



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 03:43 AM EDT

PDB ID : 7RHQ
EMDB ID : EMD-24466
Title : Cryo-EM structure of Xenopus Patched-1 in complex with GAS1 and Sonic Hedgehog
Authors : Huang, P.; Lian, T.; Wierbowski, B.; Garcia-Linares, S.; Jiang, J.; Salic, A.
Deposited on : 2021-07-18
Resolution : 3.53 Å(reported)

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

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

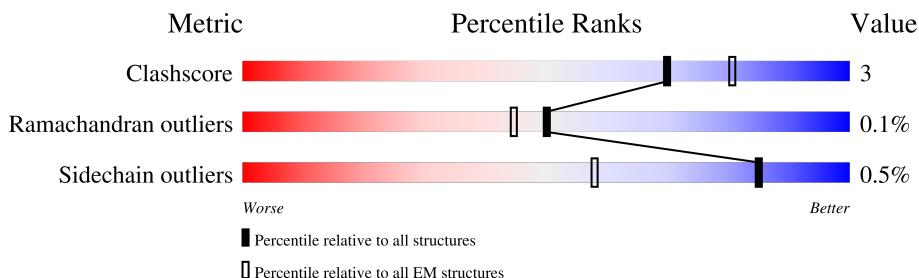
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1205	
2	C	192	
3	G	282	
4	B	2	
4	D	2	
4	E	2	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10499 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Patched-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	974	7680	5008	1261	1371	40	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1179	SER	-	expression tag	UNP Q98SW6
A	1180	SER	-	expression tag	UNP Q98SW6
A	1181	SER	-	expression tag	UNP Q98SW6
A	1182	PRO	-	expression tag	UNP Q98SW6
A	1183	ALA	-	expression tag	UNP Q98SW6
A	1184	ALA	-	expression tag	UNP Q98SW6
A	1185	ALA	-	expression tag	UNP Q98SW6
A	1186	HIS	-	expression tag	UNP Q98SW6
A	1187	HIS	-	expression tag	UNP Q98SW6
A	1188	HIS	-	expression tag	UNP Q98SW6
A	1189	HIS	-	expression tag	UNP Q98SW6
A	1190	HIS	-	expression tag	UNP Q98SW6
A	1191	HIS	-	expression tag	UNP Q98SW6
A	1192	HIS	-	expression tag	UNP Q98SW6
A	1193	HIS	-	expression tag	UNP Q98SW6
A	1194	GLU	-	expression tag	UNP Q98SW6
A	1195	ASP	-	expression tag	UNP Q98SW6
A	1196	GLN	-	expression tag	UNP Q98SW6
A	1197	VAL	-	expression tag	UNP Q98SW6
A	1198	ASP	-	expression tag	UNP Q98SW6
A	1199	PRO	-	expression tag	UNP Q98SW6
A	1200	ARG	-	expression tag	UNP Q98SW6
A	1201	LEU	-	expression tag	UNP Q98SW6
A	1202	ILE	-	expression tag	UNP Q98SW6
A	1203	ASP	-	expression tag	UNP Q98SW6
A	1204	GLY	-	expression tag	UNP Q98SW6
A	1205	LYS	-	expression tag	UNP Q98SW6

- Molecule 2 is a protein called Sonic hedgehog protein N-product.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	171	Total	C	N	O	S	0	0
			1354	844	249	255	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	130A	GLY	-	insertion	UNP Q15465
C	130B	GLY	-	insertion	UNP Q15465
C	130C	THR	-	insertion	UNP Q15465
C	130D	GLU	-	insertion	UNP Q15465
C	130E	ASP	-	insertion	UNP Q15465
C	130F	GLN	-	insertion	UNP Q15465
C	130G	VAL	-	insertion	UNP Q15465
C	130H	ASP	-	insertion	UNP Q15465
C	130I	PRO	-	insertion	UNP Q15465
C	130J	ARG	-	insertion	UNP Q15465
C	130K	LEU	-	insertion	UNP Q15465
C	130L	ILE	-	insertion	UNP Q15465
C	130M	ASP	-	insertion	UNP Q15465
C	130N	GLY	-	insertion	UNP Q15465
C	130O	LYS	-	insertion	UNP Q15465
C	130P	SER	-	insertion	UNP Q15465
C	130Q	GLY	-	insertion	UNP Q15465
C	130R	GLY	-	insertion	UNP Q15465

- Molecule 3 is a protein called Growth arrest-specific protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	160	Total	C	N	O	S	0	0
			1242	751	234	234	23		

There are 4 discrepancies between the modelled and reference sequences:

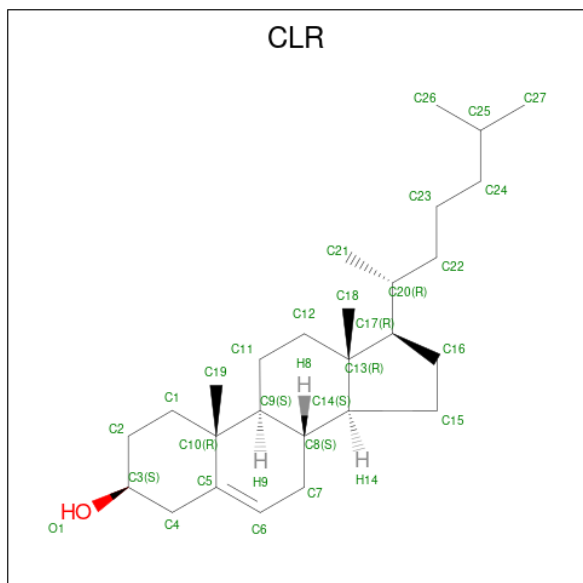
Chain	Residue	Modelled	Actual	Comment	Reference
G	36	GLY	-	expression tag	UNP P54826
G	37	PRO	-	expression tag	UNP P54826
G	38	GLY	-	expression tag	UNP P54826
G	39	SER	-	expression tag	UNP P54826

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



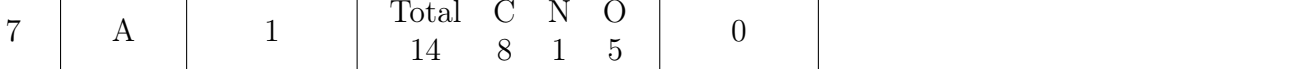
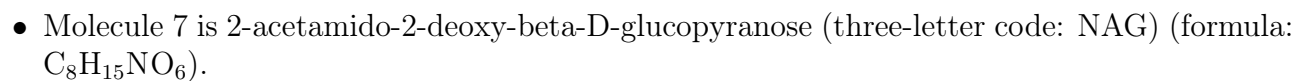
Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



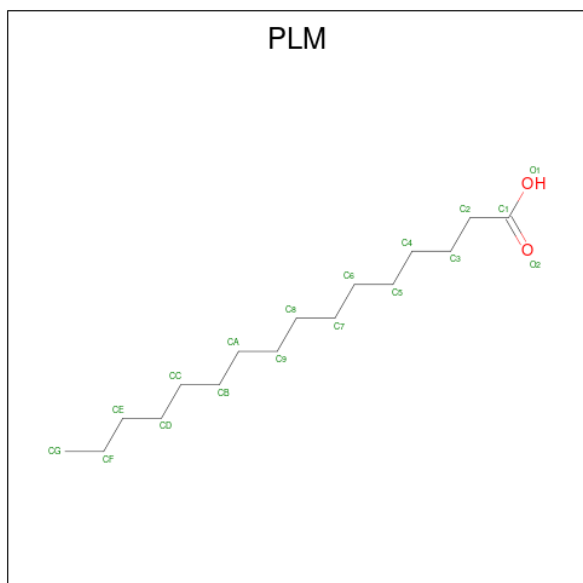
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	Zn	0
			1	1	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	C	2	Total	Ca	0
			2	2	

