



Full wwPDB EM Validation Report ⓘ

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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 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

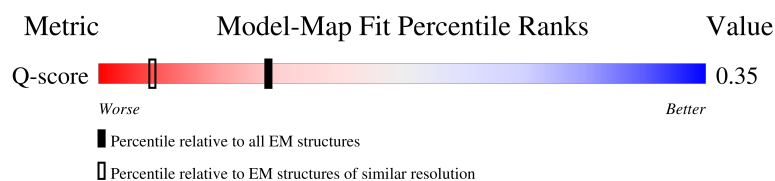
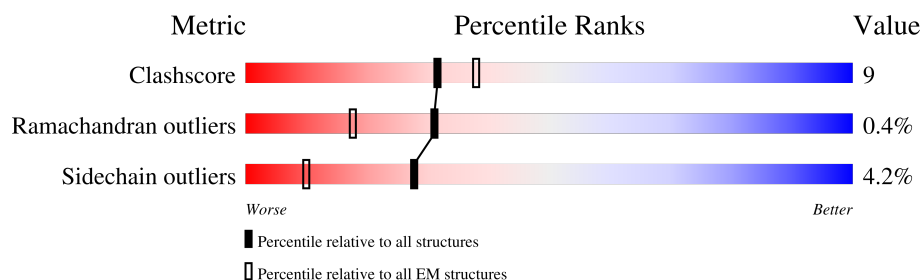
1 Overall quality at a glance i

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.



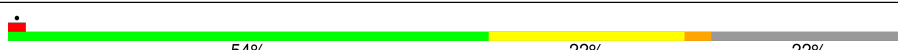
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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	
6	D	934	
7	N	680	
8	P	642	
9	R1	183	
9	R2	183	
10	U	484	
11	J	2	
11	S	2	

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

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
1	A	394	Total	C	H	N	O	S	0	0
			6269	2007	3093	528	619	22		

- Molecule 2 is a protein called Lipopolysaccharide-assembly.

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

- Molecule 3 is a protein called LptQ.

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

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
4	T	140	Total	C	H	N	O	S	0	0
			2272	747	1128	187	207	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	V	215	Total	C	H	N	O	S	0	0
			3335	1081	1648	279	321	6		

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

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

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
7	N	627	Total	C	H	N	O	S	0	0
			10116	3317	4954	879	951	15		

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

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

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

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

- Molecule 10 is a protein called Periplasmic protease.

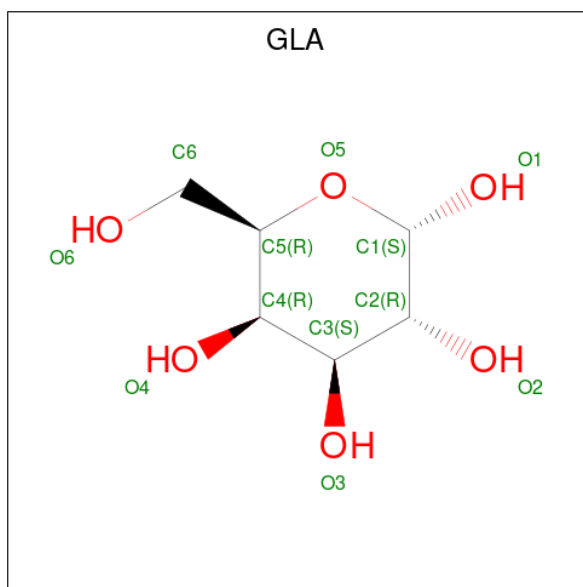
Mol	Chain	Residues	Atoms						AltConf	Trace
10	U	348	Total	C	H	N	O	S	0	0
			5465	1769	2692	444	547	13		

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



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

- Molecule 12 is alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆).



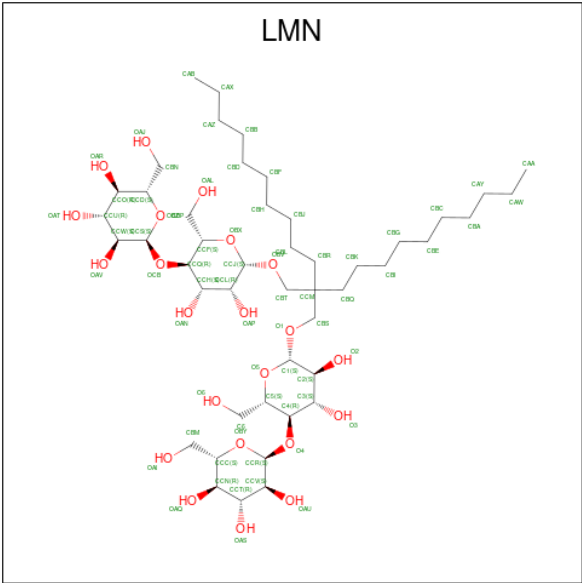
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	H	O	0
			22	6	11	5	
12	A	1	Total	C	H	O	0
			22	6	11	5	
12	A	1	Total	C	H	O	0
			22	6	11	5	
12	A	1	Total	C	H	O	0
			22	6	11	5	
12	D	1	Total	C	H	O	0
			22	6	11	5	
12	D	1	Total	C	H	O	0
			22	6	11	5	
12	P	1	Total	C	H	O	0
			22	6	11	5	
12	P	1	Total	C	H	O	0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

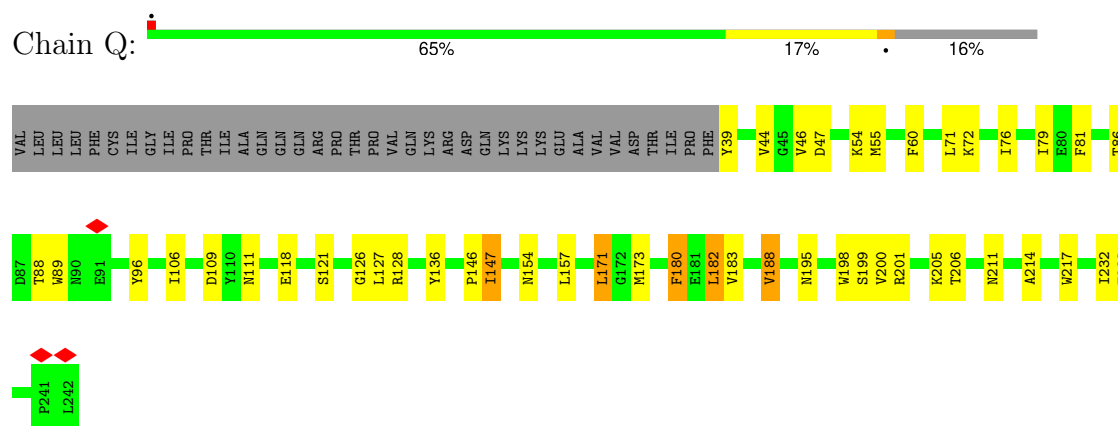
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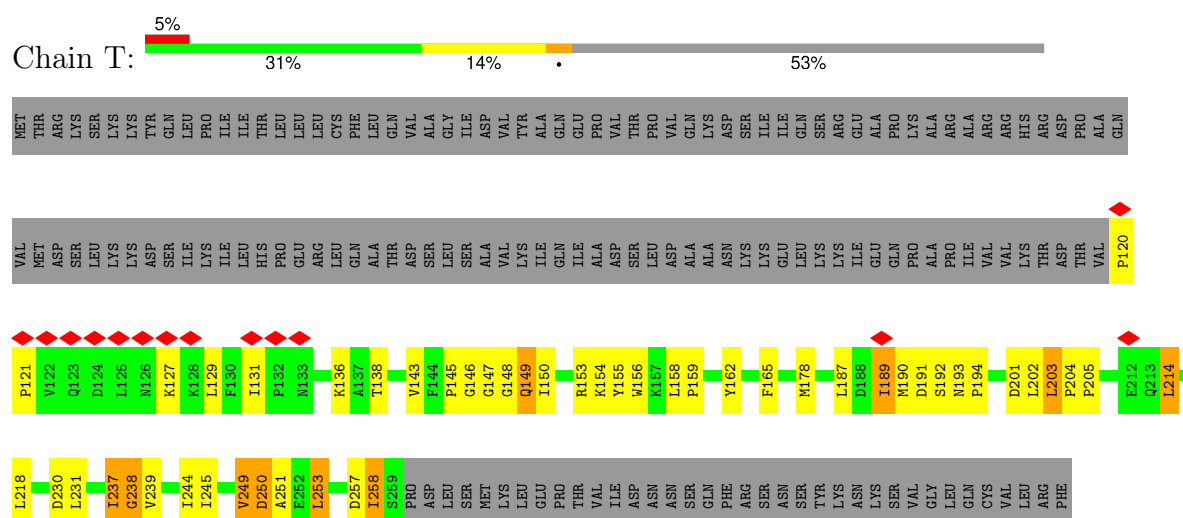
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
12	R2	1	22	6	11	5	0

- Molecule 13 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).

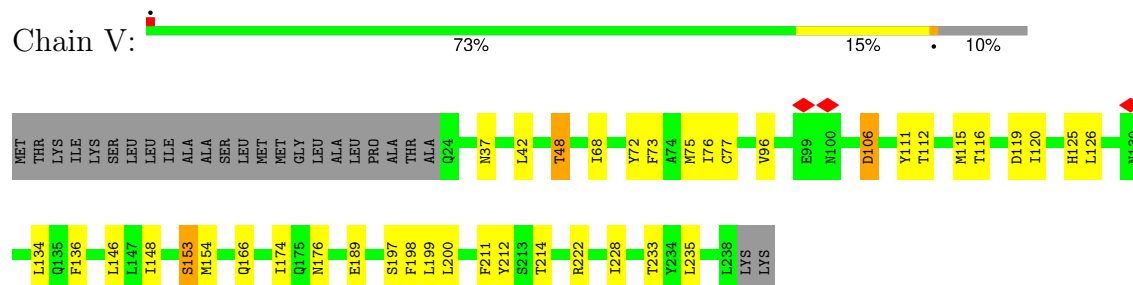




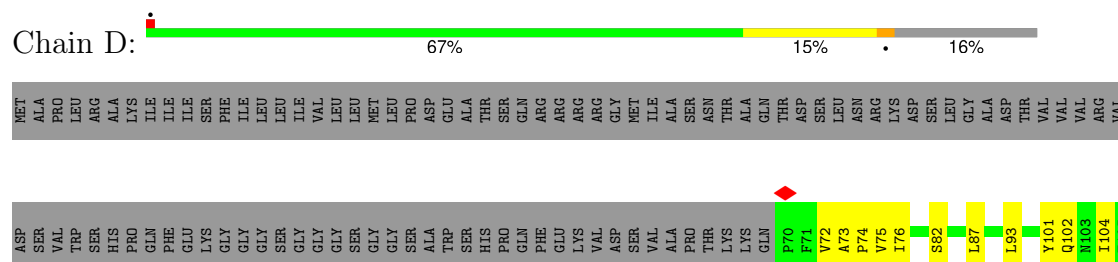
• Molecule 4: DUF5683 domain-containing protein



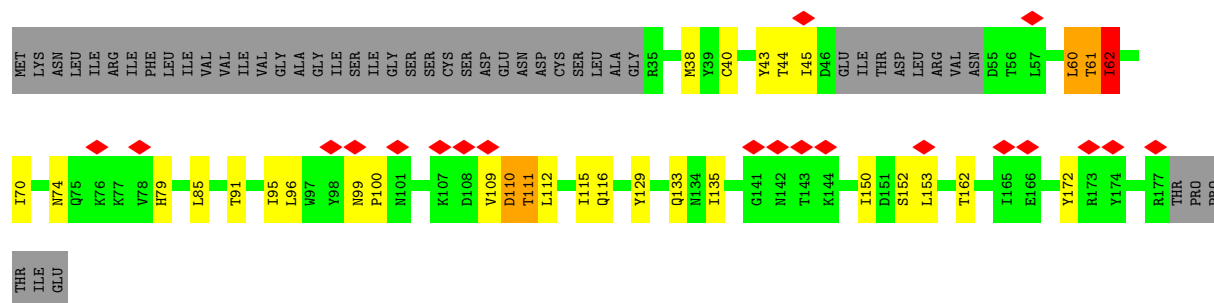
• Molecule 5: Outer membrane protein beta-barrel domain-containing protein



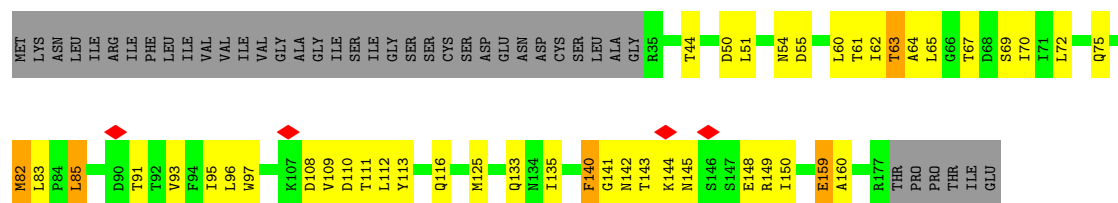
• Molecule 6: LPS-assembly protein LptD central domain-containing protein



