLU:HG2	1.72	0.54
8:8:29:LEU:HD12	8:8:78:ILE:HG13	1.89	0.54
3:3:13:ARG:HH21	6:6:110:TYR:HB2	1.73	0.54
1:1:540:THR:O	1:1:543:GLY:N	2.40	0.54
1:1:828:PRO:HA	9:10:162:VAL:HG21	1.89	0.54
1:1:290:GLN:OE1	1:1:290:GLN:N	2.38	0.54
8:8:94:GLN:OE1	8:8:105:ASN:ND2	2.40	0.54
1:1:713:LYS:HD2	1:1:738:PRO:HA	1.88	0.54
3:3:8:LEU:HD11	3:3:136:VAL:HG12	1.88	0.54
2:2:288:MET:SD	2:2:288:MET:N	2.81	0.54
1:1:771:HIS:CE1	1:1:833:VAL:HG21	2.43	0.54
1:1:203:ASN:HD21	1:1:206:ASP:HB3	1.73	0.53
3:3:78:TYR:HD2	4:4:52:VAL:HG21	1.72	0.53
1:1:714:ARG:NH2	1:1:848:GLU:OE2	2.41	0.53
1:1:629:LEU:HB3	1:1:631:VAL:HG22	1.90	0.53
2:2:250:LYS:HA	2:2:253:ASN:HD21	1.74	0.53
6:6:30:ARG:NH1	6:6:87:GLY:O	2.42	0.53
1:1:898:TYR:HE2	9:10:197:GLU:HB3	1.73	0.53
5:5:100:LEU:HB2	8:8:132:PHE:HD2	1.74	0.53
8:8:124:LEU:HD21	8:8:126:MET:HG3	1.90	0.53
1:1:687:ARG:NH1	1:1:693:GLU:OE1	2.34	0.53
2:2:155:GLN:OE1	2:2:185:ASN:ND2	2.40	0.53
1:1:182:GLY:N	1:1:284:VAL:O	2.39	0.52
4:4:109:PRO:O	4:4:111:GLN:N	2.40	0.52
5:5:88:PRO:HA	5:5:91:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:528:ASP:OD1	1:1:529:GLU:N	2.43	0.52
2:2:226:MET:HA	2:2:229:LEU:HB2	1.91	0.52
7:7:50:ARG:HA	7:7:83:SER:HA	1.91	0.52
2:2:105:ASP:N	2:2:105:ASP:OD1	2.40	0.52
5:5:7:LYS:O	5:5:10:VAL:HG12	2.08	0.52
1:1:629:LEU:HD13	1:1:641:LEU:HD13	1.90	0.52
1:1:482:GLY:O	1:1:486:LYS:HG2	2.09	0.52
1:1:683:GLY:HA3	1:1:696:TRP:NE1	2.25	0.52
1:1:870:ILE:HB	1:1:910:ILE:HG12	1.91	0.52
1:1:266:LEU:HD22	1:1:295:LEU:HD11	1.92	0.51
9:10:203:GLU:O	9:10:207:MET:HG3	2.10	0.51
3:3:149:LYS:NZ	3:3:161:LEU:O	2.38	0.51
3:3:158:LEU:HD12	3:3:161:LEU:HD22	1.91	0.51
2:2:48:LEU:HD12	2:2:51:ASP:HB3	1.92	0.51
9:10:115:ARG:HH12	9:10:125:GLY:HA3	1.75	0.51
3:3:71:GLN:N	3:3:71:GLN:OE1	2.44	0.51
1:1:590:LEU:HD21	1:1:623:ILE:HD11	1.93	0.51
8:8:92:TYR:OH	8:8:94:GLN:NE2	2.44	0.51
1:1:246:GLN:HG2	1:1:256:LEU:HD22	1.91	0.51
1:1:957:LYS:HG3	3:3:135:PHE:CE1	2.46	0.51
8:8:80:SER:HA	8:8:83:LYS:NZ	2.25	0.51
1:1:739:ASN:OD1	1:1:824:SER:OG	2.29	0.50
2:2:131:ARG:NH1	2:2:139:GLU:OE2	2.42	0.50
9:10:146:LEU:HB3	9:10:161:VAL:HG22	1.92	0.50
3:3:182:ILE:O	3:3:186:ILE:HG22	2.10	0.50
1:1:791:VAL:HG22	1:1:808:LEU:HB2	1.93	0.50
9:10:57:GLU:HG2	9:10:70:LYS:HA	1.93	0.50
1:1:249:ALA:HB3	1:1:253:GLU:HB2	1.94	0.50
1:1:728:ASP:OD1	1:1:728:ASP:O	2.29	0.50
2:2:266:ARG:O	2:2:270:PHE:HD1	1.95	0.50
8:8:135:ASP:OD1	8:8:135:ASP:N	2.38	0.50
9:10:140:SER:OG	9:10:140:SER:O	2.29	0.50
1:1:604:PHE:HB3	1:1:611:TRP:CE3	2.47	0.49
3:3:72:SER:O	3:3:76:ARG:HG2	2.12	0.49
1:1:247:THR:HG21	1:1:305:TYR:CE1	2.46	0.49
1:1:247:THR:HG21	1:1:305:TYR:HE1	1.76	0.49
3:3:65:GLY:HA2	3:3:68:ILE:HD13	1.95	0.49
1:1:231:ASP:OD1	1:1:232:GLU:N	2.46	0.49
1:1:647:TYR:O	1:1:692:THR:OG1	2.26	0.49
2:2:33:ILE:HD11	2:2:62:ALA:HB2	1.95	0.49
3:3:89:LYS:HZ2	3:3:222:TRP:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:91:SER:HA	7:7:112:ILE:HG13	1.94	0.49
1:1:577:THR:OG1	1:1:578:THR:N	2.44	0.49
1:1:27:VAL:HG13	1:1:912:TYR:CZ	2.47	0.49
2:2:200:TYR:HD2	8:8:69:PRO:HD3	1.78	0.49
1:1:279:THR:HB	1:1:324:PHE:CD2	2.44	0.49
3:3:139:LYS:HD3	6:6:104:TYR:HE2	1.78	0.49
1:1:48:SER:O	1:1:51:SER:OG	2.30	0.49
5:5:69:ASP:HB3	6:6:76:LYS:HE3	1.95	0.49
1:1:860:HIS:ND1	1:1:949:PRO:HB3	2.28	0.48
2:2:230:PHE:HA	2:2:233:TYR:HB3	1.94	0.48
8:8:16:LEU:HB3	8:8:183:LEU:HD22	1.94	0.48
8:8:23:HIS:CE1	8:8:24:CYS:HG	2.29	0.48
1:1:35:GLN:O	1:1:445:ARG:NH2	2.43	0.48
1:1:979:THR:HG21	3:3:30:ILE:HD13	1.95	0.48
3:3:45:THR:HG22	3:3:46:GLN:H	1.76	0.48
1:1:102:ASN:HB3	1:1:105:ARG:HB2	1.95	0.48
1:1:186:VAL:HB	1:1:202:PHE:HB2	1.94	0.48
1:1:242:SER:OG	1:1:244:SER:OG	2.26	0.48
1:1:550:SER:O	1:1:944:GLN:NE2	2.46	0.48
1:1:257:ARG:HH12	1:1:259:ILE:HG22	1.79	0.48
5:5:69:ASP:HB2	5:5:71:ASP:OD1	2.14	0.48
3:3:156:ILE:HG22	3:3:158:LEU:H	1.78	0.48
8:8:146:HIS:HB2	8:8:151:TRP:CE2	2.49	0.47
1:1:871:LEU:HD11	1:1:904:ILE:HA	1.96	0.47
2:2:281:SER:O	2:2:284:ALA:HB3	2.14	0.47
3:3:31:ARG:NH1	3:3:117:ASN:O	2.46	0.47
1:1:725:VAL:HG13	4:4:165:LEU:HD12	1.96	0.47
2:2:204:GLY:O	2:2:208:LEU:N	2.41	0.47
12:3:303:PCW:H322	12:3:303:PCW:H2	1.60	0.47
7:7:151:LYS:HE2	7:7:151:LYS:HB2	1.79	0.47
1:1:469:LEU:HD13	5:5:29:SER:HB3	1.95	0.47
2:2:205:LEU:HA	2:2:208:LEU:HB2	1.95	0.47
7:7:136:TYR:O	7:7:138:LEU:N	2.48	0.47
1:1:107:MET:HE3	1:1:123:LEU:HD11	1.95	0.47
3:3:81:ASN:ND2	3:3:226:GLU:HG2	2.30	0.47
3:3:175:ASN:HA	6:6:98:LEU:HD13	1.97	0.47
1:1:199:ILE:HG21	1:1:250:LEU:HD11	1.97	0.47
1:1:340:ASN:N	1:1:340:ASN:OD1	2.48	0.47
8:8:201:GLU:HB3	8:8:204:LYS:HZ1	1.79	0.47
1:1:886:PRO:HG3	1:1:897:PRO:HB3	1.96	0.46
8:8:106:GLN:O	8:8:110:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:124:ASN:ND2	7:7:130:GLU:OE2	2.30	0.46
9:10:141:HIS:ND1	9:10:177:ASP:OD2	2.48	0.46
8:8:5:LYS:HD3	8:8:6:LEU:N	2.31	0.46
5:5:52:ALA:O	5:5:56:THR:OG1	2.20	0.46
8:8:12:CYS:O	8:8:16:LEU:HD23	2.16	0.46
8:8:80:SER:HA	8:8:83:LYS:HZ3	1.81	0.46
9:10:76:TRP:HB2	9:10:83:LEU:HD13	1.98	0.46
1:1:54:LEU:O	1:1:65:ALA:HA	2.16	0.46
1:1:954:ASP:HB2	3:3:8:LEU:HD23	1.96	0.46
2:2:69:ASP:OD2	5:5:98:ARG:NH2	2.41	0.46
7:7:58:PRO:HA	7:7:61:TRP:NE1	2.31	0.46
1:1:545:LEU:HD21	1:1:589:LEU:HD22	1.98	0.46
1:1:670:PHE:CE2	1:1:685:ARG:HG2	2.51	0.46
1:1:795:TYR:CZ	1:1:804:GLU:HB2	2.51	0.46
2:2:182:MET:HE1	2:2:195:TYR:CD2	2.50	0.46
8:8:143:VAL:HG12	8:8:154:ARG:NH1	2.31	0.46
9:10:62:ILE:HD12	9:10:62:ILE:H	1.81	0.46
1:1:794:GLN:HB2	1:1:805:PHE:CE1	2.49	0.46
3:3:5:GLU:HB3	3:3:6:LEU:H	1.64	0.46
1:1:898:TYR:CE2	9:10:197:GLU:HB3	2.50	0.46
1:1:990:ARG:HA	1:1:990:ARG:HD2	1.84	0.46
3:3:126:GLY:O	3:3:130:MET:HG2	2.16	0.46
7:7:106:ASP:OD1	7:7:106:ASP:N	2.49	0.46
8:8:163:ASP:HB3	8:8:166:GLU:HB3	1.98	0.46
1:1:381:GLU:OE2	1:1:382:THR:OG1	2.33	0.46
1:1:757:ILE:HG22	1:1:778:ALA:HB3	1.98	0.46
1:1:169:GLU:OE1	1:1:172:SER:OG	2.33	0.45
1:1:534:LYS:HE3	1:1:927:SER:HA	1.98	0.45
1:1:770:ILE:HG23	1:1:831:PRO:HD2	1.98	0.45
8:8:60:LEU:HD22	8:8:74:ALA:HB1	1.97	0.45
1:1:33:ARG:HD3	1:1:914:GLN:HB3	1.98	0.45
1:1:882:ARG:HH11	1:1:896:ILE:HB	1.81	0.45
4:4:54:ASP:OD1	4:4:54:ASP:N	2.49	0.45
6:6:55:TYR:HB2	6:6:96:TYR:CZ	2.51	0.45
8:8:143:VAL:HG23	8:8:160:TYR:CE1	2.51	0.45
1:1:290:GLN:NE2	1:1:381:GLU:HA	2.31	0.45
5:5:96:ARG:HH11	8:8:22:PRO:HA	1.82	0.45
8:8:170:ILE:HD11	8:8:206:VAL:HG22	1.98	0.45
9:10:151:ASP:OD1	9:10:153:ALA:N	2.49	0.45
9:10:187:LEU:HD23	9:10:189:PRO:HD3	1.98	0.45
1:1:623:ILE:HA	1:1:644:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:10:110:VAL:HG11	9:10:161:VAL:HG21	1.98	0.45
1:1:873:LEU:HD21	1:1:902:VAL:HG11	1.99	0.45
2:2:52:ILE:HA	2:2:55:ILE:HD12	1.97	0.45
3:3:71:GLN:O	3:3:74:LEU:HD12	2.15	0.45
9:10:200:ALA:O	9:10:203:GLU:HG3	2.17	0.45
1:1:37:VAL:HB	1:1:58:THR:HG21	1.98	0.45
1:1:457:MET:HG3	1:1:925:ALA:HB2	1.99	0.45
2:2:248:LYS:HG3	2:2:249:THR:N	2.31	0.45
7:7:136:TYR:O	7:7:138:LEU:HD12	2.16	0.45
1:1:550:SER:HB2	1:1:944:GLN:HE21	1.82	0.45
7:7:67:VAL:HG21	7:7:84:PHE:CE2	2.52	0.45
8:8:93:TYR:HA	8:8:125:ILE:O	2.17	0.45
1:1:176:GLN:OE1	1:1:224:SER:N	2.33	0.45
8:8:60:LEU:HD12	8:8:60:LEU:O	2.17	0.45
1:1:469:LEU:HB2	5:5:33:LEU:HD12	1.99	0.45
2:2:270:PHE:HA	2:2:273:ARG:HG3	1.99	0.45
3:3:81:ASN:HB2	3:3:222:TRP:CE2	2.52	0.45
9:10:68:PHE:HB2	9:10:111:ARG:HH21	1.82	0.45
1:1:370:ASN:HB3	1:1:372:THR:HG23	1.99	0.44
3:3:88:PHE:HB3	3:3:222:TRP:HD1	1.81	0.44
1:1:169:GLU:OE1	1:1:173:ILE:HB	2.17	0.44
6:6:73:ARG:HH12	6:6:76:LYS:CE	2.28	0.44
7:7:172:PRO:O	7:7:176:PHE:N	2.40	0.44
5:5:53:PHE:HE2	6:6:36:LEU:HB3	1.82	0.44
6:6:43:ILE:HD13	6:6:107:VAL:HG21	1.99	0.44
