wwPDB EM Validation Summary Report (i)

Oct 12, 2026 – 05:48 PM EDT

PDB ID	:	38OL / pdb_000038ol
EMDB ID	:	EMD-79007
Title	:	LPT translocon complex from Flavobacter johnsoniae built in composite volume
Authors	:	Lea, S.M.; Berks, B.C.
Deposited on	:	2026-09-09
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

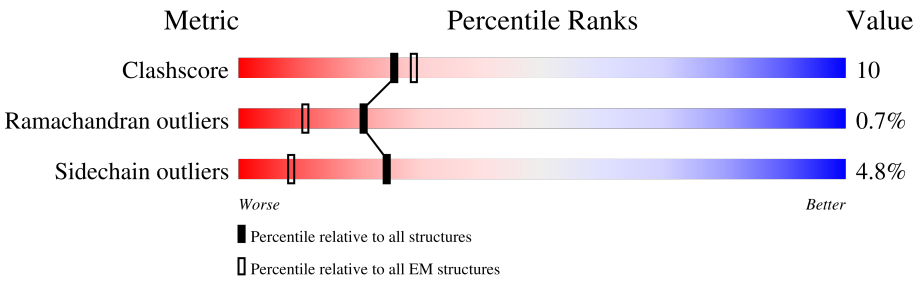
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

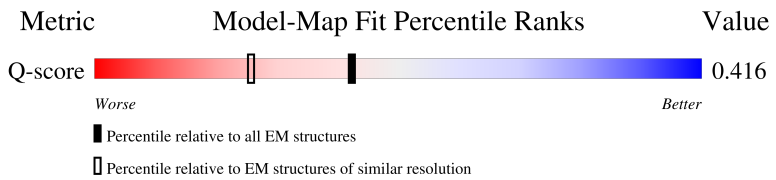
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	P	562	72% 18% • 7%
2	A	549	49% 16% • 33%
3	N	657	79% 13% • 7%
4	S1	335	73% 21% • 5%

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Mol	Chain	Length	Quality of chain
4	S2	335	13% 63% 28% 5%
5	Q	274	49% 20% 29%
6	R	182	6% 58% 28% 5% 9%
7	T	186	53% 11% 34%
8	D	926	72% 13% 13%
9	E	172	70% 18% 12%
10	G	3	67% 33%
10	I	3	33% 67%
10	J	3	67% 33%
10	O	3	67% 33% 67%
11	K	2	50% 100%
11	U	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	RAM	J	3	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 57377 atoms, of which 28352 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 Hypothetical lipoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	P	523	8596	2774	4316	683	817	6	0	0

- Molecule 2 is a protein called OstA family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	367	5959	1884	2987	511	571	6	0	0

- Molecule 3 is a protein called Porin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	N	611	9941	3273	4857	856	954	1	0	0

- Molecule 4 is a protein called Hypothetical lipoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	S2	319	4871	1555	2405	399	507	5	0	0
4	S1	319	4869	1555	2403	399	507	5	0	0

- Molecule 5 is a protein called Outer membrane protein beta-barrel domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	Q	195	3082	1024	1507	254	294	3	0	0

- Molecule 6 is a protein called Hypothetical lipoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	R	165	2532	804	1252	208	264	4	0	0

- Molecule 7 is a protein called DUF5683 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
7	T	122	2001	657	989	171	184	0	0

- Molecule 8 is a protein called Organic solvent tolerance protein OstA-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	D	805	12712	4091	6260	1097	1245	19	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	SER	-	insertion	UNP A5FB33
D	34	ALA	-	insertion	UNP A5FB33
D	35	TRP	-	insertion	UNP A5FB33
D	36	SER	-	insertion	UNP A5FB33
D	37	HIS	-	insertion	UNP A5FB33
D	38	PRO	-	insertion	UNP A5FB33
D	39	GLN	-	insertion	UNP A5FB33
D	40	PHE	-	insertion	UNP A5FB33
D	41	GLU	-	insertion	UNP A5FB33
D	42	LYS	-	insertion	UNP A5FB33
D	43	GLY	-	insertion	UNP A5FB33
D	44	GLY	-	insertion	UNP A5FB33
D	45	GLY	-	insertion	UNP A5FB33
D	46	SER	-	insertion	UNP A5FB33
D	47	GLY	-	insertion	UNP A5FB33
D	48	GLY	-	insertion	UNP A5FB33
D	49	GLY	-	insertion	UNP A5FB33
D	50	SER	-	insertion	UNP A5FB33
D	51	GLY	-	insertion	UNP A5FB33
D	52	GLY	-	insertion	UNP A5FB33
D	53	SER	-	insertion	UNP A5FB33
D	54	ALA	-	insertion	UNP A5FB33
D	55	TRP	-	insertion	UNP A5FB33
D	56	SER	-	insertion	UNP A5FB33
D	57	HIS	-	insertion	UNP A5FB33

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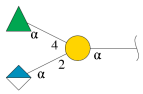
Chain	Residue	Modelled	Actual	Comment	Reference
D	58	PRO	-	insertion	UNP A5FB33
D	59	GLN	-	insertion	UNP A5FB33
D	60	PHE	-	insertion	UNP A5FB33
D	61	GLU	-	insertion	UNP A5FB33
D	62	LYS	-	insertion	UNP A5FB33
D	63	THR	-	insertion	UNP A5FB33
D	64	SER	-	insertion	UNP A5FB33

- Molecule 9 is a protein called Hypothetical lipoprotein.

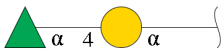
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	E	151	2354	763	1156	196	236	3	0	0

- Molecule 10 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	H	O		
10	G	3	61	18	28	15	0	0
10	I	3	61	18	28	15	0	0
10	J	3	61	18	28	15	0	0
10	O	3	61	18	28	15	0	0

- Molecule 11 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	H	O		
11	K	2	42	12	21	9	0	0

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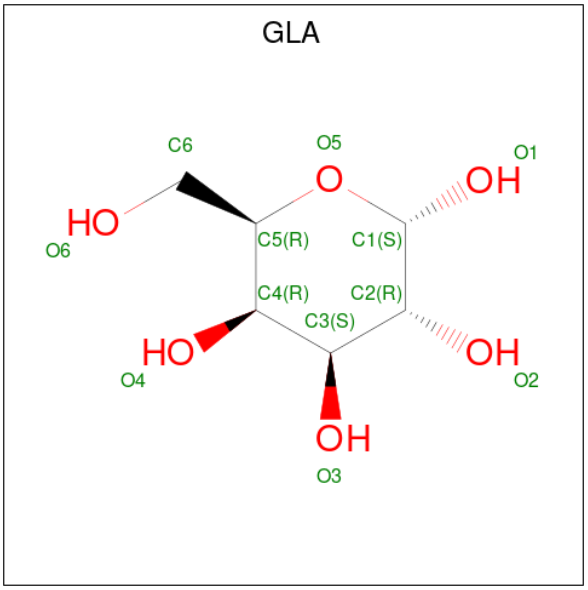
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	H	O		
11	U	2	42	12	21	9	0	0

- Molecule 12 is alpha-D-galactopyranose (CCD ID: GLA) (formula: $C_6H_{12}O_6$).



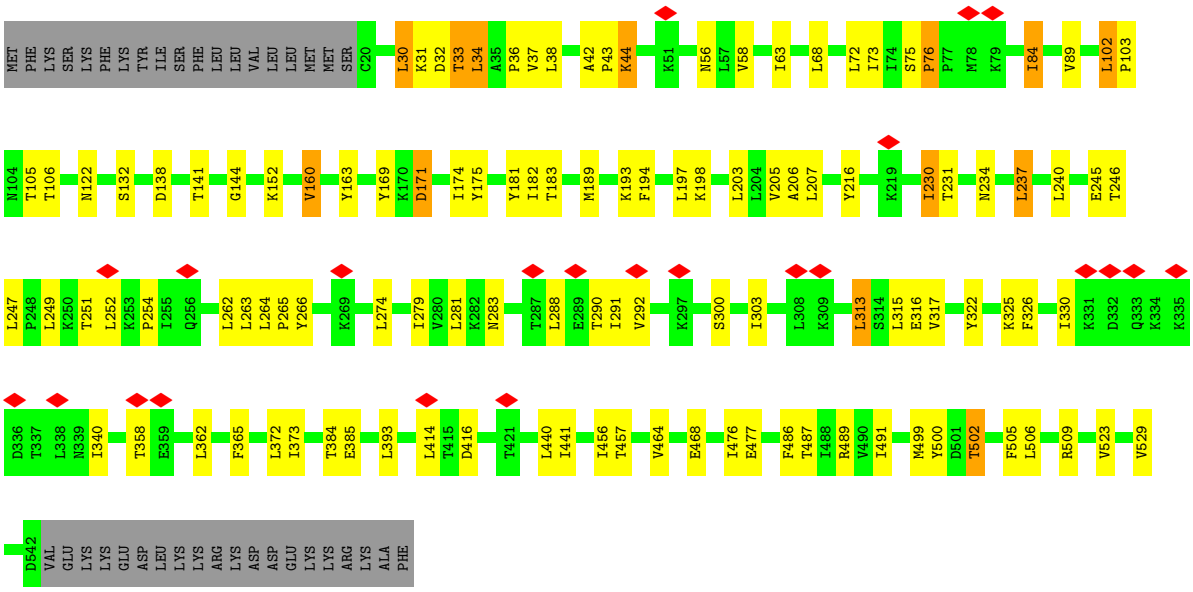
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
12	P	1	22	6	11	5	0
			Total	C	H	O	
12	P	1	22	6	11	5	0
			Total	C	H	O	
12	A	1	22	6	11	5	0
			Total	C	H	O	
12	A	1	22	6	11	5	0
			Total	C	H	O	
12	A	1	22	6	11	5	0
			Total	C	H	O	
12	A	1	22	6	11	5	0

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.

