wwPDB EM Validation Summary Report (i)

Oct 12, 2026 – 08:14 PM EDT

PDB ID	:	38QP / pdb_000038qp
EMDB ID	:	EMD-79056
Title	:	LPT translocon complex from Bacteroides thetaiotaomicron built in composite volume
Authors	:	Lea, S.M.; Berks, B.C.
Deposited on	:	2026-09-13
Resolution	:	3.10 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 (i)) were used in the production of this report:

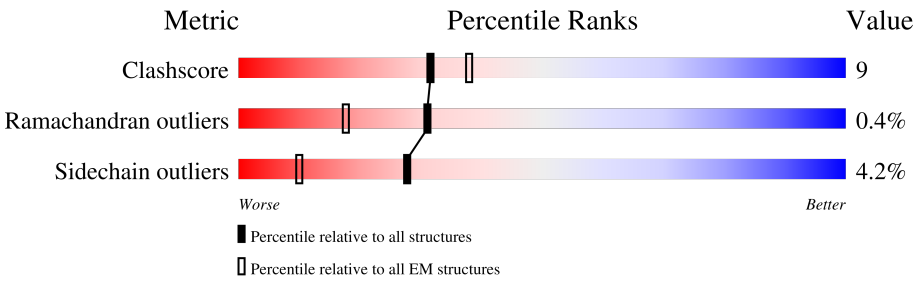
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

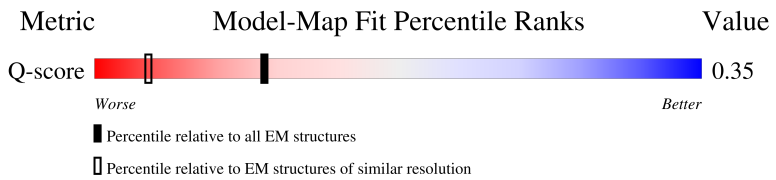
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	7%; 53%; 15%; •; 32%
2	E	175	70%; 13%; 17%
3	Q	242	•; 65%; 17%; •; 16%
4	T	295	5%; 31%; 14%; •; 53%

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Mol	Chain	Length	Quality of chain
5	V	240	73% 15% • 10%
6	D	934	67% 15% • 16%
7	N	680	80% 11% • 8%
8	P	642	10% 70% 13% • 16%
9	R1	183	11% 57% 14% • • 26%
9	R2	183	54% 22% • 22%
10	U	484	53% 62% 10% 28%
11	J	2	50% 50%
11	S	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
11	GLA	S	1	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 59038 atoms, of which 29114 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 Organic solvent tolerance-like N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	394	6269	2007	3093	528	619	22	0	0

- Molecule 2 is a protein called Lipopolysaccharide-assembly.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	145	2276	730	1117	191	237	1	0	0

- Molecule 3 is a protein called LptQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	Q	204	3206	1060	1580	259	298	9	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	VAL	-	expression tag	UNP Q89Z15
Q	2	LEU	-	expression tag	UNP Q89Z15
Q	3	LEU	-	expression tag	UNP Q89Z15
Q	4	LEU	-	expression tag	UNP Q89Z15
Q	5	PHE	-	expression tag	UNP Q89Z15
Q	6	CYS	-	expression tag	UNP Q89Z15
Q	7	ILE	-	expression tag	UNP Q89Z15
Q	8	GLY	-	expression tag	UNP Q89Z15
Q	9	ILE	-	expression tag	UNP Q89Z15
Q	10	PRO	-	expression tag	UNP Q89Z15
Q	11	THR	-	expression tag	UNP Q89Z15
Q	12	ILE	-	expression tag	UNP Q89Z15
Q	13	ALA	-	expression tag	UNP Q89Z15
Q	14	GLN	-	expression tag	UNP Q89Z15

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	15	GLN	-	expression tag	UNP Q89Z15
Q	16	GLN	-	expression tag	UNP Q89Z15
Q	17	ARG	-	expression tag	UNP Q89Z15
Q	18	PRO	-	expression tag	UNP Q89Z15
Q	19	THR	-	expression tag	UNP Q89Z15
Q	20	PRO	-	expression tag	UNP Q89Z15
Q	21	VAL	-	expression tag	UNP Q89Z15
Q	22	GLN	-	expression tag	UNP Q89Z15
Q	23	LYS	-	expression tag	UNP Q89Z15
Q	24	ARG	-	expression tag	UNP Q89Z15
Q	25	ASP	-	expression tag	UNP Q89Z15
Q	26	GLN	-	expression tag	UNP Q89Z15
Q	27	LYS	-	expression tag	UNP Q89Z15
Q	28	LYS	-	expression tag	UNP Q89Z15
Q	29	LYS	-	expression tag	UNP Q89Z15
Q	30	GLU	-	expression tag	UNP Q89Z15
Q	31	ALA	-	expression tag	UNP Q89Z15
Q	32	VAL	-	expression tag	UNP Q89Z15
Q	33	VAL	-	expression tag	UNP Q89Z15
Q	34	ASP	-	expression tag	UNP Q89Z15
Q	35	THR	-	expression tag	UNP Q89Z15
Q	36	ILE	-	expression tag	UNP Q89Z15
Q	37	PRO	-	expression tag	UNP Q89Z15
Q	38	PHE	-	expression tag	UNP Q89Z15
Q	39	TYR	-	expression tag	UNP Q89Z15
Q	40	ASN	-	expression tag	UNP Q89Z15
Q	41	GLY	-	expression tag	UNP Q89Z15
Q	42	THR	-	expression tag	UNP Q89Z15
Q	43	TYR	-	expression tag	UNP Q89Z15
Q	44	VAL	-	expression tag	UNP Q89Z15
Q	45	GLY	-	expression tag	UNP Q89Z15
Q	46	VAL	-	expression tag	UNP Q89Z15
Q	47	ASP	-	expression tag	UNP Q89Z15
Q	48	ILE	-	expression tag	UNP Q89Z15
Q	49	TYR	-	expression tag	UNP Q89Z15
Q	50	GLY	-	expression tag	UNP Q89Z15
Q	51	ILE	-	expression tag	UNP Q89Z15
Q	52	GLY	-	expression tag	UNP Q89Z15
Q	53	SER	-	expression tag	UNP Q89Z15
Q	54	LYS	-	expression tag	UNP Q89Z15

- Molecule 4 is a protein called DUF5683 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	T	140	2272	747	1128	187	207	3	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	V	215	3335	1081	1648	279	321	6	0	0

- Molecule 6 is a protein called LPS-assembly protein LptD central domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	D	784	12357	4007	6056	1056	1215	23	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	TRP	-	insertion	UNP Q8A5V3
D	33	SER	-	insertion	UNP Q8A5V3
D	34	HIS	-	insertion	UNP Q8A5V3
D	35	PRO	-	insertion	UNP Q8A5V3
D	36	GLN	-	insertion	UNP Q8A5V3
D	37	PHE	-	insertion	UNP Q8A5V3
D	38	GLU	-	insertion	UNP Q8A5V3
D	39	LYS	-	insertion	UNP Q8A5V3
D	40	GLY	-	insertion	UNP Q8A5V3
D	41	GLY	-	insertion	UNP Q8A5V3
D	42	GLY	-	insertion	UNP Q8A5V3
D	43	SER	-	insertion	UNP Q8A5V3
D	44	GLY	-	insertion	UNP Q8A5V3
D	45	GLY	-	insertion	UNP Q8A5V3
D	46	GLY	-	insertion	UNP Q8A5V3
D	47	SER	-	insertion	UNP Q8A5V3
D	48	GLY	-	insertion	UNP Q8A5V3
D	49	GLY	-	insertion	UNP Q8A5V3
D	50	SER	-	insertion	UNP Q8A5V3
D	51	ALA	-	insertion	UNP Q8A5V3
D	52	TRP	-	insertion	UNP Q8A5V3
D	53	SER	-	insertion	UNP Q8A5V3
D	54	HIS	-	insertion	UNP Q8A5V3
D	55	PRO	-	insertion	UNP Q8A5V3
D	56	GLN	-	insertion	UNP Q8A5V3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	57	PHE	-	insertion	UNP Q8A5V3
D	58	GLU	-	insertion	UNP Q8A5V3
D	59	LYS	-	insertion	UNP Q8A5V3
D	60	VAL	-	insertion	UNP Q8A5V3
D	61	ASP	-	insertion	UNP Q8A5V3
D	62	SER	-	insertion	UNP Q8A5V3
D	63	VAL	-	insertion	UNP Q8A5V3
D	72	VAL	ASP	conflict	UNP Q8A5V3

- Molecule 7 is a protein called Porin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	N	627	10116	3317	4954	879	951	15	0	0

- Molecule 8 is a protein called SbsA Ig-like domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	P	541	8672	2810	4292	728	835	7	0	0

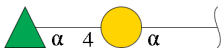
- Molecule 9 is a protein called Calcium-binding protein P.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	R1	135	2215	702	1103	186	216	8	0	0
9	R2	143	2346	742	1168	198	230	8	0	0

- Molecule 10 is a protein called Periplasmic protease.

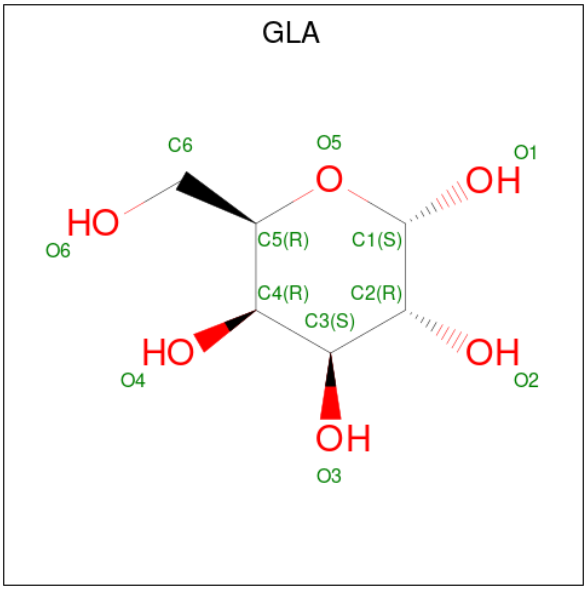
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	U	348	5465	1769	2692	444	547	13	0	0

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



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

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



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 22	C 6	H 11	O 5	0
12	A	1	Total 22	C 6	H 11	O 5	0
12	A	1	Total 22	C 6	H 11	O 5	0
12	A	1	Total 22	C 6	H 11	O 5	0
12	D	1	Total 22	C 6	H 11	O 5	0
12	D	1	Total 22	C 6	H 11	O 5	0
12	P	1	Total 22	C 6	H 11	O 5	0
12	P	1	Total 22	C 6	H 11	O 5	0
12	P	1	Total 22	C 6	H 11	O 5	0
12	R2	1	Total 22	C 6	H 11	O 5	0