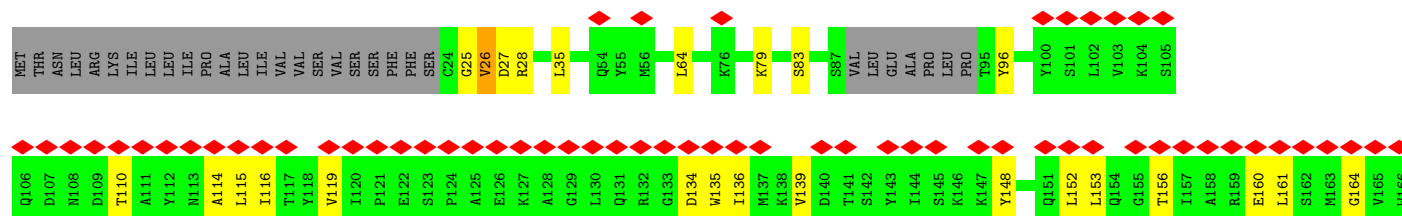
- Molecule 9: Calcium-binding protein P

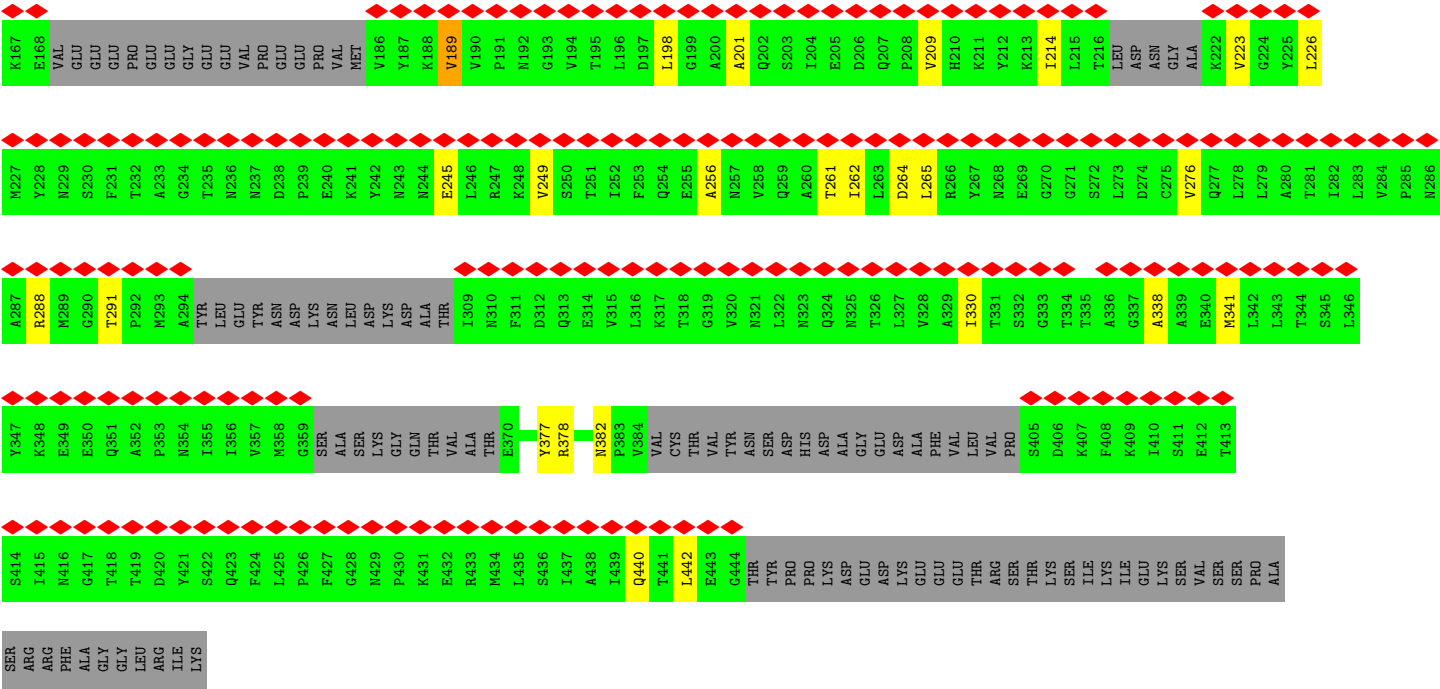


- Molecule 9: Calcium-binding protein P

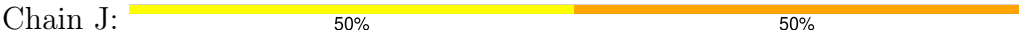


- Molecule 10: Periplasmic protease





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



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



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	228	VAL	Peptide
6	D	419	LEU	Peptide
7	N	81	PRO	Peptide
4	T	237	ILE	Peptide
4	T	249	VAL	Peptide
5	V	48	THR	Peptide

5.2 Too-close contacts

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.