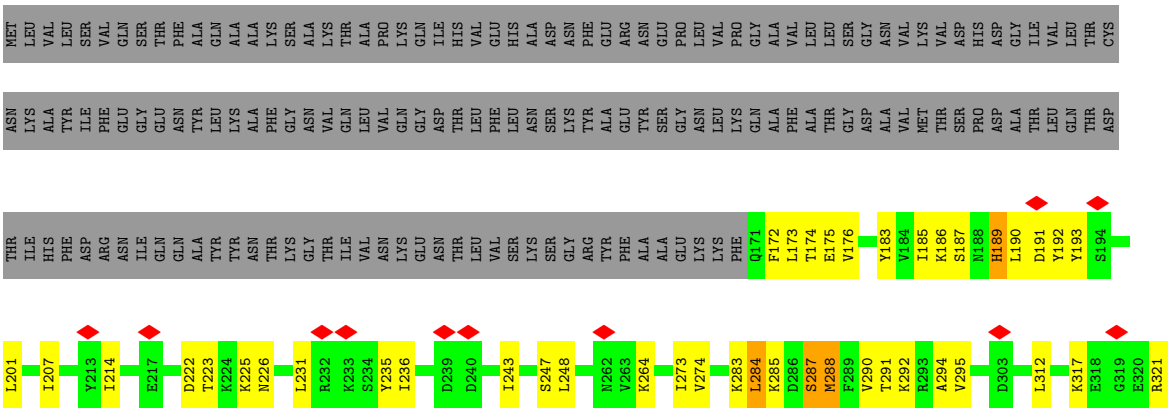
- Molecule 1: Hypothetical lipoprotein

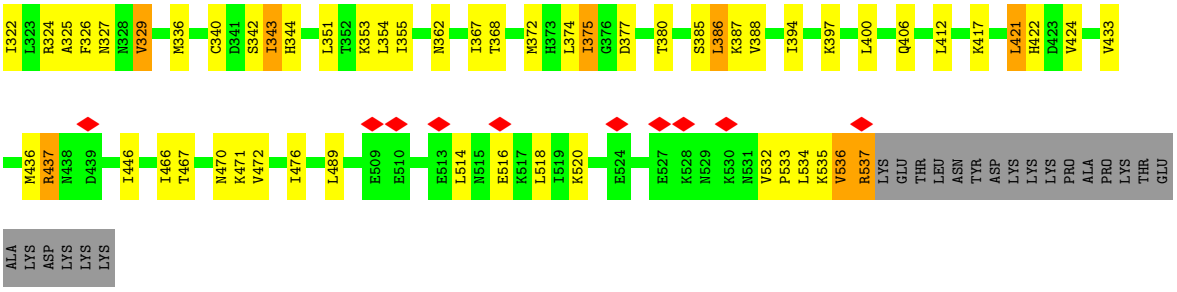
Chain P:



- Molecule 2: OstA family protein

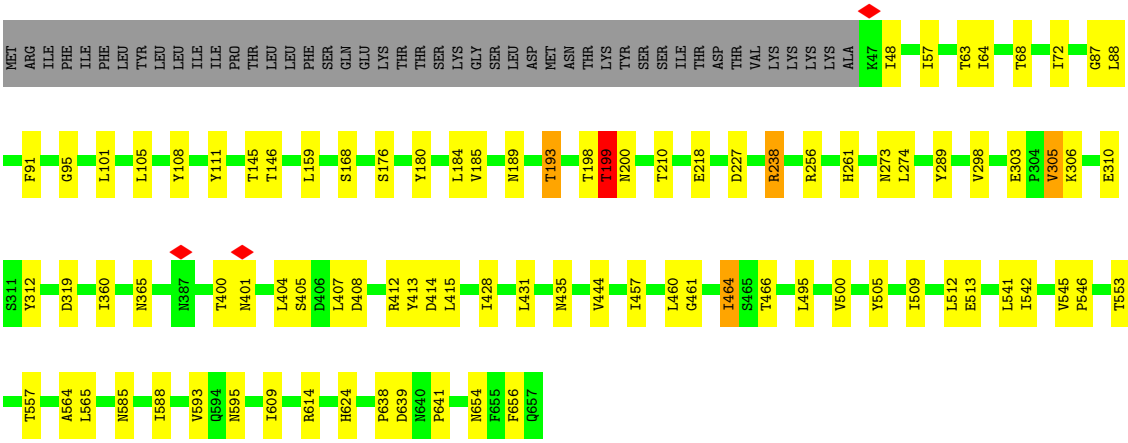
Chain A:





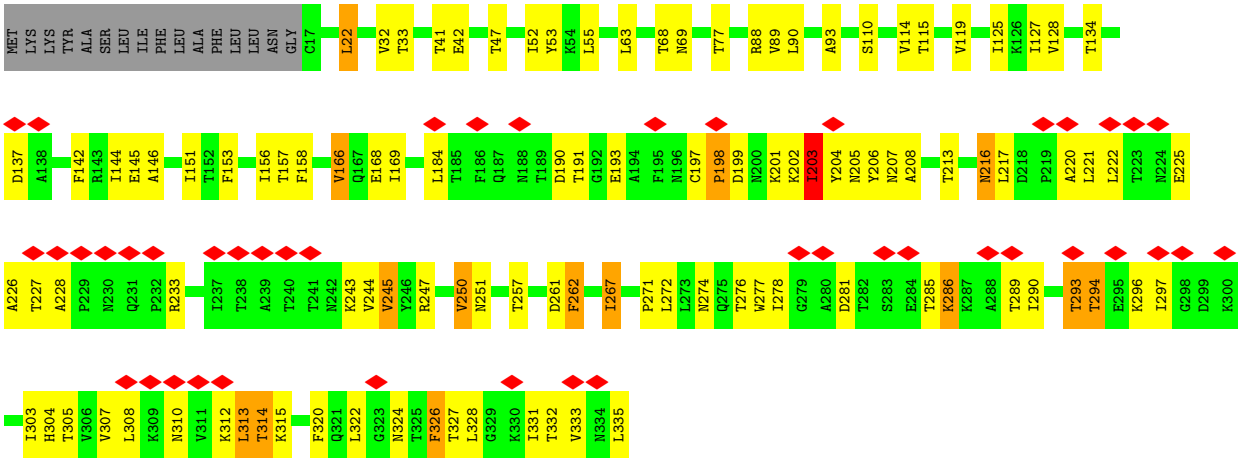
- Molecule 3: Porin

Chain N:



- Molecule 4: Hypothetical lipoprotein

Chain S2:

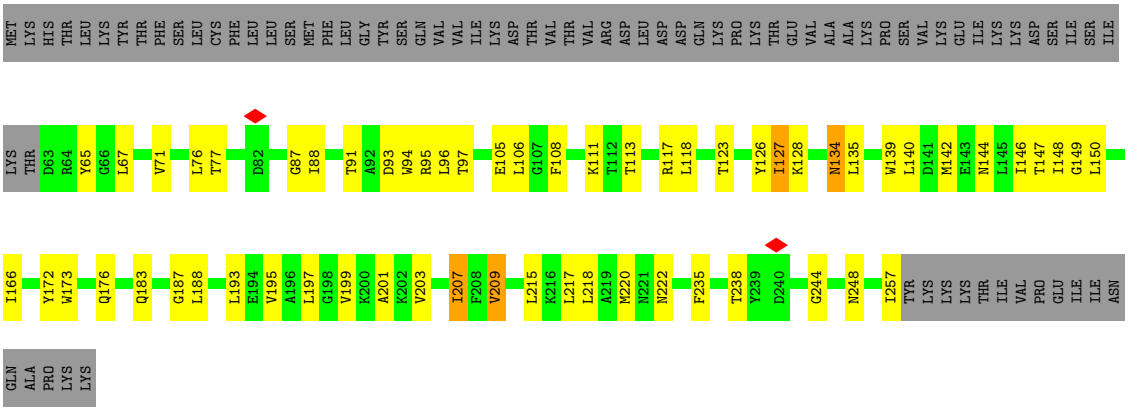


- Molecule 4: Hypothetical lipoprotein

Chain S1:

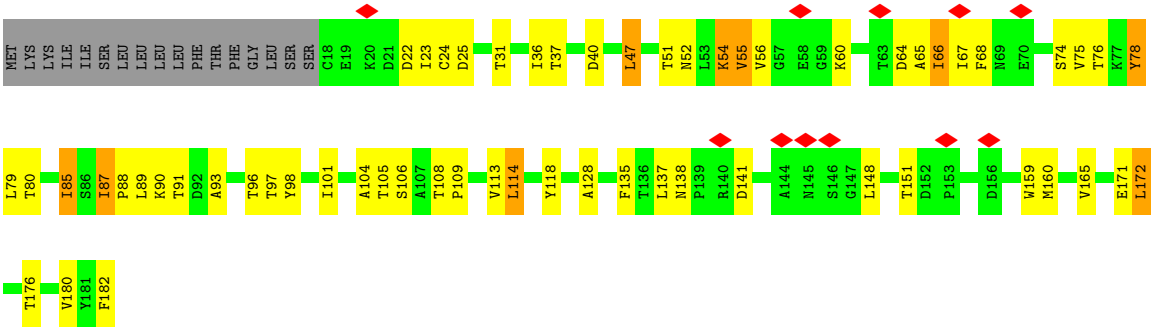
- Molecule 5: Outer membrane protein beta-barrel domain-containing protein

Chain Q:



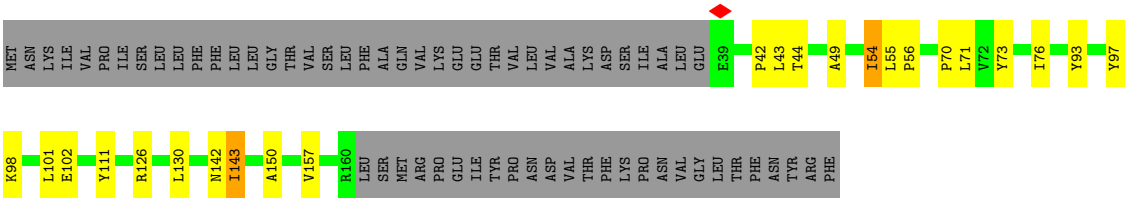
- Molecule 6: Hypothetical lipoprotein

Chain R:



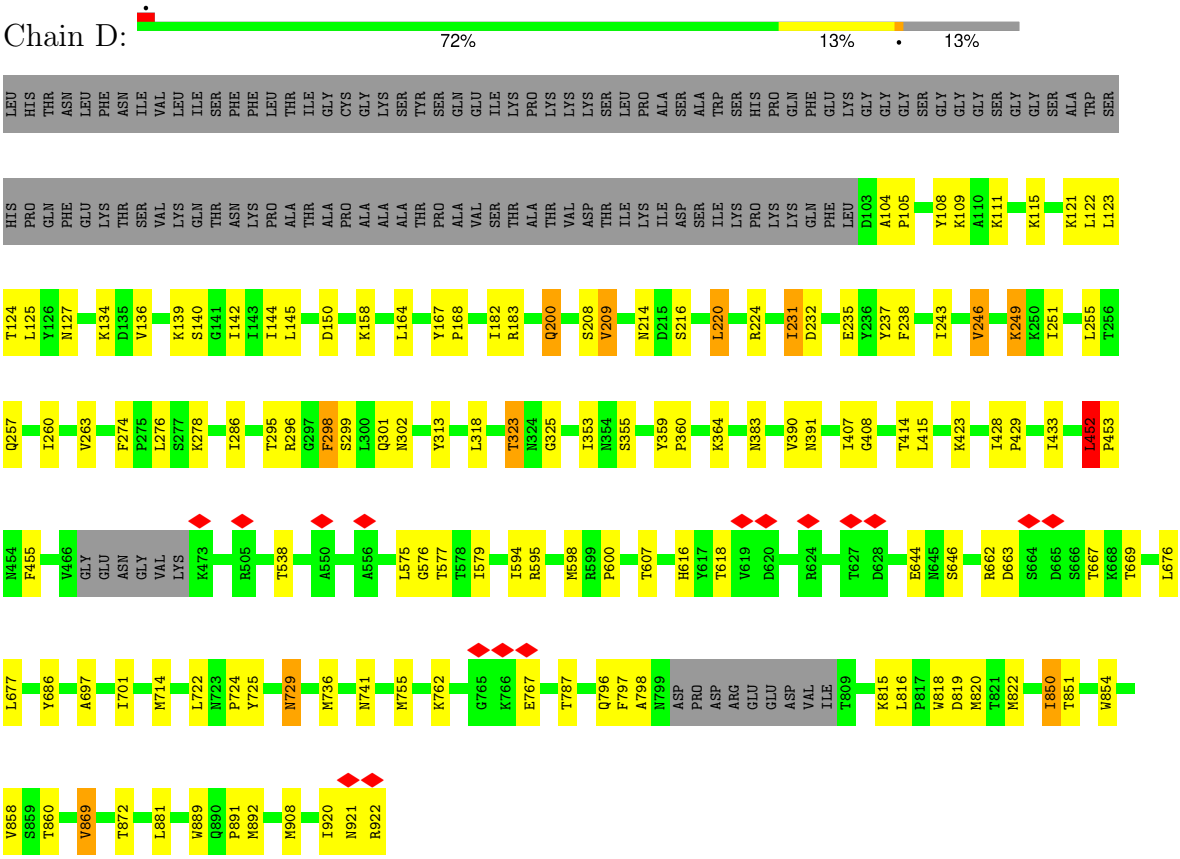
- Molecule 7: DUF5683 domain-containing protein

Chain T:



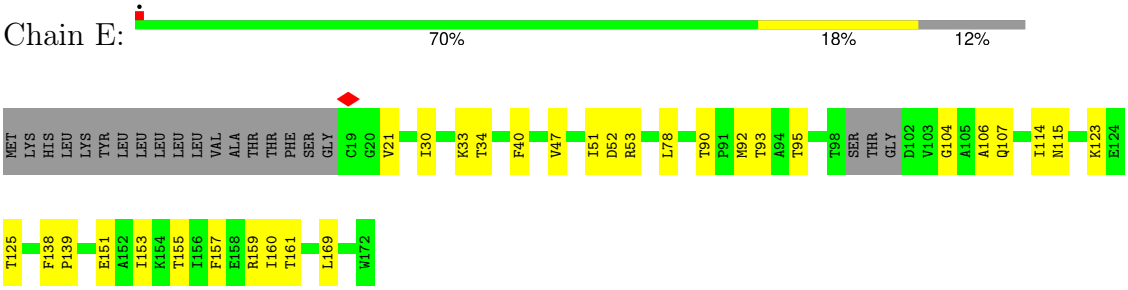
• Molecule 8: Organic solvent tolerance protein OstA-like protein

Chain D:



• Molecule 9: Hypothetical lipoprotein

Chain E:



• Molecule 10: alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-galactopyranose

Chain G:

• Molecule 10: alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-galactopyranose

Chain I:

• Molecule 10: alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-galactopyranose

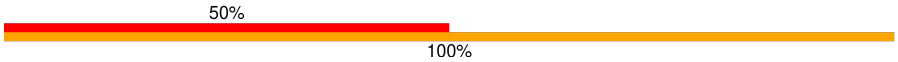
Chain J:

• Molecule 10: alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-galactopyranose

Chain O:

• Molecule 11: alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranose

Chain K:



• Molecule 11: alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranose

Chain U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218874	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.215	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	499.7, 499.7, 499.7	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.315, 1.315, 1.315	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GCU, RAM

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	P	0.17	0/4373	0.34	0/5908
2	A	0.17	0/3022	0.34	0/4067
3	N	0.37	0/5219	0.36	0/7076
4	S1	0.25	0/2515	0.33	0/3439
4	S2	0.22	0/2515	0.40	0/3439
5	Q	0.26	0/1619	0.35	0/2193
6	R	0.22	0/1303	0.39	0/1781
7	T	0.38	0/1037	0.38	0/1405
8	D	0.38	0/6600	0.38	0/8913
9	E	0.41	0/1222	0.38	0/1657
All	All	0.30	0/29425	0.36	0/39878

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
8	D	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
8	D	452	LEU	Peptide

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	P	4280	4316	4316	108	0
2	A	2972	2987	2987	60	0
3	N	5084	4857	4857	55	0
4	S1	2466	2403	2403	54	0
4	S2	2466	2405	2405	98	0
5	Q	1575	1507	1507	46	0
6	R	1280	1252	1252	57	0
7	T	1012	989	989	18	0
8	D	6452	6260	6259	84	0
9	E	1198	1156	1156	23	0
10	G	33	28	25	1	0
10	I	33	28	25	3	0
10	J	33	28	25	7	0
10	O	33	28	25	0	0
11	K	21	21	19	1	0
11	U	21	21	19	4	0
12	A	44	44	40	0	0
12	P	22	22	20	0	0
All	All	29025	28352	28329	593	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 10.

The worst 5 of 593 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)
3:N:509:ILE:HD11	3:N:542:ILE:HD11	1.49	0.94
1:P:160:VAL:HG23	1:P:183:THR:HG23	1.59	0.84
5:Q:166:ILE:HG21	6:R:91:THR:HG21	1.61	0.82
1:P:102:LEU:HD12	1:P:105:THR:HG21	1.61	0.81
10:J:1:GLA:H4	10:J:3:RAM:H5	1.63	0.80

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	P	521/562 (93%)	436 (84%)	83 (16%)	2 (0%)	30	62
2	A	365/549 (66%)	288 (79%)	75 (20%)	2 (0%)	24	59
3	N	609/657 (93%)	544 (89%)	61 (10%)	4 (1%)	18	52
4	S1	317/335 (95%)	260 (82%)	56 (18%)	1 (0%)	36	68
4	S2	317/335 (95%)	217 (68%)	92 (29%)	8 (2%)	4	27
5	Q	193/274 (70%)	154 (80%)	38 (20%)	1 (0%)	24	59
6	R	163/182 (90%)	118 (72%)	44 (27%)	1 (1%)	21	56
7	T	120/186 (64%)	108 (90%)	12 (10%)	0	100	100
8	D	799/926 (86%)	676 (85%)	117 (15%)	6 (1%)	16	50
9	E	147/172 (86%)	136 (92%)	11 (8%)	0	100	100
All	All	3551/4178 (85%)	2937 (83%)	589 (17%)	25 (1%)	20	52

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	76	PRO
2	A	536	VAL
3	N	199	THR
3	N	303	GLU
4	S2	198	PRO

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	P	485/523 (93%)	466 (96%)	19 (4%)	28	62
2	A	333/486 (68%)	301 (90%)	32 (10%)	8	32
3	N	545/589 (92%)	522 (96%)	23 (4%)	26	60
4	S1	284/297 (96%)	278 (98%)	6 (2%)	47	71
4	S2	284/297 (96%)	269 (95%)	15 (5%)	20	53
5	Q	163/238 (68%)	154 (94%)	9 (6%)	19	52
6	R	147/163 (90%)	136 (92%)	11 (8%)	12	42
7	T	103/162 (64%)	97 (94%)	6 (6%)	18	51
8	D	708/808 (88%)	679 (96%)	29 (4%)	27	60
9	E	130/148 (88%)	127 (98%)	3 (2%)	44	70
All	All	3182/3711 (86%)	3029 (95%)	153 (5%)	24	56