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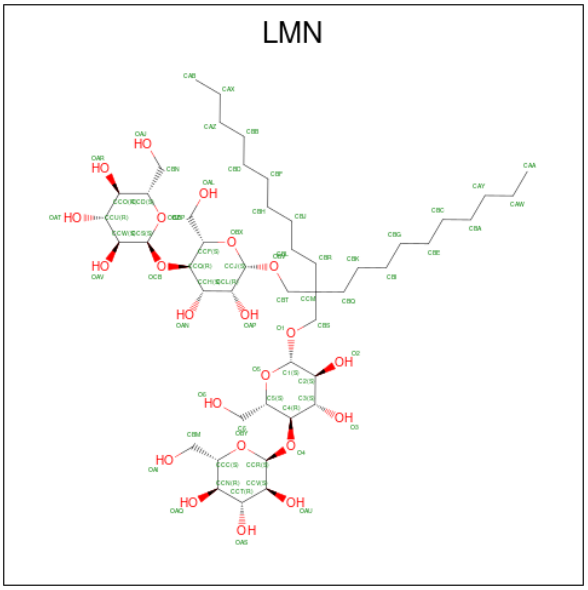
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
12	R2	1	22	6	11	5	0

- Molecule 13 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



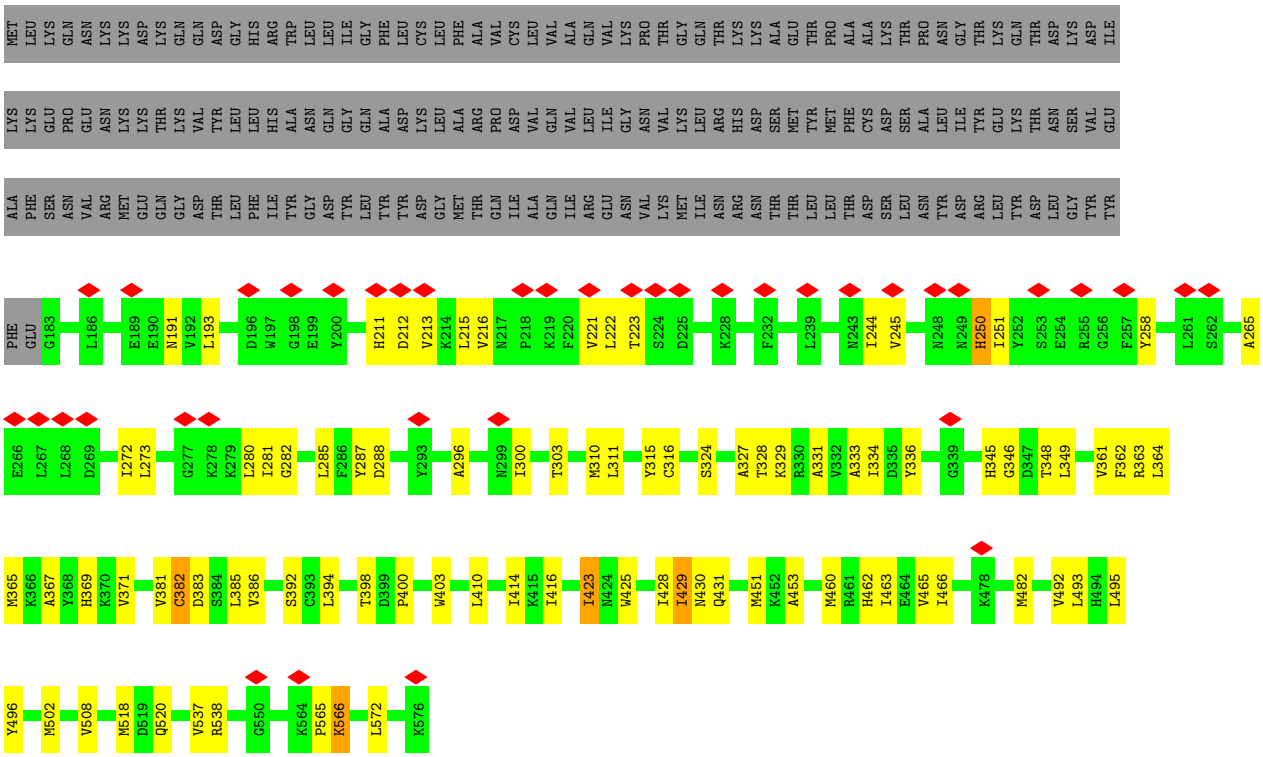
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H		
13	D	1	61	21	40		0
			Total	C	H		
13	D	1	61	21	40		0
			Total	C	H		
13	N	1	61	21	40		0

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.

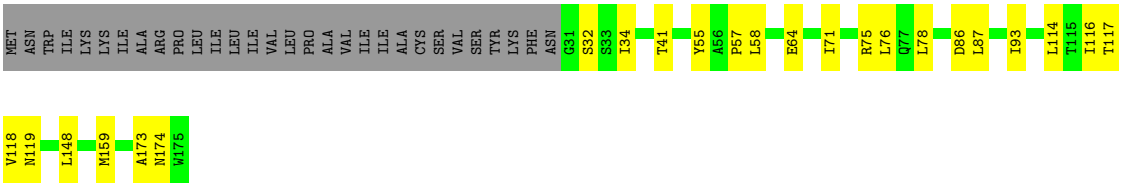
• Molecule 1: Organic solvent tolerance-like N-terminal domain-containing protein

Chain A:



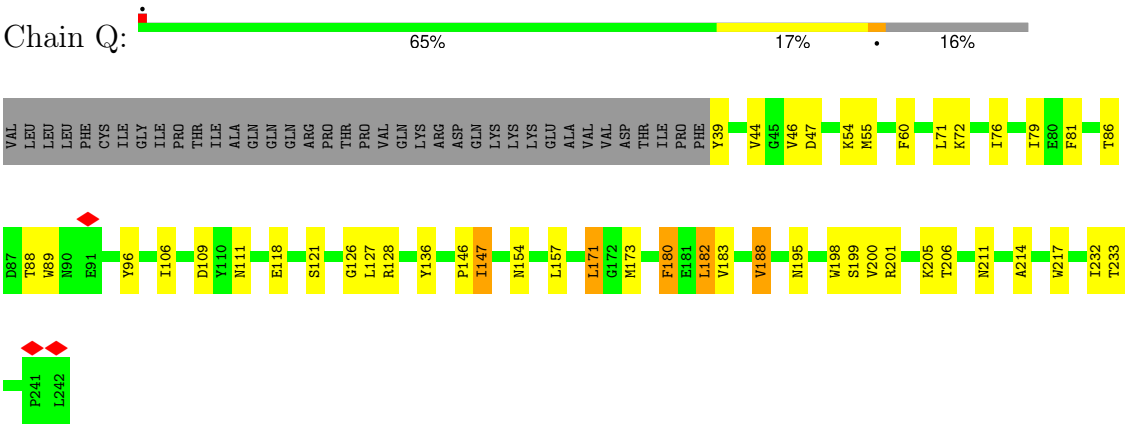
• Molecule 2: Lipopolysaccharide-assembly

Chain E:



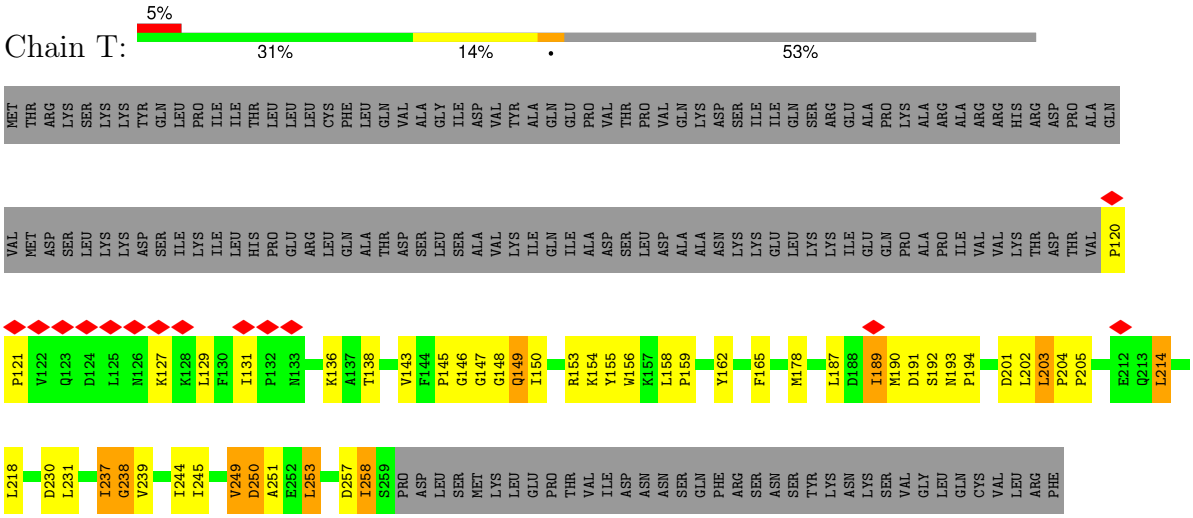
• Molecule 3: LptQ

Chain Q:



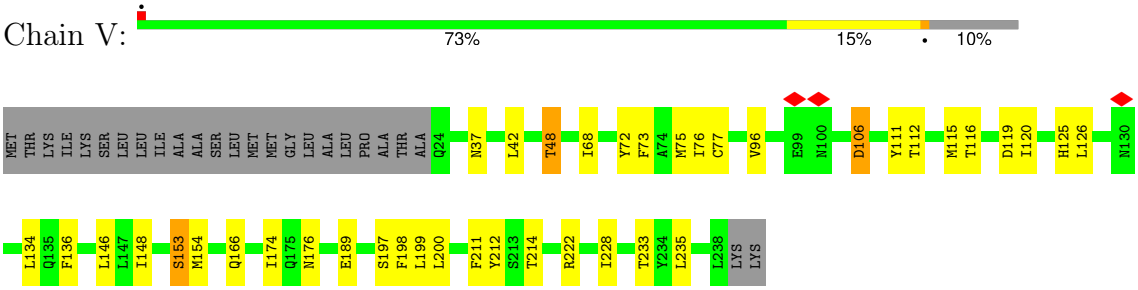
• Molecule 4: DUF5683 domain-containing protein

Chain T:



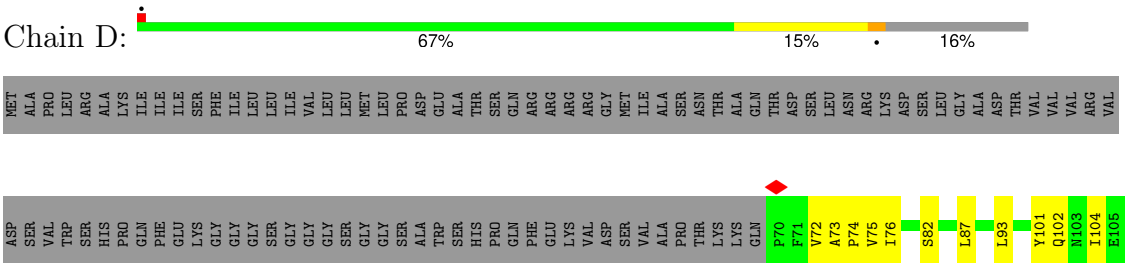
• Molecule 5: Outer membrane protein beta-barrel domain-containing protein