3:3:56:ILE:HA	3:3:59:ARG:NH1	2.32	0.44
1:1:329:GLU:OE2	1:1:329:GLU:N	2.50	0.44
8:8:186:PHE:O	8:8:190:LEU:HG	2.18	0.44
1:1:771:HIS:NE2	1:1:773:SER:HB2	2.33	0.44
2:2:283:LYS:HD3	8:8:81:TRP:HA	2.00	0.44
1:1:129:GLN:HB2	1:1:146:LEU:HD23	2.00	0.44
1:1:960:TYR:HE2	3:3:15:TRP:HB3	1.83	0.44
2:2:63:ALA:O	2:2:67:GLY:N	2.49	0.44
1:1:96:ASP:OD1	1:1:96:ASP:N	2.44	0.44
1:1:179:TYR:HD2	1:1:180:SER:H	1.66	0.44
1:1:912:TYR:HD1	1:1:913:ASN:H	1.66	0.44
2:2:199:LYS:HD3	2:2:199:LYS:HA	1.76	0.44
1:1:809:GLU:HB2	1:1:880:PRO:HG2	2.00	0.44
3:3:78:TYR:CE2	4:4:52:VAL:HG11	2.53	0.44
5:5:74:SER:OG	5:5:75:GLU:N	2.51	0.43
6:6:67:ILE:HD13	6:6:67:ILE:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:284:ALA:O	2:2:287:ASP:HB3	2.18	0.43
5:5:88:PRO:HA	5:5:91:TYR:CD1	2.53	0.43
8:8:15:VAL:HA	8:8:132:PHE:HZ	1.83	0.43
3:3:122:ILE:HD12	3:3:173:PHE:HZ	1.84	0.43
1:1:27:VAL:HG21	10:A:1:NAG:H62	2.01	0.43
1:1:167:LEU:HD12	1:1:167:LEU:H	1.84	0.43
1:1:466:GLN:HB3	5:5:33:LEU:HD11	2.01	0.43
1:1:672:TYR:CZ	1:1:741:LEU:HD21	2.53	0.43
1:1:956:LEU:HD13	3:3:12:ILE:HD12	2.01	0.43
1:1:982:LEU:HB3	3:3:37:LEU:HD11	2.01	0.43
1:1:775:GLN:OE1	1:1:795:TYR:CZ	2.71	0.43
2:2:141:ILE:HD11	2:2:164:LEU:HB3	2.01	0.43
2:2:227:ARG:HG3	8:8:190:LEU:HD13	2.01	0.43
1:1:81:GLY:HA2	1:1:918:ARG:HH21	1.83	0.43
3:3:69:PRO:HB2	3:3:71:GLN:OE1	2.19	0.43
9:10:91:SER:OG	9:10:92:GLU:N	2.51	0.43
1:1:139:SER:OG	1:1:141:ARG:NH1	2.51	0.43
1:1:960:TYR:HB3	1:1:962:TYR:CE1	2.52	0.43
9:10:148:LEU:HD11	9:10:156:VAL:HG13	1.99	0.43
9:10:132:VAL:HG21	9:10:163:THR:HG23	2.00	0.43
1:1:290:GLN:HE21	1:1:381:GLU:HA	1.83	0.43
1:1:374:THR:HA	1:1:391:ILE:O	2.18	0.43
1:1:779:LYS:HE2	1:1:779:LYS:HB3	1.79	0.43
1:1:958:ASP:OD1	7:7:152:ARG:NH2	2.33	0.43
8:8:17:HIS:ND1	8:8:93:TYR:OH	2.46	0.43
12:1:1002:PCW:H11	3:3:186:ILE:HD11	2.00	0.43
1:1:843:SER:OG	1:1:844:ILE:N	2.48	0.42
2:2:112:ARG:O	2:2:115:GLN:HG2	2.19	0.42
8:8:70:MET:HA	8:8:70:MET:CE	2.49	0.42
12:3:302:PCW:H40	12:3:302:PCW:H431	1.57	0.42
1:1:890:SER:O	1:1:894:ASN:N	2.52	0.42
12:3:303:PCW:H321	12:3:303:PCW:H351	1.59	0.42
5:5:69:ASP:HB3	6:6:76:LYS:CE	2.50	0.42
1:1:795:TYR:OH	1:1:804:GLU:OE1	2.28	0.42
1:1:797:ASN:HD22	1:1:804:GLU:CD	2.22	0.42
12:3:303:PCW:H42	12:3:303:PCW:H83	1.86	0.42
1:1:460:LEU:HD21	1:1:535:MET:HB3	2.02	0.42
1:1:663:HIS:CE1	1:1:688:LYS:HD2	2.54	0.42
1:1:777:LYS:HD3	1:1:799:LYS:HG3	2.01	0.42
3:3:129:ASN:ND2	3:3:154:GLN:OE1	2.52	0.42
5:5:10:VAL:HG21	5:5:60:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:10:143:SER:HB2	9:10:182:ASN:HD22	1.83	0.42
1:1:228:GLY:O	1:1:235:LEU:HD12	2.19	0.42
1:1:953:PHE:CZ	3:3:158:LEU:HD11	2.54	0.42
2:2:139:GLU:HB2	2:2:142:ARG:HH21	1.85	0.42
9:10:60:PHE:O	9:10:97:ARG:NH1	2.52	0.42
1:1:55:VAL:HG11	1:1:97:VAL:HG21	2.02	0.42
1:1:217:THR:O	1:1:217:THR:OG1	2.37	0.42
1:1:483:MET:HA	1:1:486:LYS:HE3	2.02	0.42
2:2:193:GLN:O	2:2:197:GLU:HG3	2.20	0.42
6:6:94:PHE:O	6:6:97:VAL:HG12	2.20	0.42
1:1:233:ALA:O	1:1:250:LEU:HB3	2.20	0.42
1:1:576:ARG:NH2	1:1:586:GLN:OE1	2.53	0.42
2:2:82:GLN:O	2:2:82:GLN:NE2	2.52	0.42
2:2:124:ARG:H	2:2:124:ARG:HG2	1.61	0.42
2:2:144:LEU:HB3	2:2:161:LEU:HD12	2.01	0.42
3:3:119:LEU:HD12	3:3:119:LEU:HA	1.91	0.42
8:8:6:LEU:HA	8:8:54:PHE:HB2	2.02	0.42
8:8:161:CYS:SG	8:8:162:GLU:N	2.93	0.42
8:8:170:ILE:HD11	8:8:206:VAL:HA	2.01	0.42
1:1:109:SER:O	1:1:118:ASN:N	2.44	0.42
1:1:303:LEU:HD13	1:1:310:LEU:HD12	2.02	0.42
8:8:202:ILE:HG13	8:8:203:ASN:N	2.35	0.42
2:2:29:ASN:OD1	2:2:29:ASN:N	2.45	0.42
7:7:103:TYR:HA	7:7:146:PRO:HD3	2.01	0.42
7:7:104:ARG:HB3	7:7:146:PRO:HG3	2.01	0.42
7:7:117:LYS:HE2	7:7:117:LYS:HB2	1.89	0.42
8:8:85:HIS:HB3	8:8:87:TYR:CE2	2.55	0.42
1:1:39:LYS:HD2	1:1:428:HIS:CD2	2.55	0.41
1:1:670:PHE:O	4:4:177:SER:HA	2.19	0.41
1:1:685:ARG:HD2	9:10:107:LEU:HD11	2.02	0.41
1:1:165:GLU:HG3	1:1:207:GLY:O	2.20	0.41
1:1:175:TYR:HA	1:1:190:GLY:HA2	2.02	0.41
1:1:179:TYR:OH	1:1:287:SER:HB3	2.19	0.41
1:1:452:VAL:HG21	1:1:538:MET:HE3	2.00	0.41
9:10:146:LEU:HG	9:10:185:VAL:HG22	2.01	0.41
1:1:47:PHE:HB3	1:1:51:SER:OG	2.21	0.41
1:1:199:ILE:HG21	1:1:250:LEU:CD1	2.51	0.41
1:1:530:PHE:O	1:1:928:GLY:HA3	2.20	0.41
1:1:573:MET:SD	1:1:640:LEU:HD13	2.60	0.41
8:8:204:LYS:HG2	8:8:205:ALA:N	2.34	0.41
2:2:183:MET:SD	3:3:61:LEU:HD13	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:68:ALA:N	8:8:69:PRO:HD2	2.35	0.41
1:1:845:SER:N	1:1:864:GLY:O	2.51	0.41
9:10:90:LEU:O	9:10:95:ARG:NH2	2.51	0.41
1:1:230:VAL:HG11	1:1:291:PHE:CG	2.55	0.41
1:1:973:VAL:HG22	3:3:26:PHE:CE2	2.55	0.41
2:2:144:LEU:HD12	2:2:144:LEU:HA	1.85	0.41
2:2:262:SER:HA	2:2:265:ASN:HD22	1.86	0.41
3:3:77:LYS:NZ	3:3:225:LEU:O	2.40	0.41
5:5:42:PRO:HB2	5:5:45:ILE:HG23	2.03	0.41
9:10:60:PHE:HB2	9:10:101:VAL:HG21	2.02	0.41
3:3:179:LEU:HD23	3:3:179:LEU:HA	1.82	0.41
8:8:145:GLU:HB3	8:8:154:ARG:NH1	2.35	0.41
8:8:154:ARG:HG3	8:8:154:ARG:HH11	1.86	0.41
8:8:96:ASN:OD1	8:8:97:GLU:N	2.48	0.41
9:10:59:SER:HB3	9:10:68:PHE:HA	2.03	0.41
1:1:134:VAL:HG12	1:1:180:SER:CB	2.51	0.41
1:1:192:VAL:HG12	1:1:195:SER:HB3	2.03	0.41
1:1:332:VAL:HG21	1:1:417:VAL:HG11	2.02	0.41
1:1:765:VAL:HG11	4:4:175:GLU:HG2	2.03	0.41
2:2:90:LYS:HB3	2:2:113:ILE:HD11	2.03	0.41
2:2:164:LEU:HD23	2:2:164:LEU:HA	1.82	0.41
5:5:28:ARG:HA	5:5:28:ARG:HD2	1.79	0.41
6:6:66:LEU:HB3	6:6:84:LEU:HD22	2.03	0.41
7:7:66:ARG:HH11	7:7:75:VAL:HG21	1.86	0.41
8:8:198:THR:OG1	8:8:200:PRO:HD3	2.21	0.41
1:1:134:VAL:O	1:1:140:VAL:HG23	2.21	0.41
1:1:442:LEU:HD12	1:1:442:LEU:HA	1.91	0.41
1:1:879:ASP:O	1:1:882:ARG:HG3	2.20	0.41
2:2:147:TYR:CD2	2:2:148:LEU:HD22	2.55	0.41
2:2:180:GLU:O	2:2:183:MET:HB2	2.20	0.41
3:3:119:LEU:O	3:3:122:ILE:HG22	2.21	0.41
6:6:81:ARG:NH2	12:6:202:PCW:H41	2.36	0.41
1:1:191:VAL:HG11	1:1:223:LEU:HD13	2.03	0.40
1:1:219:TRP:NE1	1:1:246:GLN:OE1	2.44	0.40
2:2:160:GLU:HG2	5:5:90:PHE:CD2	2.57	0.40
3:3:89:LYS:CE	3:3:222:TRP:HE1	2.34	0.40
8:8:145:GLU:HB3	8:8:154:ARG:CZ	2.51	0.40
1:1:180:SER:OG	1:1:186:VAL:HA	2.22	0.40
1:1:987:LEU:HD12	1:1:987:LEU:HA	1.97	0.40
2:2:90:LYS:HE2	2:2:112:ARG:HH22	1.86	0.40
8:8:4:VAL:HG21	8:8:123:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:452:VAL:HG11	1:1:938:TYR:HB2	2.03	0.40
1:1:916:VAL:HG13	1:1:941:ASP:HB2	2.03	0.40
1:1:987:LEU:HD13	3:3:36:ILE:HD11	2.03	0.40
2:2:60:MET:CE	2:2:76:LEU:HB2	2.51	0.40
1:1:739:ASN:O	1:1:764:GLY:N	2.54	0.40
1:1:146:LEU:HD11	1:1:175:TYR:HB3	2.03	0.40
1:1:219:TRP:HH2	1:1:237:CYS:HB3	1.86	0.40
1:1:261:LEU:HD23	1:1:261:LEU:HA	1.97	0.40
1:1:463:THR:HB	1:1:526:ALA:HB1	2.02	0.40
2:2:133:ALA:C	8:8:98:ARG:HH12	2.25	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	1	924/993 (93%)	860 (93%)	64 (7%)	0	100	100
2	2	279/297 (94%)	273 (98%)	6 (2%)	0	100	100
3	3	219/261 (84%)	206 (94%)	13 (6%)	0	100	100
4	4	138/183 (75%)	130 (94%)	8 (6%)	0	100	100
5	5	99/131 (76%)	95 (96%)	4 (4%)	0	100	100
6	6	97/110 (88%)	97 (100%)	0	0	100	100
7	7	134/242 (55%)	122 (91%)	12 (9%)	0	100	100
8	8	188/210 (90%)	182 (97%)	6 (3%)	0	100	100
9	10	150/262 (57%)	147 (98%)	3 (2%)	0	100	100
All	All	2228/2689 (83%)	2112 (95%)	116 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1	815/872 (94%)	795 (98%)	20 (2%)	47 75
2	2	236/255 (92%)	227 (96%)	9 (4%)	33 66
3	3	204/235 (87%)	193 (95%)	11 (5%)	22 57
4	4	46/149 (31%)	44 (96%)	2 (4%)	29 63
5	5	82/112 (73%)	76 (93%)	6 (7%)	14 46
6	6	78/85 (92%)	78 (100%)	0	100 100
7	7	110/207 (53%)	108 (98%)	2 (2%)	59 81
8	8	168/182 (92%)	158 (94%)	10 (6%)	19 54
9	10	129/194 (66%)	126 (98%)	3 (2%)	50 76
All	All	1868/2291 (82%)	1805 (97%)	63 (3%)	40 69