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S1	235	GLN
8	D	714	MET
4	S1	307	VAL
8	D	220	LEU
9	E	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
5	Q	134	ASN
4	S1	200	ASN
4	S1	187	GLN
8	D	490	ASN
2	A	449	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 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	GLA	G	1	10,2	11,11,12	0.98	1 (9%)	15,15,17	1.33	1 (6%)
10	GCU	G	2	10	12,12,13	1.12	1 (8%)	14,17,19	1.21	1 (7%)
10	RAM	G	3	10	10,10,11	0.96	1 (10%)	14,14,16	0.83	0
10	GLA	I	1	10,8	11,11,12	0.95	0	15,15,17	1.55	2 (13%)
10	GCU	I	2	10	12,12,13	1.15	1 (8%)	14,17,19	1.24	2 (14%)
10	RAM	I	3	10	10,10,11	0.38	0	14,14,16	0.52	0
10	GLA	J	1	10	11,11,12	1.06	1 (9%)	15,15,17	1.40	3 (20%)
10	GCU	J	2	10	12,12,13	1.16	2 (16%)	14,17,19	1.12	0
10	RAM	J	3	10	10,10,11	0.38	0	14,14,16	0.52	0
11	GLA	K	1	11	11,11,12	0.85	1 (9%)	15,15,17	2.03	5 (33%)
11	RAM	K	2	11	10,10,11	0.79	0	14,14,16	1.38	2 (14%)
10	GLA	O	1	1,10	11,11,12	0.71	0	15,15,17	1.32	1 (6%)
10	GCU	O	2	10	12,12,13	1.14	2 (16%)	14,17,19	1.03	0
10	RAM	O	3	10	10,10,11	0.38	0	14,14,16	0.52	0
11	GLA	U	1	11	11,11,12	0.64	0	15,15,17	2.54	5 (33%)
11	RAM	U	2	11	10,10,11	0.85	0	14,14,16	1.04	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	GLA	G	1	10,2	-	0/2/19/22	0/1/1/1
10	GCU	G	2	10	-	0/4/21/24	1/1/1/1
10	RAM	G	3	10	-	-	0/1/1/1
10	GLA	I	1	10,8	-	0/2/19/22	0/1/1/1
10	GCU	I	2	10	-	1/4/21/24	0/1/1/1
10	RAM	I	3	10	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GLA	J	1	10	-	0/2/19/22	0/1/1/1
10	GCU	J	2	10	-	0/4/21/24	0/1/1/1
10	RAM	J	3	10	-	-	0/1/1/1
11	GLA	K	1	11	-	2/2/19/22	0/1/1/1
11	RAM	K	2	11	-	-	1/1/1/1
10	GLA	O	1	1,10	-	2/2/19/22	0/1/1/1
10	GCU	O	2	10	-	0/4/21/24	0/1/1/1
10	RAM	O	3	10	-	-	0/1/1/1
11	GLA	U	1	11	-	2/2/19/22	0/1/1/1
11	RAM	U	2	11	-	-	1/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1	GLA	O5-C1	-2.57	1.39	1.43
10	J	2	GCU	O6B-C6	-2.30	1.23	1.30
10	G	2	GCU	O6B-C6	-2.24	1.23	1.30
10	G	1	GLA	O5-C1	-2.21	1.40	1.43
10	O	2	GCU	O6B-C6	-2.21	1.23	1.30

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	1	GLA	C1-O5-C5	6.14	120.41	112.19
11	K	1	GLA	C1-O5-C5	5.04	118.95	112.19
11	U	1	GLA	C3-C4-C5	-4.27	102.48	110.23
11	U	1	GLA	C1-C2-C3	4.01	115.48	109.64
10	O	1	GLA	C1-O5-C5	3.65	117.08	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	O	1	GLA	O5-C5-C6-O6
10	O	1	GLA	C4-C5-C6-O6
11	U	1	GLA	C4-C5-C6-O6
11	U	1	GLA	O5-C5-C6-O6
11	K	1	GLA	O5-C5-C6-O6

All (3) ring outliers are listed below:

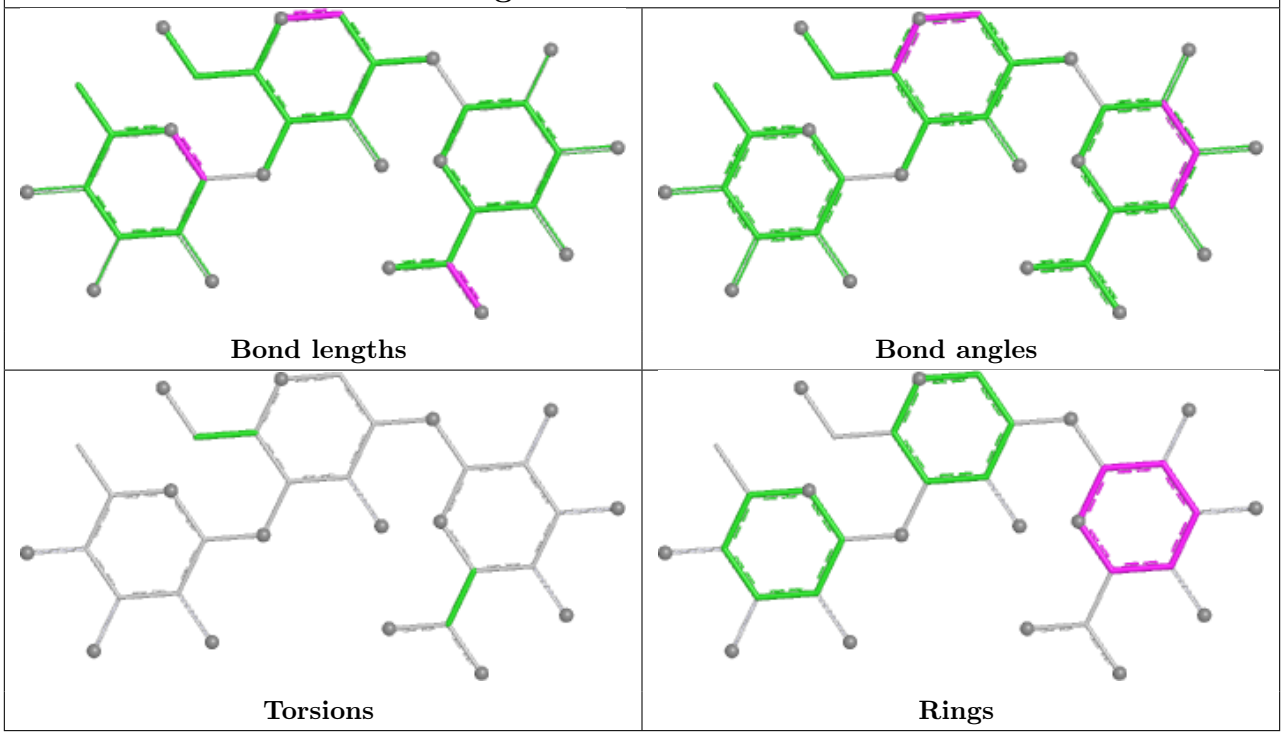
Mol	Chain	Res	Type	Atoms
11	K	2	RAM	C1-C2-C3-C4-C5-O5
11	U	2	RAM	C1-C2-C3-C4-C5-O5
10	G	2	GCU	C1-C2-C3-C4-C5-O5

10 monomers are involved in 16 short contacts:

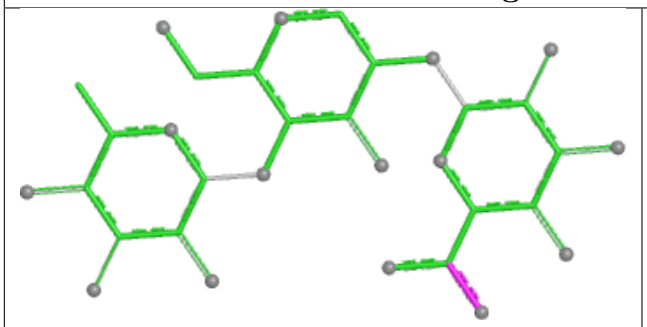
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	U	1	GLA	1	0
10	G	1	GLA	1	0
10	I	1	GLA	1	0
10	I	3	RAM	2	0
11	K	2	RAM	1	0
10	J	3	RAM	6	0
10	J	1	GLA	5	0
10	I	2	GCU	1	0
11	U	2	RAM	3	0
11	K	1	GLA	1	0