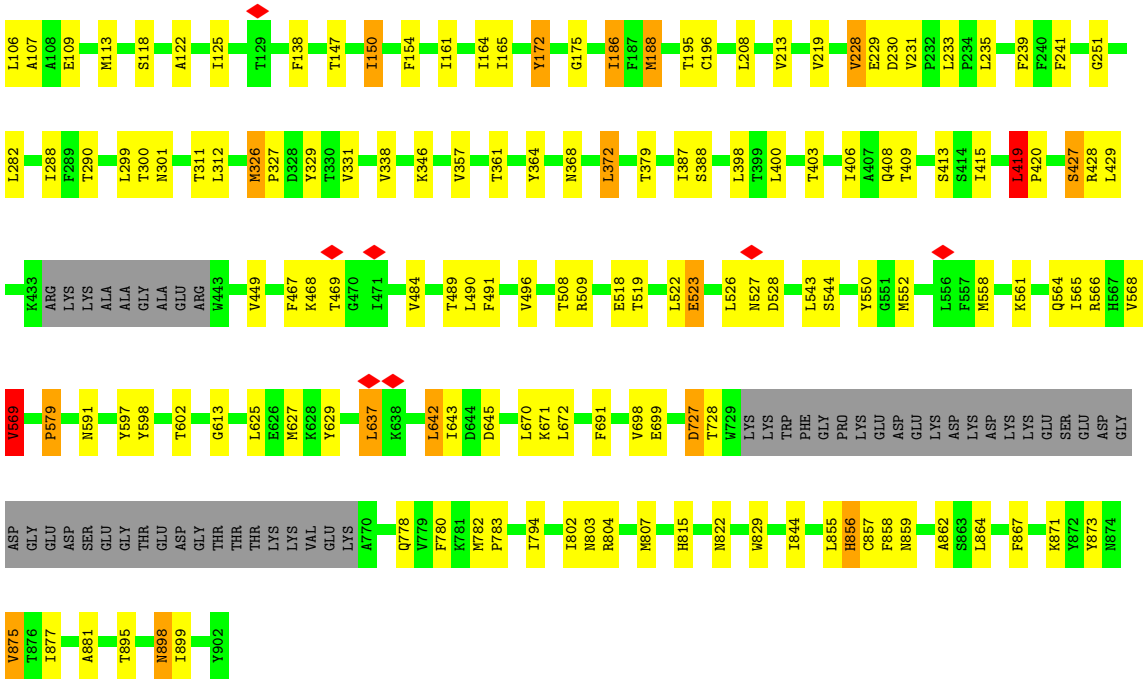
Chain V:



• Molecule 6: LPS-assembly protein LptD central domain-containing protein

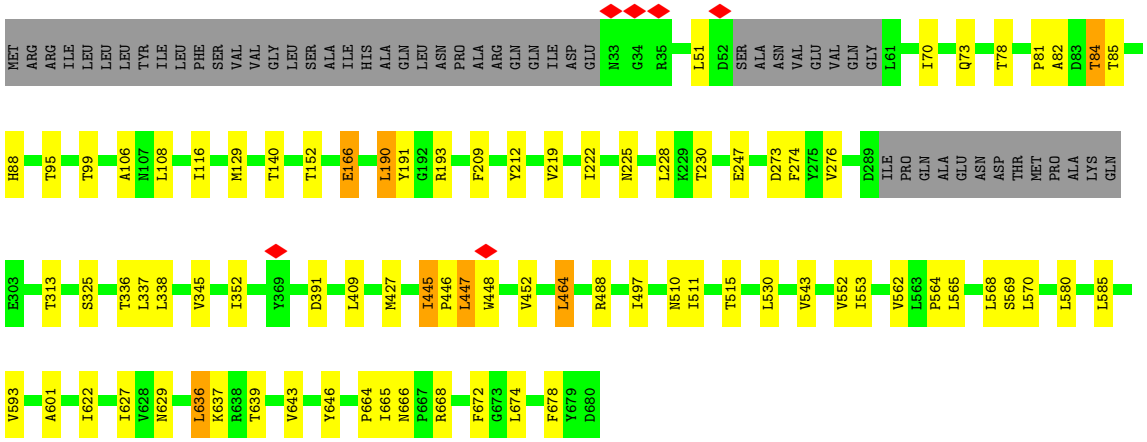
Chain D:





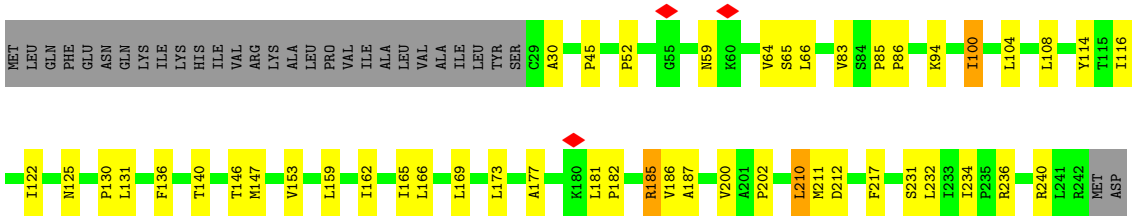
- Molecule 7: Porin

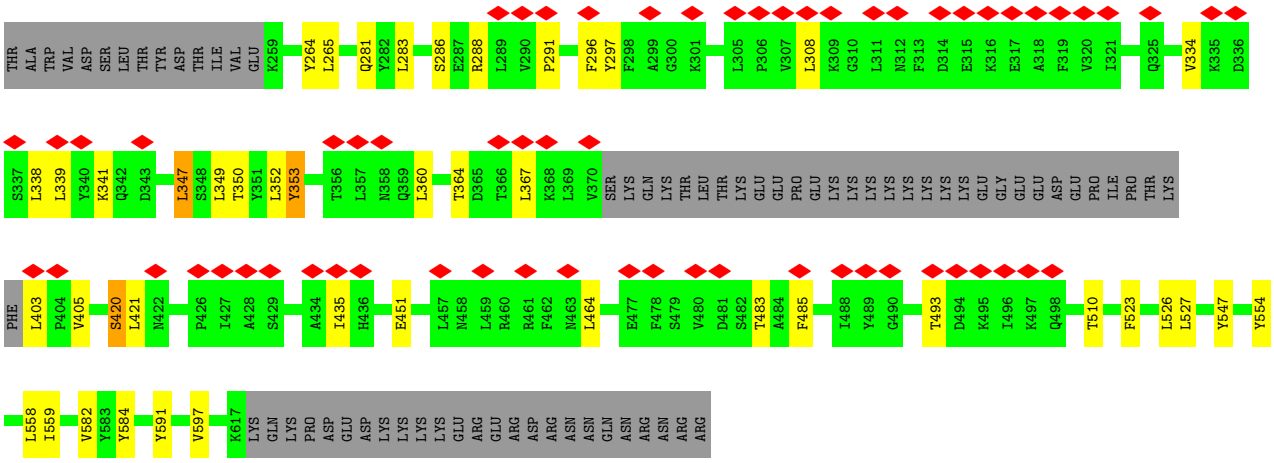
Chain N:



- Molecule 8: SbsA Ig-like domain-containing protein

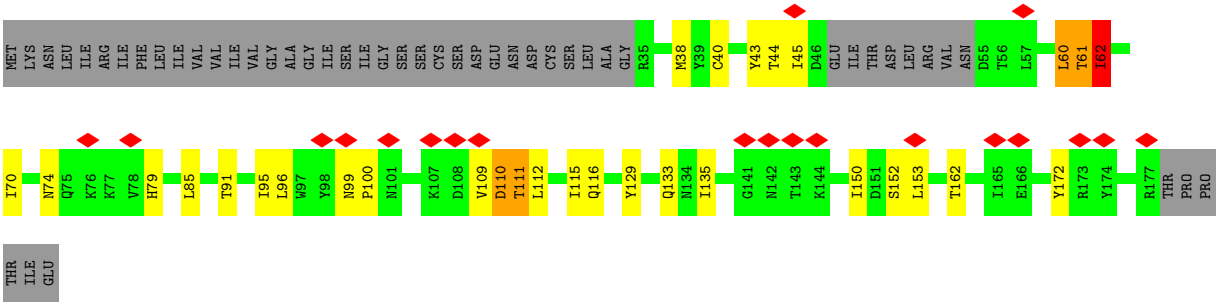
Chain P:





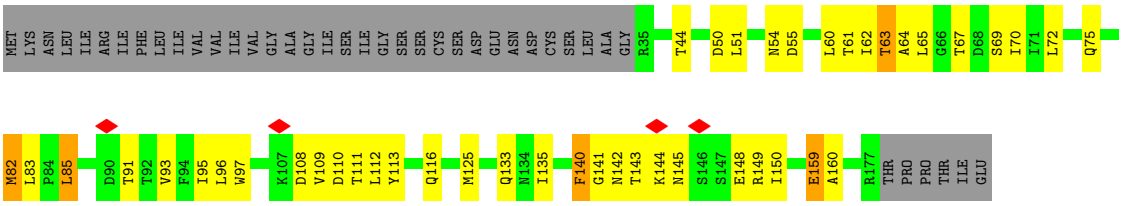
- Molecule 9: Calcium-binding protein P

Chain R1:



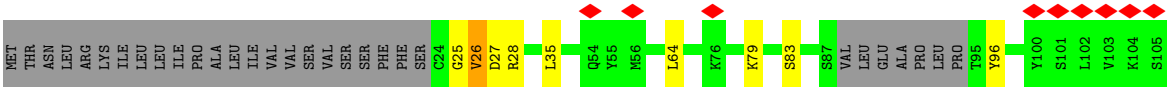
- Molecule 9: Calcium-binding protein P

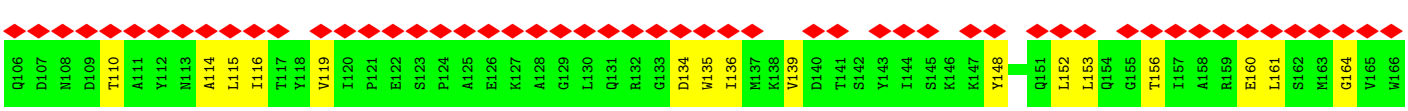
Chain R2:

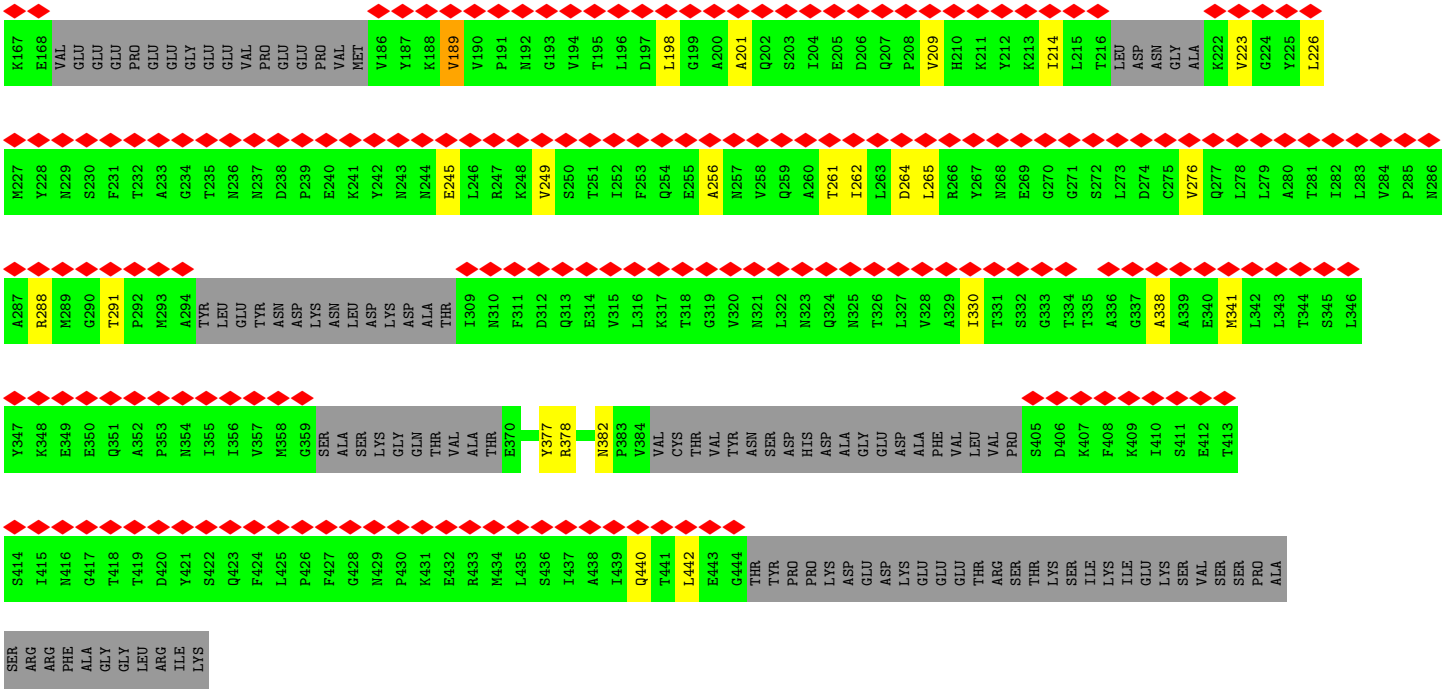


- Molecule 10: Periplasmic protease

Chain U:







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

Chain J:

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

Chain S:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130464	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	4.721	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	493.99997, 493.99997, 493.99997	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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, LMN, 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	A	0.13	0/3242	0.32	0/4373
2	E	0.29	0/1179	0.34	0/1599
3	Q	0.20	0/1676	0.37	0/2265
4	T	0.26	0/1177	0.46	0/1596
5	V	0.21	0/1724	0.36	0/2322
6	D	0.25	0/6466	0.36	0/8761
7	N	0.24	0/5307	0.31	0/7185
8	P	0.10	0/4484	0.25	0/6080
9	R1	0.14	0/1132	0.37	0/1532
9	R2	0.15	0/1199	0.36	0/1625
10	U	0.08	0/2829	0.23	0/3839
All	All	0.20	0/30415	0.33	0/41177

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	T	0	2
5	V	0	1
6	D	0	2
7	N	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	228	VAL	Peptide
6	D	419	LEU	Peptide
4	T	237	ILE	Peptide
4	T	249	VAL	Peptide
5	V	48	THR	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	A	3176	3093	3093	71	0
2	E	1159	1117	1117	13	0
3	Q	1626	1580	1580	34	0
4	T	1144	1128	1128	49	0
5	V	1687	1648	1648	26	0
6	D	6301	6056	6055	109	0
7	N	5162	4954	4954	60	0
8	P	4380	4292	4292	68	0
9	R1	1112	1103	1103	22	0
9	R2	1178	1168	1168	37	0
10	U	2773	2692	2692	38	0
11	J	21	21	19	3	0
11	S	21	21	19	6	0
12	A	44	44	40	4	0
12	D	22	22	20	0	0
12	P	33	33	30	2	0
12	R2	22	22	20	1	0
13	D	42	80	84	3	0
13	N	21	40	42	0	0
All	All	29924	29114	29104	514	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 9.

The worst 5 of 514 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:N:108:LEU:HD23	7:N:190:LEU:HD13	1.43	0.96
6:D:73:ALA:HB1	6:D:74:PRO:HD2	1.60	0.82
1:A:222:LEU:HB2	1:A:244:ILE:HG22	1.60	0.82
1:A:300:ILE:HG21	1:A:316:CYS:HB2	1.63	0.80
3:Q:121:SER:HB3	4:T:143:VAL:HG11	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/576 (68%)	347 (88%)	42 (11%)	3 (1%)	16	47
2	E	143/175 (82%)	134 (94%)	8 (6%)	1 (1%)	18	49
3	Q	202/242 (84%)	180 (89%)	21 (10%)	1 (0%)	24	57
4	T	138/295 (47%)	100 (72%)	35 (25%)	3 (2%)	5	24
5	V	213/240 (89%)	194 (91%)	19 (9%)	0	100	100
6	D	778/934 (83%)	662 (85%)	111 (14%)	5 (1%)	21	52
7	N	621/680 (91%)	586 (94%)	34 (6%)	1 (0%)	43	73
8	P	535/642 (83%)	507 (95%)	28 (5%)	0	100	100
9	R1	131/183 (72%)	101 (77%)	29 (22%)	1 (1%)	16	47
9	R2	141/183 (77%)	118 (84%)	23 (16%)	0	100	100
10	U	334/484 (69%)	315 (94%)	18 (5%)	1 (0%)	36	67
All	All	3628/4634 (78%)	3244 (89%)	368 (10%)	16 (0%)	31	61

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	LYS
3	Q	147	ILE

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Mol	Chain	Res	Type
4	T	189	ILE
6	D	523	GLU
6	D	569	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/515 (69%)	342 (97%)	12 (3%)	32	63
2	E	128/155 (83%)	125 (98%)	3 (2%)	44	70
3	Q	174/209 (83%)	164 (94%)	10 (6%)	18	49
4	T	122/263 (46%)	112 (92%)	10 (8%)	10	36
5	V	176/195 (90%)	166 (94%)	10 (6%)	18	49
6	D	693/816 (85%)	658 (95%)	35 (5%)	21	52
7	N	551/596 (92%)	528 (96%)	23 (4%)	26	58
8	P	479/575 (83%)	466 (97%)	13 (3%)	39	67
9	R1	130/172 (76%)	120 (92%)	10 (8%)	12	38
9	R2	138/172 (80%)	131 (95%)	7 (5%)	21	52
10	U	305/425 (72%)	300 (98%)	5 (2%)	55	75
All	All	3250/4093 (79%)	3112 (96%)	138 (4%)	28	58

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	P	527	LEU
9	R1	62	ILE
9	R2	140	PHE
6	D	172	TYR
6	D	150	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
9	R1	145	ASN
9	R2	163	ASN
9	R2	161	ASN
10	U	229	ASN
6	D	457	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)

4 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	$\#\|Z\| > 2$
11	GLA	J	1	11	11,11,12	1.03	1 (9%)	15,15,17	0.92	0
11	RAM	J	2	11	10,10,11	0.38	0	14,14,16	0.51	0
11	GLA	S	1	11	11,11,12	0.82	0	15,15,17	1.74	4 (26%)
11	RAM	S	2	11	10,10,11	0.38	0	14,14,16	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GLA	J	1	11	-	0/2/19/22	0/1/1/1
11	RAM	J	2	11	-	-	0/1/1/1
11	GLA	S	1	11	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	RAM	S	2	11	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1	GLA	O5-C1	-2.64	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	S	1	GLA	C1-O5-C5	4.02	117.57	112.19
11	S	1	GLA	C1-C2-C3	3.19	114.29	109.64
11	S	1	GLA	C2-C3-C4	2.33	114.95	110.86
11	S	1	GLA	O3-C3-C2	-2.08	105.81	110.05

There are no chirality outliers.

All (1) torsion outliers are listed below:

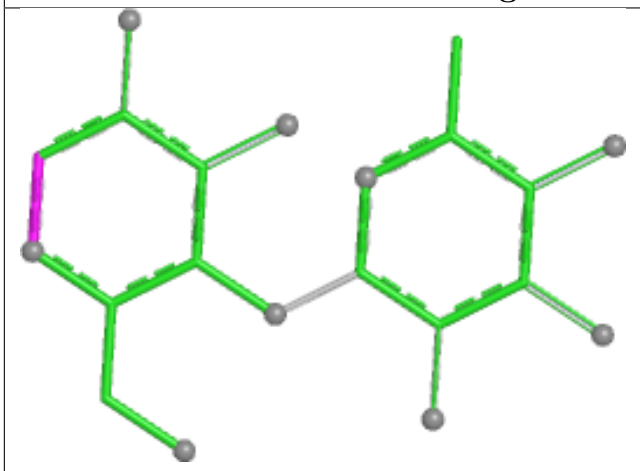
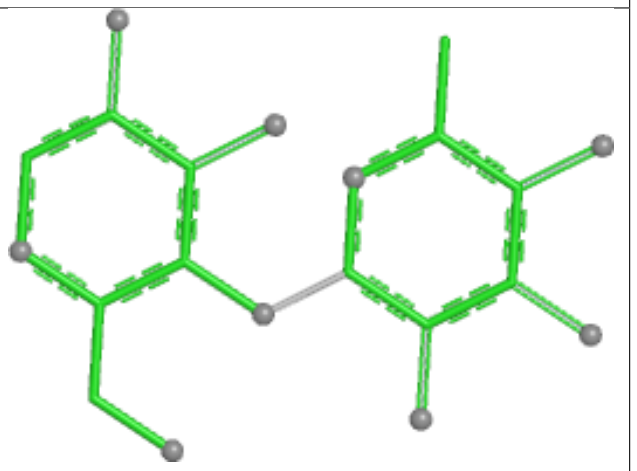
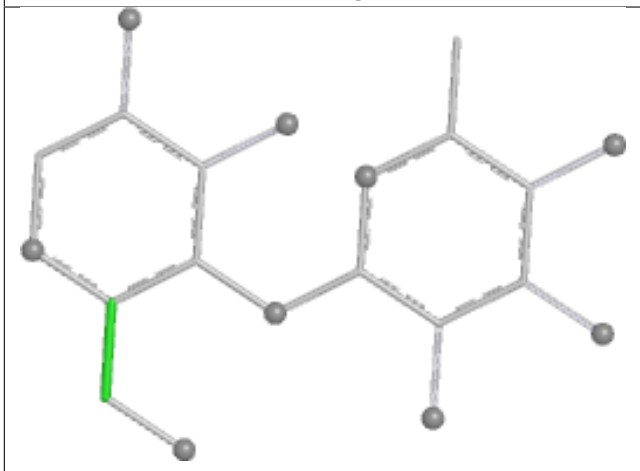
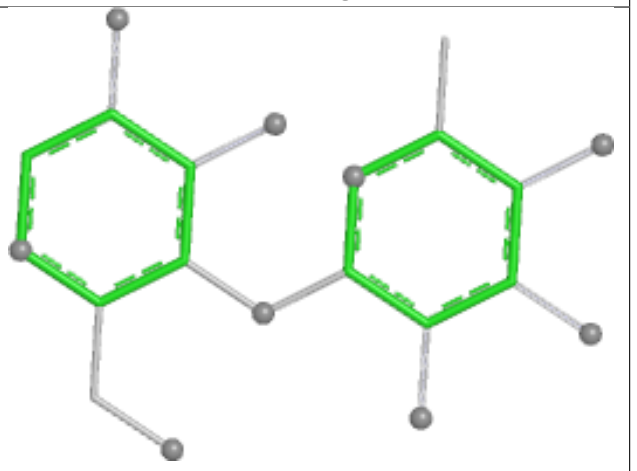
Mol	Chain	Res	Type	Atoms
11	S	1	GLA	O5-C5-C6-O6