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	90	MET
1	1	137	GLN
1	1	179	TYR
1	1	187	TRP
1	1	211	GLN
1	1	227	CYS
1	1	257	ARG
1	1	304	GLN
1	1	414	ASP
1	1	445	ARG
1	1	632	MET
1	1	665	LEU
1	1	799	LYS
1	1	801	ARG
1	1	879	ASP
1	1	894	ASN
1	1	919	MET
1	1	927	SER

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Mol	Chain	Res	Type
1	1	933	CYS
1	1	951	LYS
2	2	25	GLU
2	2	44	TYR
2	2	81	ARG
2	2	158	TRP
2	2	177	CYS
2	2	230	PHE
2	2	248	LYS
2	2	269	GLN
2	2	280	TYR
3	3	74	LEU
3	3	78	TYR
3	3	79	TYR
3	3	90	LYS
3	3	106	MET
3	3	111	MET
3	3	151	MET
3	3	173	PHE
3	3	216	LYS
3	3	222	TRP
3	3	247	HIS
4	4	49	ASP
4	4	54	ASP
5	5	7	LYS
5	5	15	PHE
5	5	69	ASP
5	5	75	GLU
5	5	76	LEU
5	5	84	LEU
7	7	118	MET
7	7	163	ASN
8	8	9	GLN
8	8	61	PHE
8	8	83	LYS
8	8	87	TYR
8	8	119	PHE
8	8	134	MET
8	8	187	ASP
8	8	195	ASN
8	8	197	TRP
8	8	204	LYS

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Mol	Chain	Res	Type
9	10	100	ASP
9	10	151	ASP
9	10	155	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	212	GLN
1	1	299	HIS
1	1	315	ASN
1	1	794	GLN
2	2	265	ASN
3	3	195	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

6 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	A	1	1,10	14,14,15	0.19	0	17,19,21	0.45	0
10	NAG	A	2	10	14,14,15	0.21	0	17,19,21	0.46	0
10	NAG	B	1	1,10	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
10	NAG	B	2	10	14,14,15	0.19	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	C	1	10,9	14,14,15	0.19	0	17,19,21	0.43	0
10	NAG	C	2	10	14,14,15	0.24	0	17,19,21	0.43	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
10	NAG	A	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	2	10	-	2/6/23/26	0/1/1/1
10	NAG	B	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	2	10	-	0/6/23/26	0/1/1/1
10	NAG	C	1	10,9	-	2/6/23/26	0/1/1/1
10	NAG	C	2	10	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	1	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2	NAG	C4-C5-C6-O6
10	C	2	NAG	O5-C5-C6-O6
10	C	1	NAG	C4-C5-C6-O6
10	A	2	NAG	O5-C5-C6-O6
10	C	2	NAG	C4-C5-C6-O6
10	C	1	NAG	O5-C5-C6-O6

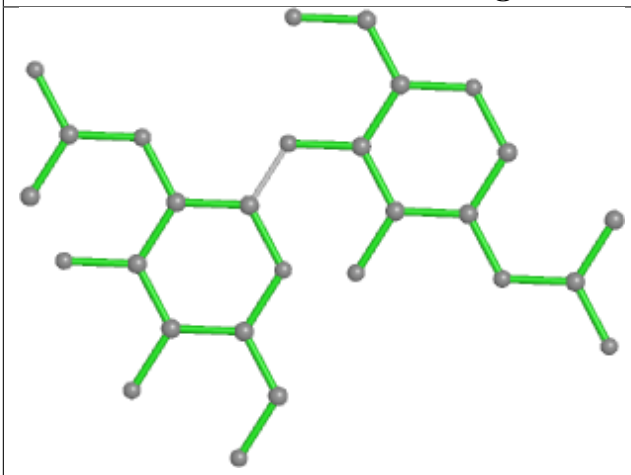
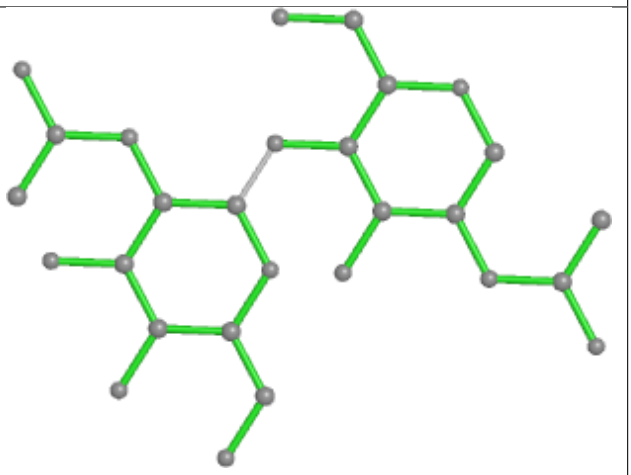
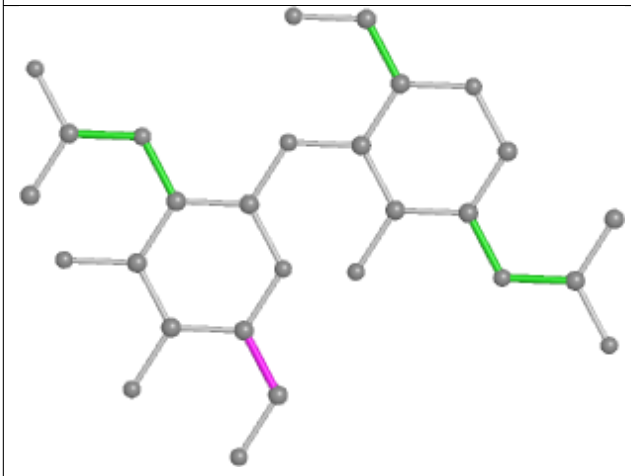
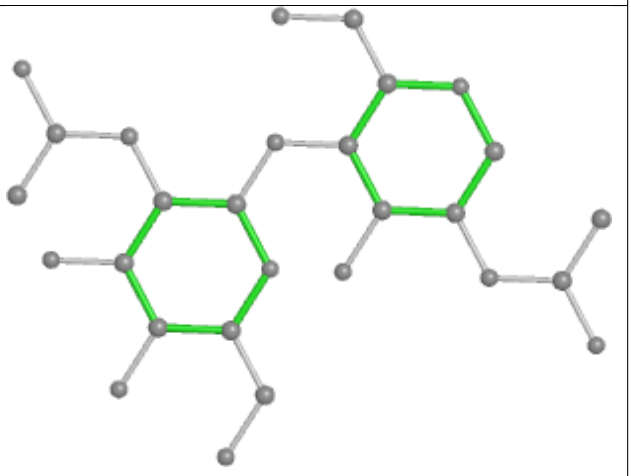
There are no ring outliers.

1 monomer is involved in 1 short contact:

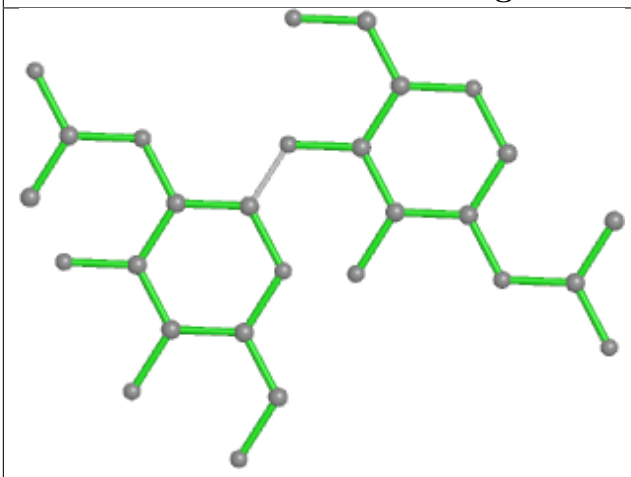
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

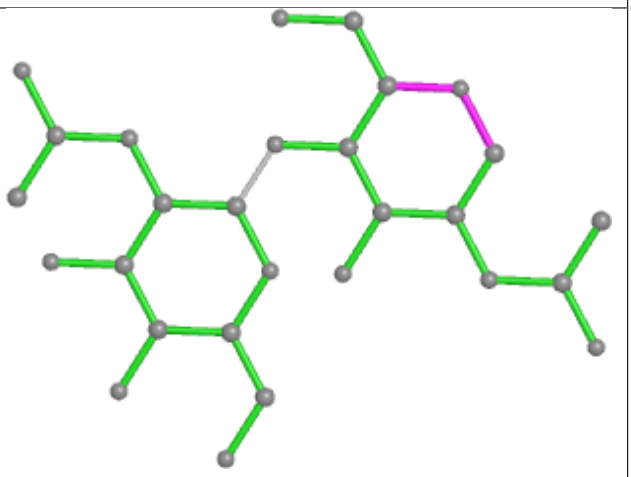
bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain A	
 Bond lengths	 Bond angles
 Torsions	 Rings

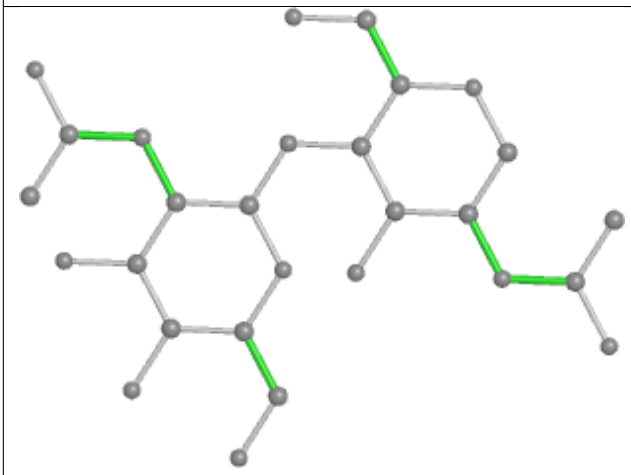
Oligosaccharide Chain B



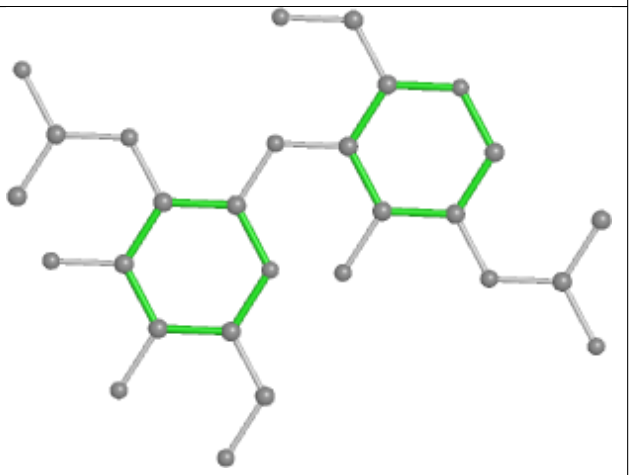
Bond lengths



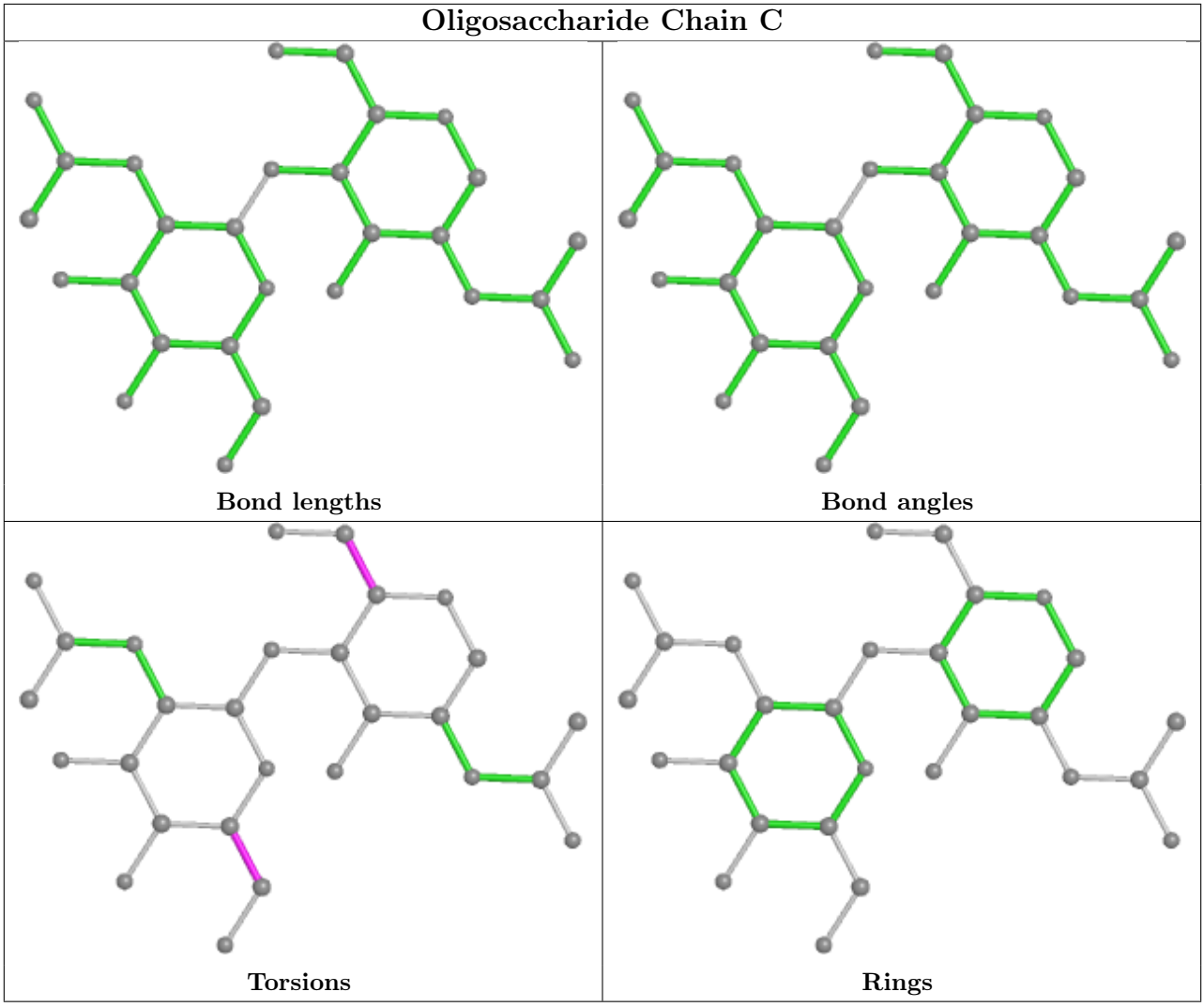
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

7 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	1	1001	1	14,14,15	0.23	0	17,19,21	0.44	0
12	PCW	3	302	-	53,53,53	1.11	3 (5%)	59,61,61	1.12	3 (5%)
12	PCW	3	301	-	37,37,53	1.25	3 (8%)	43,45,61	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PCW	3	303	-	33,33,53	1.27	3 (9%)	39,41,61	1.12	2 (5%)
12	PCW	6	202	-	29,29,53	1.32	3 (10%)	35,37,61	1.12	2 (5%)
12	PCW	6	201	-	21,21,53	1.34	3 (14%)	25,28,61	0.96	1 (4%)
12	PCW	1	1002	-	28,28,53	1.33	3 (10%)	34,36,61	1.12	2 (5%)