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

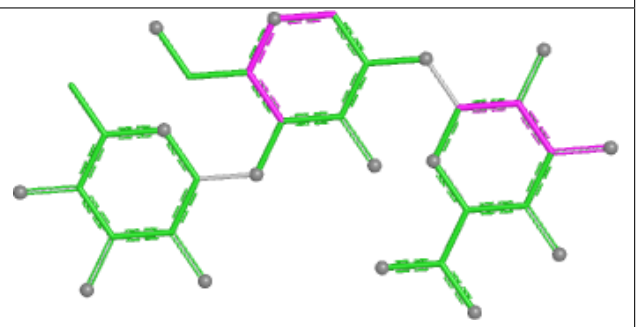
Oligosaccharide Chain G



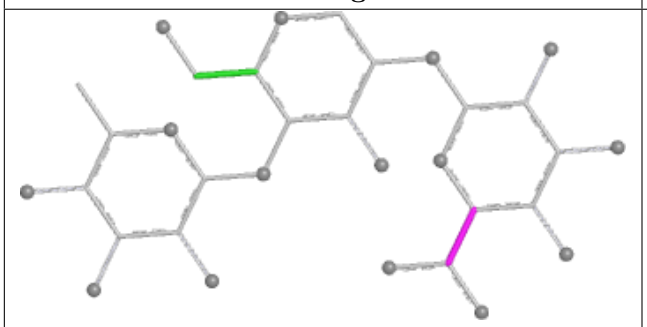
Oligosaccharide Chain I



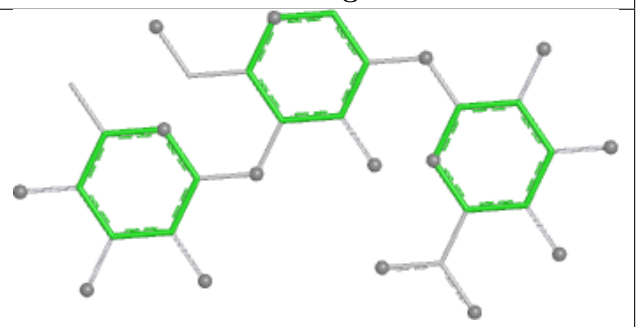
Bond lengths



Bond angles

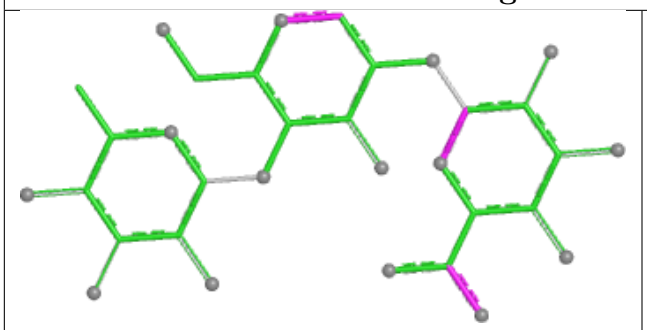


Torsions

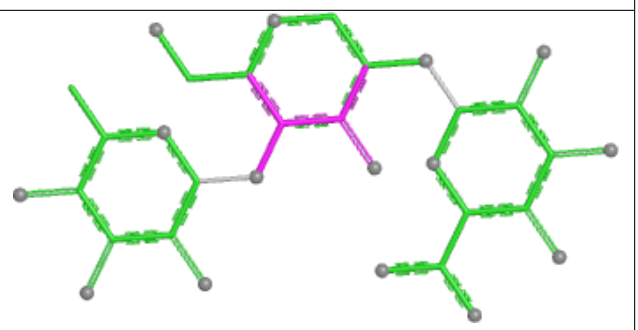


Rings

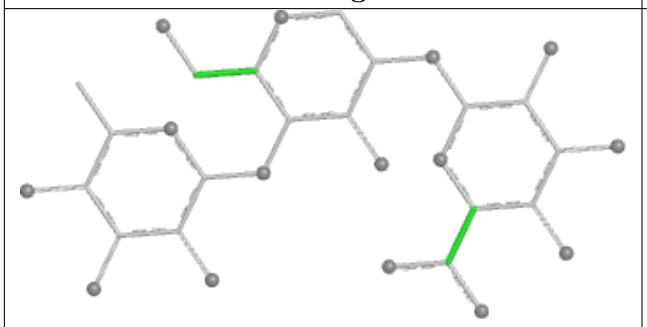
Oligosaccharide Chain J



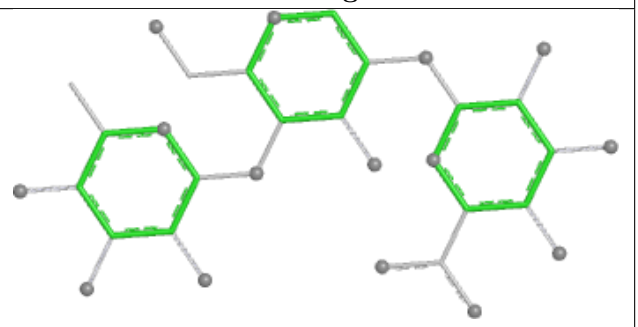
Bond lengths



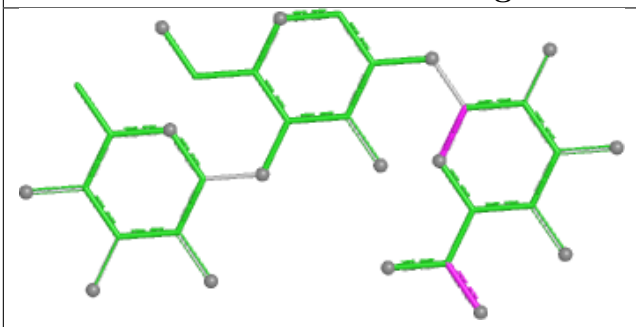
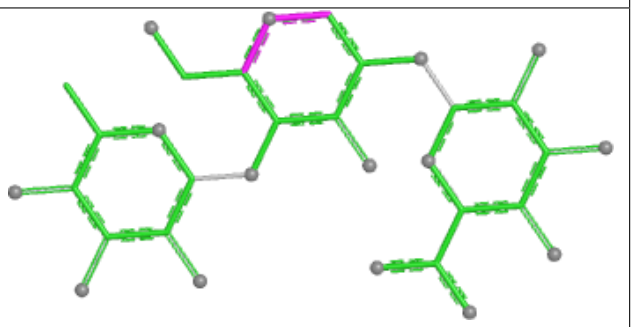
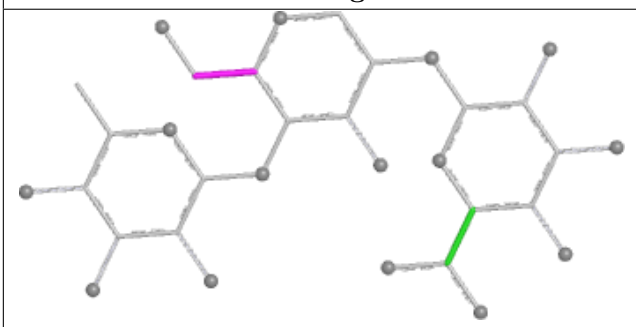
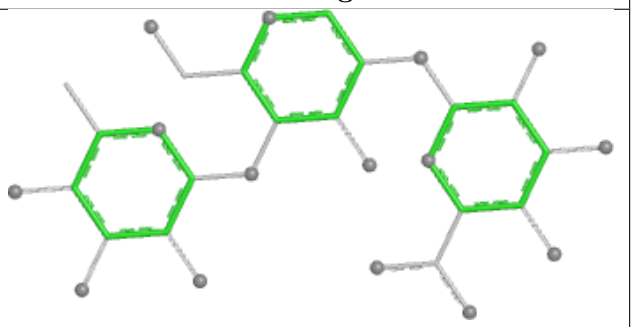
Bond angles