- Molecule 10 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

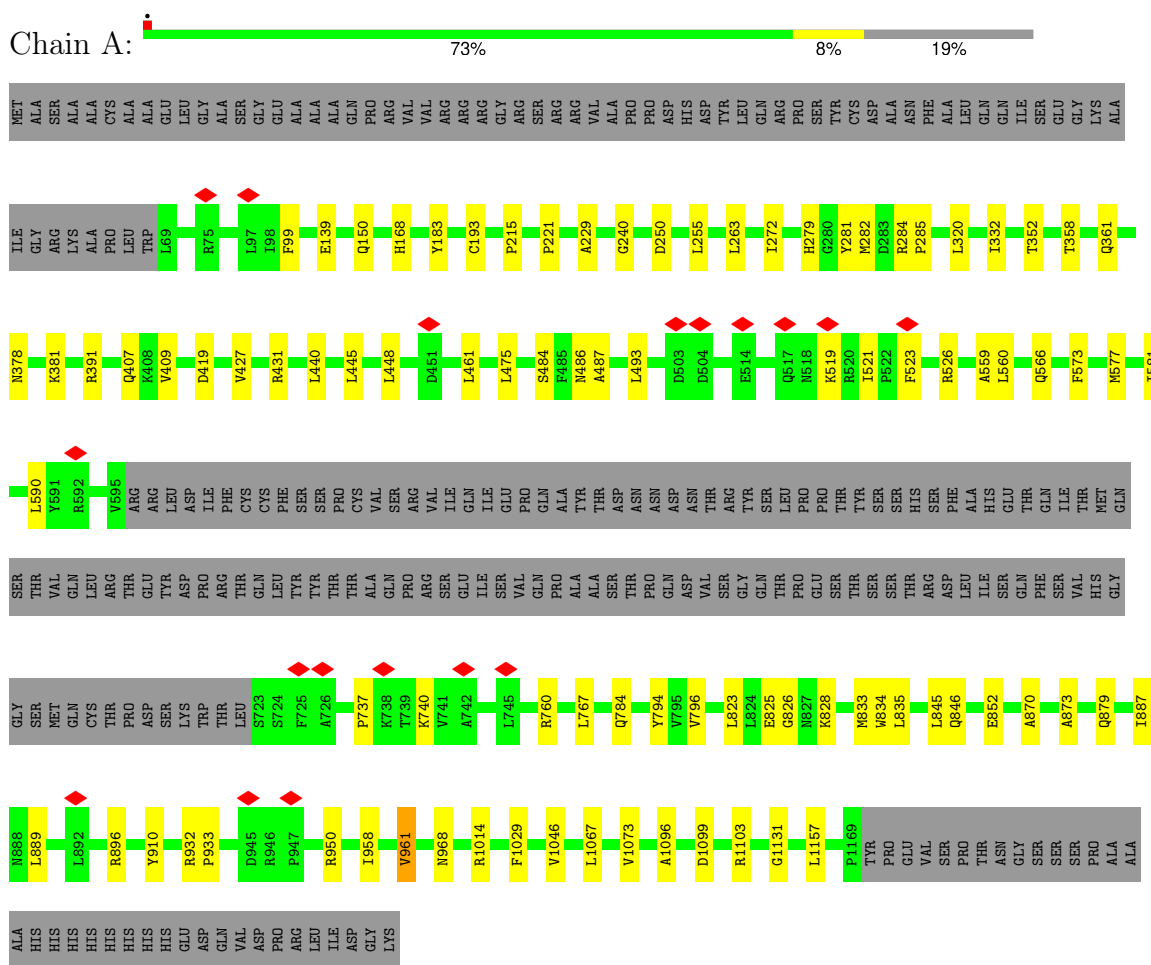


Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			17	16	1	

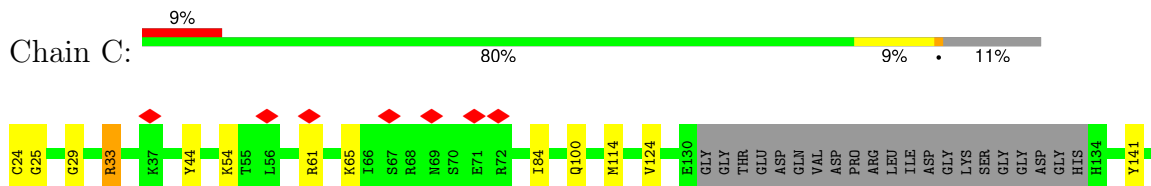
3 Residue-property plots

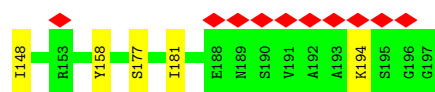
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Patched-1

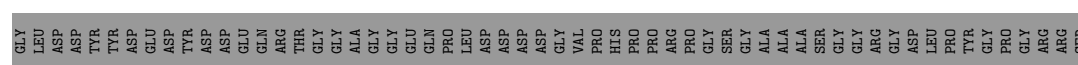
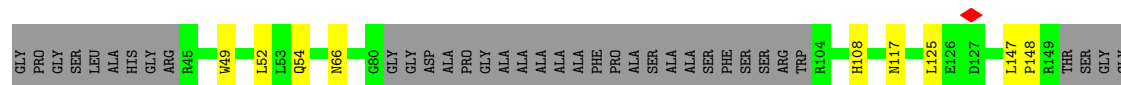


• Molecule 2: Sonic hedgehog protein N-product





- Molecule 3: Growth arrest-specific protein 1



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.356	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, Y01, CLR, PLM, CA

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	0.46	1/7864 (0.0%)	0.59	1/10696 (0.0%)
2	C	0.31	0/1382	0.52	0/1857
3	G	0.29	0/1258	0.50	0/1695
All	All	0.42	1/10504 (0.0%)	0.57	1/14248 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	796	VAL	CB-CG2	-5.02	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1157	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	828	LYS	Peptide
1	A	932	ARG	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	7680	0	7770	55	0
2	C	1354	0	1328	14	0
3	G	1242	0	1196	8	0
4	B	28	0	25	0	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	28	0	46	3	0
5	C	28	0	45	3	0
6	A	35	0	49	1	0
7	A	28	0	26	0	0
8	C	1	0	0	0	0
9	C	2	0	0	0	0
10	C	17	0	31	1	0
All	All	10499	0	10566	71	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 3.

All (71) 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)
1:A:484:SER:O	1:A:566:GLN:NE2	2.28	0.67
1:A:240:GLY:H	3:G:49:TRP:HB3	1.60	0.66
2:C:100:GLN:HE22	2:C:194:LYS:HG3	1.66	0.60
1:A:193:CYS:O	2:C:33:ARG:NH2	2.35	0.59
1:A:150:GLN:NE2	1:A:407:GLN:OE1	2.37	0.58
1:A:577:MET:HG3	1:A:581:ILE:HD12	1.88	0.56
1:A:784:GLN:HE22	2:C:25:GLY:HA2	1.71	0.55
2:C:65:LYS:HG3	2:C:141:TYR:HB3	1.88	0.55
1:A:1096:ALA:HB3	1:A:1103:ARG:HG3	1.88	0.55
2:C:54:LYS:O	2:C:61:ARG:NH1	2.40	0.55
1:A:272:ILE:HD11	6:A:1502:Y01:HAQ2	1.89	0.54
1:A:431:ARG:NH2	1:A:1131:GLY:O	2.39	0.54
1:A:737:PRO:HA	1:A:740:LYS:HB2	1.90	0.54
1:A:879:GLN:NE2	1:A:950:ARG:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:VAL:HG12	2:C:148:ILE:HG22	1.88	0.53
1:A:523:PHE:HA	1:A:526:ARG:HE	1.74	0.52
1:A:486:ASN:ND2	1:A:559:ALA:O	2.44	0.51
1:A:560:LEU:HB3	1:A:1073:VAL:HG21	1.93	0.51
3:G:147:LEU:HD12	3:G:148:PRO:HD2	1.93	0.50
2:C:158:TYR:HB3	2:C:181:ILE:HD11	1.93	0.50
1:A:845:LEU:HG	1:A:873:ALA:HB2	1.93	0.50
1:A:475:LEU:HD21	1:A:493:LEU:HD23	1.94	0.50
1:A:526:ARG:HD2	1:A:590:LEU:HD21	1.94	0.49
1:A:99:PHE:HE1	1:A:573:PHE:HD1	1.62	0.48
1:A:833:MET:HG3	1:A:835:LEU:H	1.78	0.48
1:A:221:PRO:HG3	1:A:332:ILE:HB	1.95	0.48
1:A:910:TYR:HE1	1:A:958:ILE:HG13	1.79	0.47
2:C:84:ILE:O	3:G:195:ASN:ND2	2.47	0.47
1:A:279:HIS:HB3	1:A:282:MET:HB2	1.97	0.47
1:A:250:ASP:OD1	1:A:250:ASP:N	2.48	0.47
1:A:521:ILE:O	1:A:526:ARG:NH2	2.48	0.46
1:A:139:GLU:HG3	1:A:358:THR:HG21	1.97	0.46
1:A:361:GLN:HE22	2:C:33:ARG:H	1.64	0.46
1:A:391:ARG:NH1	1:A:419:ASP:OD2	2.49	0.46
1:A:168:HIS:NE2	1:A:352:THR:OG1	2.38	0.45
1:A:846:GLN:HE22	1:A:896:ARG:HG2	1.81	0.45
1:A:361:GLN:NE2	2:C:33:ARG:H	2.15	0.45
1:A:263:LEU:HD21	3:G:54:GLN:HG2	2.00	0.44
1:A:1099:ASP:O	1:A:1103:ARG:N	2.42	0.44
1:A:240:GLY:HA3	3:G:49:TRP:HD1	1.82	0.44
2:C:44:TYR:HE1	2:C:177:SER:HA	1.82	0.44
5:C:201:CLR:H162	5:C:201:CLR:H221	1.62	0.44
1:A:958:ILE:HG21	1:A:961:VAL:HG22	1.99	0.44
1:A:834:TRP:CE2	1:A:961:VAL:HG11	2.53	0.44
5:A:1501:CLR:H213	5:A:1501:CLR:H231	1.88	0.44
5:C:201:CLR:H193	5:C:201:CLR:H111	1.78	0.44
1:A:255:LEU:HD11	1:A:272:ILE:HD12	1.99	0.43
1:A:519:LYS:HA	1:A:526:ARG:HH12	1.84	0.43
1:A:852:GLU:HG3	1:A:870:ALA:HB2	1.99	0.43
1:A:284:ARG:HA	1:A:285:PRO:HD3	1.91	0.42
1:A:215:PRO:HG3	1:A:320:LEU:HD23	2.01	0.42
1:A:1029:PHE:HB2	1:A:1046:VAL:HG21	2.01	0.42
3:G:219:LEU:O	3:G:236:LYS:NZ	2.46	0.42
2:C:114:MET:HG3	3:G:108:HIS:CE1	2.55	0.41
1:A:487:ALA:HB3	10:C:205:PLM:HD1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD12	1:A:461:LEU:HG	2.03	0.41
1:A:320:LEU:HD13	1:A:320:LEU:HA	1.93	0.41
1:A:427:VAL:HG11	5:A:1501:CLR:H111	2.02	0.41
1:A:767:LEU:HD22	2:C:24:CYS:HB3	2.03	0.41
1:A:1014:ARG:NH1	1:A:1067:LEU:HD23	2.36	0.41
1:A:445:LEU:HD13	1:A:448:LEU:HD21	2.02	0.41
1:A:794:TYR:OH	2:C:29:GLY:O	2.29	0.41
1:A:150:GLN:HB2	1:A:409:VAL:HG12	2.03	0.40
3:G:52:LEU:HA	3:G:125:LEU:HD21	2.03	0.40
1:A:183:TYR:CZ	1:A:381:LYS:HG3	2.56	0.40
1:A:229:ALA:HB2	1:A:281:TYR:CG	2.56	0.40
1:A:887:ILE:HG12	1:A:889:LEU:H	1.86	0.40
1:A:823:LEU:HD13	1:A:968:ASN:HD22	1.86	0.40
5:C:201:CLR:H183	5:C:201:CLR:H20	1.90	0.40
1:A:825:GLU:HB3	1:A:826:GLY:H	1.79	0.40
5:A:1501:CLR:H162	5:A:1501:CLR:H221	1.83	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	970/1205 (80%)	913 (94%)	56 (6%)	1 (0%)	48	79
2	C	167/192 (87%)	159 (95%)	8 (5%)	0	100	100
3	G	154/282 (55%)	145 (94%)	9 (6%)	0	100	100
All	All	1291/1679 (77%)	1217 (94%)	73 (6%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	933	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	828/1027 (81%)	825 (100%)	3 (0%)	89	95
2	C	142/157 (90%)	141 (99%)	1 (1%)	81	90
3	G	138/209 (66%)	136 (99%)	2 (1%)	62	80
All	All	1108/1393 (80%)	1102 (100%)	6 (0%)	85	93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	A	760	ARG
1	A	961	VAL
2	C	33	ARG
3	G	66	ASN
3	G	117	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	326	HIS
1	A	361	GLN
1	A	369	HIS
1	A	378	ASN
1	A	407	GLN
1	A	784	GLN
1	A	846	GLN
1	A	940	HIS
1	A	1110	HIS
2	C	35	HIS
2	C	100	GLN
3	G	195	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 ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	B	1	4,1	14,14,15	0.38	0	17,19,21	0.52	0
4	NAG	B	2	4	14,14,15	0.43	0	17,19,21	1.02	1 (5%)
4	NAG	D	1	4,1	14,14,15	0.47	0	17,19,21	0.71	0
4	NAG	D	2	4	14,14,15	0.45	0	17,19,21	0.44	0
4	NAG	E	1	4,3	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	E	2	4	14,14,15	0.43	0	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C2-N2-C7	3.33	127.36	122.90
4	E	2	NAG	C2-N2-C7	3.24	127.24	122.90