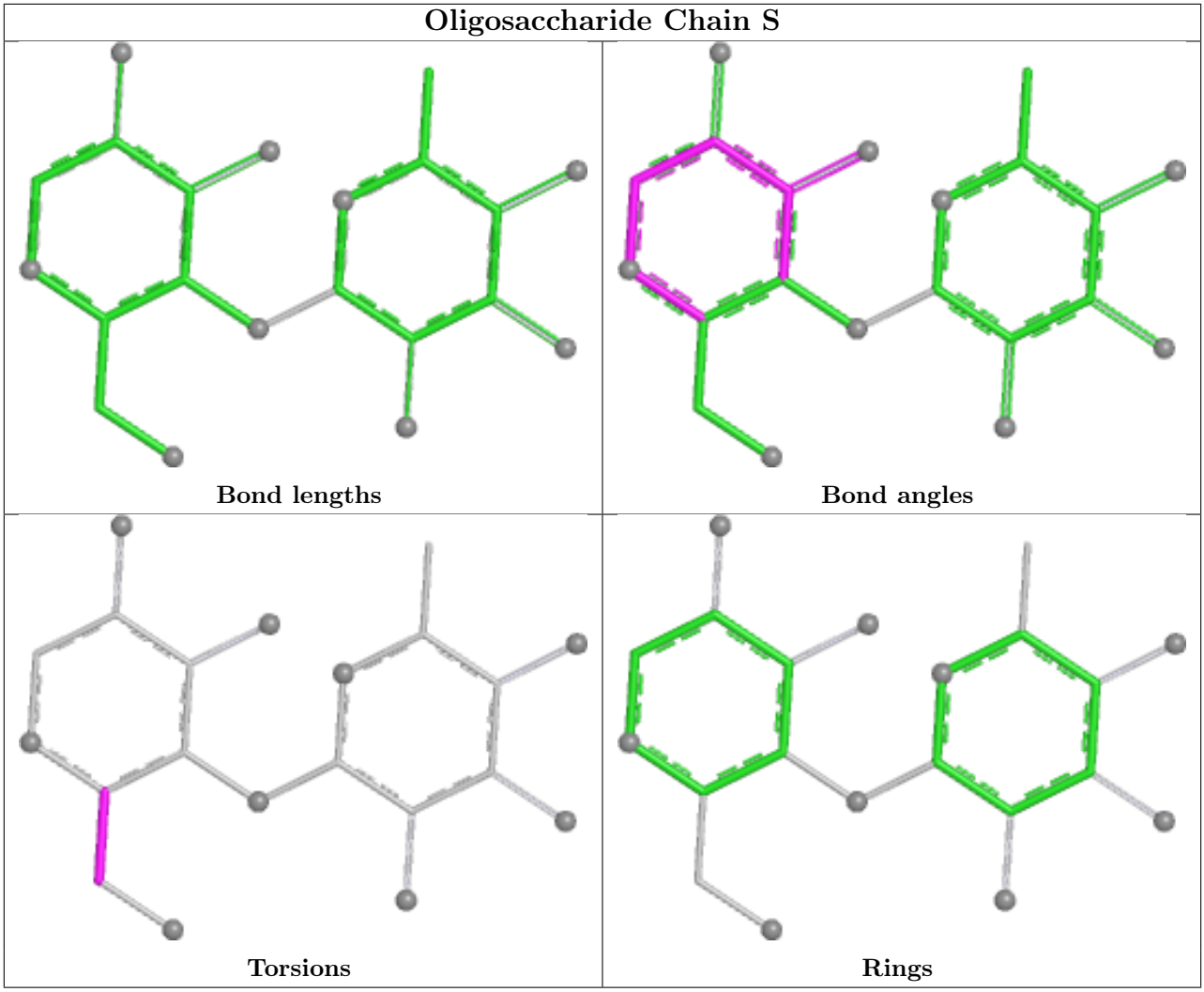
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	1	GLA	6	0
11	S	2	RAM	3	0
11	J	1	GLA	3	0
11	J	2	RAM	2	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 J	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
13	LMN	D	1002	-	20,20,72	0.25	0	19,19,98	0.41	0
12	GLA	A	604	1	11,11,12	0.82	0	15,15,17	1.05	0
12	GLA	D	1004	6	11,11,12	0.78	0	15,15,17	1.38	3 (20%)
12	GLA	R2	202	-	11,11,12	0.76	0	15,15,17	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	GLA	A	603	1	11,11,12	0.80	0	15,15,17	1.16	1 (6%)
13	LMN	D	1001	-	20,20,72	0.27	0	19,19,98	0.38	0
12	GLA	A	602	-	11,11,12	0.71	0	15,15,17	2.22	2 (13%)
13	LMN	N	701	-	20,20,72	0.30	0	19,19,98	0.53	0
12	GLA	P	701	-	11,11,12	0.66	0	15,15,17	2.14	3 (20%)
12	GLA	A	601	1	11,11,12	0.76	0	15,15,17	0.97	1 (6%)
12	GLA	D	1003	6	11,11,12	0.73	0	15,15,17	1.92	3 (20%)
12	GLA	R2	201	9	11,11,12	0.81	0	15,15,17	1.04	1 (6%)
12	GLA	P	703	8	11,11,12	0.80	0	15,15,17	1.05	0
12	GLA	P	702	8	11,11,12	0.69	0	15,15,17	1.33	1 (6%)

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
13	LMN	D	1002	-	-	7/18/18/130	-
12	GLA	A	604	1	-	0/2/19/22	0/1/1/1
12	GLA	D	1004	6	-	2/2/19/22	0/1/1/1
12	GLA	R2	202	-	-	0/2/19/22	0/1/1/1
12	GLA	A	603	1	-	0/2/19/22	0/1/1/1
13	LMN	D	1001	-	-	9/18/18/130	-
12	GLA	A	602	-	-	0/2/19/22	0/1/1/1
13	LMN	N	701	-	-	13/18/18/130	-
12	GLA	P	701	-	-	0/2/19/22	0/1/1/1
12	GLA	A	601	1	-	0/2/19/22	0/1/1/1
12	GLA	D	1003	6	-	0/2/19/22	0/1/1/1
12	GLA	R2	201	9	-	0/2/19/22	0/1/1/1
12	GLA	P	703	8	-	0/2/19/22	0/1/1/1
12	GLA	P	702	8	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	602	GLA	C1-O5-C5	7.24	121.89	112.19
12	P	701	GLA	C1-O5-C5	6.39	120.75	112.19
12	D	1003	GLA	C1-O5-C5	5.77	119.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	702	GLA	C1-O5-C5	3.82	117.30	112.19
12	P	701	GLA	C1-C2-C3	3.54	114.80	109.64

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	N	701	LMN	CBI-CBK-CBQ-CCM
13	N	701	LMN	CBL-CBR-CCM-CBQ
13	D	1002	LMN	CBG-CBI-CBK-CBQ
13	D	1002	LMN	CAY-CBA-CBC-CBE
13	D	1001	LMN	CAY-CBA-CBC-CBE

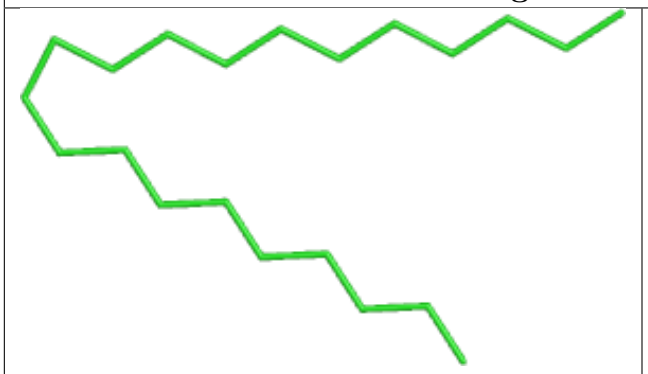
There are no ring outliers.

7 monomers are involved in 10 short contacts:

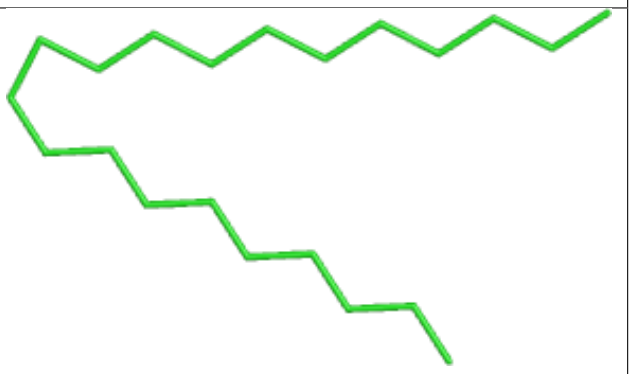
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	1002	LMN	2	0
12	A	603	GLA	1	0
13	D	1001	LMN	1	0
12	A	602	GLA	3	0
12	P	701	GLA	1	0
12	R2	201	GLA	1	0
12	P	703	GLA	1	0