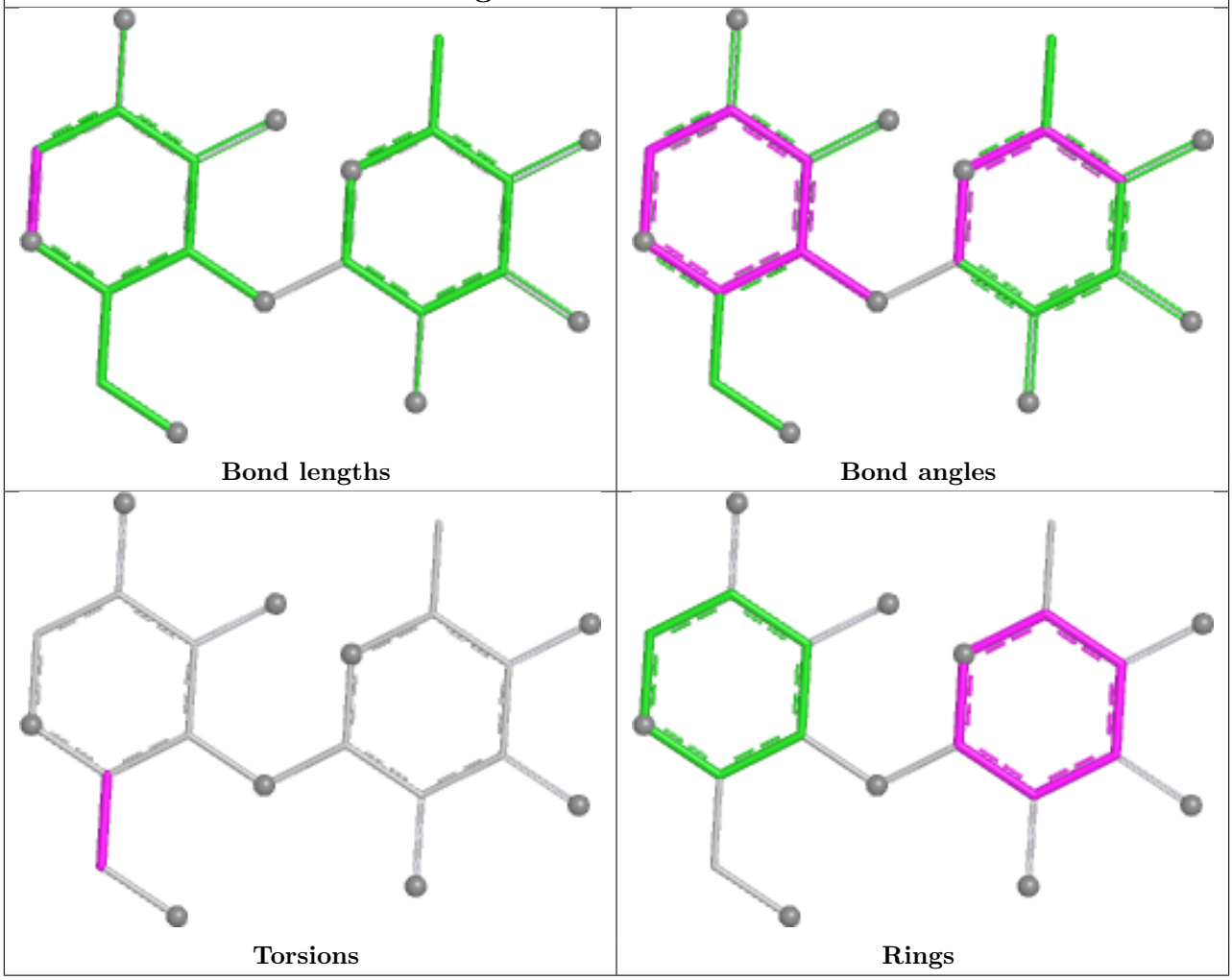
Torsions

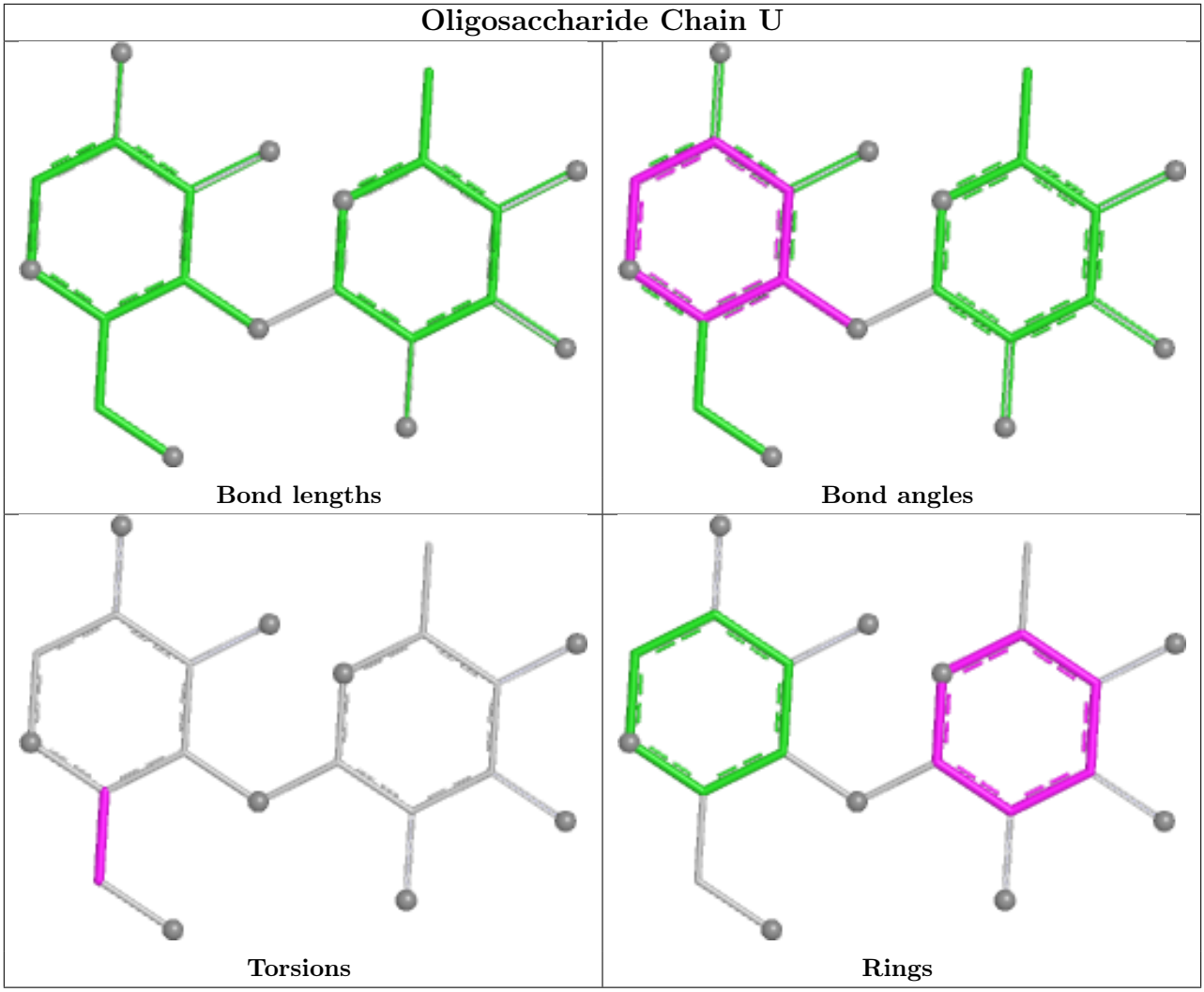


Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain K





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	$\#\|Z\| > 2$
12	GLA	P	601	1	11,11,12	0.83	0	15,15,17	0.83	0
12	GLA	P	602	-	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
12	GLA	A	604	2	11,11,12	0.74	0	15,15,17	1.62	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	GLA	A	601	2	11,11,12	0.76	0	15,15,17	1.21	1 (6%)
12	GLA	A	603	2	11,11,12	0.79	0	15,15,17	1.50	1 (6%)
12	GLA	A	602	2	11,11,12	0.83	0	15,15,17	0.98	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
12	GLA	P	601	1	-	1/2/19/22	0/1/1/1
12	GLA	P	602	-	-	2/2/19/22	0/1/1/1
12	GLA	A	604	2	-	0/2/19/22	0/1/1/1
12	GLA	A	601	2	-	0/2/19/22	0/1/1/1
12	GLA	A	603	2	-	0/2/19/22	0/1/1/1
12	GLA	A	602	2	-	0/2/19/22	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})
12	A	604	GLA	C1-O5-C5	5.04	118.94	112.19
12	A	603	GLA	C1-O5-C5	4.17	117.77	112.19
12	A	601	GLA	C1-O5-C5	3.30	116.61	112.19
12	P	602	GLA	C1-O5-C5	2.63	115.71	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	P	602	GLA	O5-C5-C6-O6
12	P	602	GLA	C4-C5-C6-O6
12	P	601	GLA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

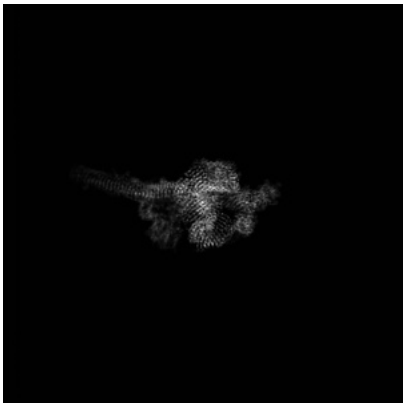
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-79007. These allow visual inspection of the internal detail of the map and identification of artifacts.

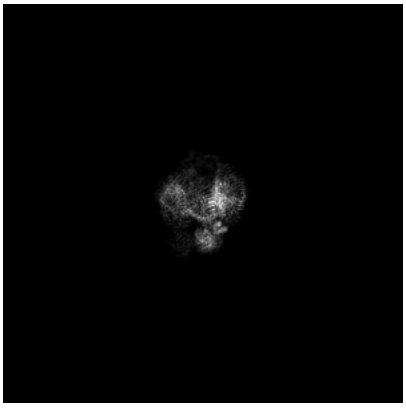
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

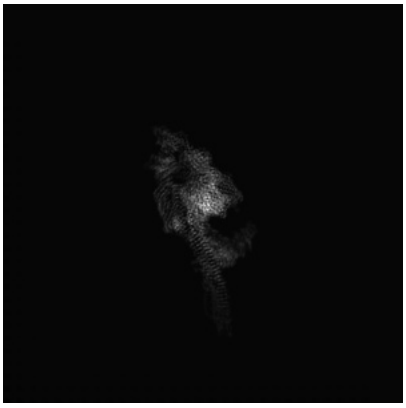
6.1.1 Primary map



X



Y



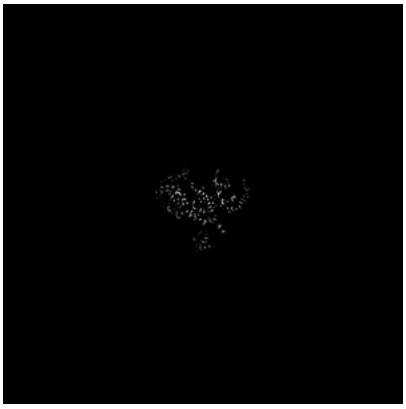
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 190



Y Index: 190

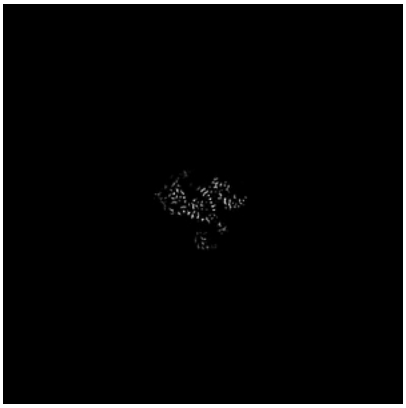
Z Index: 190

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: 191

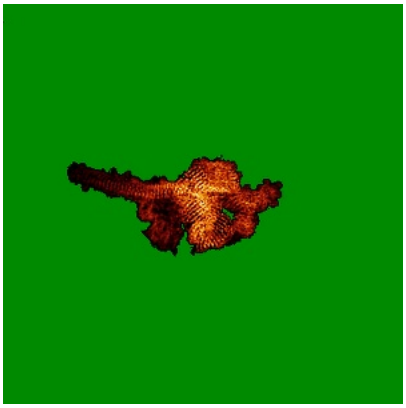

Y Index: 187

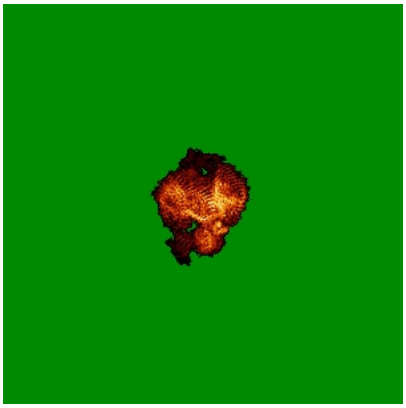
Z Index: 205

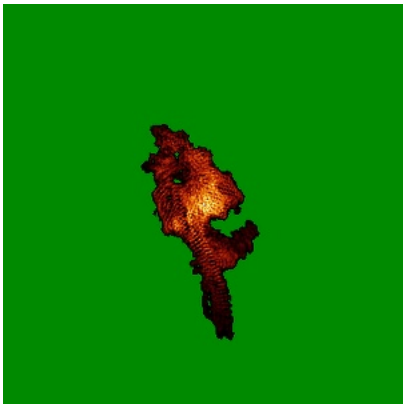
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