There are no chirality outliers.

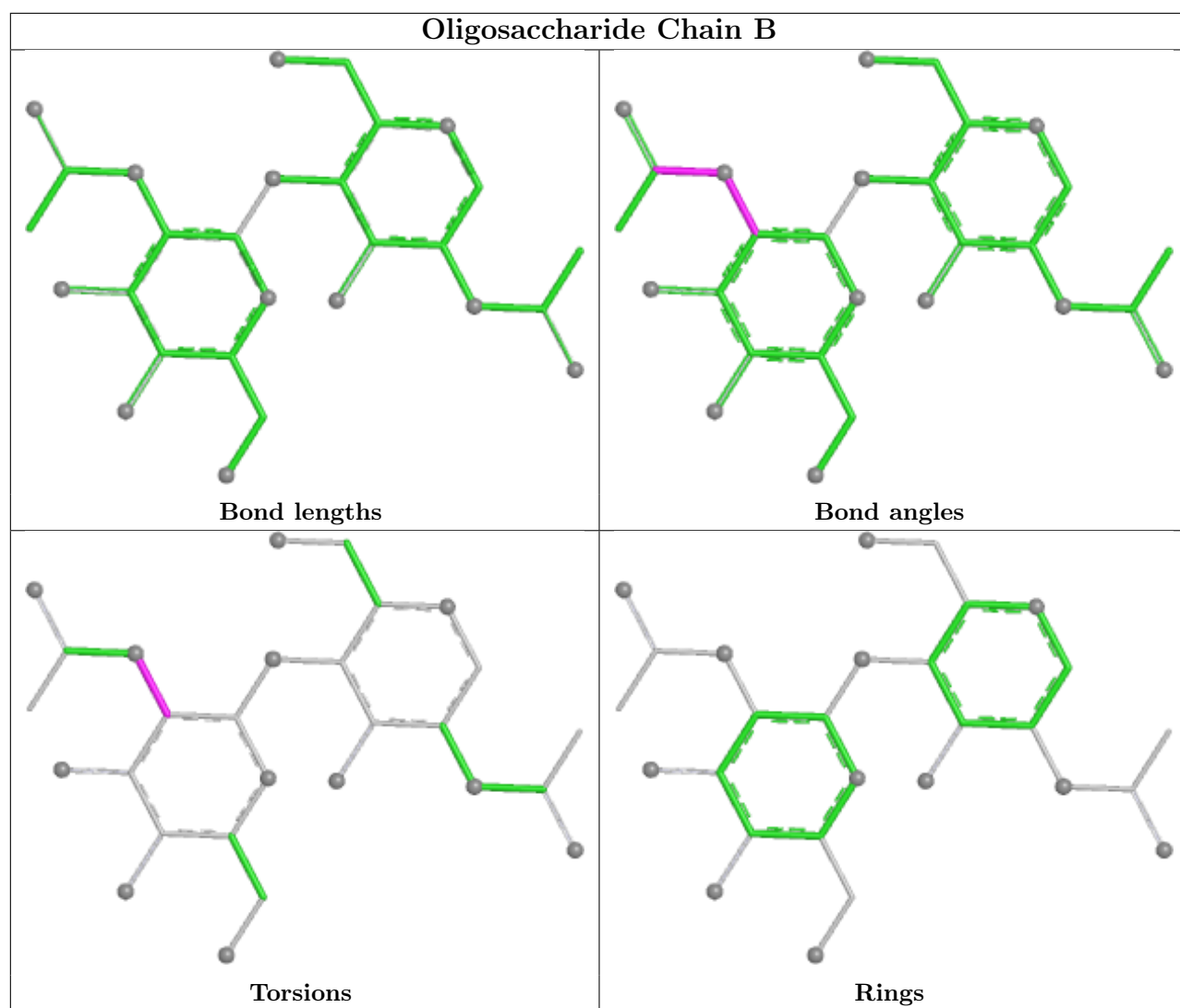
All (10) torsion outliers are listed below:

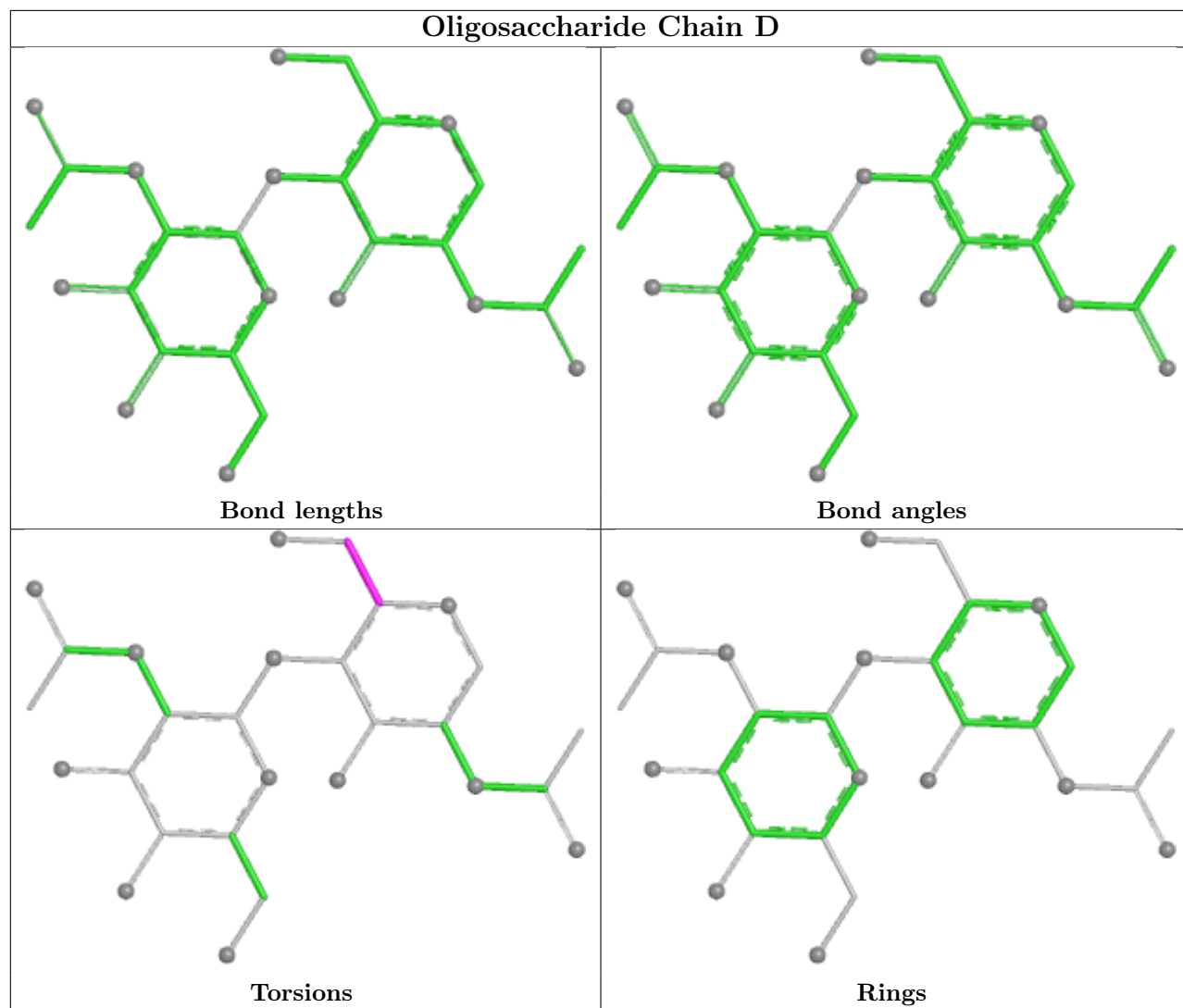
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