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

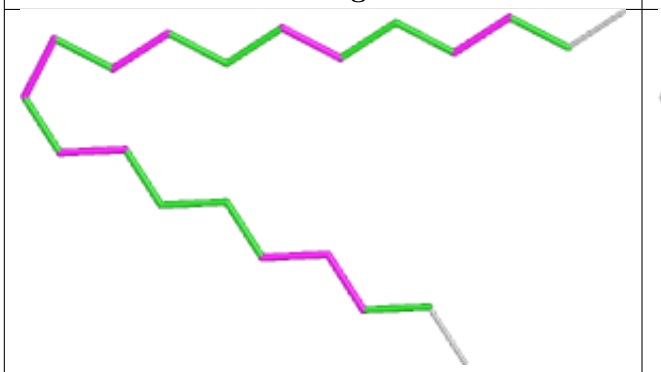
Ligand LMN D 1002



Bond lengths



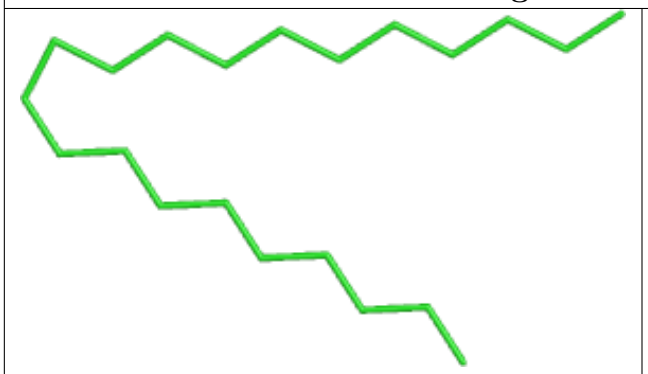
Bond angles



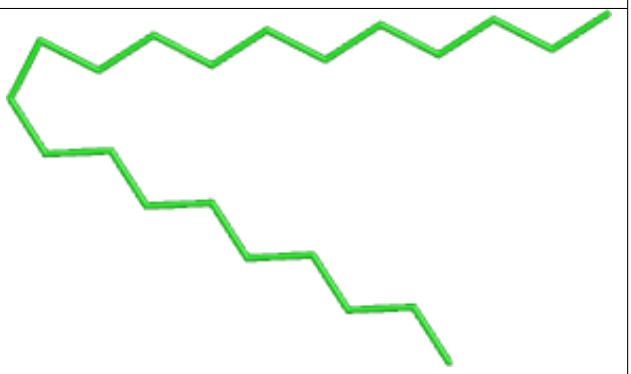
Torsions

Rings

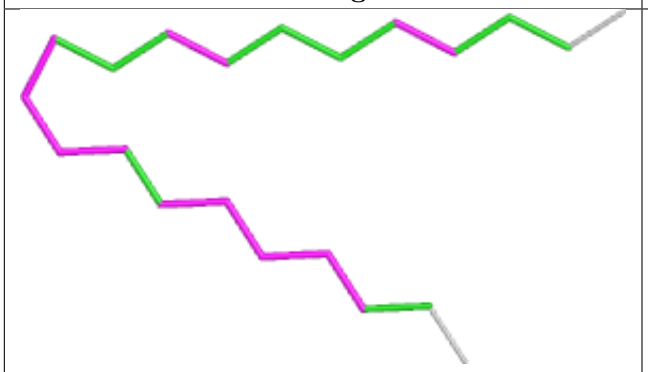
Ligand LMN D 1001



Bond lengths

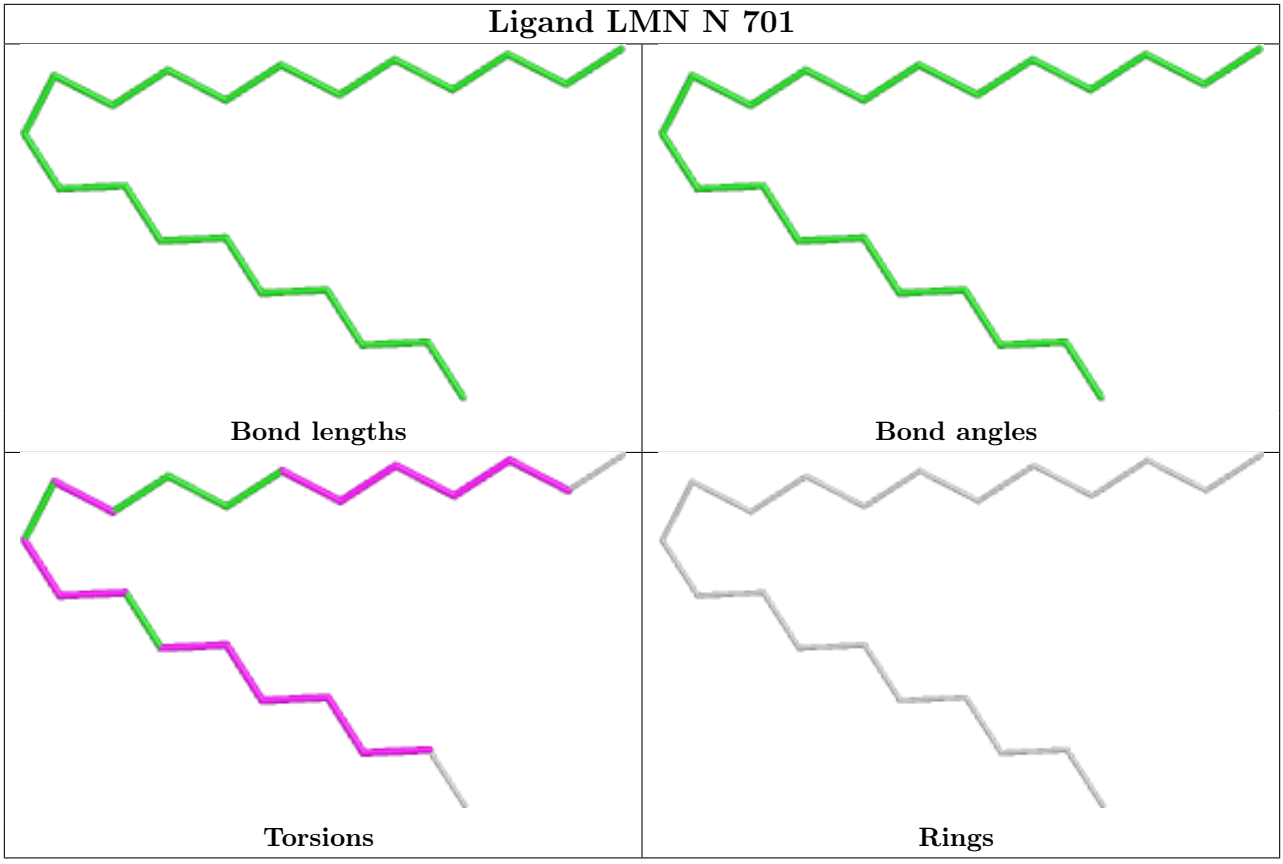


Bond angles



Torsions

Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

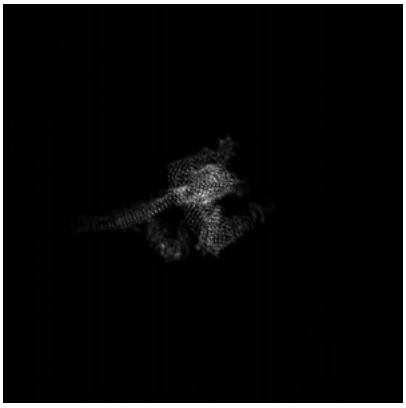
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-79056. These allow visual inspection of the internal detail of the map and identification of artifacts.

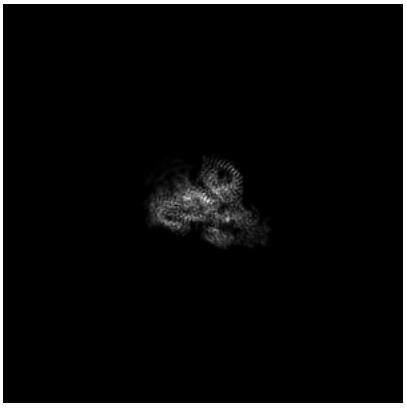
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



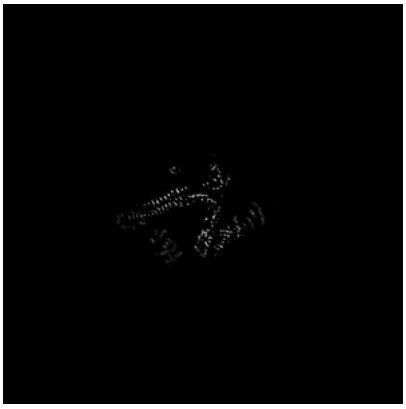
Y

Z

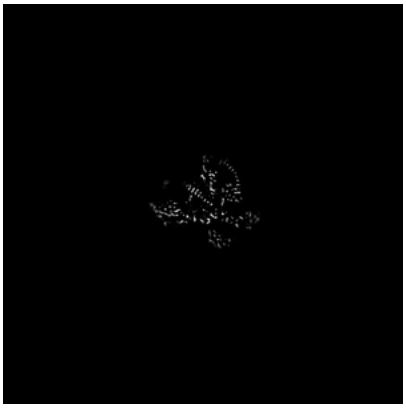
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

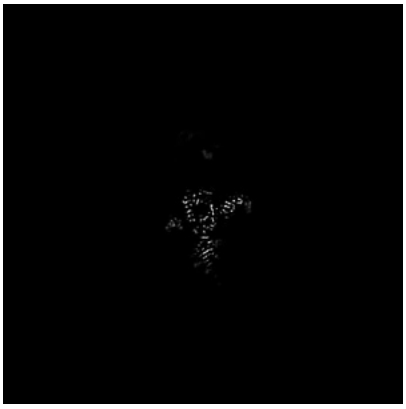
6.2.1 Primary map



X Index: 190



Y Index: 190



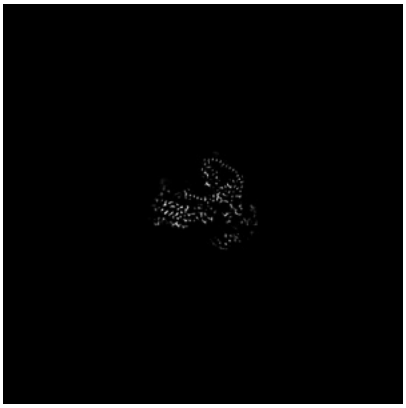
Z Index: 190

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

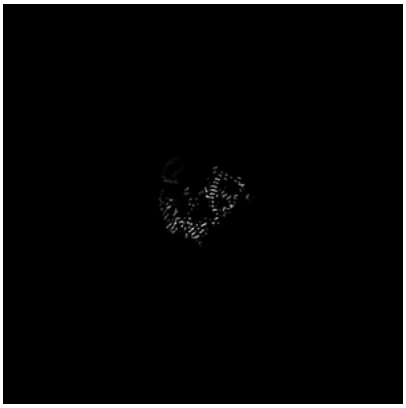
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 176



Y Index: 196

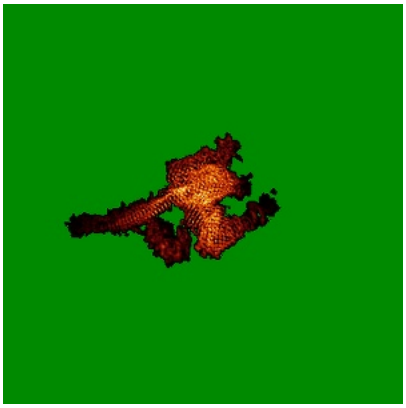


Z Index: 203

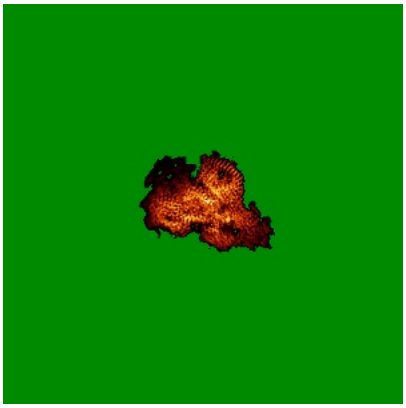
The images above show the largest variance slices of the map in three orthogonal directions.