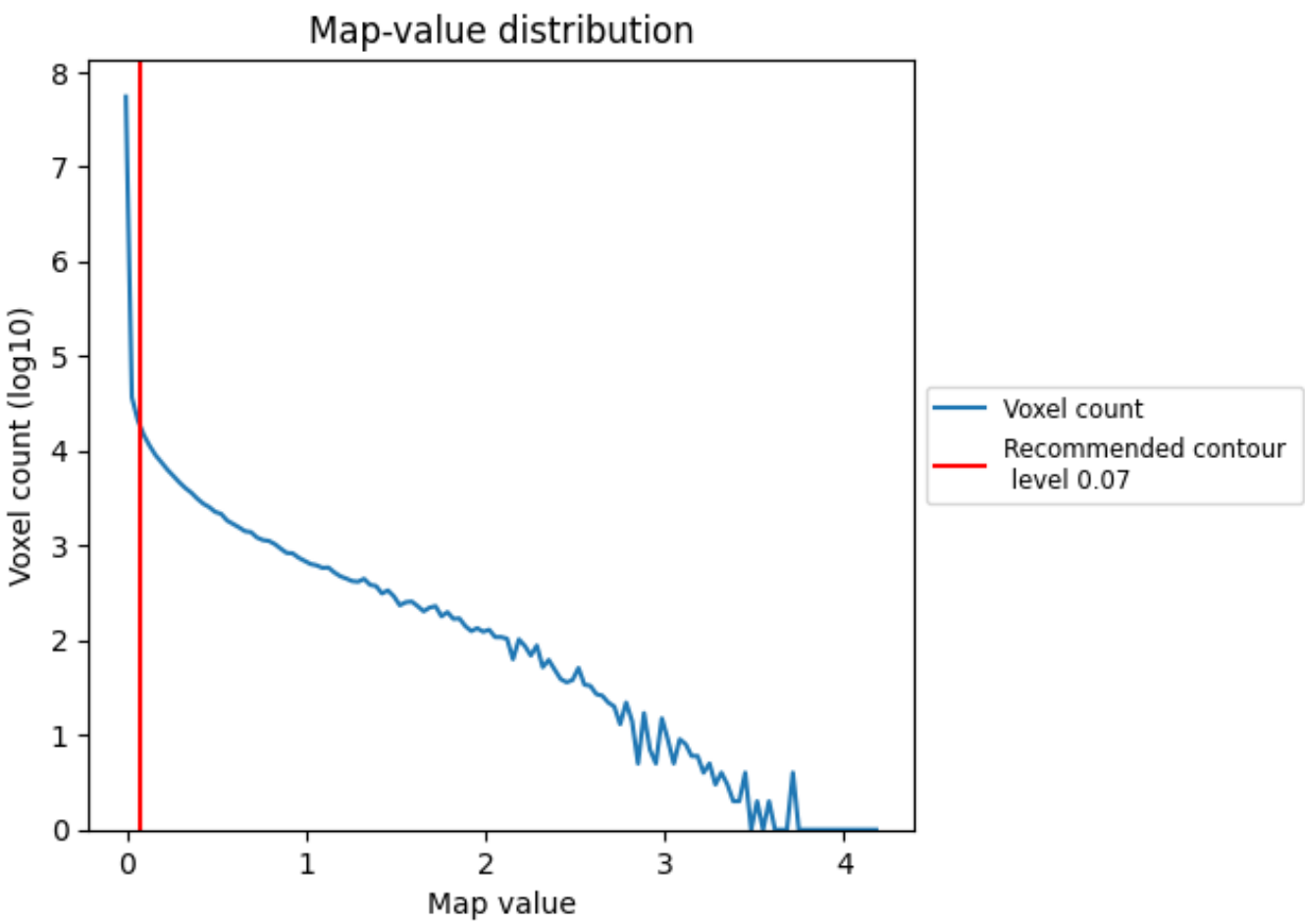
6.6 Mask visualisation (i)

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

7 Map analysis (i)

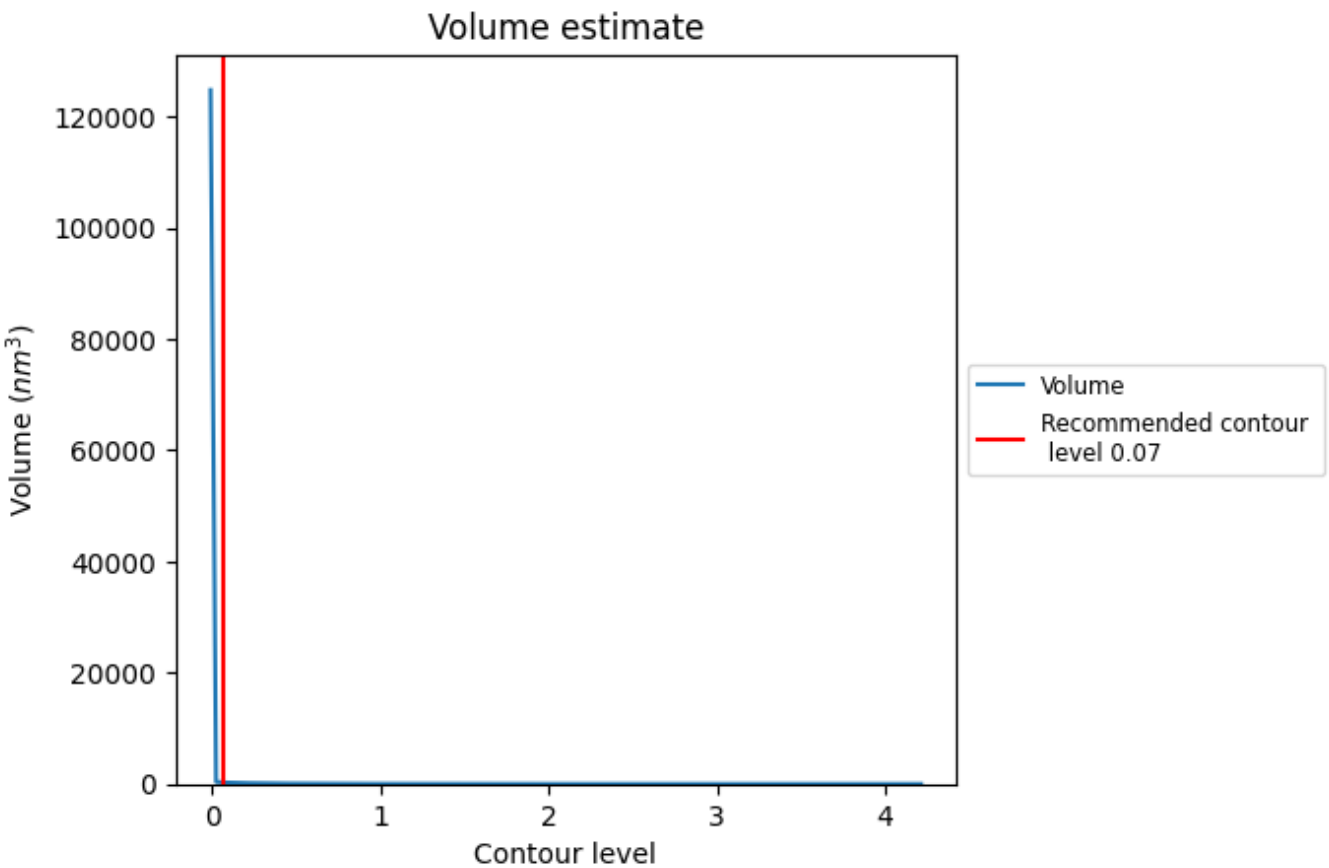
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

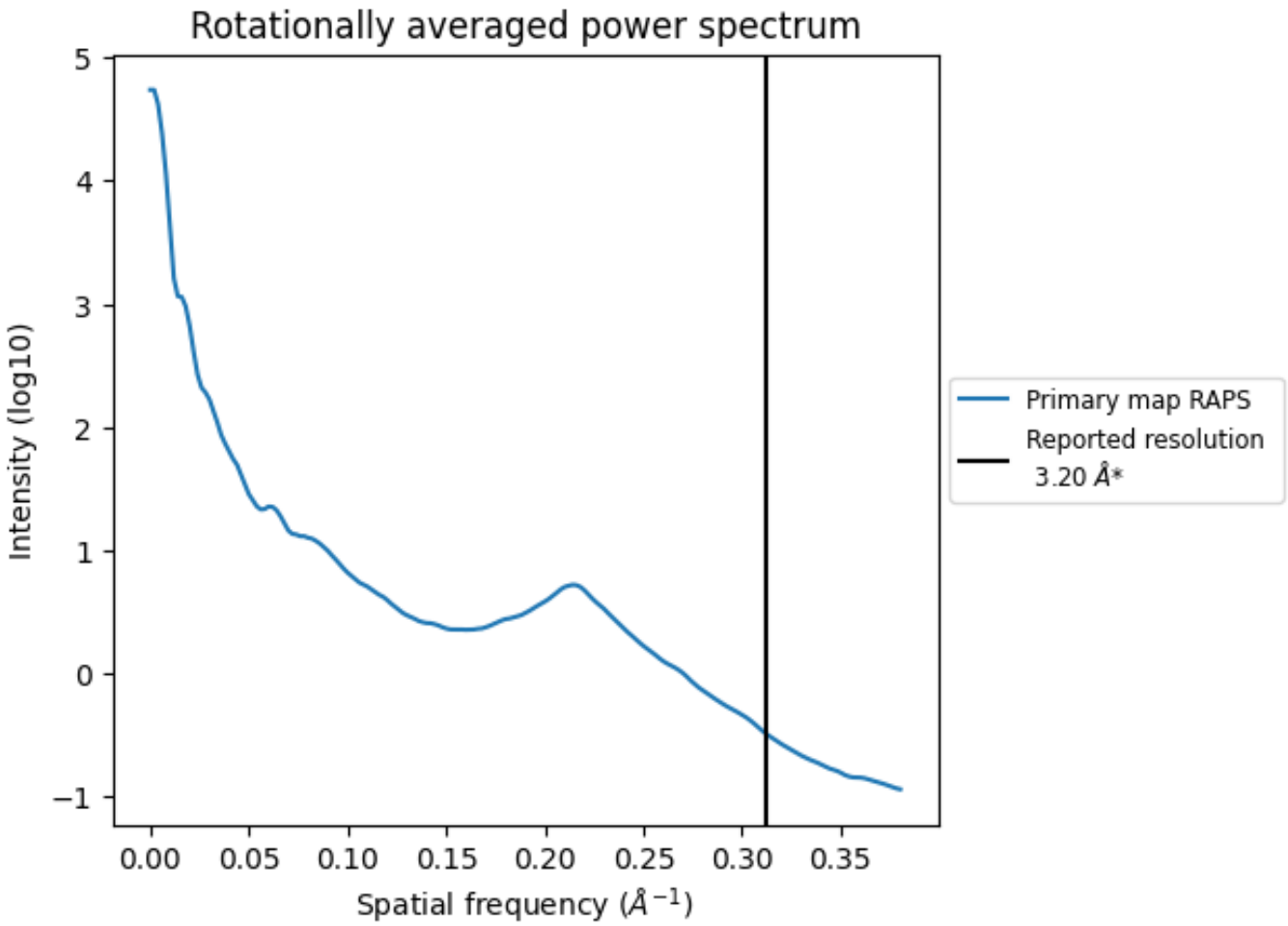
7.2 Volume estimate (i)