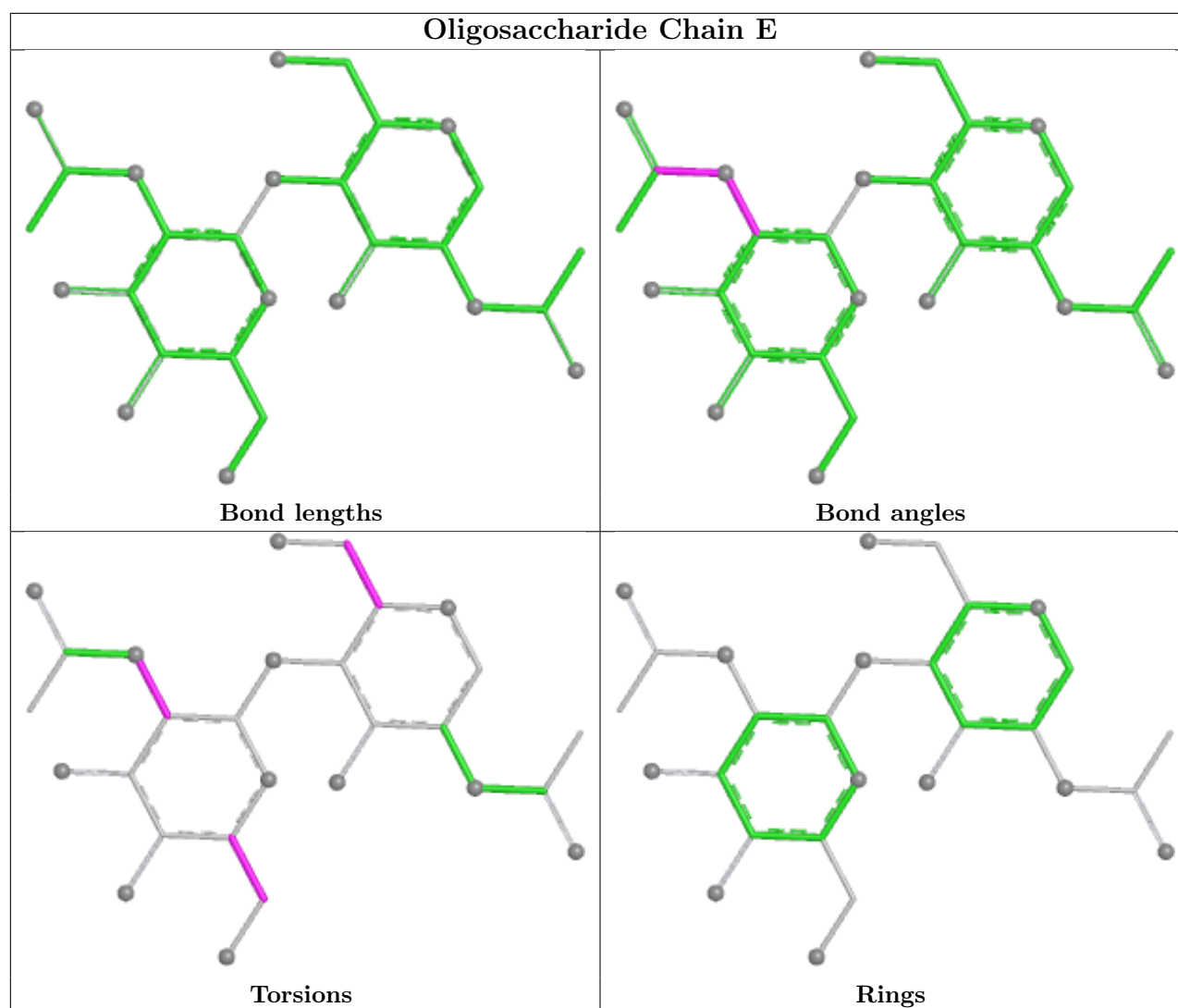
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
7	NAG	A	1503	1	14,14,15	0.46	0	17,19,21	0.47	0
7	NAG	A	1504	1	14,14,15	0.68	0	17,19,21	0.63	0
10	PLM	C	205	2	15,16,17	0.26	0	14,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	Y01	A	1502	-	38,38,38	1.10	2 (5%)	57,57,57	1.63	9 (15%)
5	CLR	C	201	2	31,31,31	0.63	0	48,48,48	1.27	7 (14%)
5	CLR	A	1501	-	31,31,31	0.61	0	48,48,48	1.12	3 (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
7	NAG	A	1503	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1504	1	-	4/6/23/26	0/1/1/1
10	PLM	C	205	2	-	6/14/14/15	-
6	Y01	A	1502	-	-	5/19/77/77	0/4/4/4
5	CLR	C	201	2	-	8/10/68/68	0/4/4/4
5	CLR	A	1501	-	-	5/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1502	Y01	OAW-CAY	4.06	1.45	1.34
6	A	1502	Y01	CBI-CBG	-2.12	1.51	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	Y01	CAV-CAZ-CBH	5.23	123.11	116.42
6	A	1502	Y01	OAW-CAY-CAM	4.03	120.19	111.48
6	A	1502	Y01	CBD-CAK-CAI	-3.41	108.04	112.76
6	A	1502	Y01	CAR-CBC-CAV	-3.31	106.37	110.97
5	C	201	CLR	C8-C7-C6	-3.29	108.21	112.76
6	A	1502	Y01	CAK-CAI-CAZ	-3.11	119.76	125.02
5	A	1501	CLR	C18-C13-C17	-2.59	106.97	111.68
6	A	1502	Y01	CAC-CBB-CBE	2.49	116.62	112.88
5	A	1501	CLR	C4-C5-C10	2.45	119.56	116.42
6	A	1502	Y01	CAV-CAZ-CAI	-2.40	117.31	120.57
6	A	1502	Y01	CBH-CAZ-CAI	-2.34	119.52	122.93
6	A	1502	Y01	CAK-CBD-CBG	-2.22	107.78	110.93
5	C	201	CLR	C17-C13-C14	2.18	102.61	100.10
5	C	201	CLR	C13-C17-C20	-2.15	116.18	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1501	CLR	C17-C13-C14	2.14	102.55	100.10
5	C	201	CLR	C22-C20-C17	2.11	114.70	110.33
5	C	201	CLR	C10-C9-C8	-2.08	109.68	112.71
5	C	201	CLR	C12-C11-C9	2.07	116.65	113.14
5	C	201	CLR	C9-C10-C5	2.01	112.59	109.65

There are no chirality outliers.

All (29) torsion outliers are listed below:

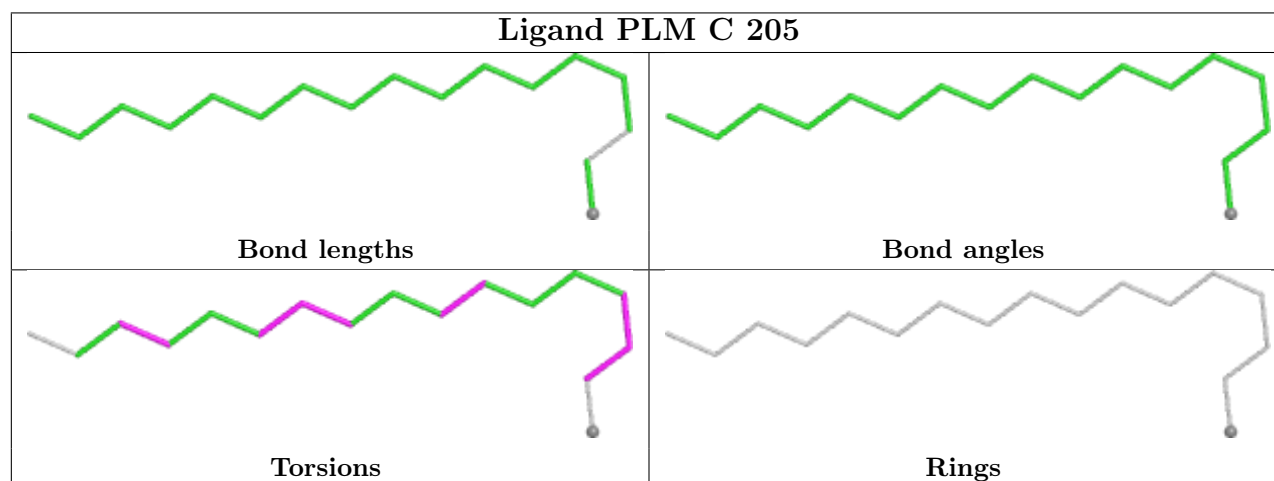
Mol	Chain	Res	Type	Atoms
10	C	205	PLM	O2-C1-C2-C3
10	C	205	PLM	C1-C2-C3-C4
5	C	201	CLR	C13-C17-C20-C22
5	C	201	CLR	C21-C20-C22-C23
5	C	201	CLR	C17-C20-C22-C23
5	A	1501	CLR	C17-C20-C22-C23
7	A	1504	NAG	C8-C7-N2-C2
7	A	1504	NAG	O7-C7-N2-C2
7	A	1504	NAG	O5-C5-C6-O6
6	A	1502	Y01	CAO-CAJ-CAN-CBA
5	C	201	CLR	C20-C22-C23-C24
5	A	1501	CLR	C20-C22-C23-C24
5	C	201	CLR	C16-C17-C20-C22
10	C	205	PLM	CC-CD-CE-CF
5	C	201	CLR	C13-C17-C20-C21
5	C	201	CLR	C16-C17-C20-C21
10	C	205	PLM	C9-CA-CB-CC
5	A	1501	CLR	C13-C17-C20-C22
6	A	1502	Y01	CAN-CAJ-CAO-CBB
6	A	1502	Y01	CAJ-CAO-CBB-CBE
5	A	1501	CLR	C13-C17-C20-C21
5	A	1501	CLR	C16-C17-C20-C22
7	A	1503	NAG	C4-C5-C6-O6
5	C	201	CLR	C22-C23-C24-C25
10	C	205	PLM	C8-C9-CA-CB
6	A	1502	Y01	CAM-CAL-CAX-OAH
6	A	1502	Y01	CAM-CAL-CAX-OAF
7	A	1504	NAG	C4-C5-C6-O6
10	C	205	PLM	C5-C6-C7-C8