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

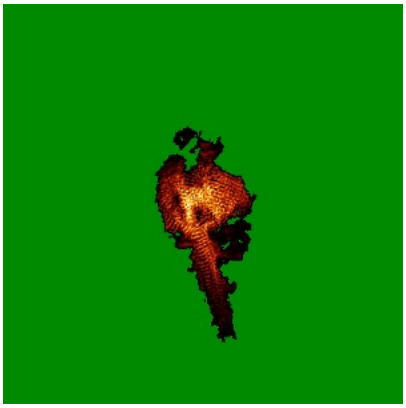
6.4.1 Primary map



X



Y

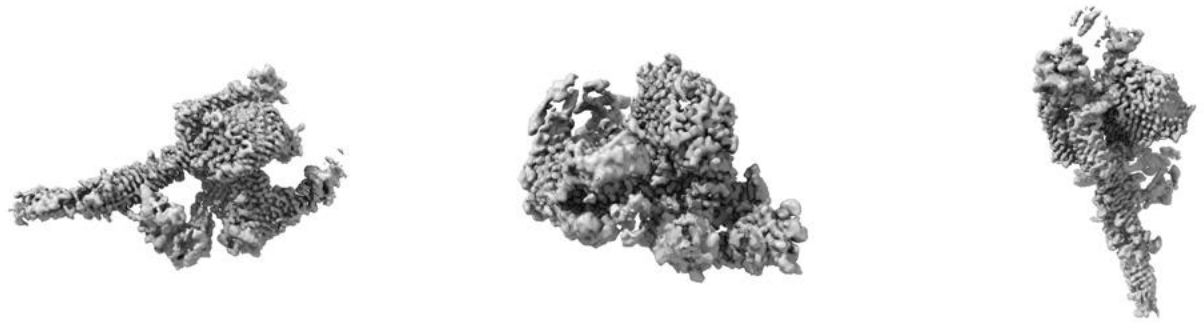


Z

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

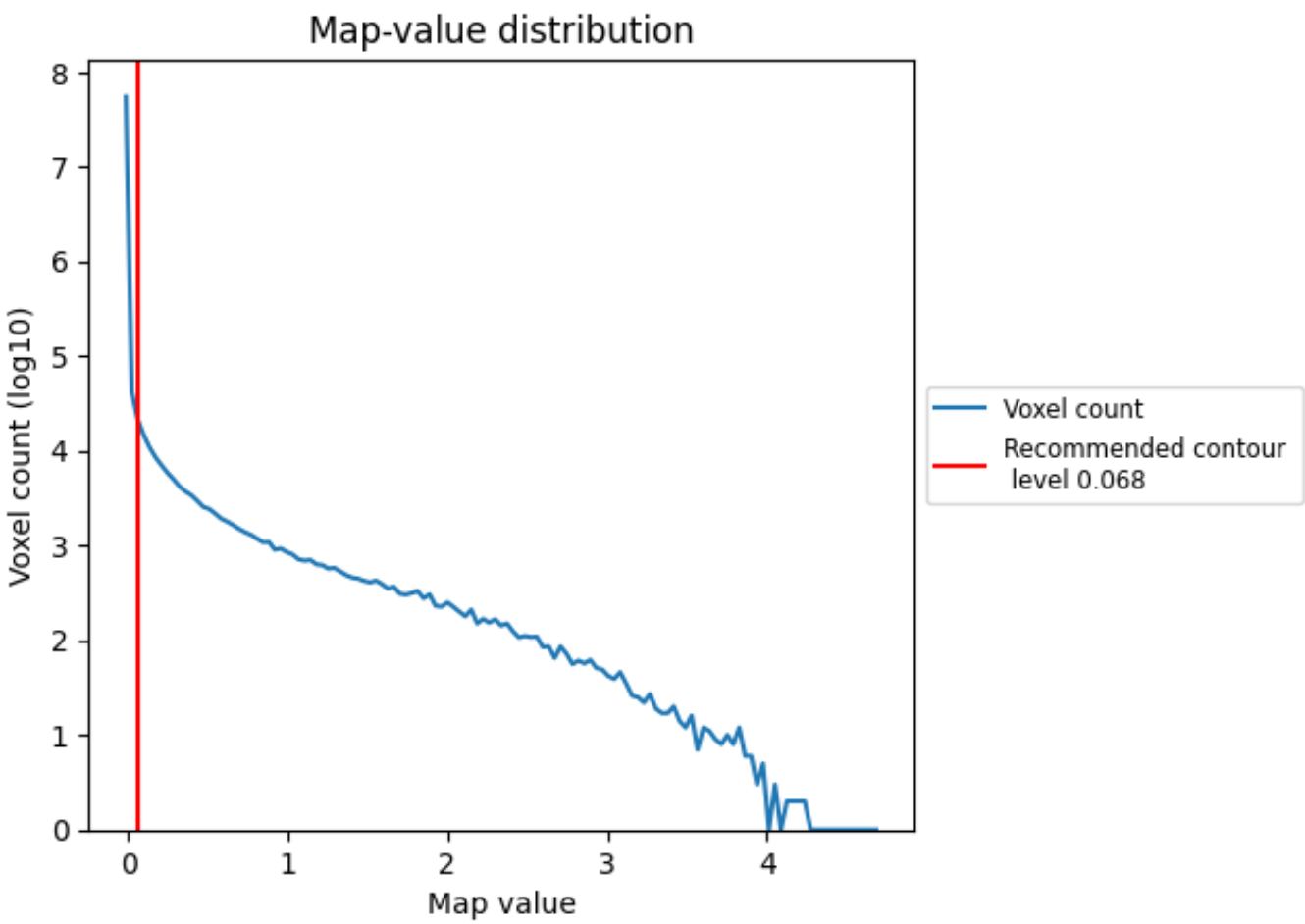
6.6 Mask visualisation (i)

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

7 Map analysis (i)

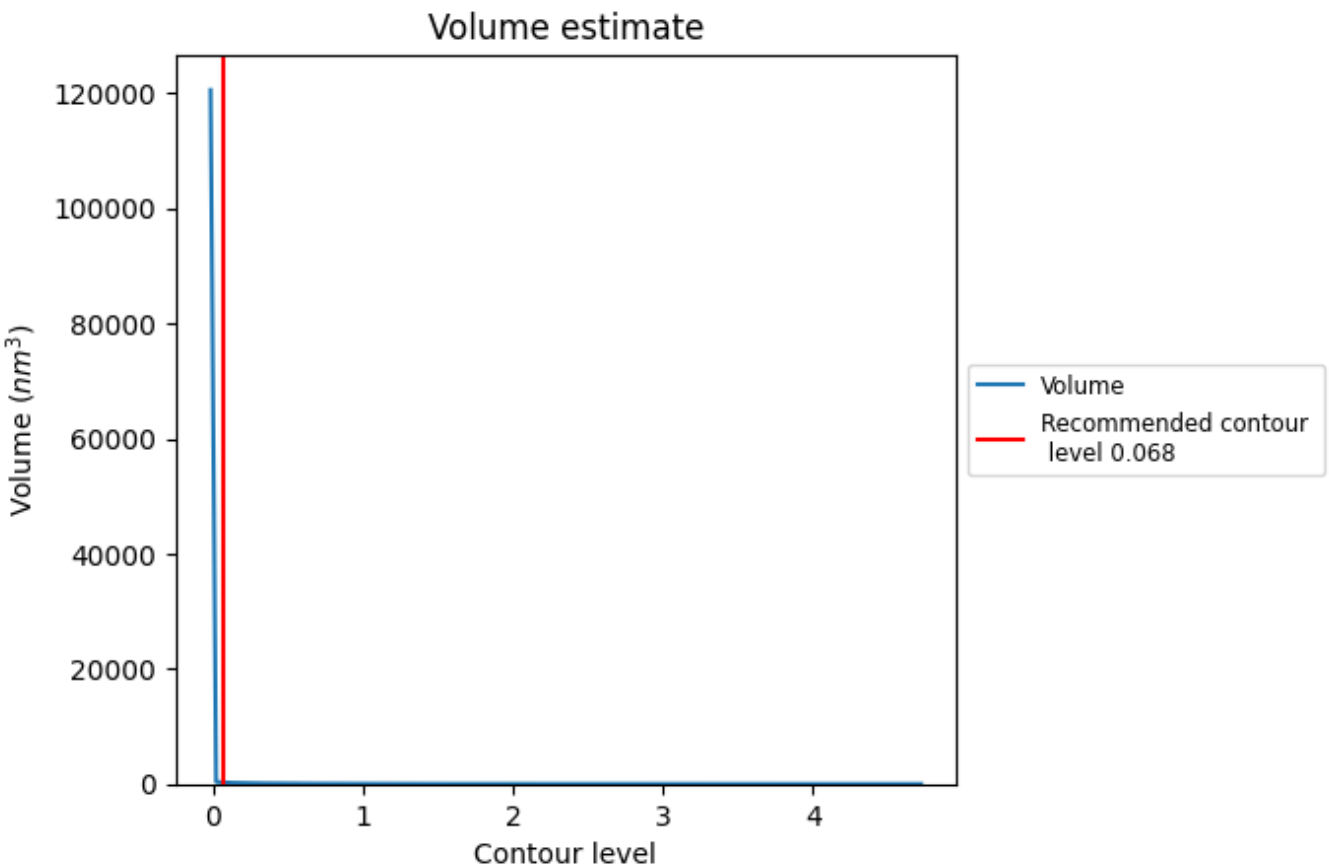
This section contains the results of statistical analysis of the map.

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.

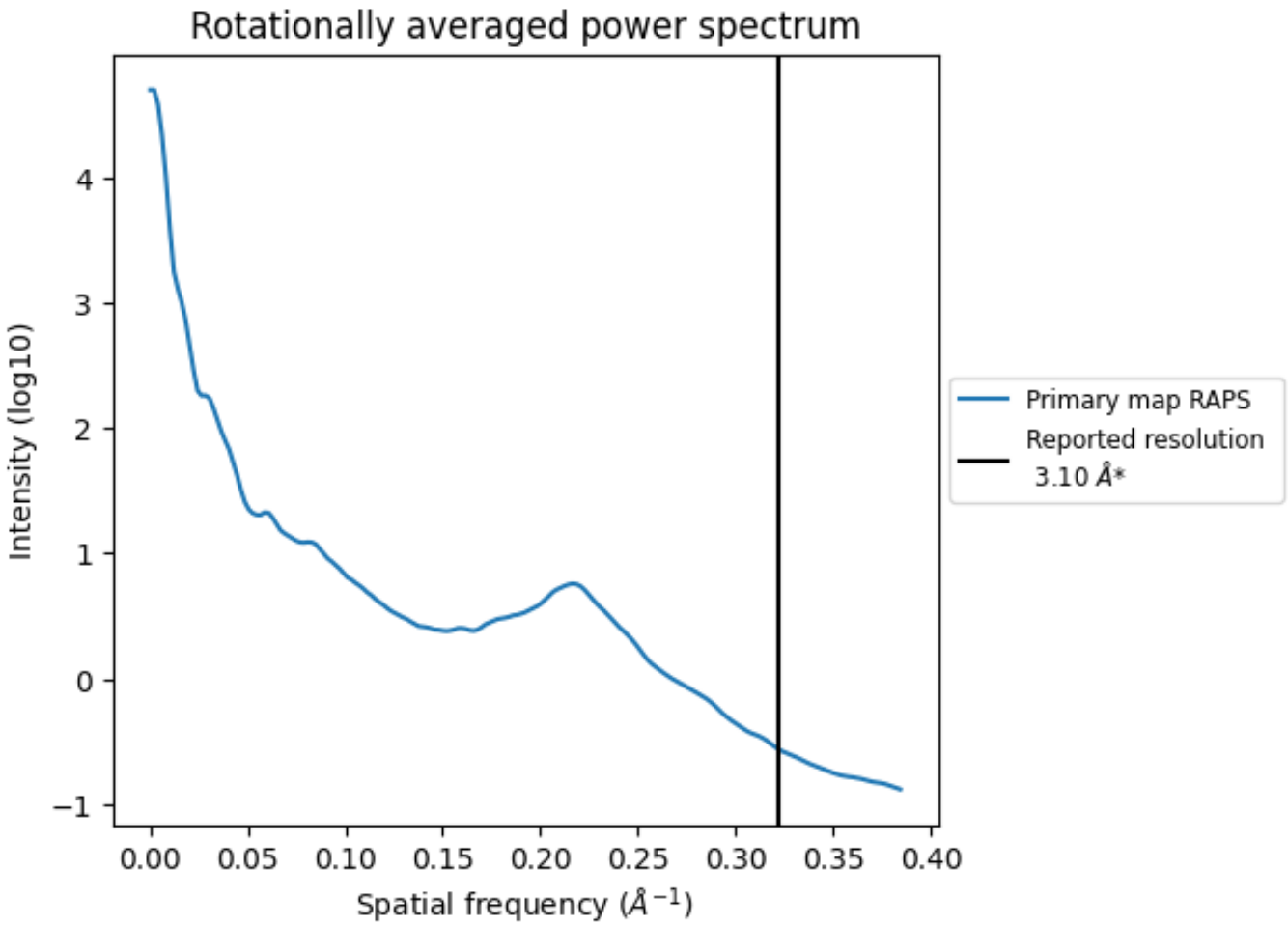
7.2 Volume estimate (i)