All (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
11:S:1:GLA:O5	11:S:2:RAM:H2	1.82	0.77
6:D:372:LEU:HD23	6:D:895:THR:HG21	1.66	0.77
8:P:173:LEU:HD22	8:P:232:LEU:HD11	1.69	0.74
8:P:147:MET:HE3	8:P:202:PRO:HG3	1.70	0.74
3:Q:173:MET:HE2	3:Q:211:ASN:HB2	1.69	0.74
7:N:568:LEU:HD22	7:N:570:LEU:HD21	1.68	0.73
8:P:59:ASN:O	8:P:140:THR:HG22	1.88	0.73
7:N:627:ILE:HD12	7:N:665:ILE:HD12	1.71	0.72
5:V:96:VAL:HG13	5:V:106:ASP:OD2	1.88	0.72
8:P:146:THR:HG21	12:P:701:GLA:H3	1.70	0.72
1:A:300:ILE:HG21	1:A:316:CYS:CB	2.20	0.71
9:R2:65:LEU:HD22	9:R2:93:VAL:HB	1.72	0.71
3:Q:200:VAL:HG12	3:Q:232:ILE:HD13	1.72	0.70
4:T:145:PRO:HA	4:T:244:ILE:HD11	1.73	0.70
7:N:73:GLN:O	7:N:313:THR:HG21	1.92	0.70
9:R1:38:MET:HB2	9:R1:85:LEU:HD21	1.72	0.70
8:P:308:LEU:HD11	8:P:347:LEU:HD12	1.74	0.69
7:N:209:PHE:HB3	7:N:222:ILE:HG22	1.74	0.69
7:N:108:LEU:HD22	7:N:166:GLU:CG	2.22	0.69
1:A:416:ILE:HG22	1:A:423:ILE:HD13	1.74	0.68
1:A:281:ILE:O	1:A:300:ILE:HG23	1.93	0.68
8:P:181:LEU:HD12	8:P:182:PRO:HD2	1.76	0.68
8:P:45:PRO:HG2	8:P:131:LEU:HD21	1.74	0.68
4:T:202:LEU:O	4:T:202:LEU:HD12	1.92	0.68
6:D:228:VAL:HG12	6:D:229:GLU:H	1.57	0.68
3:Q:121:SER:CB	4:T:143:VAL:HG11	2.24	0.67
1:A:348:THR:HG21	12:A:602:GLA:O2	1.94	0.67
10:U:209:VAL:HG11	10:U:249:VAL:HG21	1.76	0.67
4:T:249:VAL:HG12	4:T:249:VAL:O	1.94	0.67
8:P:236:ARG:NH1	8:P:265:LEU:HD13	2.10	0.67
6:D:783:PRO:HB2	7:N:51:LEU:HD23	1.76	0.67
6:D:822:ASN:O	7:N:51:LEU:HD22	1.95	0.67
1:A:328:THR:HG22	1:A:329:LYS:H	1.60	0.66
6:D:558:MET:HE1	6:D:561:LYS:HB2	1.77	0.66
7:N:447:LEU:HD23	7:N:448:TRP:N	2.11	0.65
6:D:518:GLU:HG2	6:D:519:THR:HG23	1.78	0.65
6:D:899:ILE:HD11	7:N:193:ARG:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R1:91:THR:HG22	9:R1:115:ILE:HD12	1.79	0.65
8:P:264:TYR:C	8:P:265:LEU:HD12	2.22	0.65
7:N:601:ALA:HB3	7:N:622:ILE:HG21	1.78	0.64
8:P:45:PRO:CG	8:P:131:LEU:HD21	2.28	0.64
7:N:209:PHE:CB	7:N:222:ILE:HG22	2.27	0.64
6:D:186:ILE:HG23	6:D:213:VAL:HB	1.80	0.64
1:A:346:GLY:HA3	1:A:371:VAL:HG12	1.80	0.63
1:A:385:LEU:HG	1:A:394:LEU:HD11	1.79	0.63
4:T:249:VAL:HG11	6:D:239:PHE:HB2	1.80	0.63
4:T:150:ILE:HD13	4:T:162:TYR:HE1	1.62	0.63
1:A:462:HIS:C	1:A:463:ILE:HD12	2.24	0.63
1:A:265:ALA:HB3	1:A:287:TYR:CD2	2.33	0.63
3:Q:55:MET:HE2	3:Q:55:MET:HA	1.81	0.63
3:Q:54:LYS:HE3	3:Q:55:MET:HE3	1.81	0.62
7:N:129:MET:HE1	7:N:228:LEU:HD13	1.81	0.62
7:N:447:LEU:HD22	7:N:452:VAL:HG13	1.81	0.62
1:A:364:LEU:HD23	1:A:365:MET:N	2.14	0.62
6:D:195:THR:HG21	6:D:881:ALA:CB	2.29	0.62
7:N:325:SER:HB3	7:N:345:VAL:HG12	1.81	0.62
5:V:42:LEU:HD12	5:V:42:LEU:O	2.00	0.62
3:Q:88:THR:HG21	3:Q:217:TRP:CZ3	2.35	0.62
9:R2:96:LEU:O	9:R2:109:VAL:HA	2.00	0.62
1:A:251:ILE:HG23	1:A:273:LEU:HG	1.81	0.61
7:N:129:MET:HE1	7:N:228:LEU:CD1	2.31	0.61
9:R1:109:VAL:HG13	9:R1:110:ASP:H	1.65	0.61
6:D:164:ILE:C	6:D:165:ILE:HD12	2.25	0.61
5:V:119:ASP:C	5:V:120:ILE:HD12	2.25	0.61
9:R2:82:MET:C	9:R2:83:LEU:HD22	2.25	0.61
9:R2:64:ALA:HB3	9:R2:67:THR:HG21	1.82	0.60
6:D:106:LEU:HD23	6:D:107:ALA:N	2.17	0.60
7:N:580:LEU:HD11	7:N:585:LEU:HD23	1.84	0.60
9:R2:112:LEU:HD12	9:R2:112:LEU:C	2.25	0.60
4:T:145:PRO:CA	4:T:244:ILE:HD11	2.31	0.60
6:D:93:LEU:HD11	6:D:113:MET:HE3	1.84	0.60
3:Q:173:MET:HE1	3:Q:214:ALA:N	2.17	0.60
4:T:257:ASP:O	4:T:258:ILE:HD12	2.01	0.60
8:P:166:LEU:HD22	8:P:212:ASP:HB3	1.84	0.60
8:P:283:LEU:HD12	8:P:297:TYR:O	2.02	0.60
1:A:482:MET:HE2	1:A:482:MET:HA	1.83	0.59
1:A:414:ILE:CG2	1:A:416:ILE:HD11	2.32	0.59
9:R1:133:GLN:HE21	9:R1:135:ILE:HG23	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:308:LEU:HD11	8:P:347:LEU:CD1	2.33	0.58
9:R2:108:ASP:O	9:R2:109:VAL:HG23	2.04	0.58
11:J:1:GLA:H4	11:J:2:RAM:H5	1.84	0.58
1:A:482:MET:C	1:A:518:MET:HE1	2.29	0.58
9:R1:112:LEU:HD13	9:R1:150:ILE:HG21	1.86	0.58
6:D:807:MET:HE1	10:U:28:ARG:NE	2.18	0.57
8:P:352:LEU:HG	8:P:360:LEU:HD12	1.85	0.57
10:U:160:GLU:C	10:U:161:LEU:HD22	2.29	0.57
4:T:245:ILE:O	4:T:249:VAL:HG23	2.04	0.57
10:U:264:ASP:C	10:U:265:LEU:HD12	2.30	0.57
6:D:195:THR:HG21	6:D:881:ALA:HB2	1.85	0.57
5:V:120:ILE:HG22	5:V:120:ILE:O	2.04	0.56
6:D:300:THR:HG22	6:D:312:LEU:O	2.05	0.56
7:N:108:LEU:HD22	7:N:166:GLU:HG2	1.85	0.56
8:P:334:VAL:HG13	8:P:339:LEU:HD23	1.87	0.56
5:V:42:LEU:HD11	5:V:228:ILE:HD12	1.86	0.56
9:R1:96:LEU:HD12	9:R1:150:ILE:HD11	1.86	0.56
4:T:155:TYR:O	4:T:156:TRP:CD1	2.58	0.56
4:T:202:LEU:HD22	4:T:218:LEU:HD21	1.88	0.56
3:Q:47:ASP:CG	3:Q:233:THR:HG23	2.31	0.56
4:T:149:GLN:C	4:T:150:ILE:HD12	2.30	0.56
3:Q:200:VAL:HG12	3:Q:232:ILE:CD1	2.36	0.56
5:V:115:MET:CE	5:V:174:ILE:HD11	2.36	0.56
9:R1:133:GLN:NE2	9:R1:135:ILE:HG23	2.20	0.56
9:R2:60:LEU:HD12	9:R2:97:TRP:O	2.06	0.56
7:N:190:LEU:C	7:N:190:LEU:HD12	2.31	0.56
6:D:829:TRP:NE1	7:N:152:THR:HG21	2.20	0.56
6:D:794:ILE:HG22	6:D:794:ILE:O	2.06	0.55
9:R2:140:PHE:HE1	9:R2:150:ILE:HG23	1.71	0.55
3:Q:128:ARG:NH1	3:Q:183:VAL:HG11	2.21	0.55
9:R2:62:ILE:HG22	9:R2:72:LEU:CB	2.36	0.55
9:R2:91:THR:HG23	9:R2:91:THR:O	2.06	0.55
11:J:1:GLA:H4	11:J:2:RAM:C5	2.36	0.55
4:T:202:LEU:HD13	4:T:214:LEU:HD21	1.87	0.55
1:A:285:LEU:HD23	1:A:296:ALA:HA	1.88	0.55
7:N:445:ILE:HD12	7:N:446:PRO:HD2	1.87	0.55
1:A:328:THR:HG21	12:A:602:GLA:O6	2.07	0.55
4:T:136:LYS:HG3	4:T:253:LEU:HD23	1.89	0.55
6:D:552:MET:HE1	6:D:564:GLN:HG2	1.88	0.55
7:N:447:LEU:HD23	7:N:448:TRP:H	1.70	0.55
2:E:75:ARG:CZ	6:D:489:THR:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:198:TRP:CZ3	3:Q:200:VAL:HG13	2.42	0.54
10:U:35:LEU:H	10:U:35:LEU:HD23	1.73	0.54
5:V:68:ILE:HD12	5:V:76:ILE:HG12	1.90	0.54
8:P:122:ILE:HG13	8:P:131:LEU:HD23	1.89	0.54
8:P:52:PRO:HD2	8:P:64:VAL:HG13	1.89	0.54
1:A:222:LEU:HD12	1:A:223:THR:N	2.23	0.54
9:R1:109:VAL:HG13	9:R1:110:ASP:N	2.23	0.54
6:D:568:VAL:HG23	6:D:569:VAL:N	2.23	0.54
9:R1:43:TYR:CG	9:R1:43:TYR:O	2.61	0.54
7:N:336:THR:C	7:N:337:LEU:HD12	2.33	0.54
7:N:152:THR:HG23	7:N:678:PHE:HB2	1.90	0.53
7:N:190:LEU:HD12	7:N:191:TYR:N	2.23	0.53
8:P:166:LEU:CD1	8:P:211:MET:HE2	2.37	0.53
8:P:159:LEU:HD11	8:P:582:VAL:CG1	2.38	0.53
5:V:48:THR:HG22	5:V:222:ARG:HB3	1.91	0.53
8:P:165:ILE:HA	8:P:211:MET:HE3	1.91	0.53
9:R2:65:LEU:HD23	9:R2:65:LEU:O	2.08	0.53
6:D:301:ASN:OD1	6:D:311:THR:HG22	2.08	0.53
6:D:829:TRP:HE1	7:N:152:THR:HG21	1.73	0.53
6:D:780:PHE:CZ	6:D:782:MET:HE2	2.43	0.53
1:A:333:ALA:C	1:A:334:ILE:HD12	2.34	0.52
8:P:181:LEU:HD12	8:P:182:PRO:CD	2.40	0.52
3:Q:205:LYS:O	3:Q:206:THR:HG23	2.10	0.52
8:P:283:LEU:HD11	8:P:296:PHE:HB3	1.90	0.52
7:N:564:PRO:O	7:N:565:LEU:HD12	2.10	0.52
1:A:414:ILE:HG22	1:A:416:ILE:HD11	1.91	0.52
6:D:526:LEU:HD12	6:D:528:ASP:H	1.74	0.52
3:Q:171:LEU:HD22	3:Q:171:LEU:N	2.25	0.51
6:D:419:LEU:O	6:D:420:PRO:C	2.53	0.51
8:P:85:PRO:N	8:P:86:PRO:HA	2.25	0.51
3:Q:60:PHE:H	3:Q:86:THR:HG22	1.76	0.51
3:Q:198:TRP:HZ3	3:Q:200:VAL:HG13	1.76	0.51
5:V:68:ILE:HG21	5:V:76:ILE:HD11	1.93	0.51
5:V:75:MET:CE	5:V:126:LEU:HD22	2.41	0.51
8:P:236:ARG:HH12	8:P:265:LEU:HD13	1.75	0.51
10:U:139:VAL:HG11	10:U:152:LEU:CB	2.40	0.51
1:A:310:MET:O	1:A:311:LEU:HD22	2.11	0.51
4:T:143:VAL:O	4:T:143:VAL:HG12	2.11	0.51
6:D:543:LEU:HD23	6:D:544:SER:N	2.25	0.51
7:N:337:LEU:O	7:N:338:LEU:HD12	2.10	0.51
10:U:139:VAL:HG11	10:U:152:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:79:ILE:HG13	3:Q:106:ILE:HD12	1.92	0.51
3:Q:157:LEU:HD21	9:R1:129:TYR:CG	2.46	0.51
8:P:286:SER:OG	8:P:367:LEU:HD21	2.10	0.51
8:P:147:MET:HE3	8:P:202:PRO:CG	2.40	0.51
9:R1:91:THR:HG22	9:R1:115:ILE:CD1	2.39	0.51
9:R2:44:THR:HG23	9:R2:55:ASP:CG	2.36	0.51
6:D:508:THR:O	6:D:509:ARG:C	2.53	0.50
7:N:212:TYR:HB3	7:N:219:VAL:HG12	1.93	0.50
10:U:338:ALA:HA	10:U:341:MET:HE2	1.93	0.50
1:A:565:PRO:O	1:A:566:LYS:C	2.55	0.50
6:D:233:LEU:HB3	6:D:235:LEU:HD12	1.93	0.50
6:D:419:LEU:HD12	6:D:420:PRO:HD3	1.93	0.50
9:R2:140:PHE:CE1	9:R2:150:ILE:HG23	2.46	0.50
6:D:419:LEU:HB3	6:D:420:PRO:CD	2.41	0.50
7:N:129:MET:HE3	7:N:273:ASP:CG	2.36	0.50
4:T:250:ASP:O	4:T:251:ALA:HB3	2.11	0.50
3:Q:79:ILE:N	3:Q:79:ILE:HD12	2.26	0.50
4:T:129:LEU:HD12	4:T:154:LYS:HD3	1.94	0.50
8:P:159:LEU:HD11	8:P:582:VAL:HG13	1.93	0.50
3:Q:88:THR:HG21	3:Q:217:TRP:HZ3	1.77	0.50
6:D:490:LEU:HD23	6:D:496:VAL:HG21	1.94	0.50
3:Q:188:VAL:CG1	4:T:143:VAL:HG12	2.41	0.50
6:D:228:VAL:HG11	13:D:1002:LMN:HBAA	1.93	0.50
6:D:543:LEU:HD23	6:D:543:LEU:C	2.37	0.50
6:D:625:LEU:HD13	6:D:643:ILE:HD11	1.92	0.50
8:P:162:ILE:HD12	8:P:162:ILE:N	2.27	0.50
11:S:1:GLA:C1	11:S:2:RAM:H2	2.41	0.50
6:D:429:LEU:HD23	6:D:449:VAL:O	2.12	0.50
9:R1:99:ASN:HB3	9:R1:100:PRO:HD3	1.94	0.50
10:U:214:ILE:HD13	10:U:256:ALA:HB2	1.94	0.50
6:D:109:GLU:OE1	6:D:125:ILE:HG23	2.13	0.49
6:D:419:LEU:HB3	6:D:420:PRO:HD2	1.94	0.49
8:P:420:SER:O	8:P:421:LEU:HD22	2.11	0.49
2:E:75:ARG:NH2	6:D:489:THR:HG23	2.27	0.49
3:Q:39:TYR:N	3:Q:72:LYS:HZ2	2.10	0.49
7:N:409:LEU:C	7:N:409:LEU:HD23	2.37	0.49
8:P:231:SER:HB3	12:P:703:GLA:O2	2.12	0.49
10:U:214:ILE:HD13	10:U:256:ALA:CB	2.42	0.49
5:V:197:SER:O	5:V:199:LEU:HD12	2.13	0.49
1:A:244:ILE:HG13	1:A:244:ILE:O	2.13	0.49
1:A:371:VAL:HG22	1:A:382:CYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:HG2	1:A:465:VAL:HG22	1.94	0.49
8:P:83:VAL:HG12	8:P:116:ILE:HG23	1.94	0.49
6:D:147:THR:HB	6:D:161:ILE:HG23	1.95	0.49
9:R1:61:THR:C	9:R1:62:ILE:HG23	2.38	0.49
7:N:452:VAL:HG12	7:N:497:ILE:HG12	1.93	0.49
4:T:189:ILE:C	4:T:190:MET:HE2	2.38	0.49
10:U:152:LEU:HD12	10:U:153:LEU:HB2	1.95	0.49
5:V:200:LEU:C	5:V:200:LEU:HD23	2.38	0.49
10:U:262:ILE:HD11	10:U:442:LEU:CD1	2.43	0.49
1:A:215:LEU:HD21	1:A:222:LEU:HD23	1.95	0.48
5:V:111:TYR:HB2	5:V:154:MET:HE1	1.95	0.48
6:D:526:LEU:HD12	6:D:527:ASN:N	2.28	0.48
6:D:856:HIS:CE1	6:D:857:CYS:SG	3.05	0.48
8:P:83:VAL:HG12	8:P:116:ILE:HD12	1.95	0.48
8:P:420:SER:C	8:P:421:LEU:HD22	2.38	0.48
8:P:483:THR:HG22	8:P:483:THR:O	2.12	0.48
6:D:873:TYR:OH	13:D:1001:LMN:HAAB	2.13	0.48
4:T:136:LYS:CG	4:T:253:LEU:HD23	2.43	0.48
8:P:523:PHE:O	8:P:558:LEU:HD12	2.13	0.48
6:D:195:THR:HG22	6:D:195:THR:O	2.12	0.48
6:D:565:ILE:HG22	6:D:627:MET:CB	2.44	0.48
1:A:367:ALA:O	1:A:371:VAL:HG11	2.13	0.48
10:U:209:VAL:HG13	10:U:226:LEU:HD11	1.95	0.48
6:D:467:PHE:O	6:D:468:LYS:C	2.56	0.48
8:P:108:LEU:HB3	8:P:140:THR:HG21	1.96	0.48
8:P:186:VAL:HG21	8:P:217:PHE:CD2	2.49	0.48
9:R2:50:ASP:O	9:R2:51:LEU:HD23	2.13	0.48
9:R2:85:LEU:HD22	9:R2:116:GLN:HG2	1.96	0.48
5:V:72:TYR:O	5:V:73:PHE:C	2.57	0.48
6:D:864:LEU:HD23	6:D:864:LEU:H	1.78	0.48
8:P:66:LEU:HB2	8:P:100:ILE:HG23	1.94	0.48
7:N:108:LEU:CD2	7:N:190:LEU:HD13	2.31	0.47
8:P:451:GLU:O	8:P:464:LEU:HD12	2.14	0.47
8:P:559:ILE:N	8:P:559:ILE:HD12	2.30	0.47
4:T:129:LEU:HD23	4:T:129:LEU:O	2.14	0.47
6:D:859:ASN:O	6:D:877:ILE:HD12	2.14	0.47
6:D:164:ILE:HD13	6:D:186:ILE:HD11	1.97	0.47
6:D:364:TYR:O	6:D:368:ASN:HB2	2.14	0.47
6:D:637:LEU:HD22	6:D:637:LEU:H	1.79	0.47
7:N:116:ILE:HD12	7:N:553:ILE:HG21	1.96	0.47
10:U:377:TYR:O	10:U:378:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:862:ALA:HB2	6:D:875:VAL:HG22	1.95	0.47
4:T:202:LEU:C	4:T:203:LEU:HD22	2.39	0.47
6:D:388:SER:HB2	6:D:403:THR:HG22	1.97	0.47
6:D:802:ILE:HD11	6:D:807:MET:HB3	1.96	0.47
7:N:636:LEU:HD12	7:N:637:LYS:HG2	1.95	0.47
8:P:159:LEU:N	8:P:159:LEU:HD12	2.30	0.47
8:P:435:ILE:HD11	8:P:485:PHE:CE1	2.50	0.47
10:U:25:GLY:O	10:U:26:VAL:O	2.32	0.47
10:U:245:GLU:O	10:U:249:VAL:HG23	2.15	0.47
10:U:262:ILE:HG23	10:U:330:ILE:HD11	1.96	0.47
1:A:245:VAL:HA	1:A:250:HIS:HA	1.97	0.47
6:D:508:THR:HG22	6:D:509:ARG:H	1.79	0.47
7:N:95:THR:O	7:N:95:THR:HG22	2.15	0.47
4:T:257:ASP:C	4:T:258:ILE:HD12	2.40	0.47
6:D:288:ILE:HG23	6:D:288:ILE:O	2.14	0.47
7:N:129:MET:HE3	7:N:273:ASP:OD1	2.14	0.47