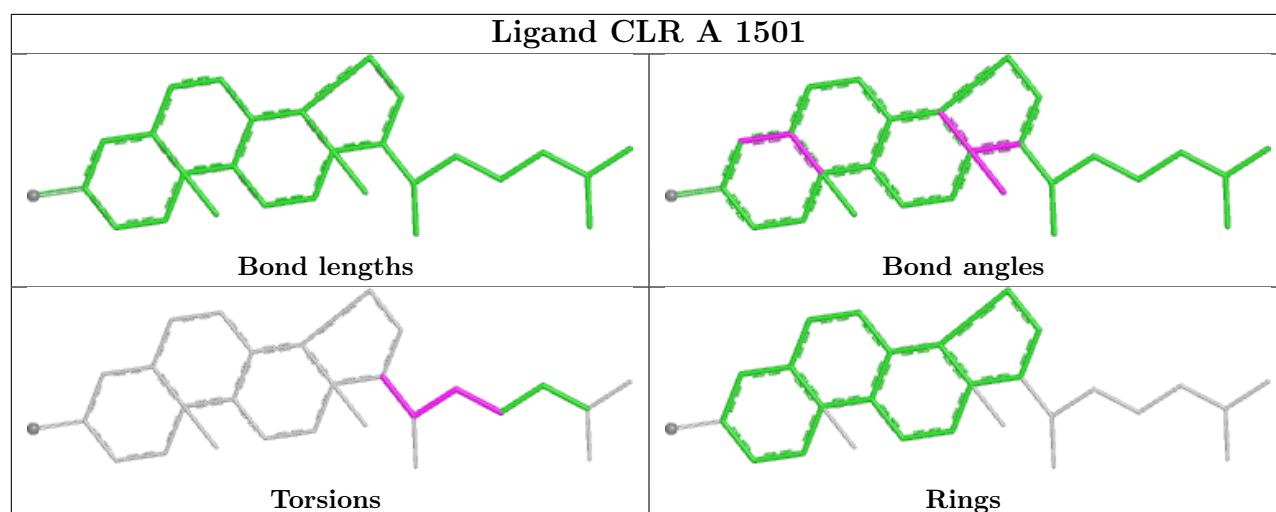
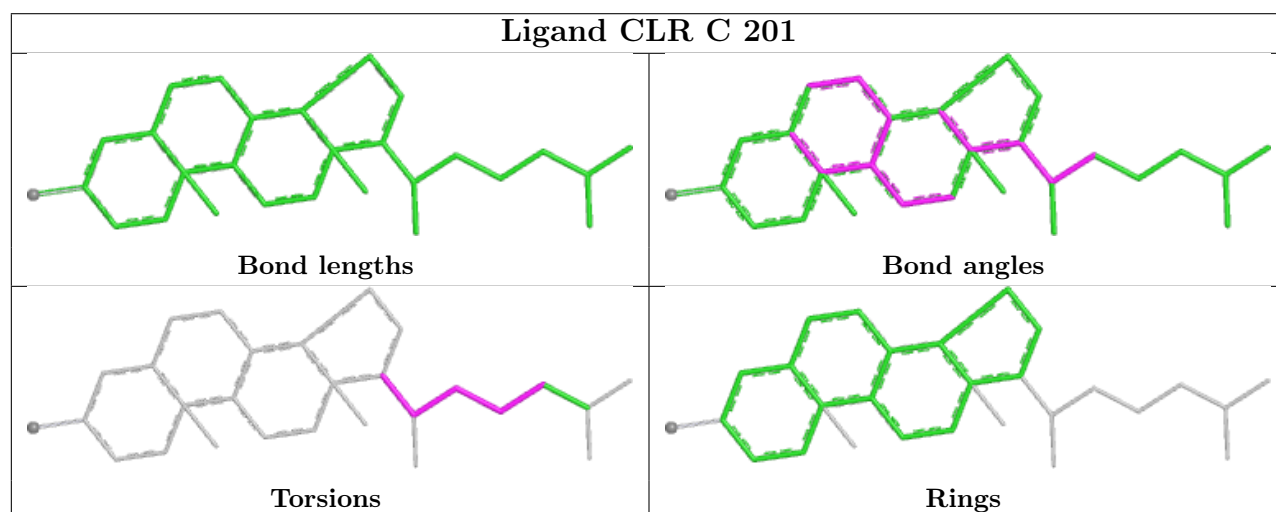
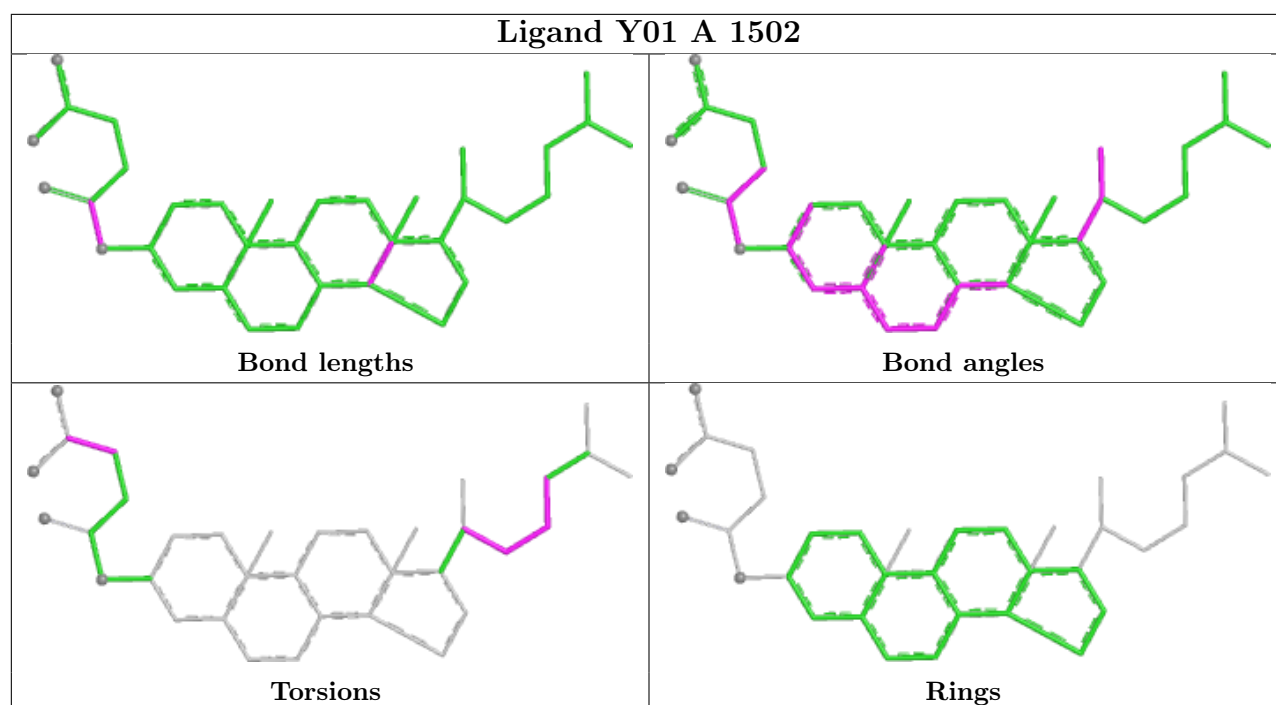
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	205	PLM	1	0
6	A	1502	Y01	1	0
5	C	201	CLR	3	0
5	A	1501	CLR	3	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

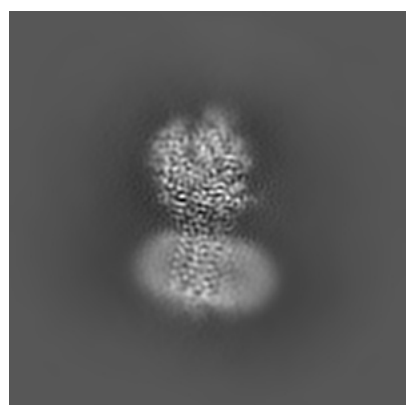
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24466. These allow visual inspection of the internal detail of the map and identification of artifacts.