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 242 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 0.323 Å^{-1}

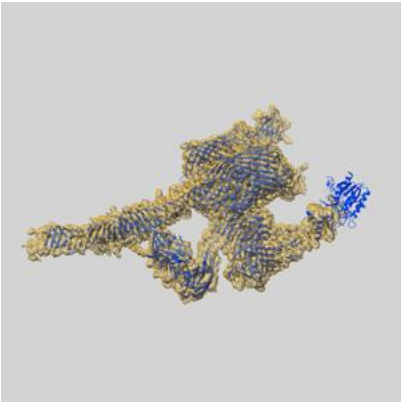
8 Fourier-Shell correlation (i)

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

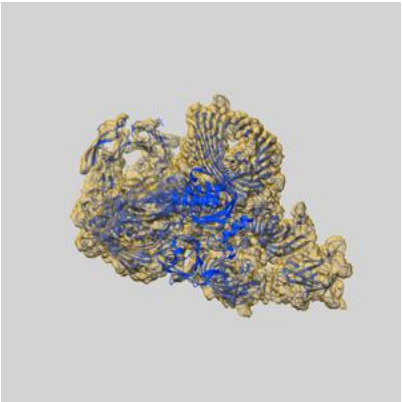
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-79056 and PDB model 38QP. Per-residue inclusion information can be found in section 3 on page 10.

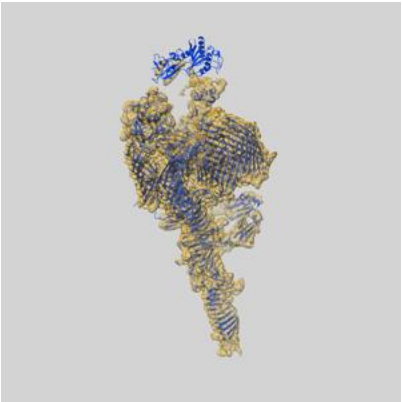
9.1 Map-model overlay (i)



X



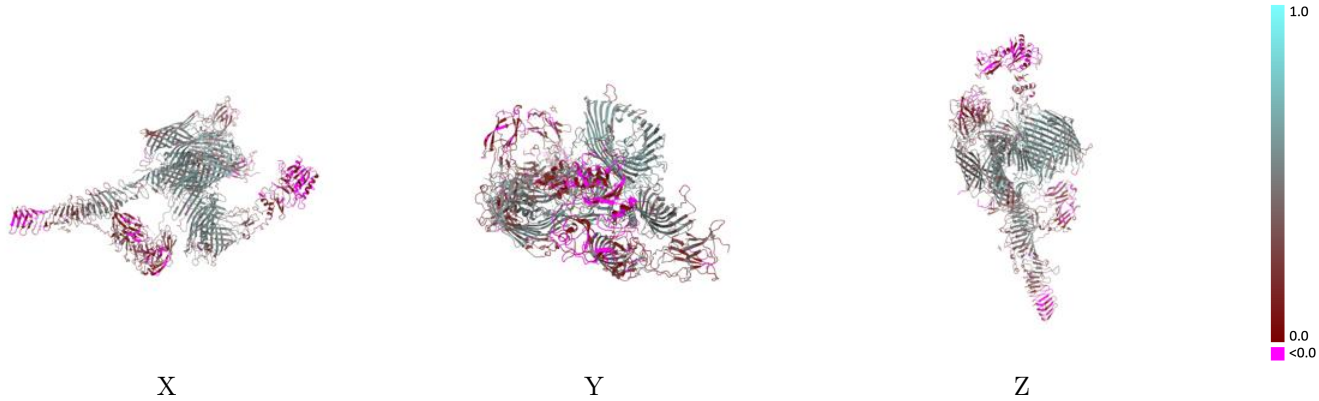
Y



Z

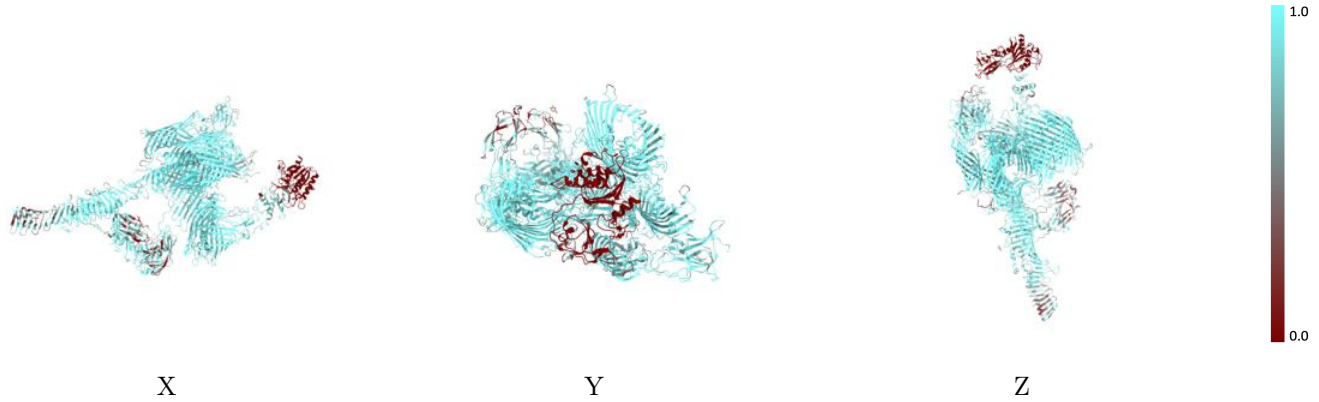
The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



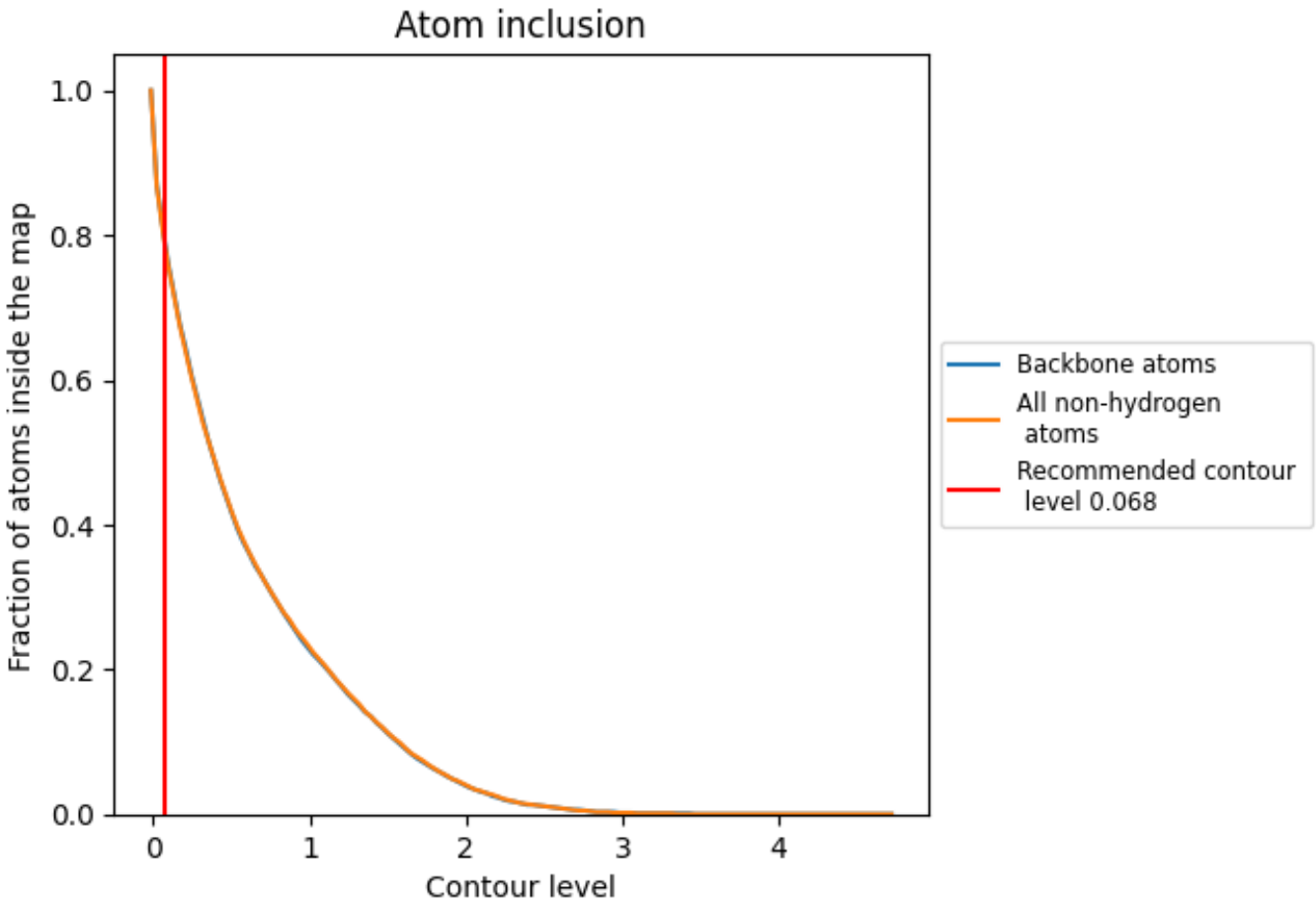
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.068).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.3500
A	0.7640	0.2510
D	0.9260	0.4560
E	0.9590	0.5030
J	0.9050	0.3910
N	0.9440	0.5240
P	0.7330	0.2250
Q	0.9000	0.3970
R1	0.6790	0.1640
R2	0.8240	0.2690
S	0.8570	0.3710
T	0.8260	0.3770
U	0.2310	0.0400
V	0.9110	0.4480