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	1	1001	1	-	2/6/23/26	0/1/1/1
12	PCW	3	302	-	-	34/57/57/57	-
12	PCW	3	301	-	-	22/41/41/57	-
12	PCW	3	303	-	-	19/37/37/57	-
12	PCW	6	202	-	-	21/33/33/57	-
12	PCW	6	201	-	-	13/24/24/57	-
12	PCW	1	1002	-	-	17/32/32/57	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	302	PCW	O3-C11	3.12	1.42	1.33
12	6	202	PCW	O3-C11	3.12	1.42	1.33
12	3	301	PCW	O3-C11	3.12	1.42	1.33
12	3	303	PCW	O3-C11	3.10	1.42	1.33
12	1	1002	PCW	O3-C11	3.09	1.42	1.33
12	3	303	PCW	O2-C31	3.04	1.42	1.34
12	3	301	PCW	O2-C31	2.98	1.42	1.34
12	3	302	PCW	O2-C31	2.96	1.42	1.34
12	6	202	PCW	O2-C31	2.95	1.42	1.34
12	1	1002	PCW	O2-C31	2.95	1.42	1.34
12	6	201	PCW	O2-C31	2.94	1.42	1.34
12	6	201	PCW	O3-C11	2.34	1.42	1.33
12	1	1002	PCW	O2-C2	-2.16	1.41	1.46
12	6	201	PCW	O2-C2	-2.15	1.41	1.46
12	3	302	PCW	O2-C2	-2.14	1.41	1.46
12	3	301	PCW	O2-C2	-2.14	1.41	1.46
12	6	202	PCW	O2-C2	-2.13	1.41	1.46
12	3	303	PCW	O2-C2	-2.10	1.41	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	3	303	PCW	O2-C31-C32	4.34	120.85	111.50
12	6	202	PCW	O2-C31-C32	3.99	120.09	111.50
12	3	301	PCW	O2-C31-C32	3.96	120.04	111.50
12	3	302	PCW	O2-C31-C32	3.96	120.04	111.50
12	1	1002	PCW	O2-C31-C32	3.84	119.78	111.50
12	3	302	PCW	C21-C20-C19	3.69	153.05	124.73
12	6	201	PCW	O2-C31-C32	3.31	120.04	110.80
12	6	202	PCW	O3-C11-C12	2.62	120.12	111.91
12	1	1002	PCW	O3-C11-C12	2.61	120.11	111.91
12	3	302	PCW	O3-C11-C12	2.57	119.97	111.91
12	3	301	PCW	O3-C11-C12	2.56	119.93	111.91
12	3	303	PCW	O3-C11-C12	2.55	119.91	111.91
12	3	301	PCW	C18-C19-C20	-2.15	112.19	126.84

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	3	301	PCW	O4P-C4-C5-N
12	3	301	PCW	C32-C31-O2-C2
12	3	301	PCW	C1-O3P-P-O1P
12	3	301	PCW	C1-O3P-P-O2P
12	3	302	PCW	O4P-C4-C5-N
12	3	302	PCW	C1-O3P-P-O1P
12	3	302	PCW	C1-O3P-P-O2P
12	3	302	PCW	C4-O4P-P-O1P
12	3	302	PCW	C4-O4P-P-O3P
12	3	303	PCW	O4P-C4-C5-N
12	3	303	PCW	C32-C31-O2-C2
12	3	303	PCW	O31-C31-O2-C2
12	3	303	PCW	C1-O3P-P-O1P
12	6	201	PCW	O4P-C4-C5-N
12	6	202	PCW	C2-C1-O3P-P
12	6	202	PCW	O2-C2-C3-O3
12	6	202	PCW	O4P-C4-C5-N
12	6	202	PCW	C32-C31-O2-C2
12	6	202	PCW	C1-O3P-P-O1P
12	6	202	PCW	C4-O4P-P-O2P
12	3	301	PCW	O31-C31-O2-C2
12	3	302	PCW	O31-C31-O2-C2
12	6	202	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
12	3	301	PCW	C12-C11-O3-C3
12	3	302	PCW	C32-C31-O2-C2
12	3	302	PCW	C12-C11-O3-C3
12	3	302	PCW	O11-C11-O3-C3
12	6	202	PCW	O11-C11-O3-C3
12	6	202	PCW	C12-C11-O3-C3
12	3	301	PCW	O11-C11-O3-C3
11	1	1001	NAG	O5-C5-C6-O6
12	1	1002	PCW	C12-C11-O3-C3
12	3	302	PCW	C42-C43-C44-C45
12	1	1002	PCW	O11-C11-O3-C3
11	1	1001	NAG	C4-C5-C6-O6
12	1	1002	PCW	C1-O3P-P-O4P
12	3	301	PCW	C1-O3P-P-O4P
12	3	302	PCW	C1-O3P-P-O4P
12	3	303	PCW	C1-O3P-P-O4P
12	6	201	PCW	C1-O3P-P-O4P
12	6	201	PCW	C4-O4P-P-O3P
12	6	202	PCW	C1-O3P-P-O4P
12	6	202	PCW	C4-O4P-P-O3P
12	6	202	PCW	C11-C12-C13-C14
12	3	302	PCW	C20-C21-C22-C23
12	3	302	PCW	C40-C41-C42-C43
12	3	302	PCW	C22-C23-C24-C25
12	3	301	PCW	C14-C15-C16-C17
12	3	302	PCW	C35-C36-C37-C38
12	3	303	PCW	C35-C36-C37-C38
12	3	301	PCW	C11-C12-C13-C14
12	3	303	PCW	C13-C14-C15-C16
12	3	301	PCW	C13-C14-C15-C16
12	3	302	PCW	C43-C44-C45-C46
12	3	301	PCW	C33-C34-C35-C36
12	3	301	PCW	C35-C36-C37-C38
12	3	302	PCW	C23-C24-C25-C26
12	1	1002	PCW	C1-C2-C3-O3
12	6	201	PCW	C32-C31-O2-C2
12	3	302	PCW	C14-C15-C16-C17
12	3	303	PCW	C31-C32-C33-C34
12	6	201	PCW	O31-C31-O2-C2
12	1	1002	PCW	C32-C31-O2-C2
12	1	1002	PCW	C11-C12-C13-C14
12	3	303	PCW	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
12	3	301	PCW	C16-C17-C18-C19
12	3	302	PCW	C16-C17-C18-C19
12	3	302	PCW	C36-C37-C38-C39
12	1	1002	PCW	O31-C31-O2-C2
12	3	303	PCW	O3P-C1-C2-C3
12	6	201	PCW	O3P-C1-C2-C3
12	3	302	PCW	C41-C42-C43-C44
12	3	303	PCW	C1-C2-C3-O3
12	3	303	PCW	C12-C13-C14-C15
12	3	301	PCW	C31-C32-C33-C34
12	3	302	PCW	C13-C14-C15-C16
12	3	303	PCW	C14-C15-C16-C17
12	3	303	PCW	O2-C2-C3-O3
12	1	1002	PCW	C14-C15-C16-C17
12	3	302	PCW	C45-C46-C47-C48
12	6	202	PCW	C1-C2-C3-O3
12	1	1002	PCW	C2-C1-O3P-P
12	3	303	PCW	C36-C37-C38-C39
12	3	303	PCW	C32-C33-C34-C35
12	3	301	PCW	C1-C2-C3-O3
12	3	302	PCW	C33-C34-C35-C36
12	3	301	PCW	C37-C38-C39-C40
12	3	302	PCW	C24-C25-C26-C27
12	3	302	PCW	O2-C2-C3-O3
12	6	201	PCW	C2-C3-O3-C11
12	3	301	PCW	C32-C33-C34-C35
12	3	301	PCW	C34-C35-C36-C37
12	3	301	PCW	C2-C1-O3P-P
12	1	1002	PCW	C1-O3P-P-O2P
12	3	301	PCW	C4-O4P-P-O1P
12	3	302	PCW	C4-O4P-P-O2P
12	3	303	PCW	C4-O4P-P-O2P
12	6	201	PCW	C1-O3P-P-O1P
12	6	201	PCW	C1-O3P-P-O2P
12	6	201	PCW	C4-O4P-P-O2P
12	1	1002	PCW	C5-C4-O4P-P
12	6	202	PCW	C5-C4-O4P-P
12	3	303	PCW	O3P-C1-C2-O2
12	6	202	PCW	O3P-C1-C2-O2
12	3	302	PCW	C25-C26-C27-C28
12	1	1002	PCW	O4P-C4-C5-N
12	6	201	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
12	1	1002	PCW	O2-C2-C3-O3
12	6	201	PCW	O3P-C1-C2-O2
12	1	1002	PCW	C12-C13-C14-C15
12	1	1002	PCW	C31-C32-C33-C34
12	6	202	PCW	O3P-C1-C2-C3
12	6	202	PCW	C32-C33-C34-C35
12	6	202	PCW	C13-C14-C15-C16
12	3	302	PCW	C1-C2-C3-O3
12	3	301	PCW	C36-C37-C38-C39
12	3	302	PCW	C19-C20-C21-C22
12	3	302	PCW	C39-C40-C41-C42
12	3	302	PCW	O2-C31-C32-C33
12	6	202	PCW	C12-C13-C14-C15
12	1	1002	PCW	O3-C11-C12-C13
12	6	201	PCW	C4-O4P-P-O1P
12	6	202	PCW	O2-C31-C32-C33
12	3	302	PCW	C5-C4-O4P-P
12	3	302	PCW	O31-C31-C32-C33
12	1	1002	PCW	O11-C11-C12-C13
12	3	303	PCW	O2-C31-C32-C33
12	6	202	PCW	O3-C11-C12-C13

There are no ring outliers.

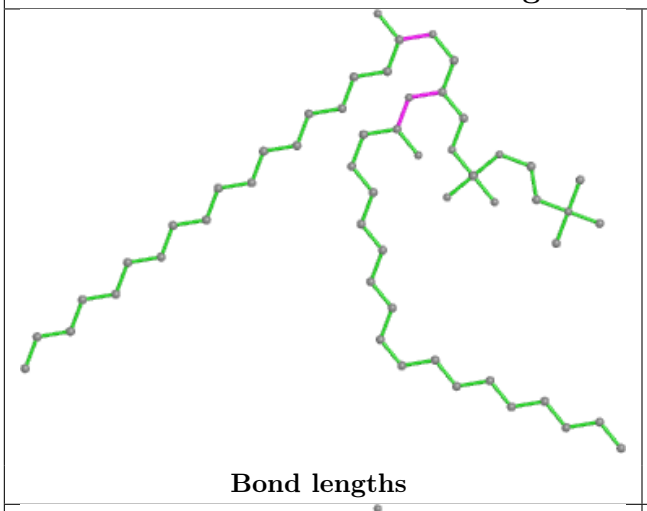
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	3	302	PCW	1	0
12	3	303	PCW	4	0
12	6	202	PCW	1	0
12	1	1002	PCW	1	0

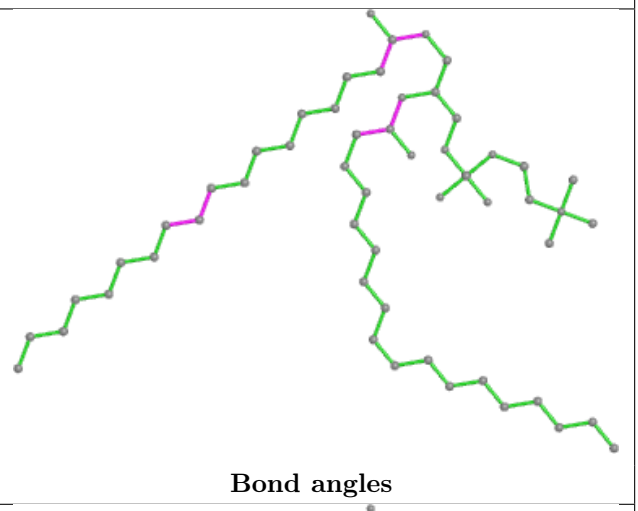
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