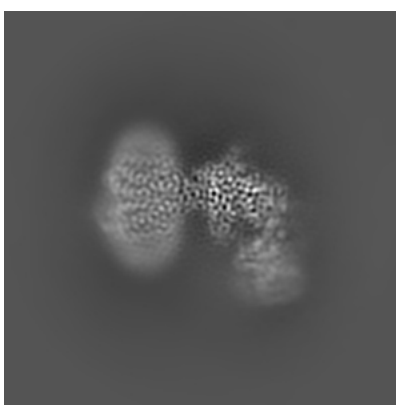
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

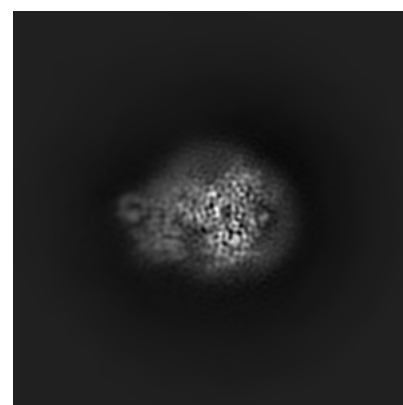
6.1.1 Primary map



X



Y



Z

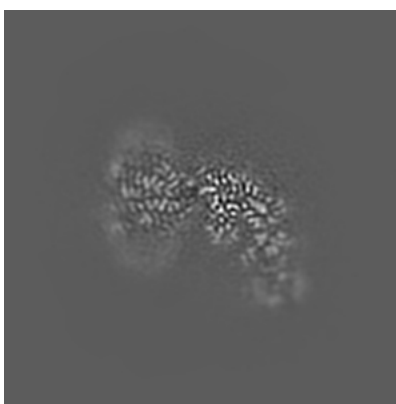
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

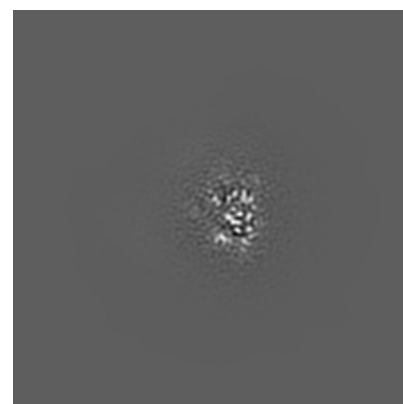
6.2.1 Primary map



X Index: 120



Y Index: 120

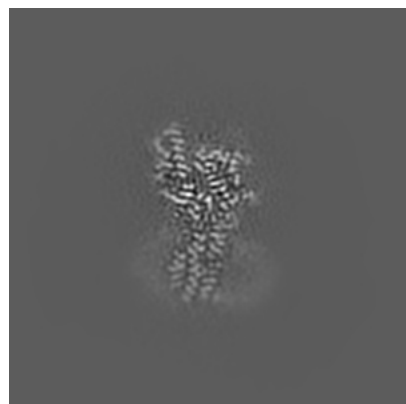


Z Index: 120

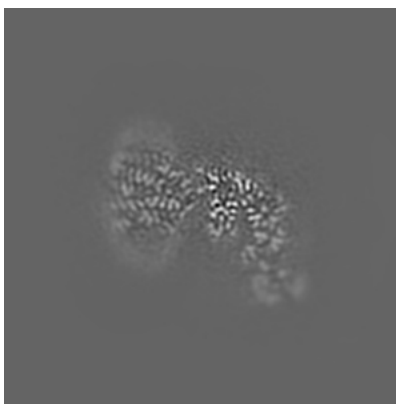
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

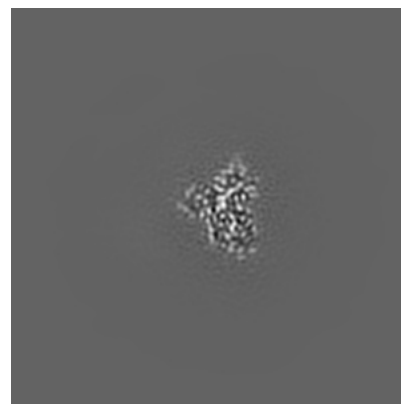
6.3.1 Primary map



X Index: 132



Y Index: 119

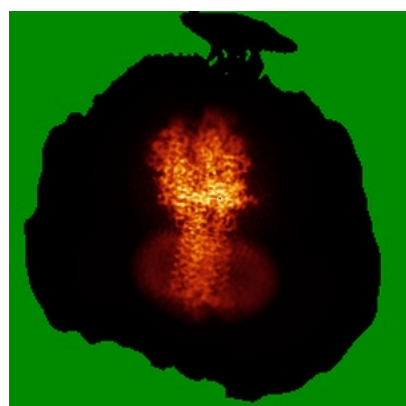


Z Index: 127

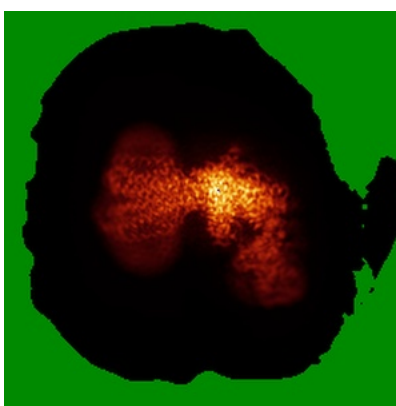
The images above show the largest variance slices of the map in three orthogonal directions.

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

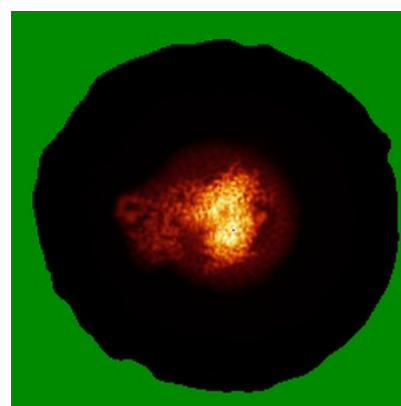
6.4.1 Primary map



X



Y

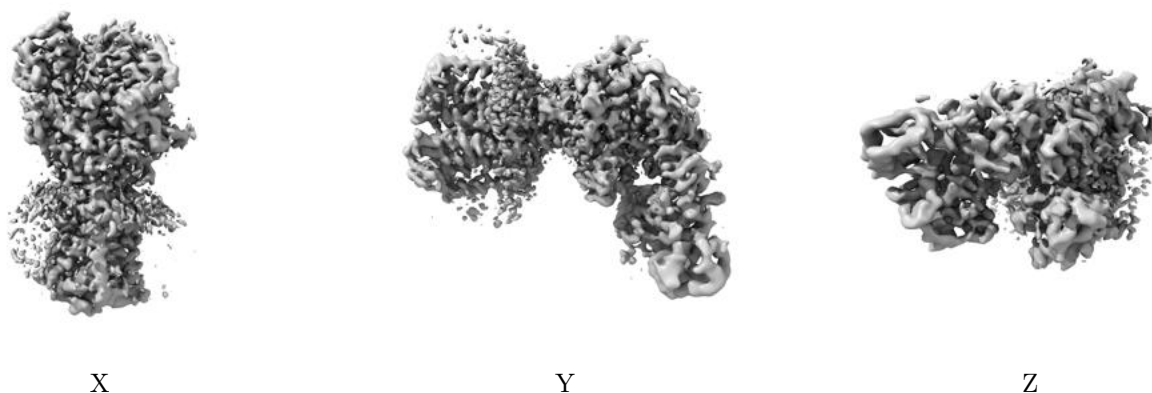


Z

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

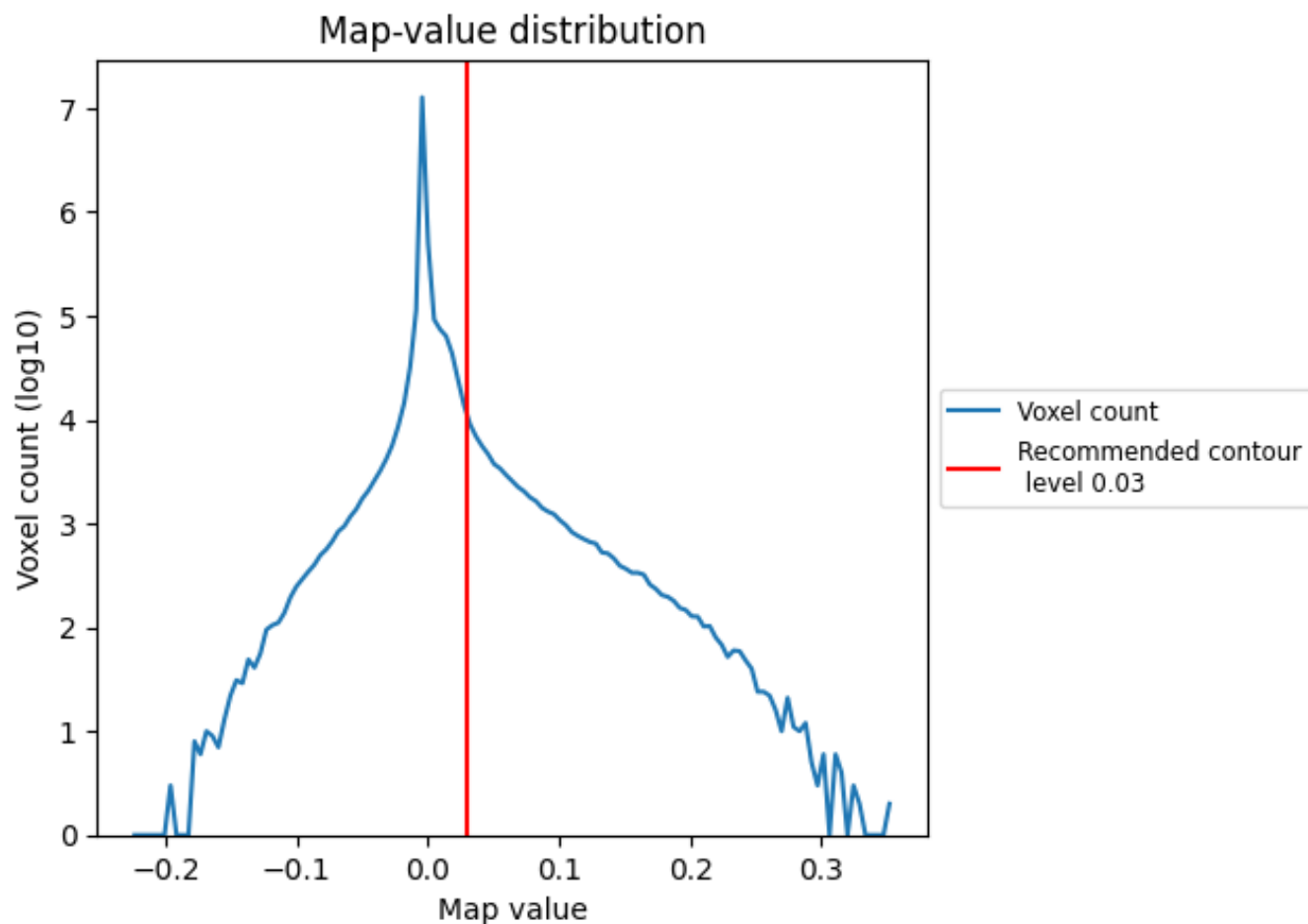
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