10:U:116:ILE:HG23	10:U:116:ILE:O	2.14	0.47
6:D:195:THR:HG21	6:D:881:ALA:HB1	1.96	0.47
6:D:855:LEU:O	6:D:858:PHE:O	2.32	0.47
8:P:353:TYR:C	8:P:360:LEU:HD13	2.40	0.47
8:P:526:LEU:HD21	8:P:554:TYR:CD1	2.49	0.47
1:A:334:ILE:HD12	1:A:334:ILE:N	2.30	0.46
3:Q:76:ILE:HD12	3:Q:109:ASP:O	2.15	0.46
4:T:129:LEU:HG	4:T:153:ARG:HB2	1.97	0.46
6:D:338:VAL:HG23	6:D:338:VAL:O	2.14	0.46
7:N:108:LEU:HD22	7:N:166:GLU:HG3	1.95	0.46
8:P:153:VAL:HG12	8:P:162:ILE:HD13	1.96	0.46
1:A:383:ASP:OD1	1:A:398:THR:HG21	2.15	0.46
9:R2:62:ILE:HG22	9:R2:72:LEU:HB3	1.96	0.46
1:A:300:ILE:HD13	1:A:316:CYS:HB2	1.98	0.46
1:A:386:VAL:O	1:A:386:VAL:HG23	2.15	0.46
4:T:193:ASN:N	4:T:194:PRO:HD3	2.30	0.46
4:T:201:ASP:O	4:T:202:LEU:HG	2.15	0.46
7:N:562:VAL:O	7:N:562:VAL:HG12	2.16	0.46
2:E:55:TYR:CZ	2:E:57:PRO:HG2	2.50	0.46
2:E:114:LEU:HD21	2:E:148:LEU:CD1	2.46	0.46
10:U:262:ILE:HD12	10:U:262:ILE:N	2.30	0.46
6:D:698:VAL:HG22	6:D:699:GLU:N	2.31	0.46
7:N:488:ARG:HG3	7:N:511:ILE:HG22	1.96	0.46
1:A:193:LEU:HD11	1:A:213:VAL:CG1	2.45	0.46
5:V:115:MET:HE2	5:V:174:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:MET:HG3	6:D:87:LEU:HD11	1.97	0.46
2:E:118:VAL:HG22	2:E:119:ASN:H	1.80	0.46
3:Q:88:THR:HG23	3:Q:96:TYR:HB3	1.98	0.46
5:V:112:THR:HG22	5:V:153:SER:HB2	1.97	0.46
6:D:76:ILE:HD12	6:D:76:ILE:N	2.31	0.46
6:D:228:VAL:O	6:D:230:ASP:N	2.49	0.46
8:P:130:PRO:C	8:P:131:LEU:HD22	2.41	0.46
9:R1:162:THR:O	9:R1:162:THR:HG22	2.16	0.46
1:A:410:LEU:HD23	1:A:410:LEU:C	2.41	0.45
3:Q:154:ASN:HB2	3:Q:157:LEU:HD12	1.98	0.45
5:V:112:THR:HG23	5:V:112:THR:O	2.15	0.45
6:D:104:ILE:HG23	6:D:138:PHE:CE1	2.51	0.45
1:A:216:VAL:HG23	1:A:221:VAL:HG22	1.97	0.45
10:U:291:THR:O	10:U:291:THR:HG23	2.16	0.45
1:A:258:TYR:CD1	1:A:265:ALA:HB2	2.51	0.45
7:N:569:SER:C	7:N:570:LEU:HD23	2.42	0.45
8:P:131:LEU:HD22	8:P:131:LEU:N	2.30	0.45
2:E:75:ARG:O	2:E:76:LEU:HD23	2.17	0.45
1:A:400:PRO:HG2	1:A:414:ILE:HG12	1.98	0.45
2:E:41:THR:HG23	2:E:86:ASP:H	1.82	0.45
5:V:199:LEU:HD13	5:V:235:LEU:CD1	2.46	0.45
10:U:83:SER:HA	10:U:382:ASN:O	2.16	0.45
9:R2:110:ASP:OD2	9:R2:150:ILE:HG21	2.17	0.45
4:T:145:PRO:C	4:T:147:GLY:N	2.73	0.45
4:T:178:MET:HE2	4:T:178:MET:HA	1.99	0.45
8:P:166:LEU:N	8:P:166:LEU:HD12	2.32	0.45
8:P:186:VAL:HG12	8:P:187:ALA:N	2.32	0.45
6:D:122:ALA:HB3	6:D:150:ILE:HG23	1.98	0.45
8:P:185:ARG:HD2	8:P:200:VAL:HG12	1.98	0.45
3:Q:180:PHE:CZ	3:Q:182:LEU:HD11	2.52	0.45
13:D:1002:LMN:HBCA	7:N:639:THR:HG21	1.99	0.45
1:A:281:ILE:HG22	1:A:282:GLY:N	2.32	0.45
6:D:728:THR:O	6:D:728:THR:HG22	2.16	0.45
8:P:114:TYR:HE2	8:P:140:THR:HG23	1.82	0.45
4:T:230:ASP:OD2	6:D:290:THR:HG21	2.17	0.44
6:D:579:PRO:O	6:D:613:GLY:HA2	2.17	0.44
1:A:537:VAL:HG12	1:A:537:VAL:O	2.16	0.44
3:Q:126:GLY:C	3:Q:127:LEU:HD22	2.42	0.44
5:V:96:VAL:HG22	5:V:106:ASP:OD1	2.16	0.44
6:D:568:VAL:C	6:D:569:VAL:HG13	2.43	0.44
2:E:71:ILE:HD11	2:E:78:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:104:ILE:HG23	6:D:138:PHE:HE1	1.82	0.44
1:A:423:ILE:HD11	1:A:425:TRP:O	2.17	0.44
4:T:129:LEU:HG	4:T:153:ARG:CB	2.48	0.44
1:A:348:THR:HB	12:A:602:GLA:H5	1.98	0.44
6:D:101:TYR:O	6:D:102:GLN:C	2.60	0.44
7:N:552:VAL:HG12	7:N:570:LEU:HD22	1.99	0.44
1:A:331:ALA:HB3	1:A:349:LEU:HD13	2.00	0.44
4:T:155:TYR:O	4:T:156:TRP:CG	2.71	0.44
8:P:308:LEU:HD13	8:P:349:LEU:HD13	1.99	0.44
8:P:338:LEU:HD13	8:P:341:LYS:HD2	1.99	0.44
10:U:96:TYR:CG	10:U:198:LEU:HD21	2.52	0.44
10:U:114:ALA:HB3	10:U:136:ILE:HB	2.00	0.44
5:V:116:THR:HG23	5:V:116:THR:O	2.17	0.44
7:N:646:TYR:O	7:N:668:ARG:HA	2.18	0.44
8:P:104:LEU:HD12	8:P:108:LEU:HD11	2.00	0.44
9:R2:109:VAL:HG11	11:S:1:GLA:O6	2.17	0.44
4:T:250:ASP:O	4:T:251:ALA:CB	2.65	0.44
6:D:73:ALA:HB1	6:D:74:PRO:CD	2.40	0.44
6:D:379:THR:HG23	6:D:379:THR:O	2.18	0.44
10:U:116:ILE:HG22	10:U:134:ASP:O	2.18	0.44
11:S:1:GLA:H2	11:S:2:RAM:C1	2.48	0.44
6:D:489:THR:HG22	6:D:491:PHE:O	2.18	0.43
10:U:262:ILE:CG2	10:U:330:ILE:HD11	2.48	0.43
6:D:671:LYS:O	6:D:672:LEU:C	2.61	0.43
7:N:337:LEU:C	7:N:338:LEU:HD12	2.44	0.43
4:T:138:THR:O	4:T:138:THR:HG22	2.17	0.43
6:D:72:VAL:HB	6:D:101:TYR:CE1	2.54	0.43
9:R1:70:ILE:HD12	9:R1:70:ILE:N	2.33	0.43
10:U:64:LEU:H	10:U:64:LEU:HD23	1.83	0.43
1:A:324:SER:HB2	12:A:603:GLA:O2	2.18	0.43
2:E:58:LEU:CD2	2:E:93:ILE:HD13	2.48	0.43
3:Q:44:VAL:HG23	3:Q:44:VAL:O	2.18	0.43
7:N:228:LEU:N	7:N:228:LEU:HD12	2.33	0.43
4:T:204:PRO:N	4:T:205:PRO:HD2	2.33	0.43
9:R2:96:LEU:N	9:R2:96:LEU:HD12	2.33	0.43
1:A:315:TYR:O	1:A:327:ALA:HA	2.18	0.43
1:A:403:TRP:CG	1:A:538:ARG:HE	2.37	0.43
4:T:129:LEU:HB2	4:T:154:LYS:HD3	2.01	0.43
4:T:136:LYS:CD	4:T:253:LEU:HD23	2.49	0.43
6:D:228:VAL:O	6:D:229:GLU:C	2.61	0.43
6:D:565:ILE:HG22	6:D:627:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:625:LEU:CB	6:D:642:LEU:HD11	2.49	0.43
9:R2:72:LEU:HD11	9:R2:75:GLN:HB2	1.99	0.43
9:R2:93:VAL:HG22	9:R2:113:TYR:CD1	2.54	0.43
9:R2:159:GLU:O	9:R2:160:ALA:HB2	2.19	0.43
10:U:115:LEU:N	10:U:115:LEU:HD22	2.33	0.43
1:A:495:LEU:N	1:A:495:LEU:HD12	2.33	0.43
4:T:165:PHE:CE1	4:T:239:VAL:HG13	2.54	0.43
6:D:106:LEU:HD23	6:D:106:LEU:C	2.44	0.43
6:D:346:LYS:HE3	8:P:125:ASN:O	2.18	0.43
2:E:116:ILE:HD12	2:E:159:MET:HE3	2.01	0.43
6:D:449:VAL:HG22	6:D:484:VAL:HG22	2.01	0.43
3:Q:89:TRP:CE2	9:R2:125:MET:HE3	2.53	0.43
5:V:75:MET:HE1	5:V:126:LEU:HD22	2.00	0.43
6:D:625:LEU:CD1	6:D:643:ILE:HD11	2.49	0.43
6:D:803:ASN:O	6:D:804:ARG:HB3	2.18	0.43
7:N:84:THR:HB	11:J:1:GLA:O2	2.19	0.43
7:N:629:ASN:HB3	7:N:646:TYR:HA	2.00	0.43
8:P:186:VAL:HG21	8:P:217:PHE:HD2	1.83	0.43
6:D:898:ASN:O	6:D:898:ASN:CG	2.62	0.42
9:R2:111:THR:HG21	11:S:1:GLA:O2	2.18	0.42
9:R2:148:GLU:O	9:R2:149:ARG:C	2.62	0.42
10:U:164:GLY:O	10:U:189:VAL:HG23	2.18	0.42
6:D:118:SER:HG	6:D:154:PHE:HD1	1.66	0.42
8:P:94:LYS:O	8:P:100:ILE:HD12	2.18	0.42
9:R1:44:THR:O	9:R1:45:ILE:C	2.61	0.42
9:R2:144:LYS:O	9:R2:145:ASN:C	2.62	0.42
1:A:251:ILE:HA	1:A:273:LEU:HA	2.00	0.42
4:T:143:VAL:C	4:T:145:PRO:CD	2.93	0.42
4:T:190:MET:HE2	4:T:190:MET:N	2.35	0.42
4:T:191:ASP:C	4:T:192:SER:HG	2.26	0.42
8:P:403:LEU:HB3	8:P:493:THR:HG22	2.01	0.42
9:R2:133:GLN:HB2	9:R2:160:ALA:HB2	2.00	0.42
1:A:272:ILE:HG22	1:A:273:LEU:N	2.35	0.42
1:A:381:VAL:HG13	1:A:381:VAL:O	2.20	0.42
1:A:428:ILE:O	1:A:429:ILE:HB	2.19	0.42
4:T:189:ILE:HB	4:T:190:MET:HE2	2.01	0.42
9:R1:153:LEU:N	9:R1:153:LEU:HD23	2.34	0.42
10:U:288:ARG:O	10:U:291:THR:HG22	2.19	0.42
3:Q:146:PRO:O	3:Q:147:ILE:HB	2.18	0.42
7:N:84:THR:O	7:N:85:THR:C	2.62	0.42
1:A:244:ILE:CG1	1:A:251:ILE:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:HB3	1:A:316:CYS:HB3	2.01	0.42
3:Q:111:ASN:OD1	3:Q:111:ASN:C	2.63	0.42
5:V:134:LEU:C	5:V:134:LEU:HD23	2.45	0.42
6:D:331:VAL:O	6:D:331:VAL:HG13	2.20	0.42
6:D:727:ASP:O	6:D:728:THR:C	2.62	0.42
7:N:601:ALA:CB	7:N:622:ILE:HG21	2.48	0.42
9:R1:110:ASP:CG	9:R1:111:THR:N	2.78	0.42
10:U:261:THR:C	10:U:262:ILE:HD12	2.43	0.42
1:A:362:PHE:O	1:A:363:ARG:HB3	2.18	0.42
5:V:212:TYR:O	5:V:214:THR:HG23	2.19	0.42
6:D:282:LEU:C	6:D:282:LEU:HD12	2.45	0.42
7:N:464:LEU:HD12	7:N:464:LEU:O	2.19	0.42
9:R1:61:THR:O	9:R1:62:ILE:HG13	2.18	0.42
2:E:173:ALA:O	2:E:174:ASN:C	2.62	0.42
6:D:844:ILE:HD13	6:D:867:PHE:CD2	2.55	0.42
8:P:177:ALA:O	8:P:181:LEU:HB3	2.20	0.42
5:V:176:ASN:HB2	5:V:211:PHE:HA	2.02	0.42
6:D:175:GLY:HA3	6:D:188:MET:HE2	2.02	0.42
6:D:251:GLY:HA3	8:P:30:ALA:HB2	2.02	0.42
6:D:357:VAL:HG21	6:D:387:ILE:HD11	2.01	0.42
6:D:522:LEU:O	6:D:523:GLU:C	2.62	0.42
9:R1:60:LEU:HD11	9:R1:96:LEU:HD22	2.02	0.42
9:R2:125:MET:N	9:R2:125:MET:HE2	2.35	0.42
4:T:145:PRO:O	4:T:147:GLY:N	2.53	0.42
5:V:125:HIS:O	5:V:126:LEU:HD23	2.20	0.42
6:D:408:GLN:HG2	6:D:415:ILE:HG22	2.01	0.42
8:P:591:TYR:OH	8:P:597:VAL:HG11	2.20	0.42
1:A:280:LEU:HD13	1:A:316:CYS:SG	2.60	0.41
4:T:145:PRO:O	4:T:148:GLY:N	2.53	0.41
4:T:158:LEU:HB2	4:T:159:PRO:HD3	2.01	0.41
6:D:172:TYR:CD1	6:D:172:TYR:N	2.85	0.41
6:D:400:LEU:N	6:D:400:LEU:HD12	2.34	0.41
6:D:552:MET:HE1	6:D:564:GLN:CG	2.50	0.41
8:P:350:THR:HG22	8:P:364:THR:OG1	2.20	0.41
9:R2:141:GLY:O	9:R2:143:THR:HG23	2.20	0.41
4:T:249:VAL:O	4:T:249:VAL:CG1	2.66	0.41
6:D:219:VAL:O	6:D:241:PHE:HA	2.21	0.41
6:D:468:LYS:O	6:D:469:THR:C	2.62	0.41
7:N:568:LEU:HD22	7:N:570:LEU:CD2	2.44	0.41
7:N:636:LEU:HD12	7:N:637:LYS:CG	2.49	0.41
10:U:110:THR:O	10:U:110:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:330:ILE:HD12	10:U:330:ILE:H	1.85	0.41
3:Q:71:LEU:O	3:Q:72:LYS:C	2.61	0.41
7:N:70:ILE:O	7:N:140:THR:HG23	2.19	0.41
7:N:643:VAL:HG13	7:N:672:PHE:CE1	2.56	0.41
10:U:276:VAL:HG11	10:U:341:MET:HE3	2.01	0.41
1:A:348:THR:HG23	1:A:348:THR:O	2.18	0.41
1:A:453:ALA:HB1	1:A:460:MET:HE3	2.02	0.41
2:E:118:VAL:HG22	2:E:119:ASN:N	2.36	0.41
6:D:388:SER:CB	6:D:403:THR:HG22	2.50	0.41
7:N:106:ALA:HB2	7:N:664:PRO:O	2.20	0.41
8:P:288:ARG:HE	8:P:291:PRO:HA	1.86	0.41
1:A:345:HIS:CG	1:A:346:GLY:N	2.87	0.41
1:A:496:TYR:N	1:A:496:TYR:CD1	2.88	0.41
3:Q:47:ASP:OD2	3:Q:233:THR:HG23	2.21	0.41
6:D:228:VAL:HG12	6:D:229:GLU:N	2.29	0.41
4:T:120:PRO:N	4:T:121:PRO:CD	2.84	0.41
6:D:490:LEU:HD23	6:D:496:VAL:CG2	2.50	0.41
6:D:643:ILE:HG22	6:D:670:LEU:CD2	2.50	0.41
9:R1:95:ILE:HG22	9:R1:109:VAL:HG22	2.03	0.41
10:U:116:ILE:HD11	10:U:119:VAL:HB	2.03	0.41
1:A:193:LEU:C	1:A:193:LEU:HD23	2.45	0.41
1:A:211:HIS:O	1:A:212:ASP:CG	2.64	0.41
1:A:258:TYR:HA	1:A:265:ALA:HA	2.01	0.41
1:A:429:ILE:HG22	1:A:430:ASN:N	2.35	0.41
4:T:156:TRP:O	4:T:156:TRP:CE3	2.74	0.41
8:P:405:VAL:HG21	8:P:493:THR:HG21	2.02	0.41
1:A:251:ILE:N	1:A:251:ILE:HD12	2.36	0.41
1:A:369:HIS:O	1:A:371:VAL:HG13	2.20	0.41
5:V:146:LEU:C	5:V:146:LEU:HD12	2.46	0.41
6:D:326:MET:HG2	6:D:327:PRO:HD2	2.02	0.41
7:N:543:VAL:HG13	7:N:543:VAL:O	2.20	0.41
8:P:159:LEU:HD13	8:P:584:TYR:CZ	2.56	0.41
8:P:510:THR:HG23	8:P:547:TYR:CD1	2.56	0.41
9:R1:44:THR:HG22	9:R1:172:TYR:N	2.36	0.41
9:R2:62:ILE:HD12	9:R2:95:ILE:O	2.21	0.41
9:R2:110:ASP:OD1	9:R2:110:ASP:C	2.64	0.41
9:R2:111:THR:C	9:R2:141:GLY:HA3	2.46	0.41
10:U:148:TYR:O	10:U:152:LEU:HD23	2.20	0.41
2:E:117:THR:O	2:E:117:THR:HG23	2.21	0.41
6:D:780:PHE:HZ	6:D:782:MET:HE2	1.85	0.41
7:N:627:ILE:HD12	7:N:665:ILE:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R2:61:THR:HG1	9:R2:97:TRP:CD1	2.39	0.41
9:R2:111:THR:CB	11:S:1:GLA:O2	2.68	0.41
9:R2:135:ILE:O	9:R2:135:ILE:HG22	2.19	0.41
1:A:429:ILE:HD12	1:A:429:ILE:N	2.36	0.40
1:A:465:VAL:O	1:A:466:ILE:HD13	2.21	0.40
1:A:492:VAL:CG2	1:A:508:VAL:HB	2.52	0.40
7:N:209:PHE:HB2	7:N:222:ILE:HG22	2.03	0.40
7:N:530:LEU:HD23	7:N:530:LEU:C	2.46	0.40
8:P:166:LEU:HB2	8:P:210:LEU:HD12	2.03	0.40
4:T:237:ILE:O	4:T:238:GLY:C	2.64	0.40
3:Q:183:VAL:HG23	3:Q:199:SER:HB2	2.03	0.40
9:R2:63:THR:HG22	9:R2:70:ILE:HG22	2.02	0.40
1:A:463:ILE:HD12	1:A:463:ILE:N	2.35	0.40
6:D:427:SER:OG	6:D:428:ARG:N	2.54	0.40
9:R2:69:SER:HB2	12:R2:201:GLA:O2	2.21	0.40
10:U:27:ASP:CG	10:U:28:ARG:H	2.30	0.40
10:U:28:ARG:CD	10:U:28:ARG:N	2.84	0.40
10:U:156:THR:HG23	10:U:201:ALA:HB3	2.03	0.40
1:A:385:LEU:HD23	1:A:385:LEU:C	2.47	0.40
6:D:409:THR:O	6:D:413:SER:HA	2.22	0.40
8:P:52:PRO:HD2	8:P:64:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	LYS
3	Q	147	ILE
4	T	189	ILE
6	D	523	GLU
6	D	569	VAL
9	R1	62	ILE
10	U	26	VAL
1	A	361	VAL
2	E	34	ILE
6	D	361	THR
7	N	82	ALA
4	T	238	GLY
4	T	146	GLY
6	D	326	MET
1	A	429	ILE
6	D	579	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	250	HIS
1	A	288	ASP
1	A	303	THR
1	A	336	TYR
1	A	382	CYS
1	A	392	SER
1	A	423	ILE
1	A	431	GLN
1	A	493	LEU
1	A	520	GLN
1	A	572	LEU
2	E	32	SER
2	E	64	GLU
2	E	87	LEU
3	Q	46	VAL
3	Q	81	PHE
3	Q	118	GLU
3	Q	136	TYR
3	Q	171	LEU
3	Q	180	PHE
3	Q	182	LEU
3	Q	188	VAL