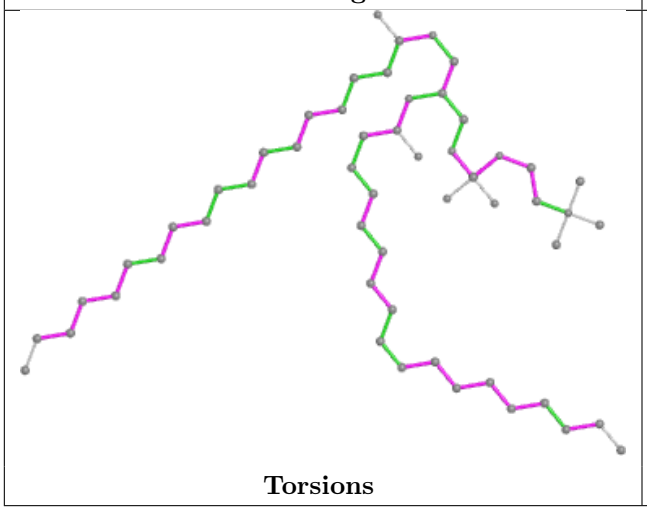
Ligand PCW 3 302



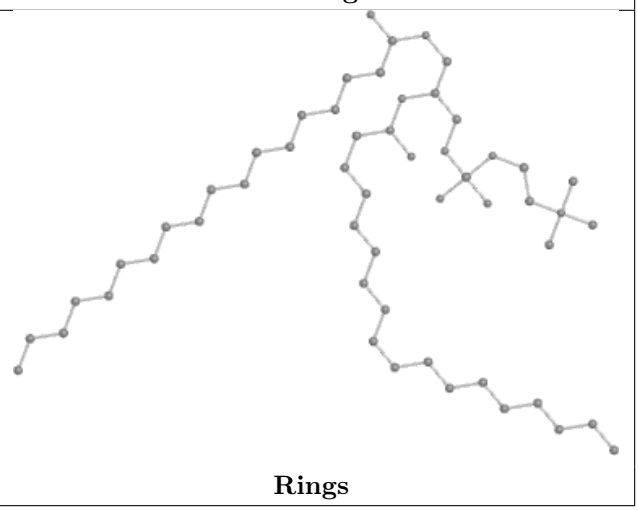
Bond lengths



Bond angles

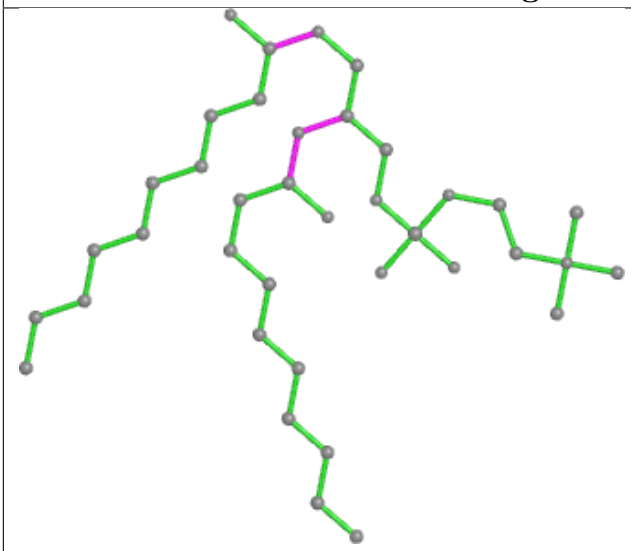


Torsions

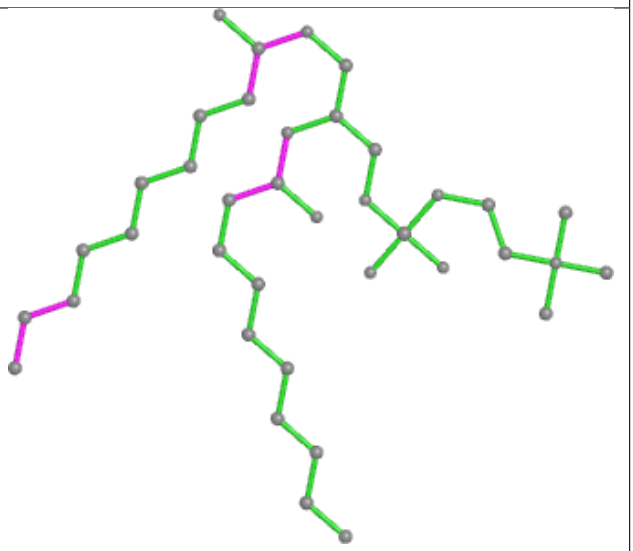


Rings

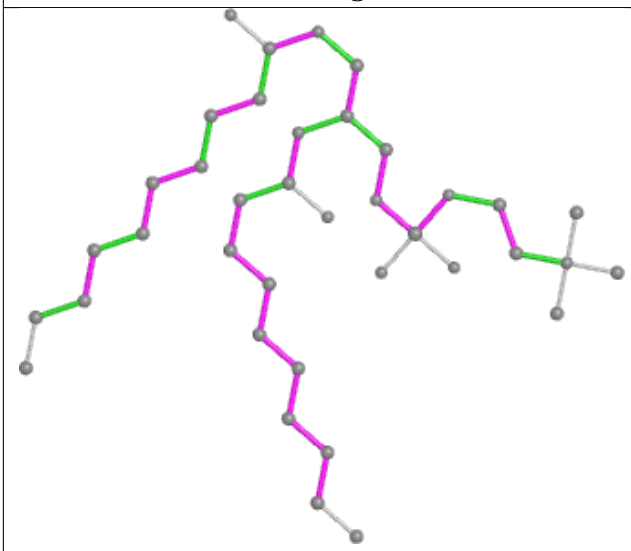
Ligand PCW 3 301



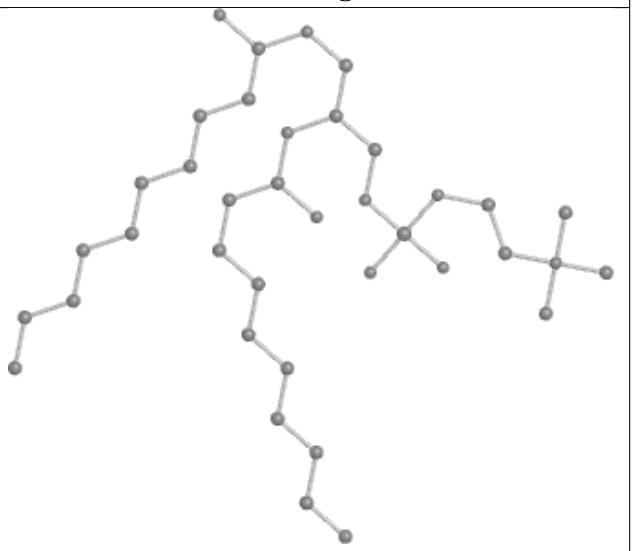
Bond lengths



Bond angles

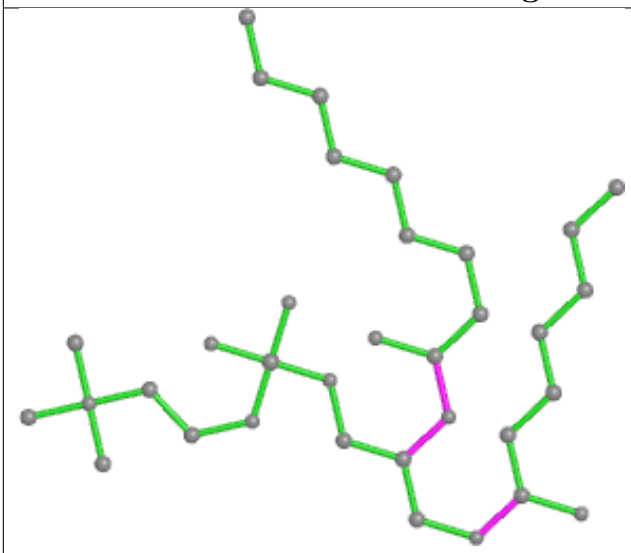


Torsions

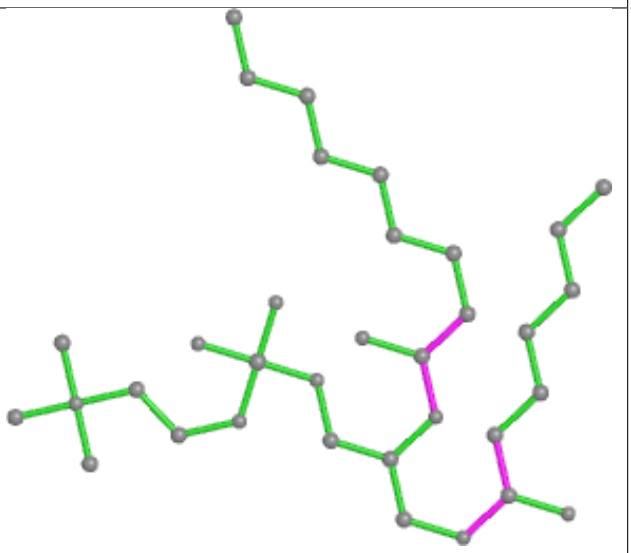


Rings

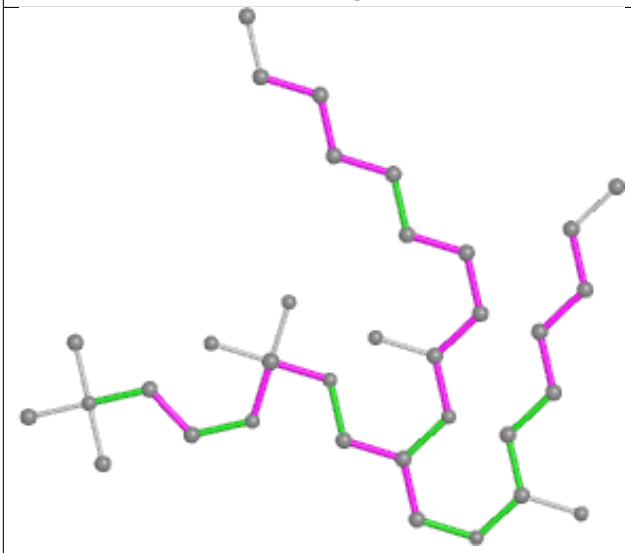
Ligand PCW 3 303



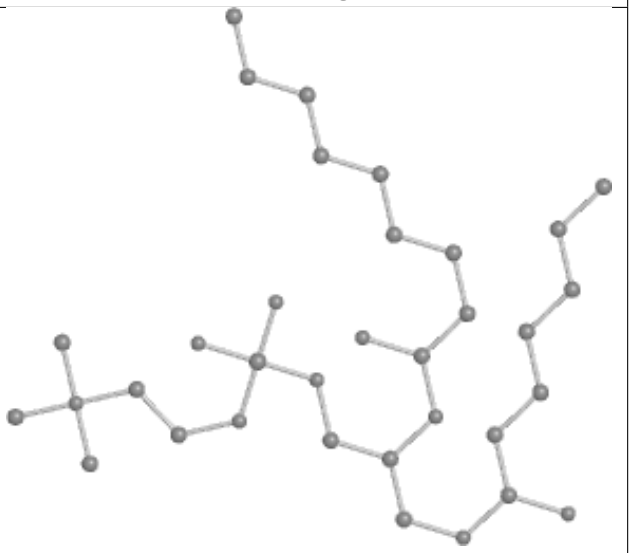
Bond lengths



Bond angles

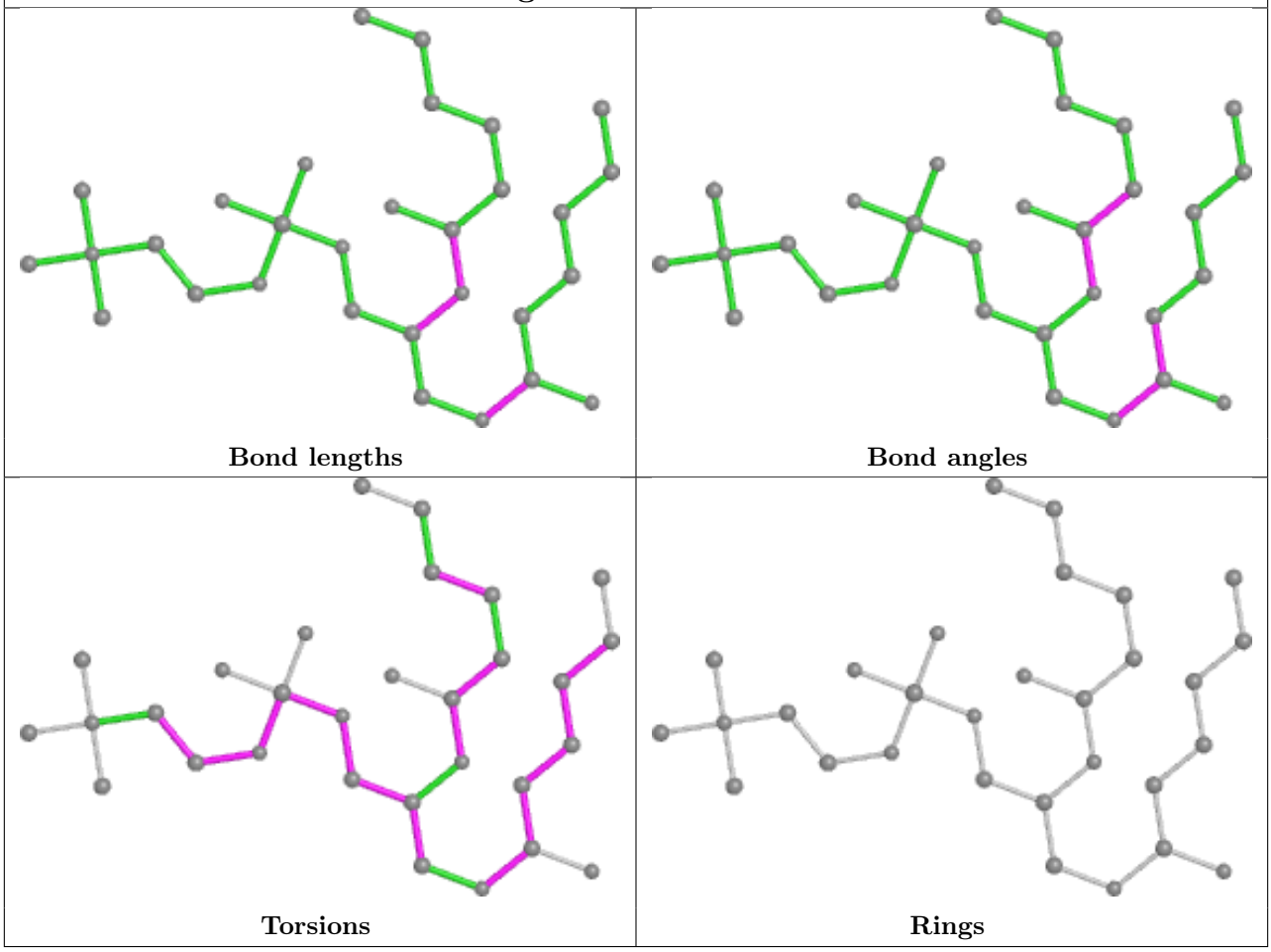


Torsions

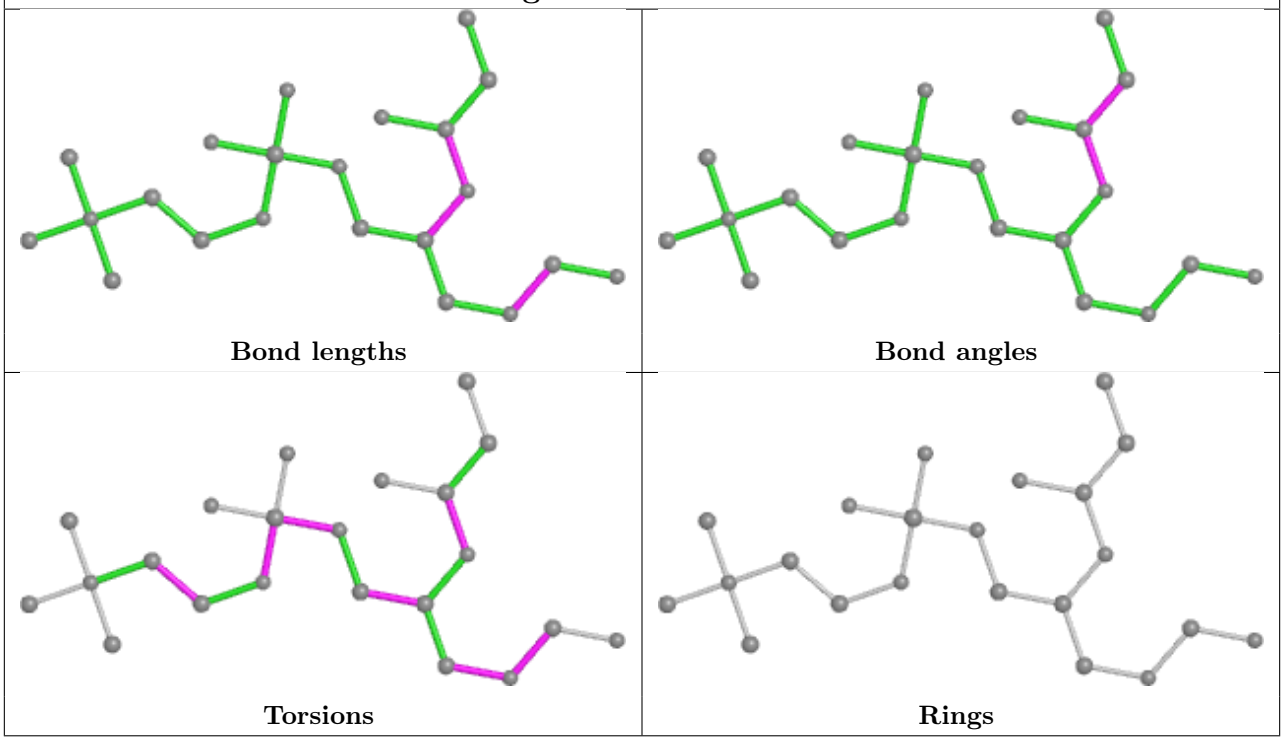


Rings

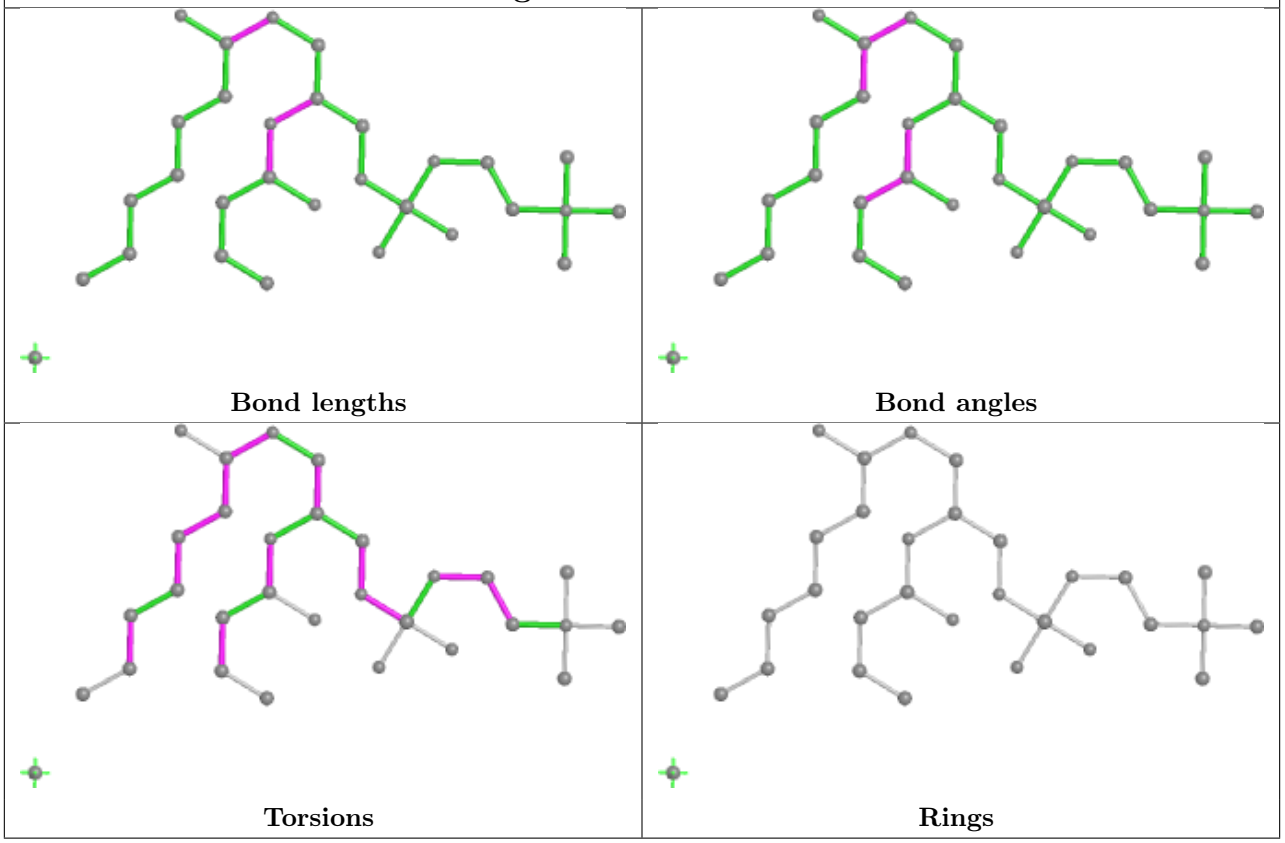
Ligand PCW 6 202



Ligand PCW 6 201



Ligand PCW 1 1002



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

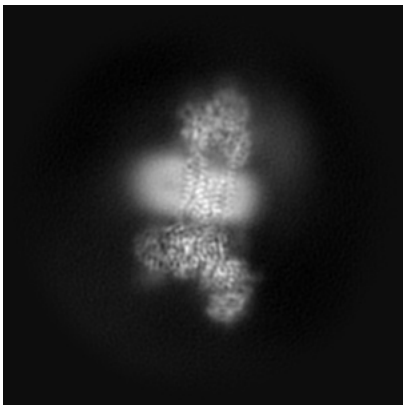
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40245. These allow visual inspection of the internal detail of the map and identification of artifacts.

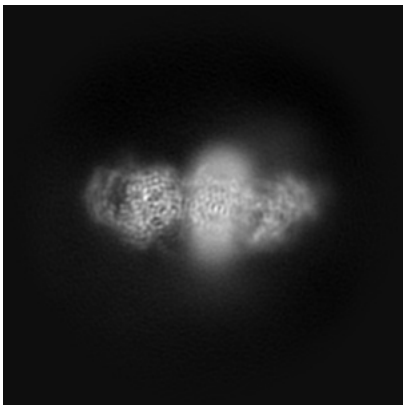
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

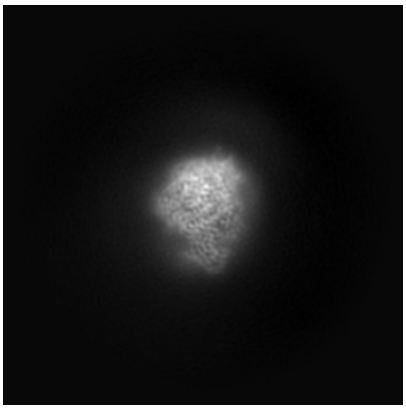
6.1.1 Primary map