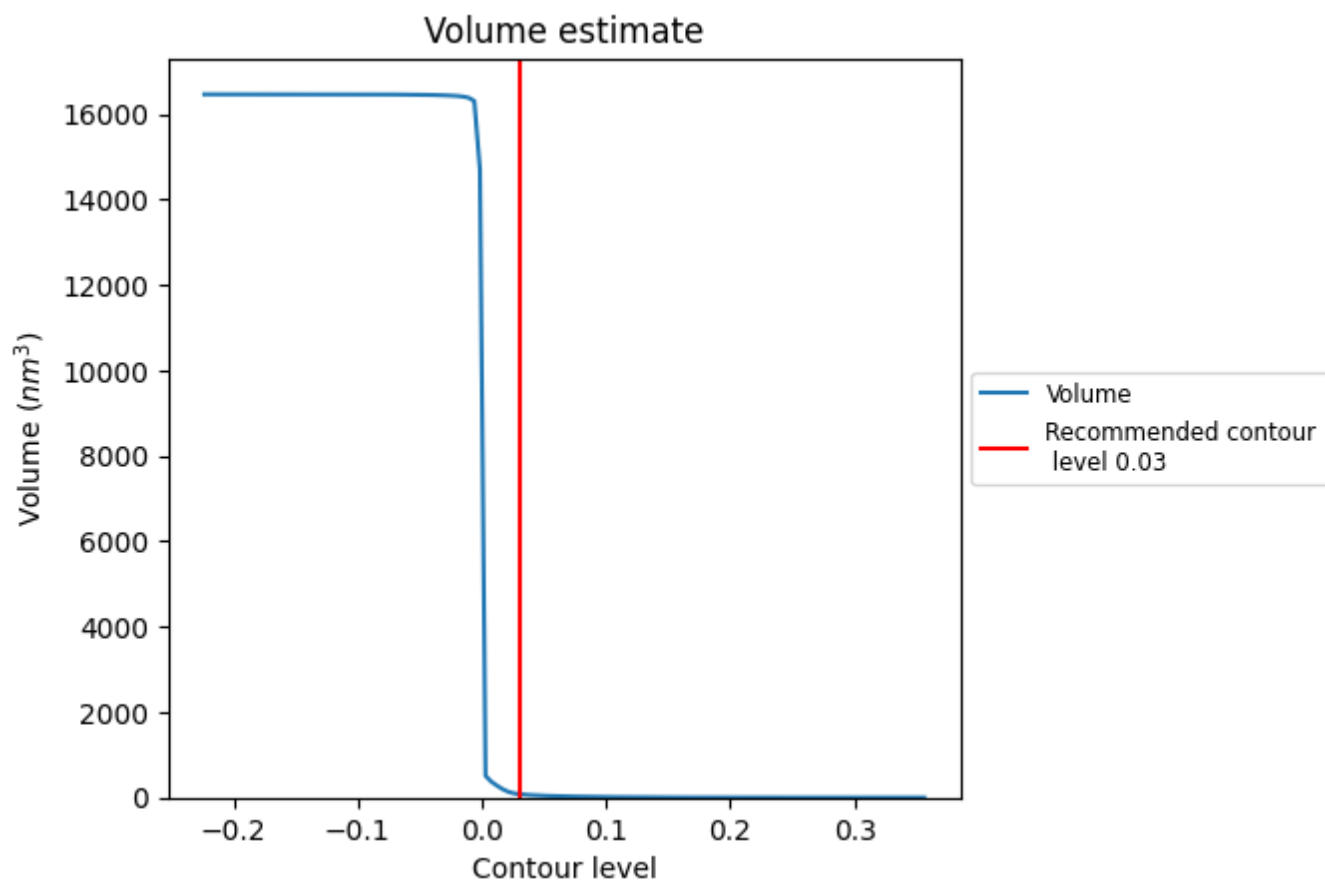
This section contains the results of statistical analysis of the map.

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.

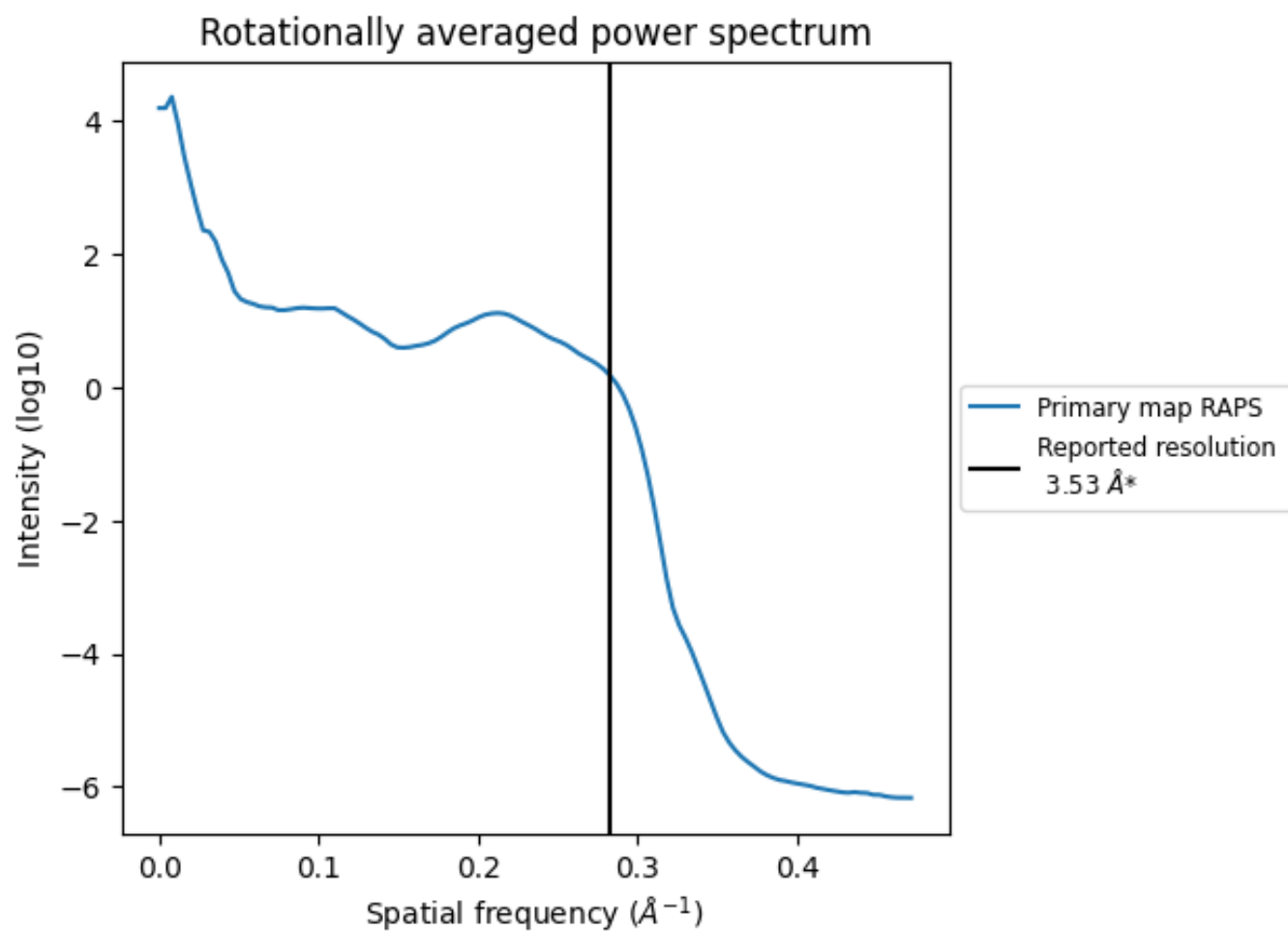
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 73 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 0.283 Å⁻¹