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Mol	Chain	Res	Type
3	Q	195	ASN
3	Q	201	ARG
4	T	127	LYS
4	T	131	ILE
4	T	149	GLN
4	T	187	LEU
4	T	203	LEU
4	T	214	LEU
4	T	231	LEU
4	T	250	ASP
4	T	253	LEU
4	T	258	ILE
5	V	37	ASN
5	V	77	CYS
5	V	106	ASP
5	V	136	PHE
5	V	148	ILE
5	V	153	SER
5	V	166	GLN
5	V	189	GLU
5	V	198	PHE
5	V	233	THR
6	D	75	VAL
6	D	82	SER
6	D	150	ILE
6	D	172	TYR
6	D	186	ILE
6	D	188	MET
6	D	196	CYS
6	D	208	LEU
6	D	231	VAL
6	D	299	LEU
6	D	329	TYR
6	D	372	LEU
6	D	398	LEU
6	D	406	ILE
6	D	419	LEU
6	D	427	SER
6	D	550	TYR
6	D	566	ARG
6	D	569	VAL
6	D	591	ASN

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Mol	Chain	Res	Type
6	D	597	TYR
6	D	598	TYR
6	D	602	THR
6	D	629	TYR
6	D	637	LEU
6	D	642	LEU
6	D	645	ASP
6	D	691	PHE
6	D	727	ASP
6	D	778	GLN
6	D	815	HIS
6	D	856	HIS
6	D	871	LYS
6	D	875	VAL
6	D	898	ASN
7	N	78	THR
7	N	84	THR
7	N	88	HIS
7	N	99	THR
7	N	166	GLU
7	N	190	LEU
7	N	225	ASN
7	N	230	THR
7	N	247	GLU
7	N	274	PHE
7	N	276	VAL
7	N	352	ILE
7	N	391	ASP
7	N	427	MET
7	N	445	ILE
7	N	447	LEU
7	N	464	LEU
7	N	510	ASN
7	N	515	THR
7	N	593	VAL
7	N	636	LEU
7	N	666	ASN
7	N	674	LEU
8	P	65	SER
8	P	100	ILE
8	P	136	PHE
8	P	169	LEU

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Mol	Chain	Res	Type
8	P	185	ARG
8	P	210	LEU
8	P	234	ILE
8	P	240	ARG
8	P	281	GLN
8	P	347	LEU
8	P	353	TYR
8	P	420	SER
8	P	527	LEU
9	R1	40	CYS
9	R1	60	LEU
9	R1	61	THR
9	R1	62	ILE
9	R1	74	ASN
9	R1	79	HIS
9	R1	110	ASP
9	R1	111	THR
9	R1	116	GLN
9	R1	152	SER
9	R2	54	ASN
9	R2	63	THR
9	R2	82	MET
9	R2	85	LEU
9	R2	140	PHE
9	R2	142	ASN
9	R2	159	GLU
10	U	79	LYS
10	U	135	TRP
10	U	189	VAL
10	U	223	VAL
10	U	440	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
3	Q	90	ASN
4	T	213	GLN
5	V	125	HIS
6	D	203	HIS
6	D	423	ASN
6	D	457	ASN

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Mol	Chain	Res	Type
6	D	594	ASN
6	D	675	ASN
6	D	771	GLN
6	D	859	ASN
6	D	898	ASN
7	N	225	ASN
7	N	555	GLN
9	R1	145	ASN
9	R2	157	ASN
9	R2	161	ASN
9	R2	163	ASN
10	U	229	ASN
10	U	243	ASN
10	U	257	ASN
10	U	382	ASN

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 ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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(°)	Ideal(°)
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:

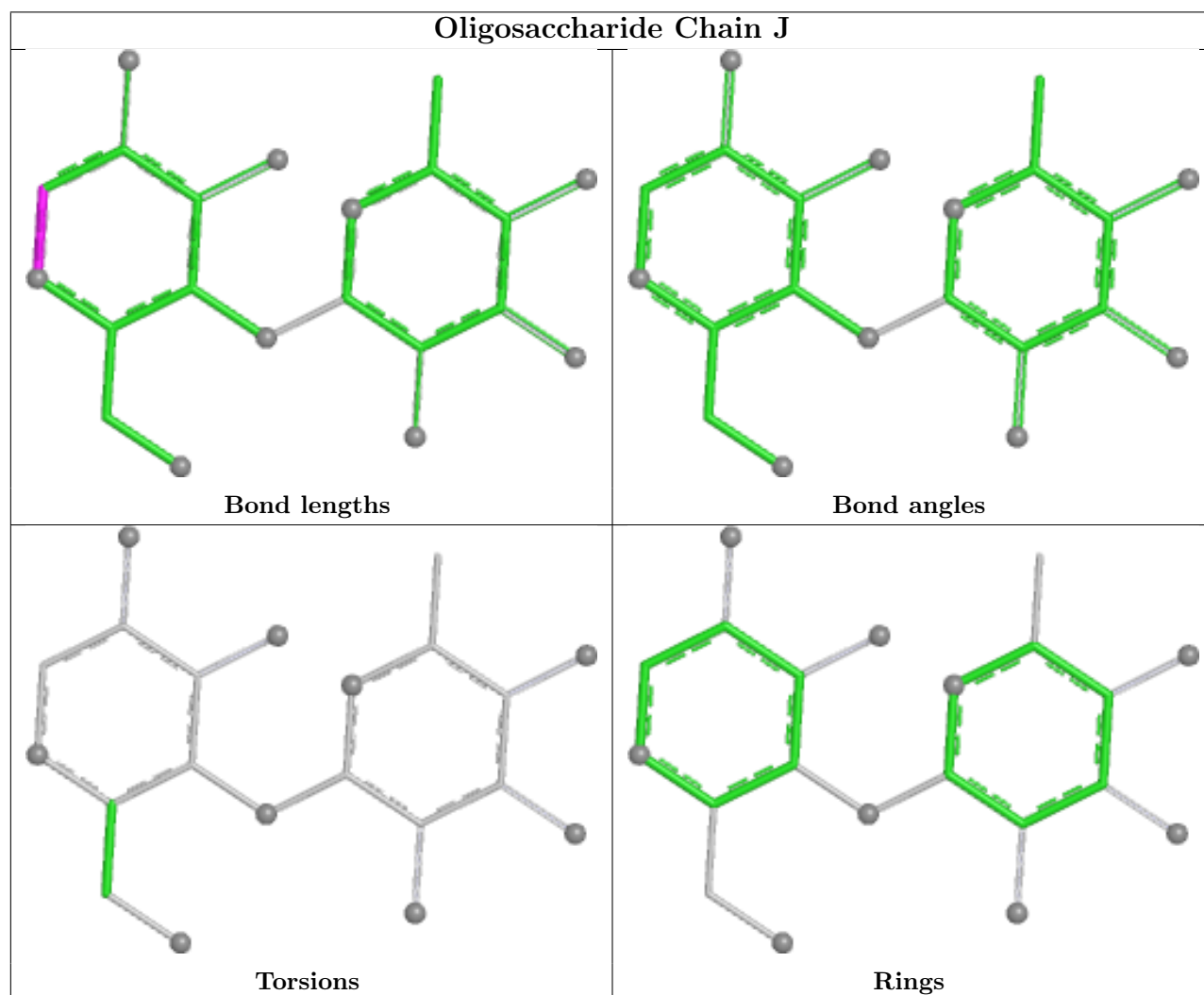
Mol	Chain	Res	Type	Atoms
11	S	1	GLA	O5-C5-C6-O6