X

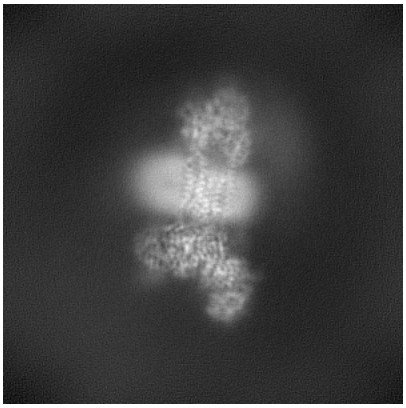


Y

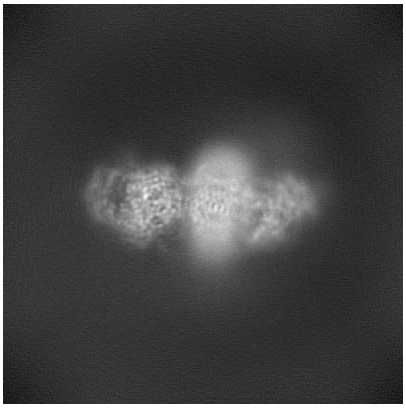


Z

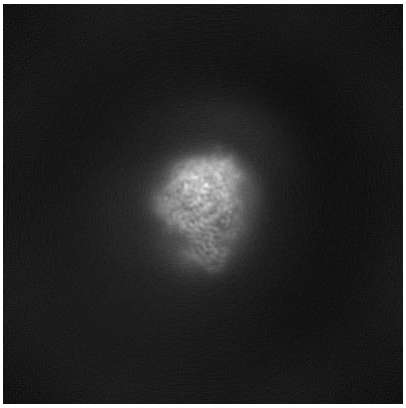
6.1.2 Raw map



X



Y

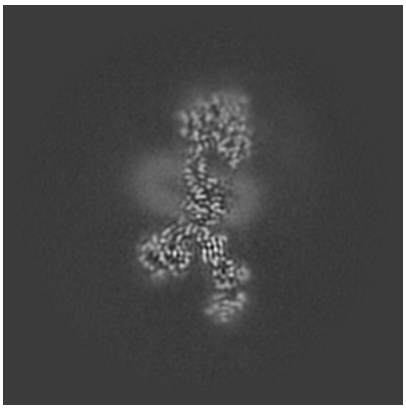


Z

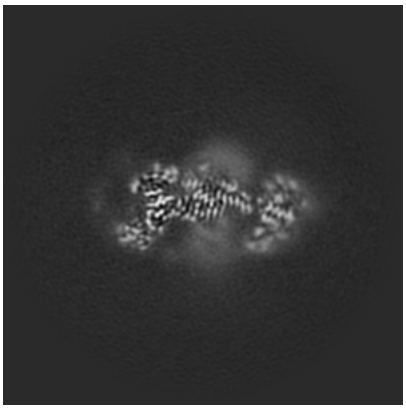
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

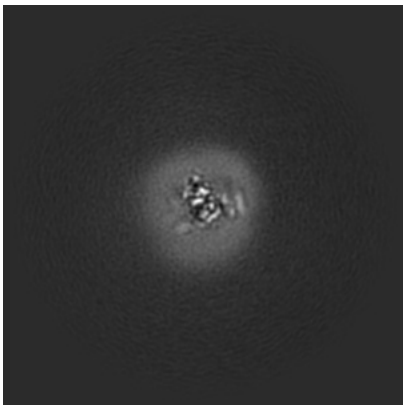
6.2.1 Primary map



X Index: 200

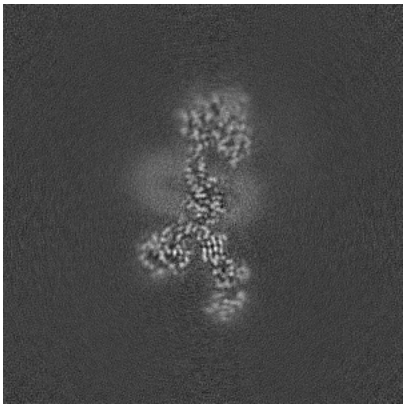


Y Index: 200

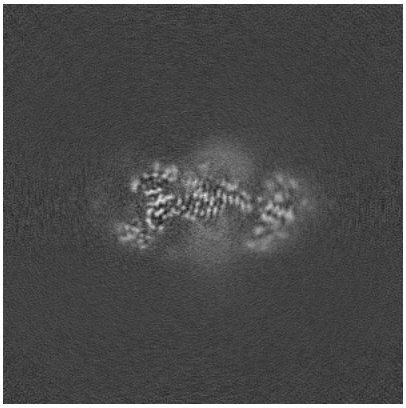


Z Index: 200

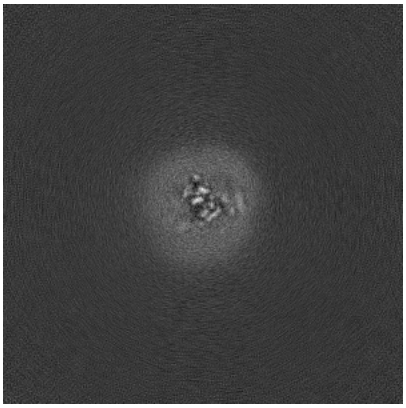
6.2.2 Raw map



X Index: 200



Y Index: 200

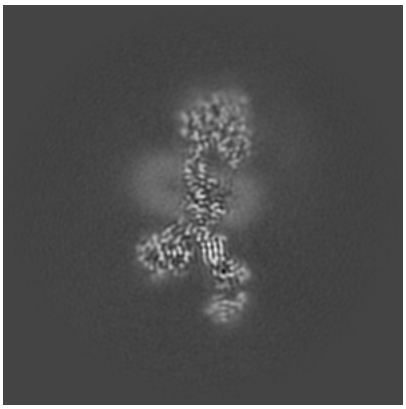


Z Index: 200

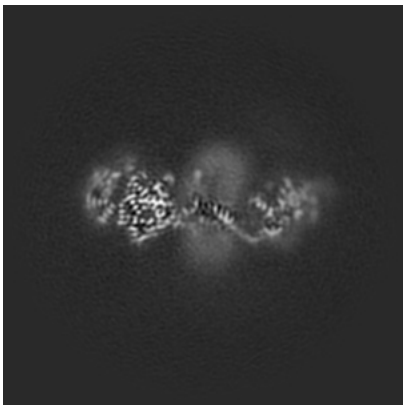
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

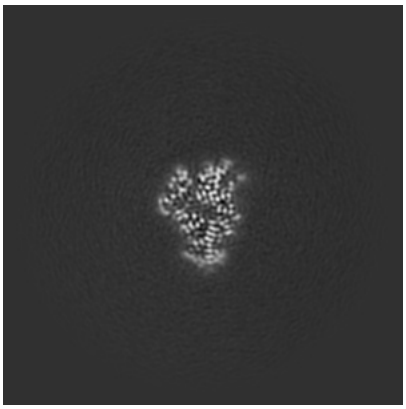
6.3.1 Primary map



X Index: 201

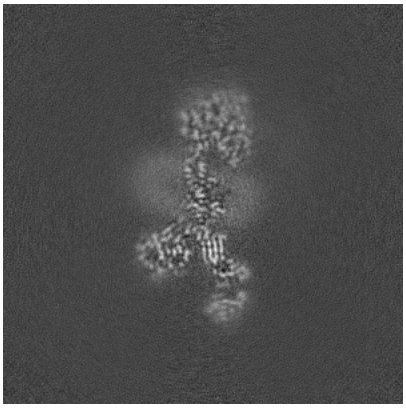


Y Index: 218

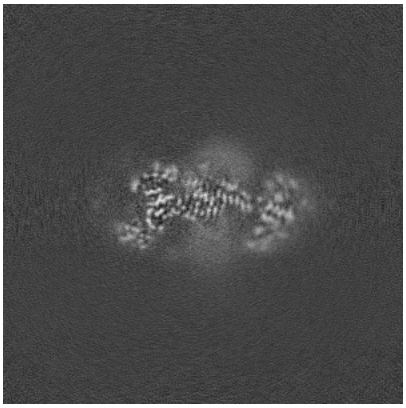


Z Index: 142

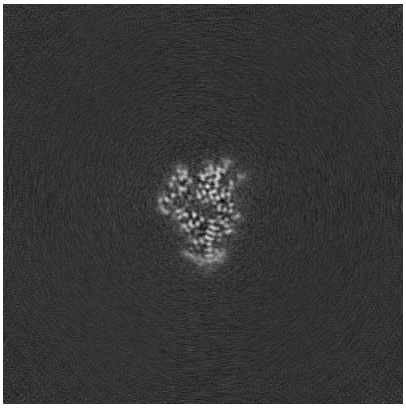
6.3.2 Raw map



X Index: 201



Y Index: 200

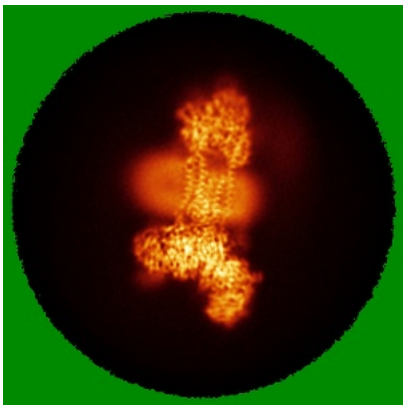


Z Index: 142

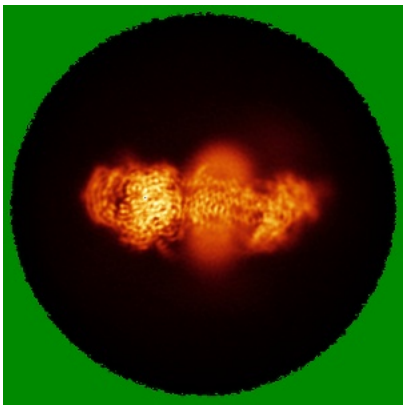
The images above show the largest variance slices of the map in three orthogonal directions.