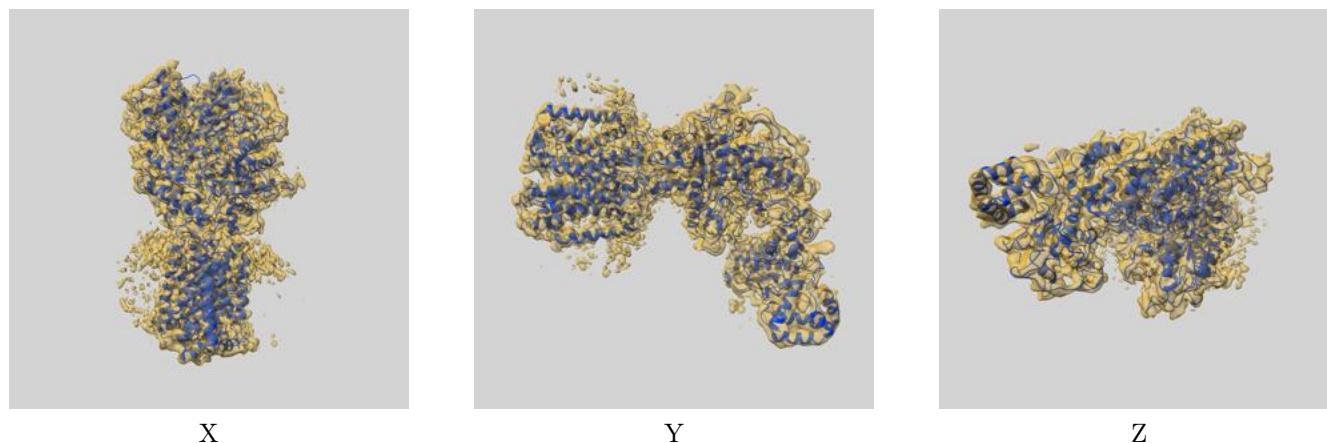
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

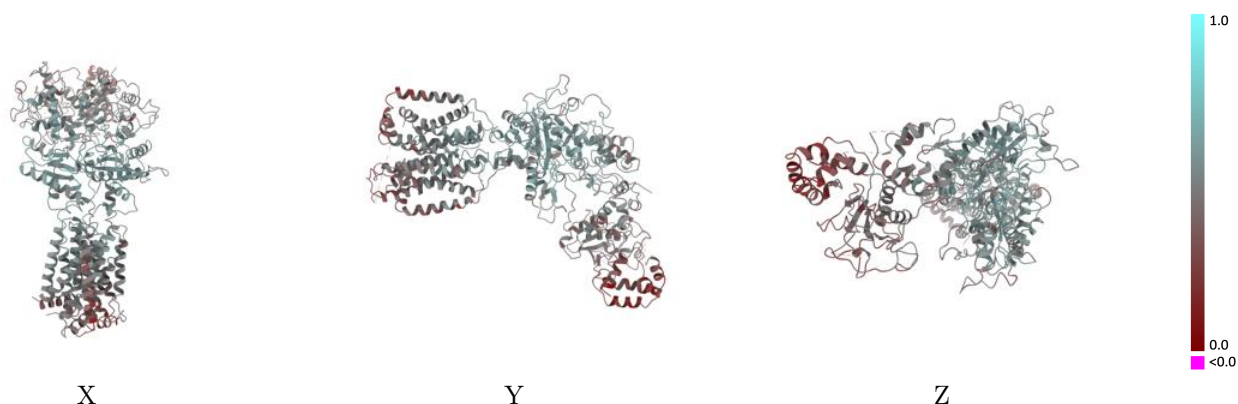
This section contains information regarding the fit between EMDB map EMD-24466 and PDB model 7RHQ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



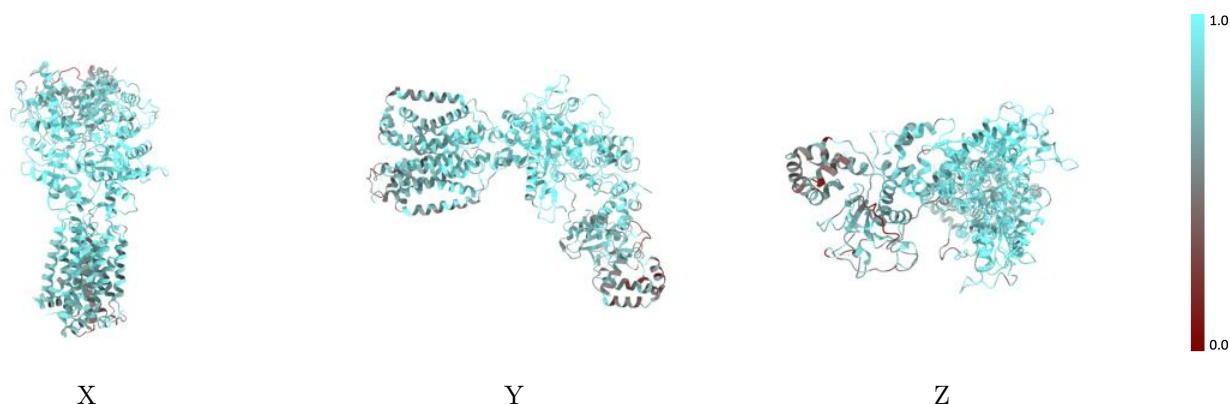
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



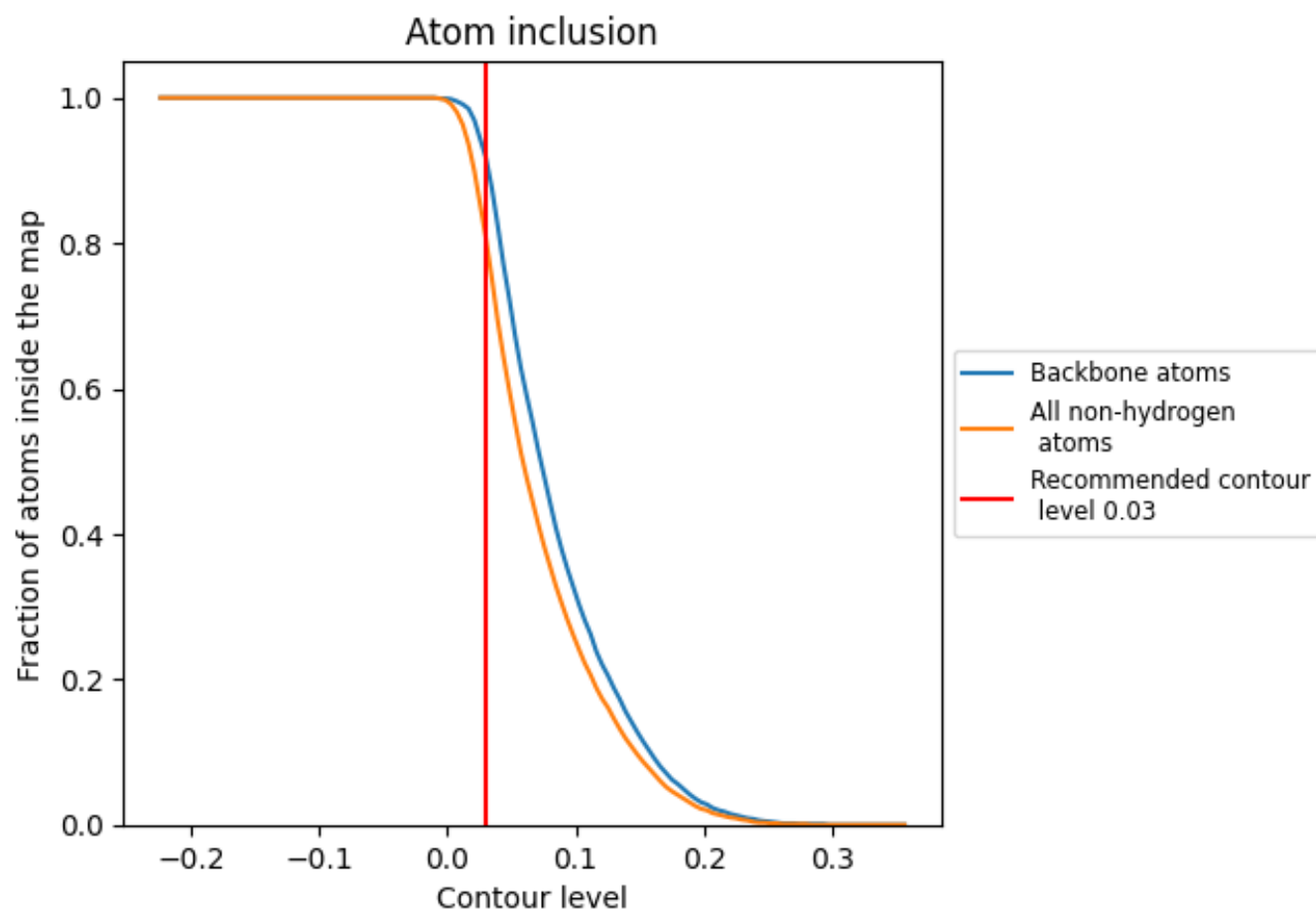
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8070</div>	<div><div></div>0.4710</div>
A	<div><div></div>0.8460</div>	<div><div></div>0.5000</div>
B	<div><div></div>0.6790</div>	<div><div></div>0.5240</div>
C	<div><div></div>0.6900</div>	<div><div></div>0.4060</div>
D	<div><div></div>0.8570</div>	<div><div></div>0.5070</div>
E	<div><div></div>0.6070</div>	<div><div></div>0.4530</div>
G	<div><div></div>0.7010</div>	<div><div></div>0.3610</div>

1.0

0.0

<0.0