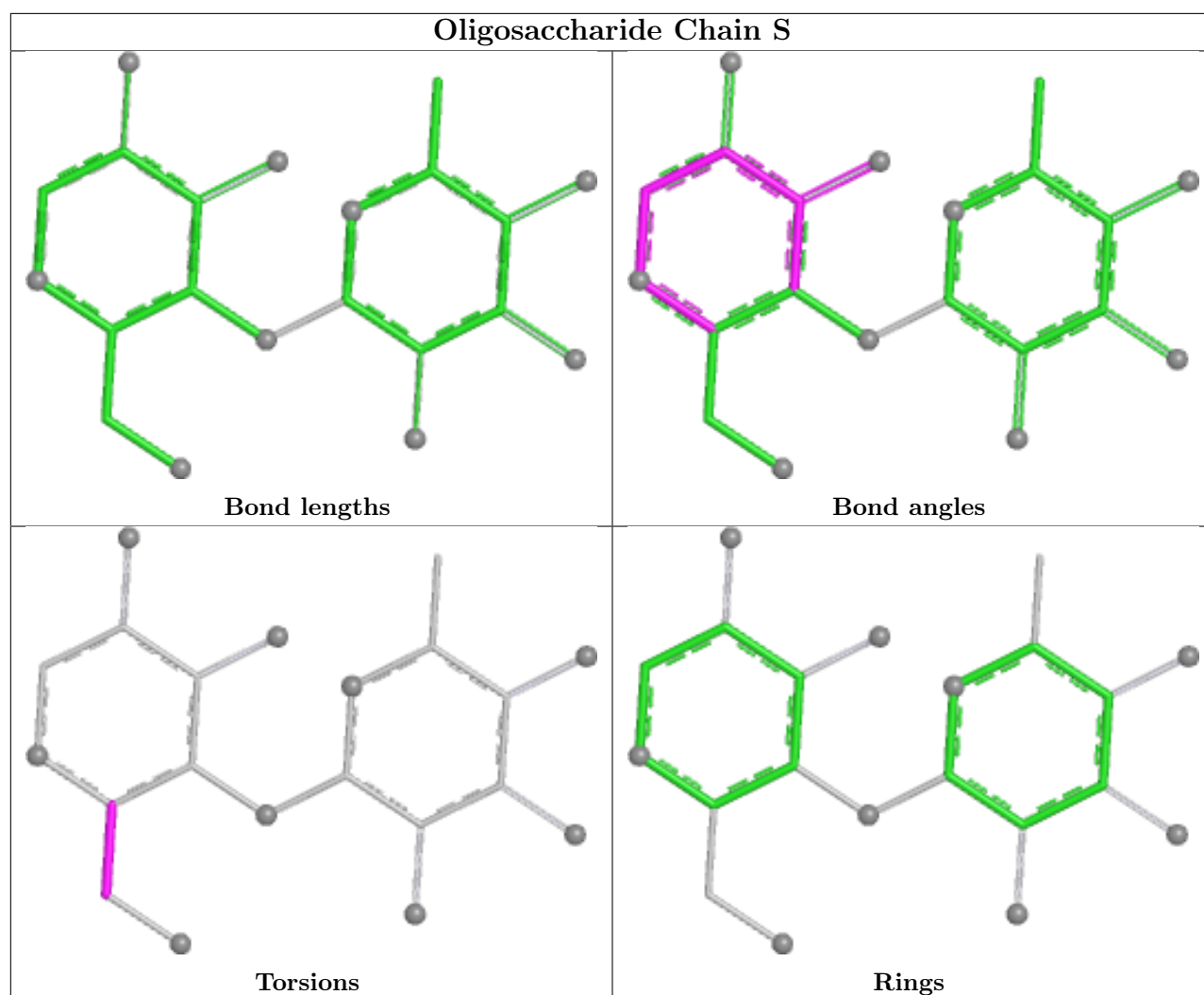
There are no ring outliers.

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.





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.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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(°)	Ideal(°)
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
12	R2	202	GLA	C1-O5-C5	3.17	116.44	112.19
12	A	602	GLA	C1-C2-C3	3.09	114.15	109.64
12	A	603	GLA	C1-O5-C5	3.01	116.22	112.19
12	D	1004	GLA	C3-C4-C5	-2.57	105.57	110.23
12	R2	201	GLA	C1-O5-C5	2.48	115.50	112.19
12	D	1003	GLA	C1-C2-C3	2.34	113.06	109.64
12	D	1003	GLA	C3-C4-C5	-2.23	106.19	110.23
12	D	1004	GLA	C1-O5-C5	2.22	115.16	112.19
12	D	1004	GLA	C1-C2-C3	2.15	112.77	109.64
12	A	601	GLA	C1-O5-C5	2.15	115.07	112.19
12	P	701	GLA	C3-C4-C5	-2.10	106.43	110.23

There are no chirality outliers.

All (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
13	D	1001	LMN	CBK-CBQ-CCM-CBR
13	D	1001	LMN	CBC-CBE-CBG-CBI
12	D	1004	GLA	C4-C5-C6-O6
13	N	701	LMN	CBC-CBE-CBG-CBI
13	N	701	LMN	CAW-CAY-CBA-CBC
13	N	701	LMN	CAZ-CBB-CBD-CBF
13	N	701	LMN	CBD-CBF-CBH-CBJ
13	D	1002	LMN	CBJ-CBL-CBR-CCM
13	N	701	LMN	CBG-CBI-CBK-CBQ
12	D	1004	GLA	O5-C5-C6-O6
13	N	701	LMN	CBA-CBC-CBE-CBG
13	D	1002	LMN	CAX-CAZ-CBB-CBD
13	D	1001	LMN	CAZ-CBB-CBD-CBF
13	D	1002	LMN	CBD-CBF-CBH-CBJ
13	N	701	LMN	CAB-CAX-CAZ-CBB
13	D	1002	LMN	CAW-CAY-CBA-CBC
13	D	1001	LMN	CBG-CBI-CBK-CBQ
13	N	701	LMN	CAA-CAW-CAY-CBA
13	N	701	LMN	CAY-CBA-CBC-CBE

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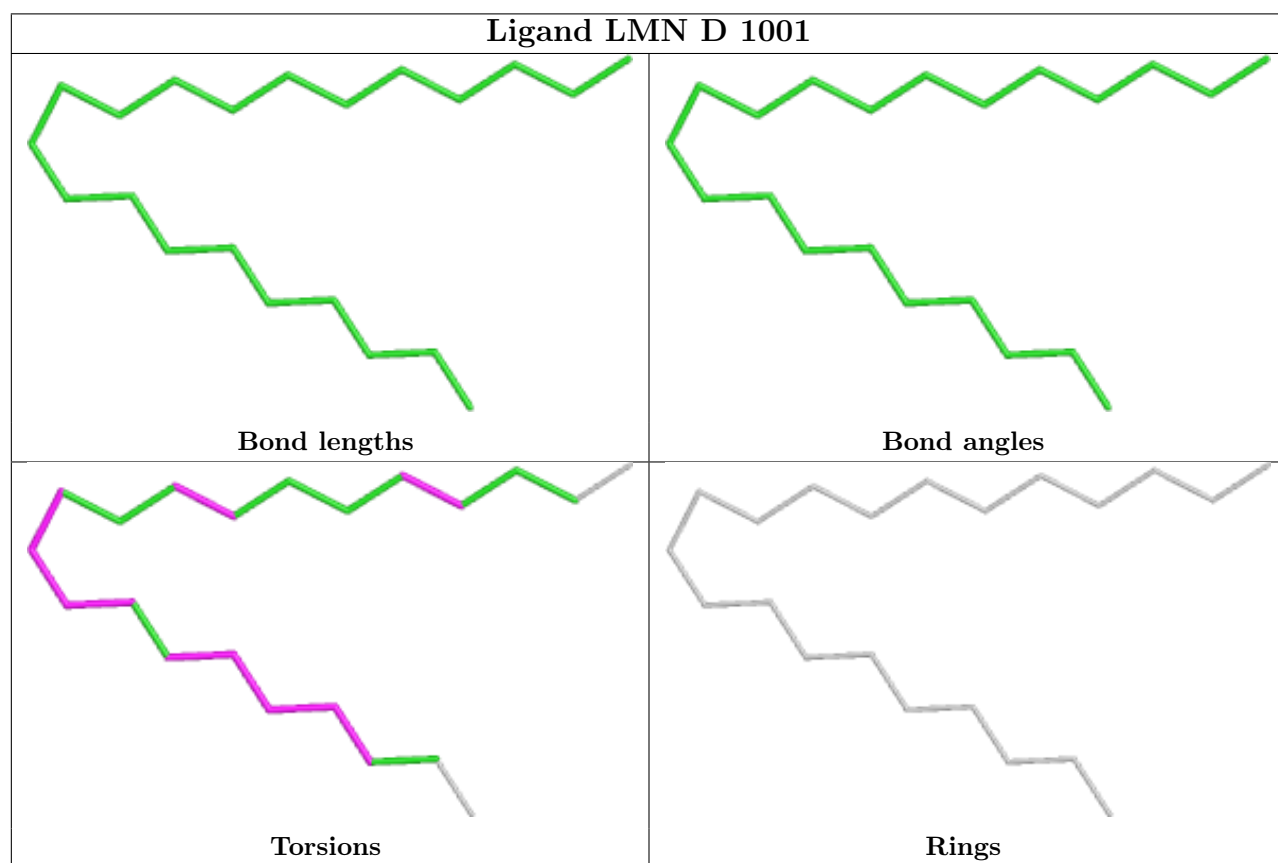
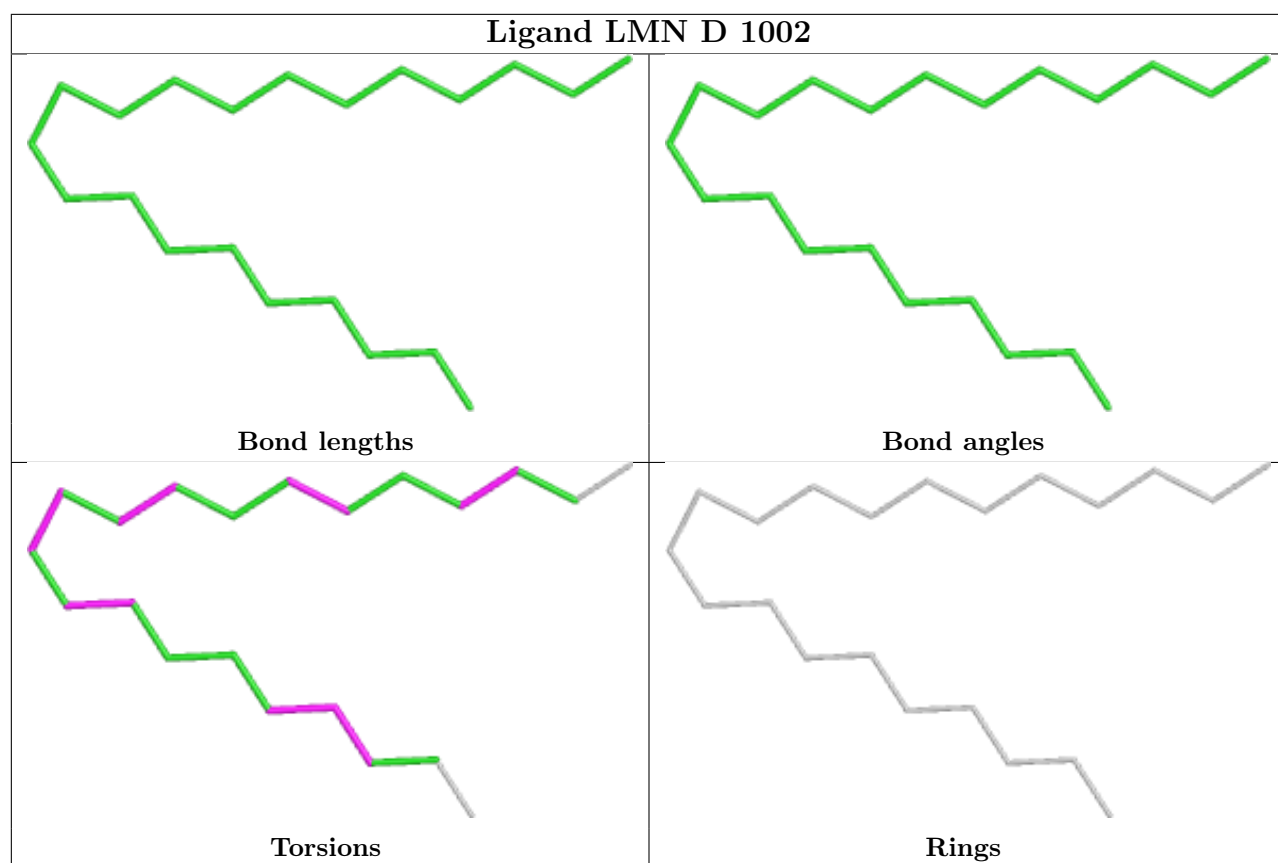
Mol	Chain	Res	Type	Atoms
13	D	1002	LMN	CBK-CBQ-CCM-CBR
13	D	1001	LMN	CBA-CBC-CBE-CBG
13	D	1001	LMN	CBH-CBJ-CBL-CBR
13	D	1001	LMN	CBI-CBK-CBQ-CCM
13	D	1001	LMN	CAW-CAY-CBA-CBC
13	N	701	LMN	CBB-CBD-CBF-CBH
12	P	702	GLA	C4-C5-C6-O6
13	N	701	LMN	CAX-CAZ-CBB-CBD

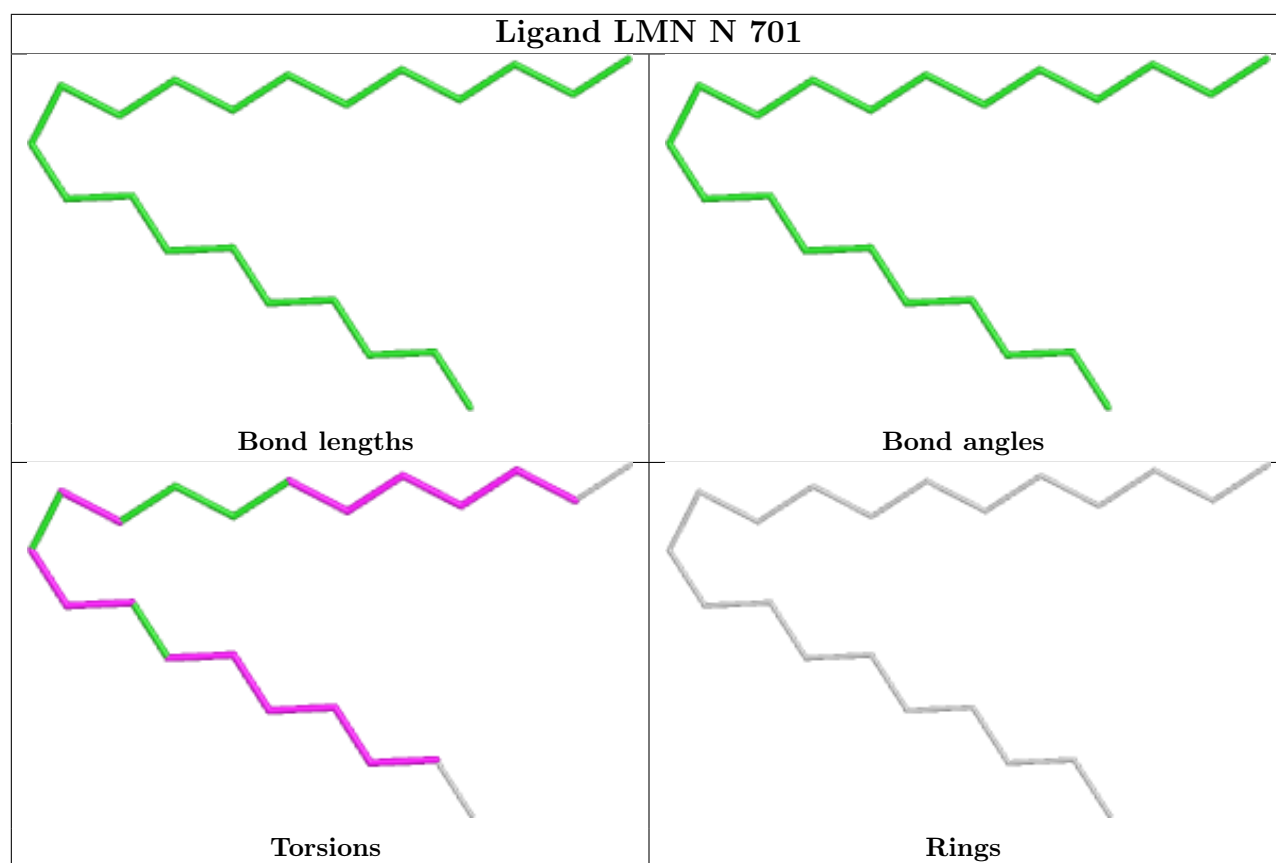
There are no ring outliers.