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

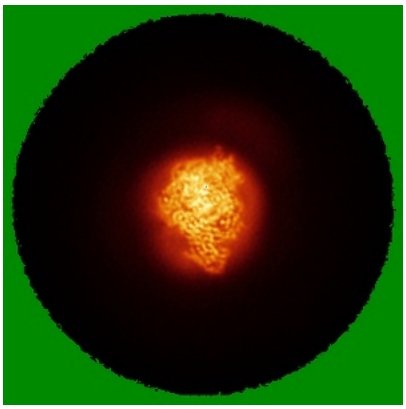
6.4.1 Primary map



X

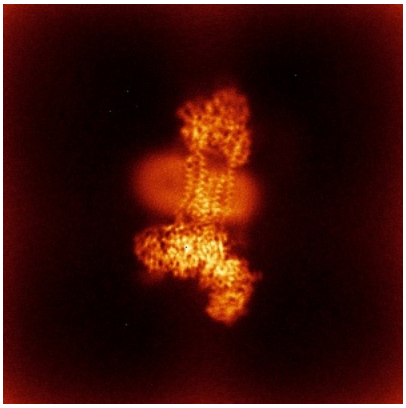


Y

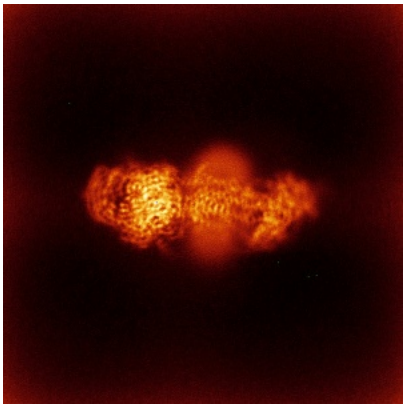


Z

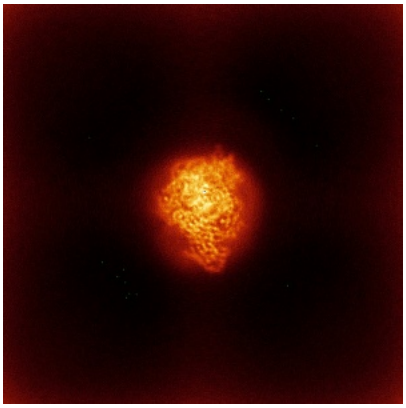
6.4.2 Raw map



X



Y

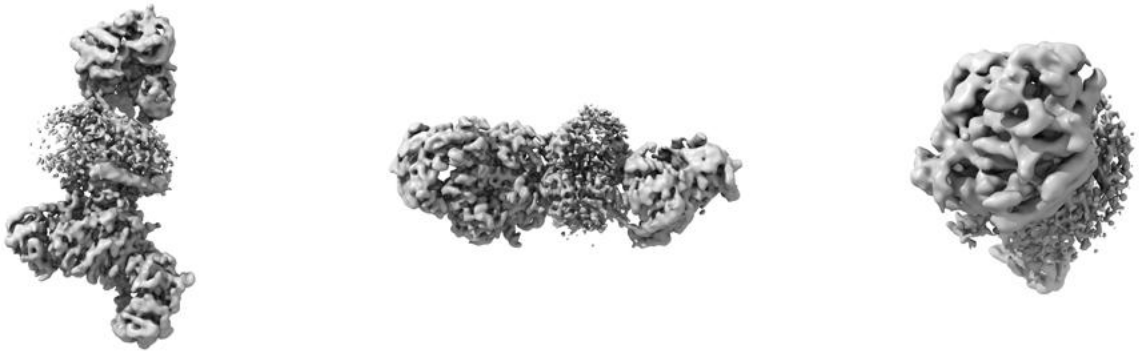


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.101. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

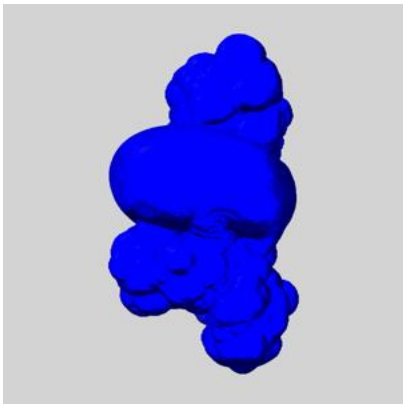
6.6 Mask visualisation (i)

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

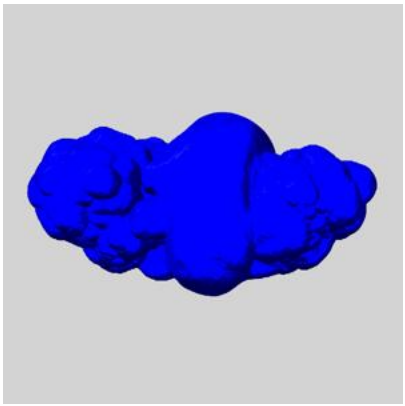
A mask typically either:

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

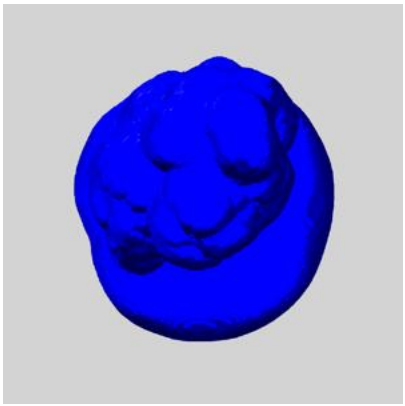
6.6.1 emd_40245_msk_1.map (i)



X



Y

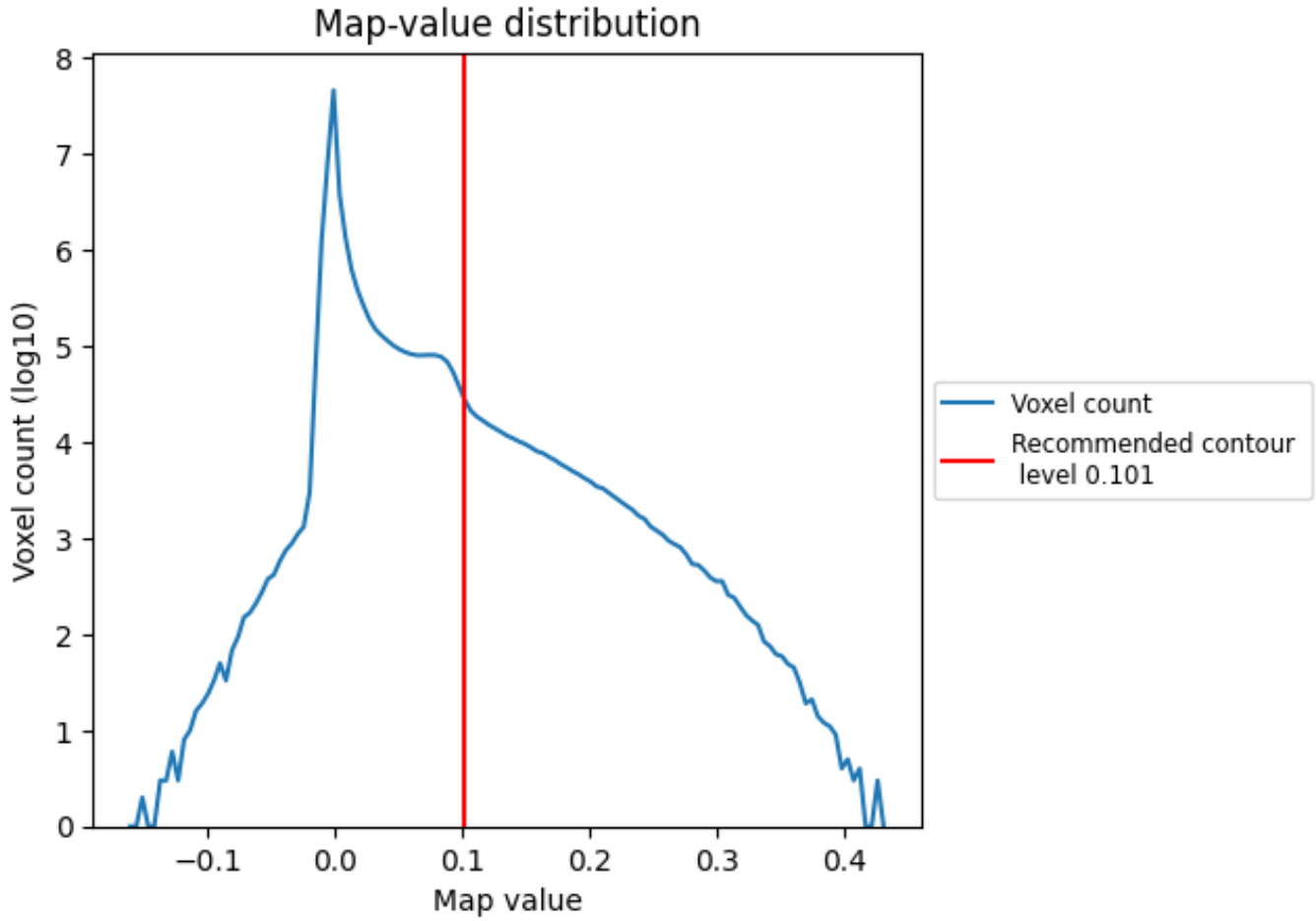


Z

7 Map analysis

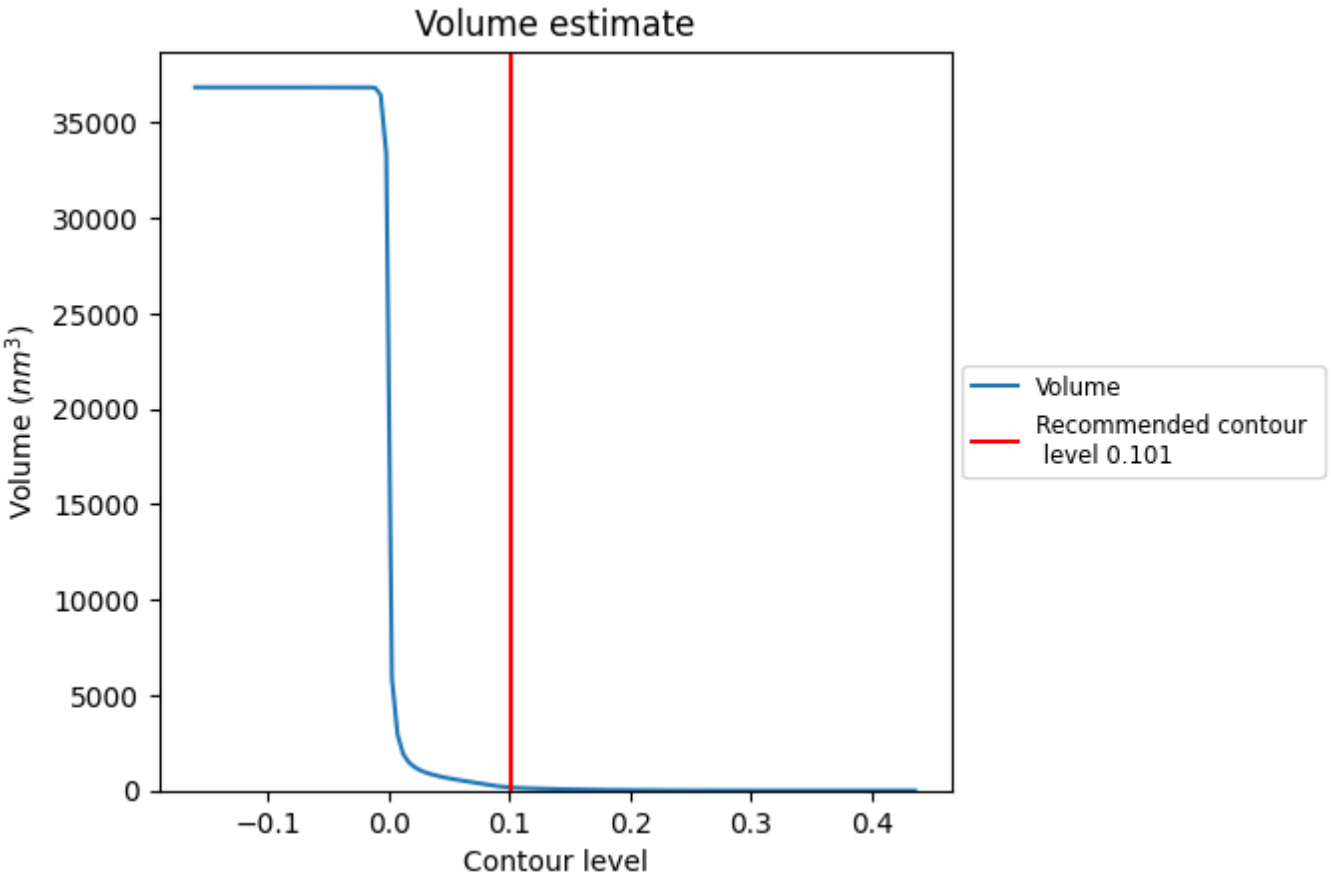
This section contains the results of statistical analysis of the map.

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.