The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 247 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 0.312 Å^{-1}

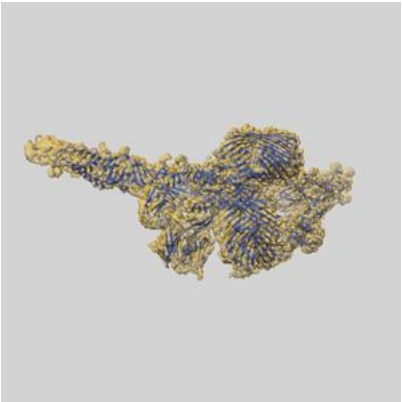
8 Fourier-Shell correlation (i)

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

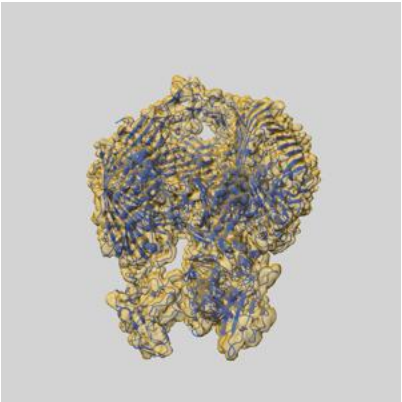
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-79007 and PDB model 38OL. Per-residue inclusion information can be found in section 3 on page 8.

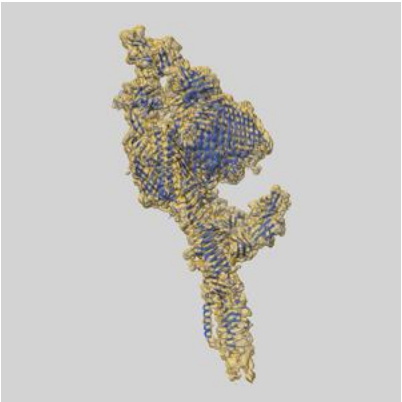
9.1 Map-model overlay (i)



X



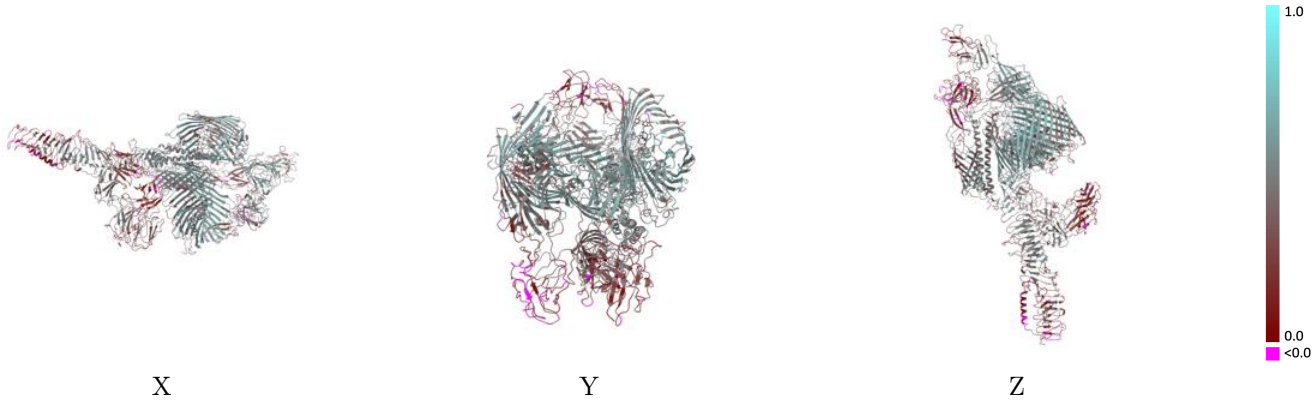
Y



Z

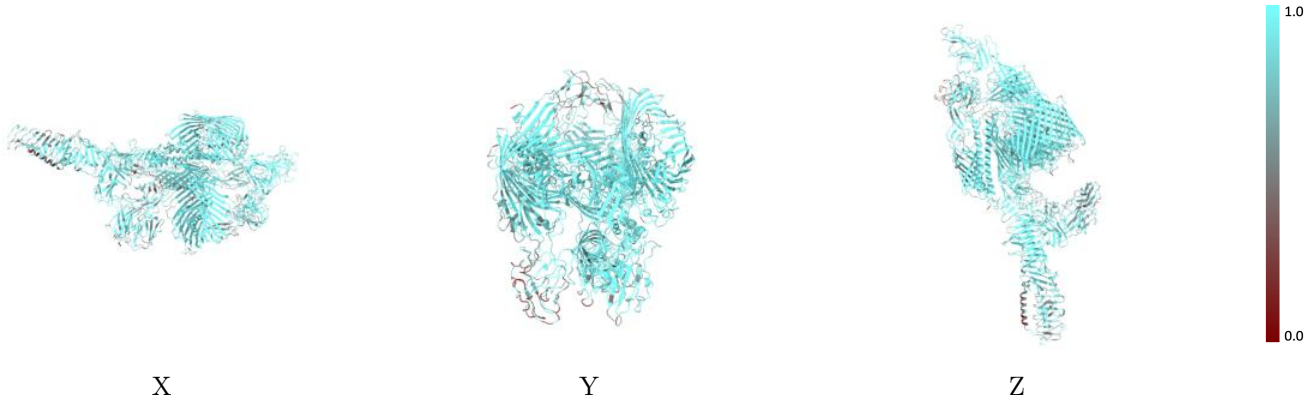
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



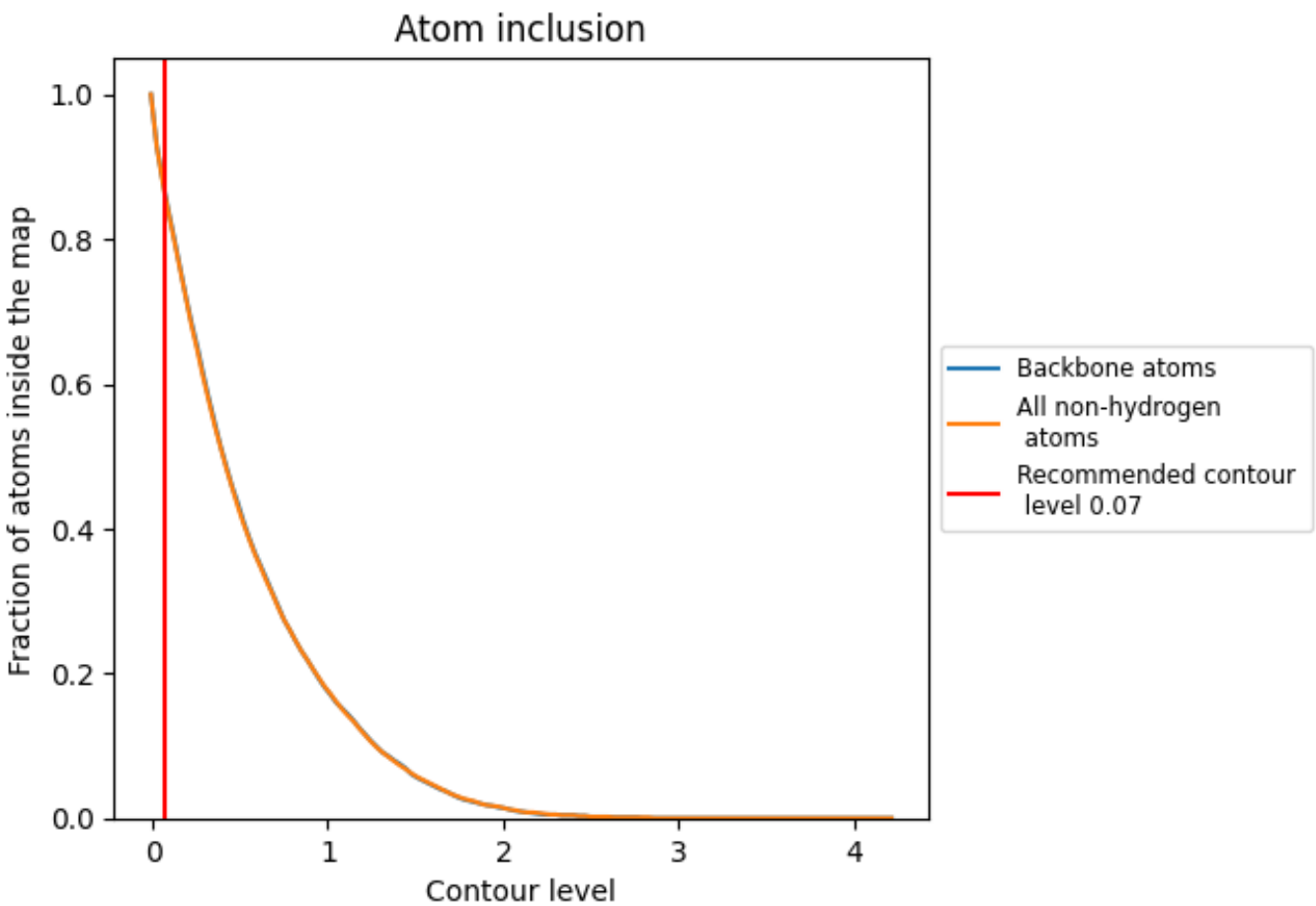
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.4160
A	0.7790	0.3230
D	0.9100	0.4910
E	0.9440	0.5350
G	0.7580	0.3190
I	0.7880	0.2110
J	0.8790	0.3730
K	0.6190	0.2000
N	0.9360	0.5320
O	0.4850	0.1820
P	0.7920	0.3110
Q	0.8840	0.3980
R	0.8050	0.2400
S1	0.9090	0.4310
S2	0.7490	0.2980
T	0.9430	0.4760
U	0.7140	0.1390