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 than 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.





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.

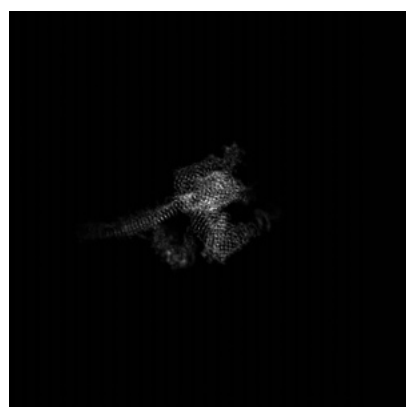
6 Map visualisation [i](#)

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.

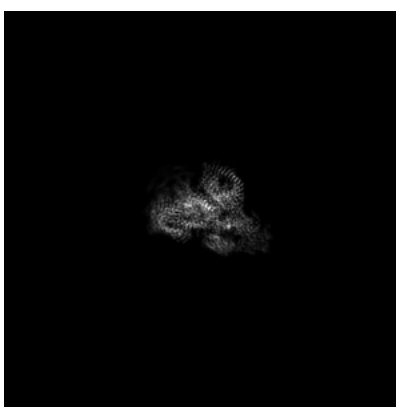
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

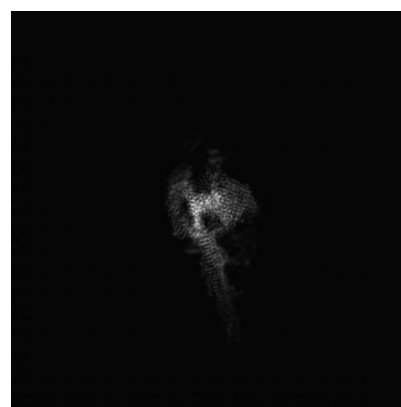
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

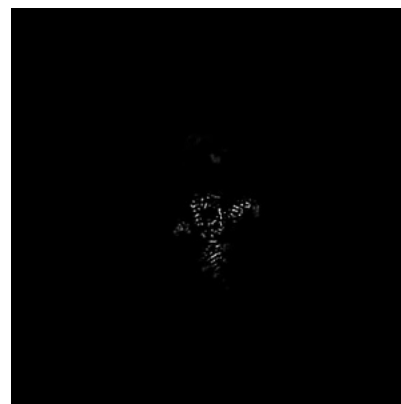
6.2.1 Primary map



X Index: 190



Y Index: 190

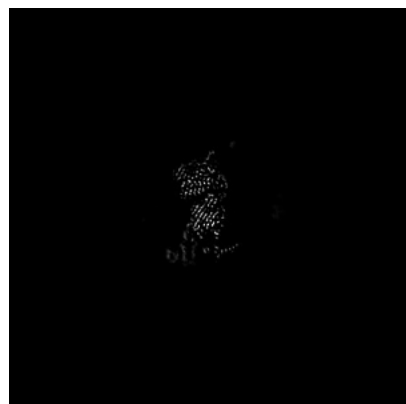


Z Index: 190

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

6.3 Largest variance slices [i](#)

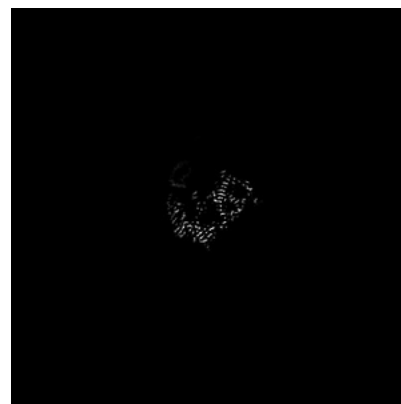
6.3.1 Primary map



X Index: 176



Y Index: 196

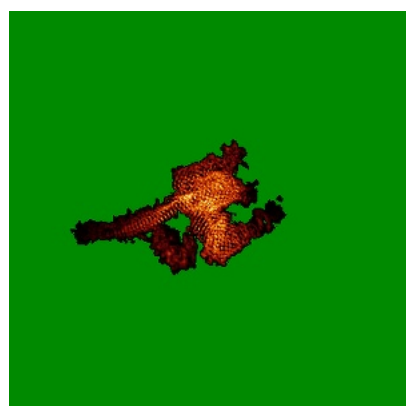


Z Index: 203

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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

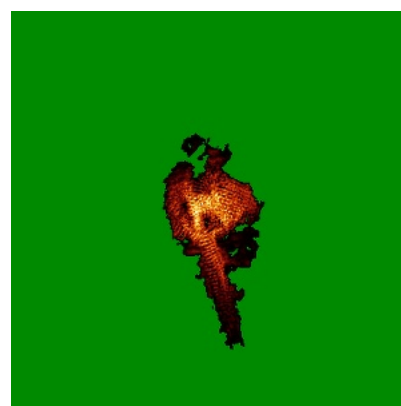
6.4.1 Primary map



X



Y

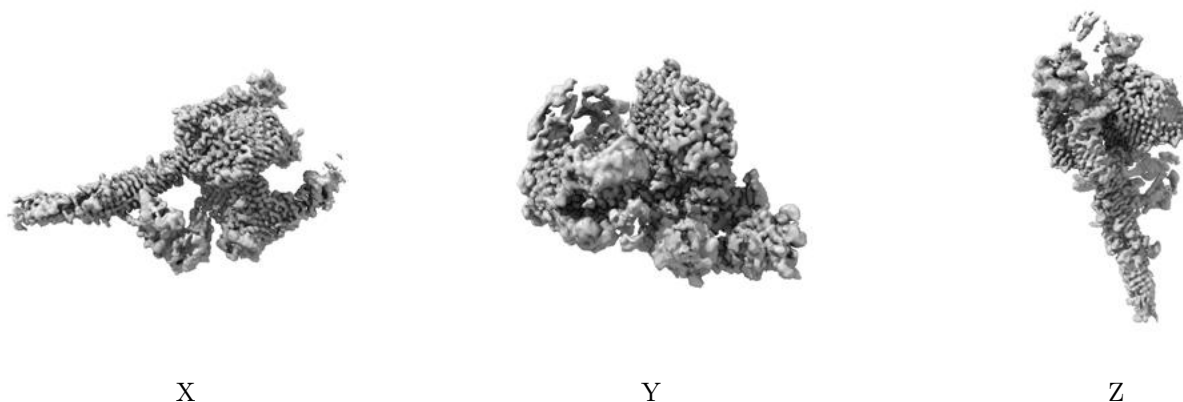


Z

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



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.

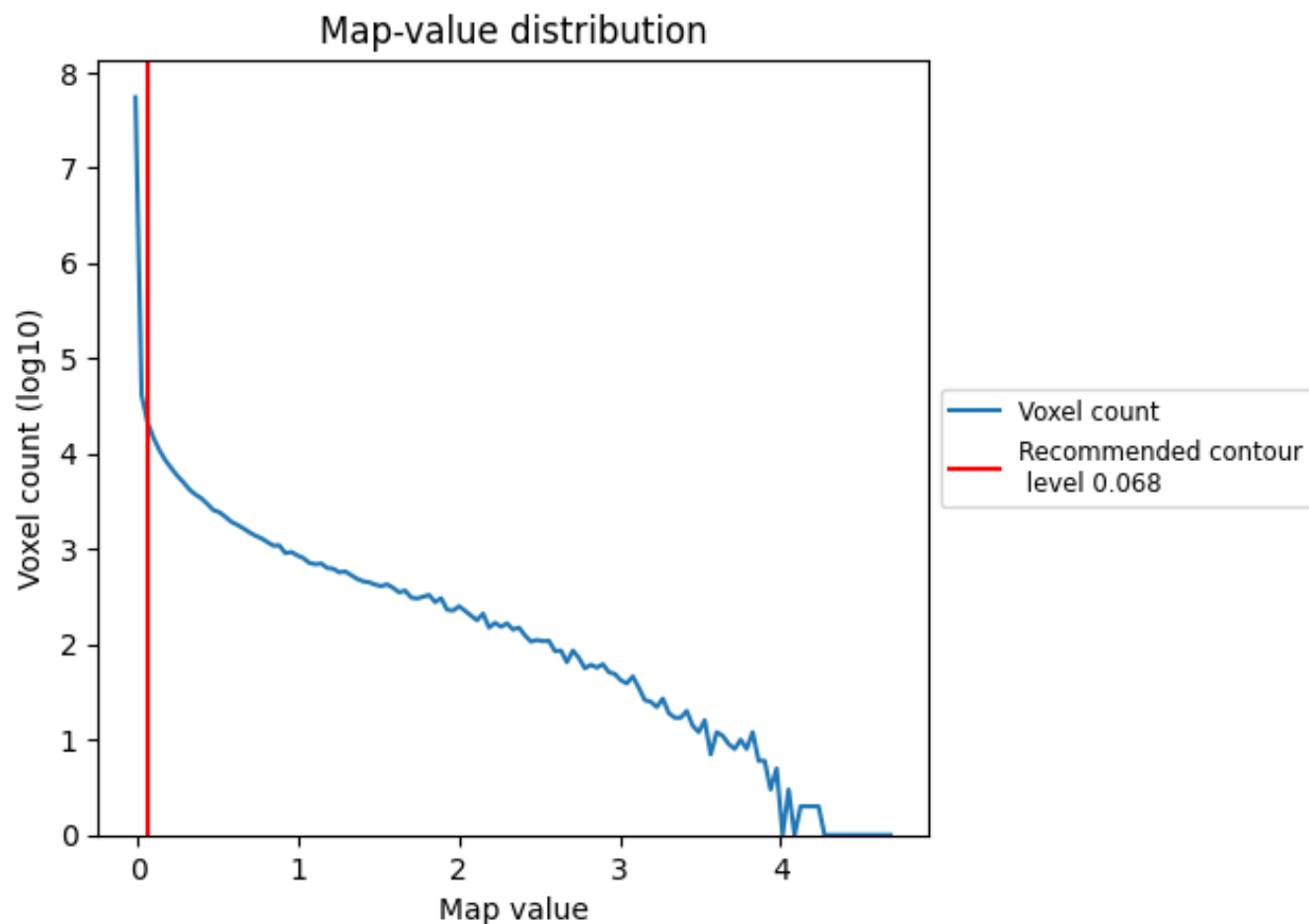
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

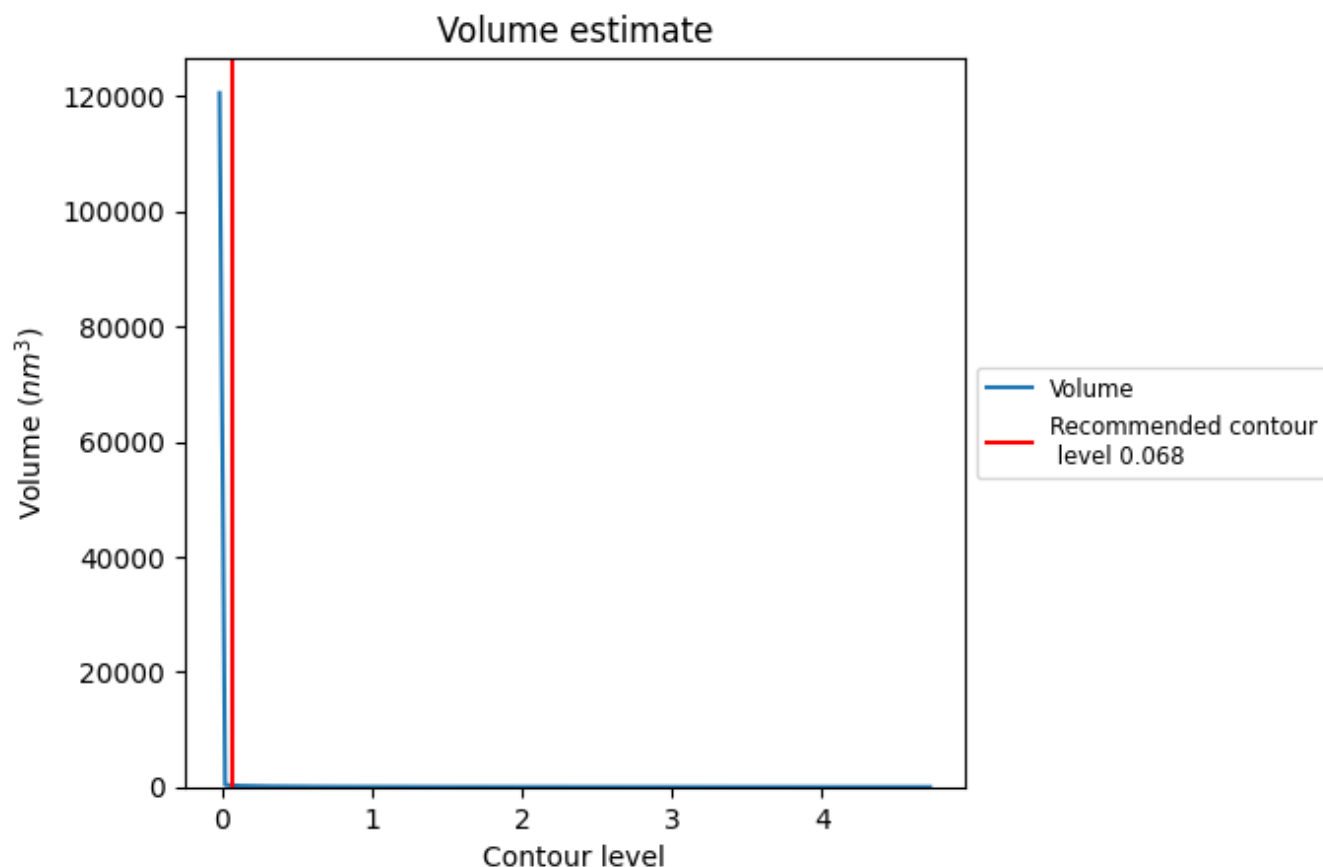
This section contains the results of statistical analysis of the map.