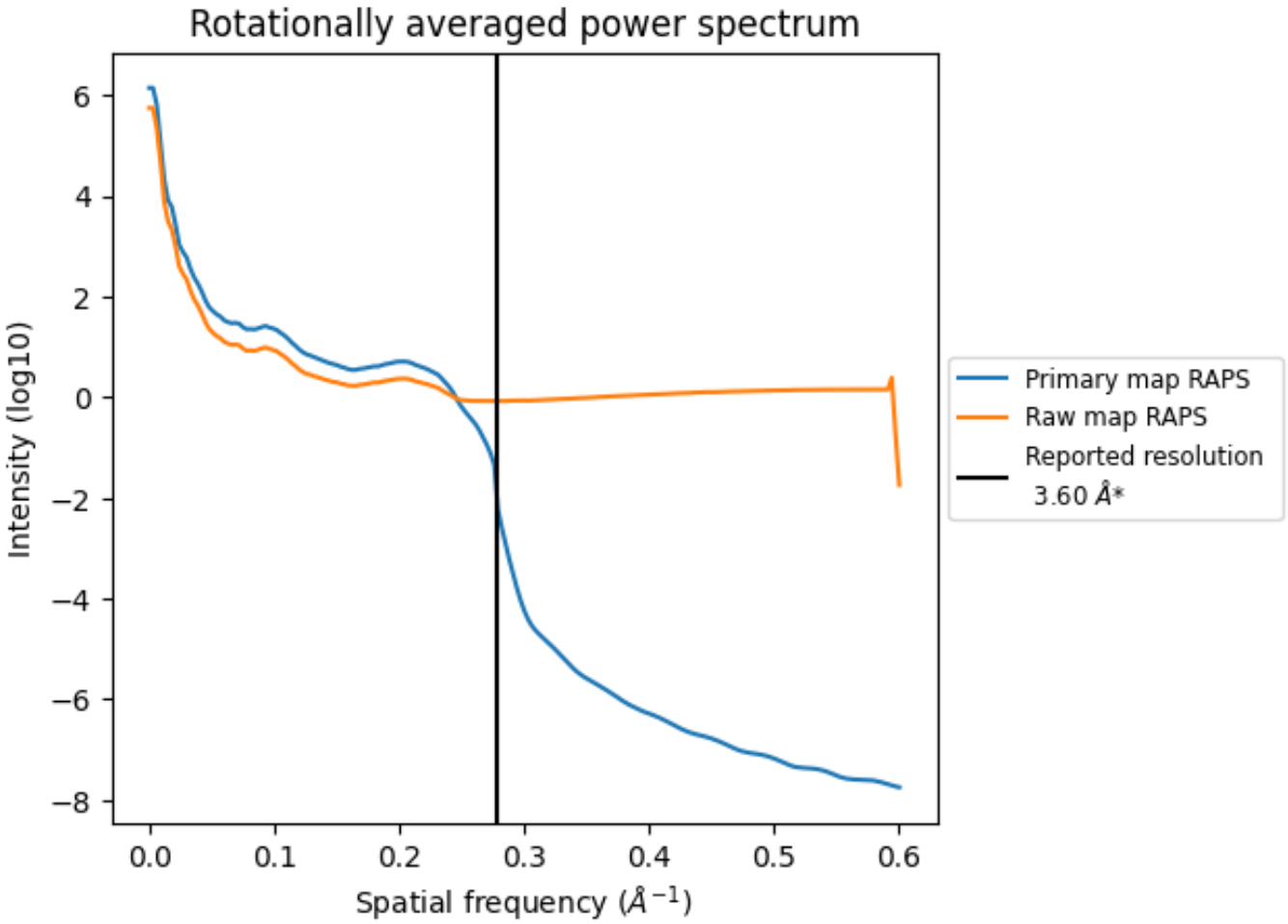
7.2 Volume estimate



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 145 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)

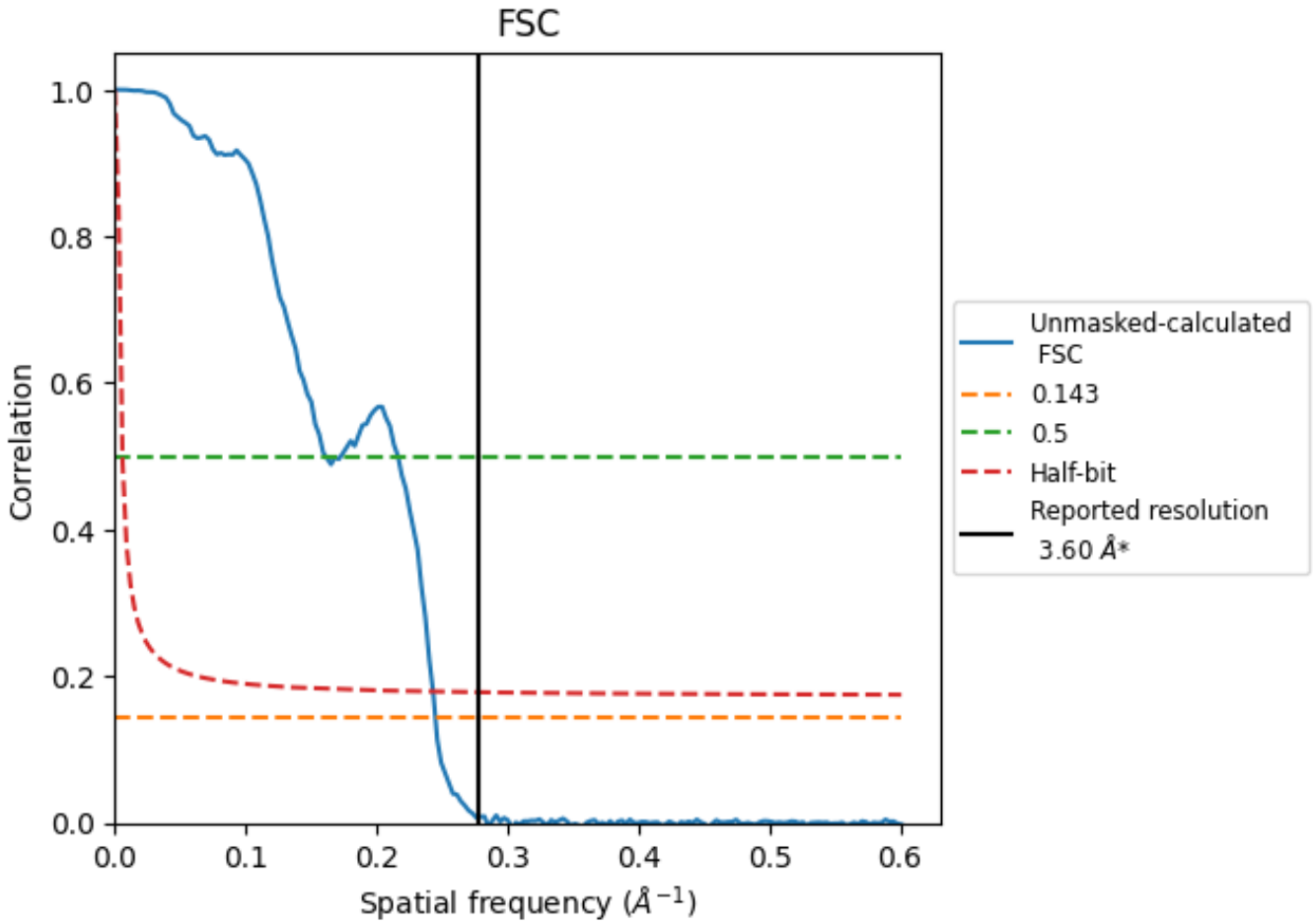


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

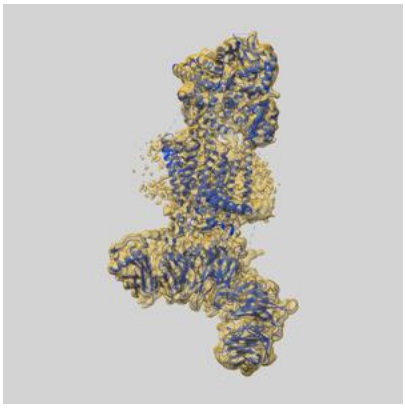
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.21	4.11

*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 4.08 differs from the reported value 3.6 by more than 10 %

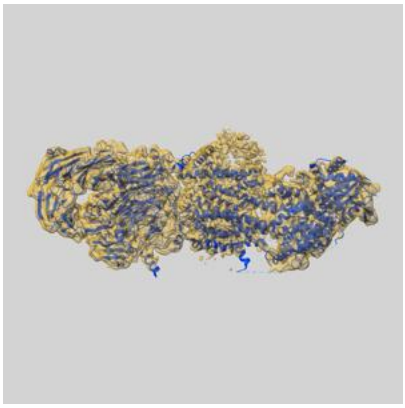
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40245 and PDB model 8S9S. Per-residue inclusion information can be found in section 3 on page 8.

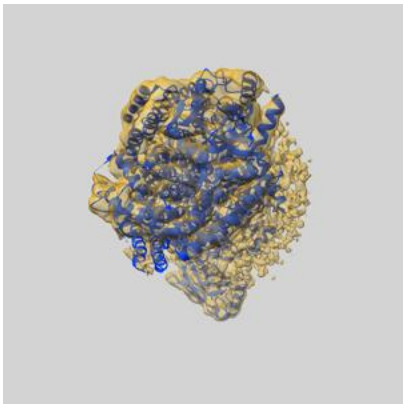
9.1 Map-model overlay



X



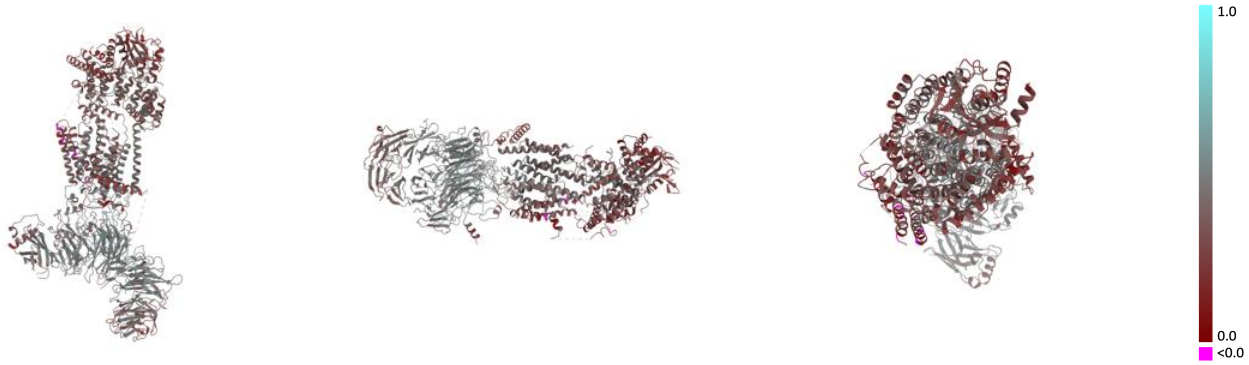
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.101 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



X Y Z

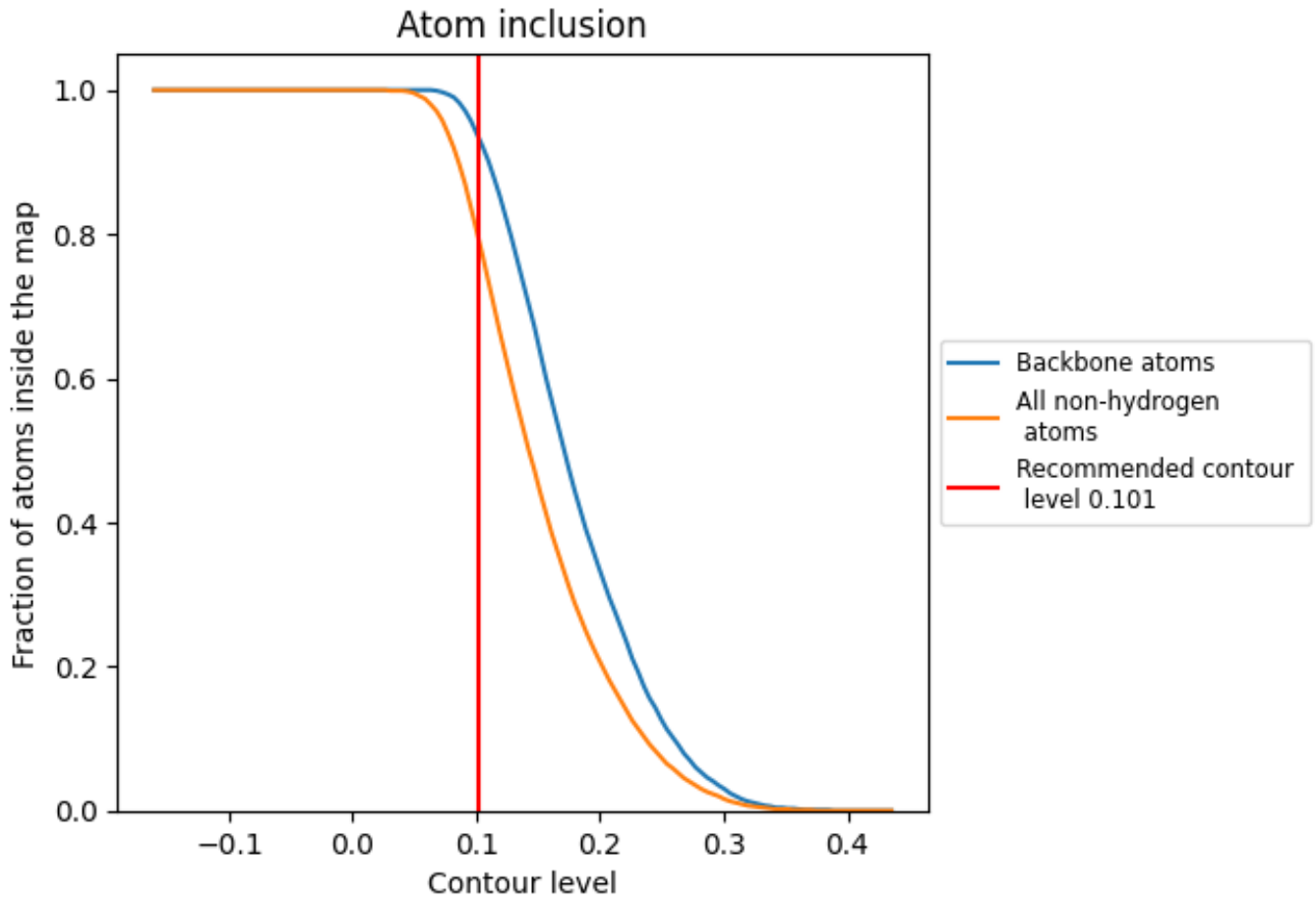
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.101).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.4040
1	0.8480	0.4490
10	0.8140	0.4240
2	0.7810	0.3360
3	0.7550	0.3720
4	0.5780	0.3280
5	0.8010	0.4020
6	0.8710	0.4480
7	0.8220	0.4410
8	0.6970	0.3040
A	0.7860	0.4530
B	0.7500	0.3870
C	0.5360	0.4000