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.

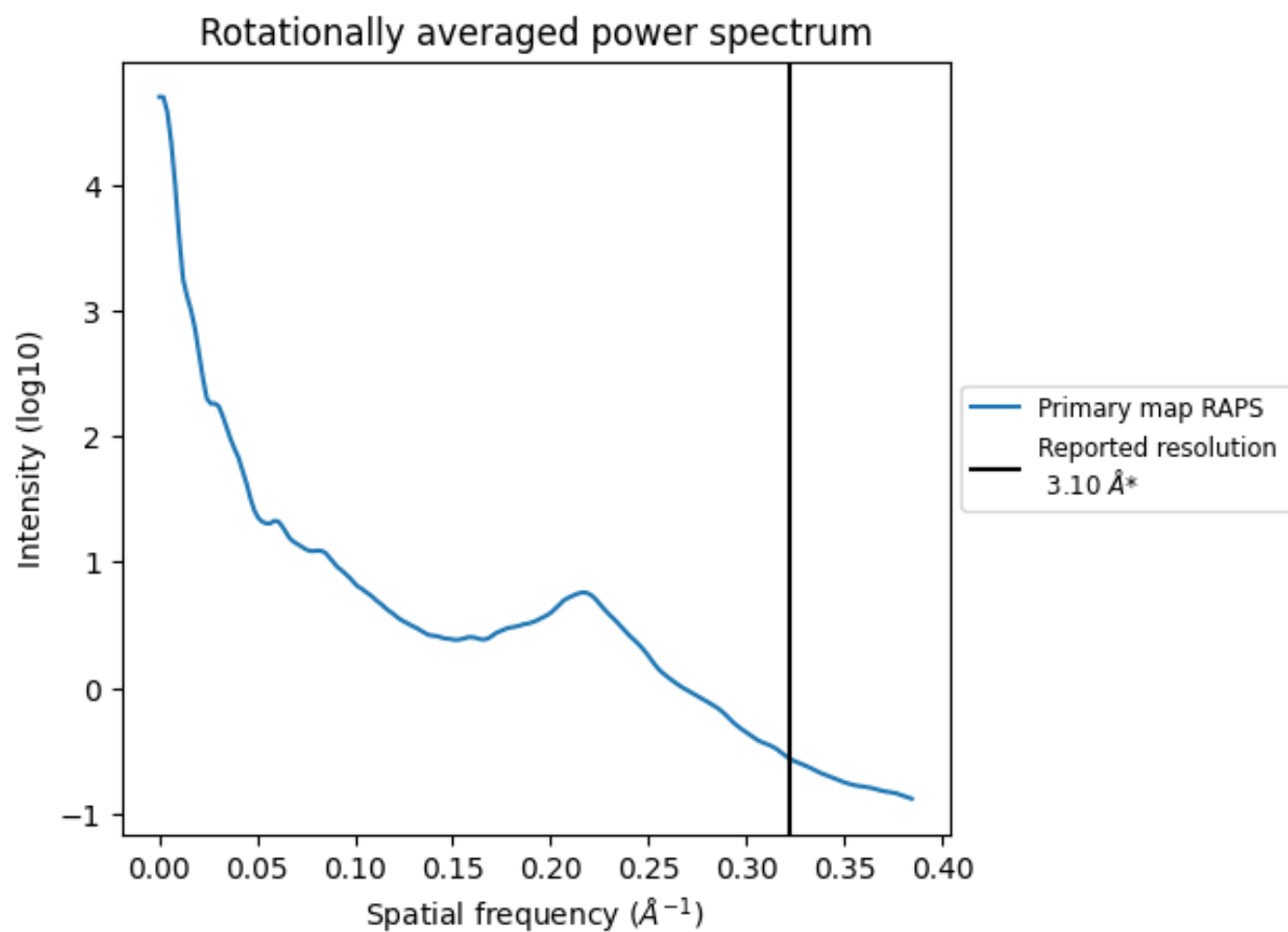
7.2 Volume estimate [i](#)



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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

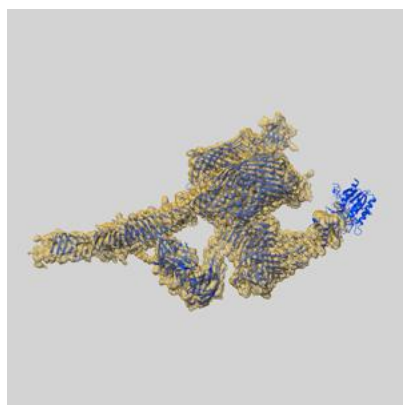
8 Fourier-Shell correlation ⓘ

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

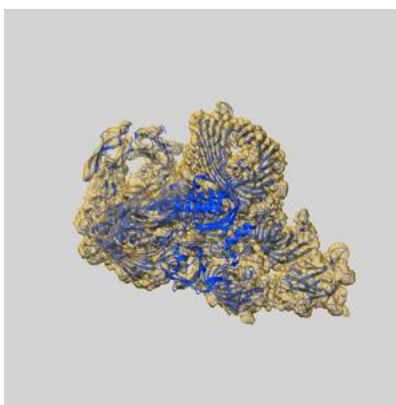
9 Map-model fit [i](#)

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](#).

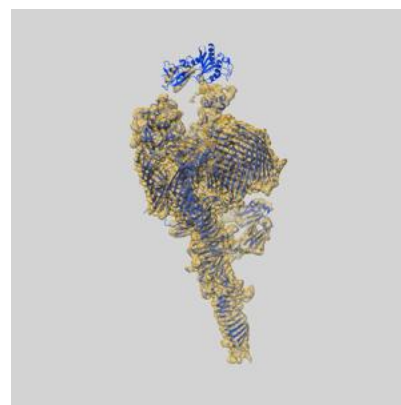
9.1 Map-model overlay [i](#)



X



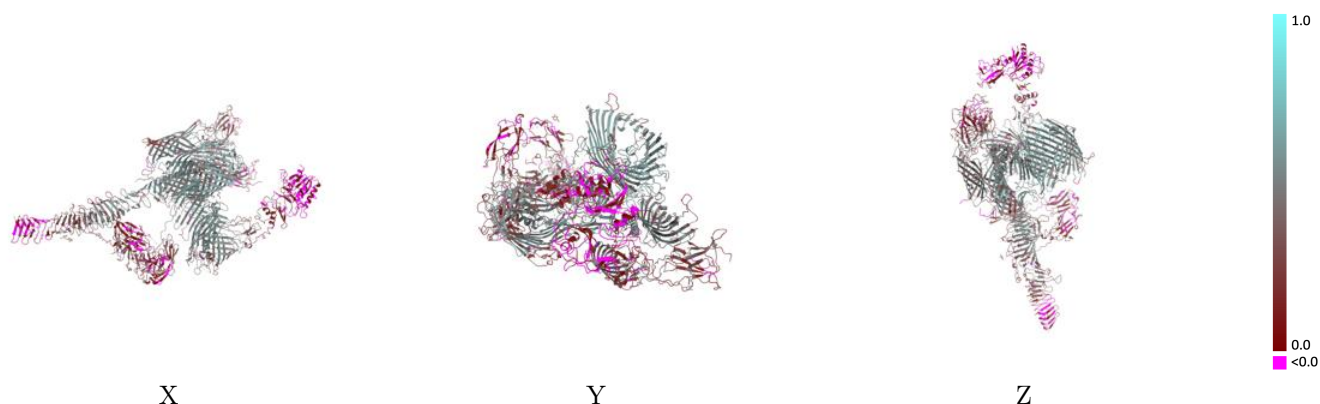
Y



Z

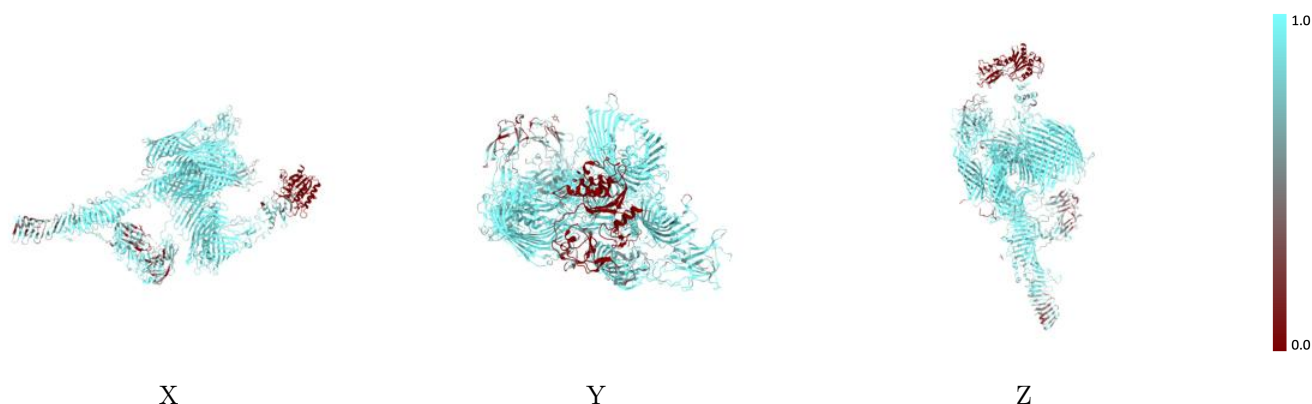
The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



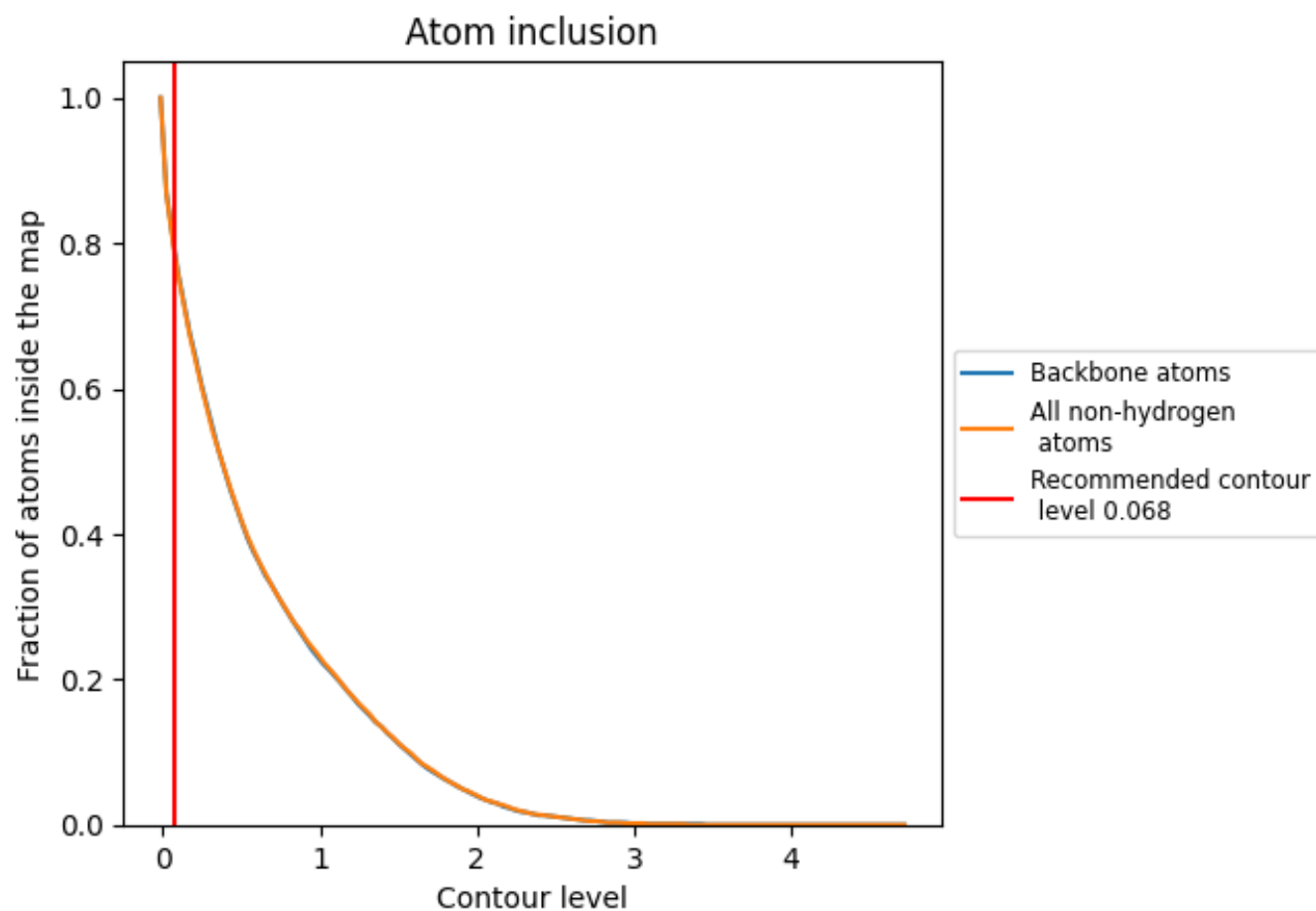
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.068).

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

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

