



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 06:16 PM JST

PDB ID : 7V6Z
EMDB ID : EMD-31754
Title : Cryo-EM structure of Patched1 (V1084A mutant) in lipid nanodisc, 3.64 angstrom (reprocessed with the dataset of 7dzp)
Authors : Luo, Y.; Zhao, Y.; Qu, Q.; Li, D.
Deposited on : 2021-08-20
Resolution : 3.64 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

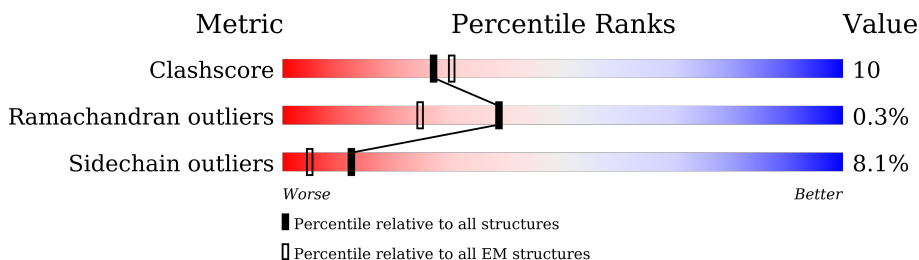
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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	1090	 50% 72% 19% 8%
2	B	2	 50% 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7082 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 Protein patched homolog 1, Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1008	6984	4559	1190	1203	32	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q61115
A	0	GLY	-	expression tag	UNP Q61115
A	1	SER	-	expression tag	UNP Q61115
A	1084	ALA	VAL	engineered mutation	UNP Q61115
A	1176	THR	-	expression tag	UNP Q61115
A	1177	LEU	-	expression tag	UNP Q61115
A	1178	GLU	-	expression tag	UNP Q61115
A	1179	VAL	-	expression tag	UNP Q61115
A	1180	LEU	-	expression tag	UNP Q61115
A	1181	PHE	-	expression tag	UNP Q61115
A	1182	GLN	-	expression tag	UNP Q61115
A	1183	GLY	-	expression tag	UNP Q61115

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



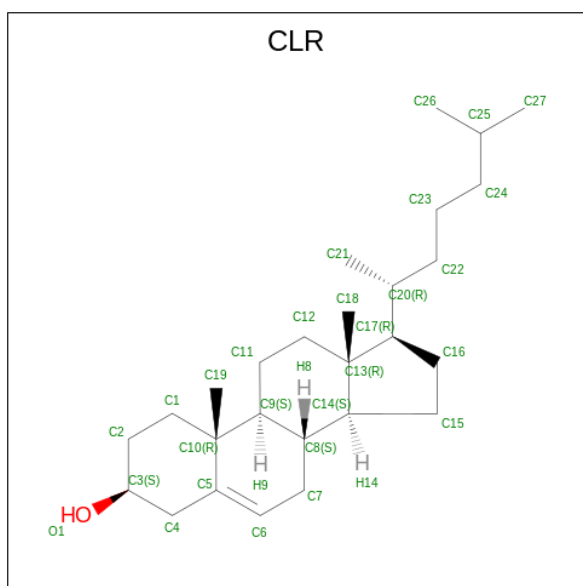
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

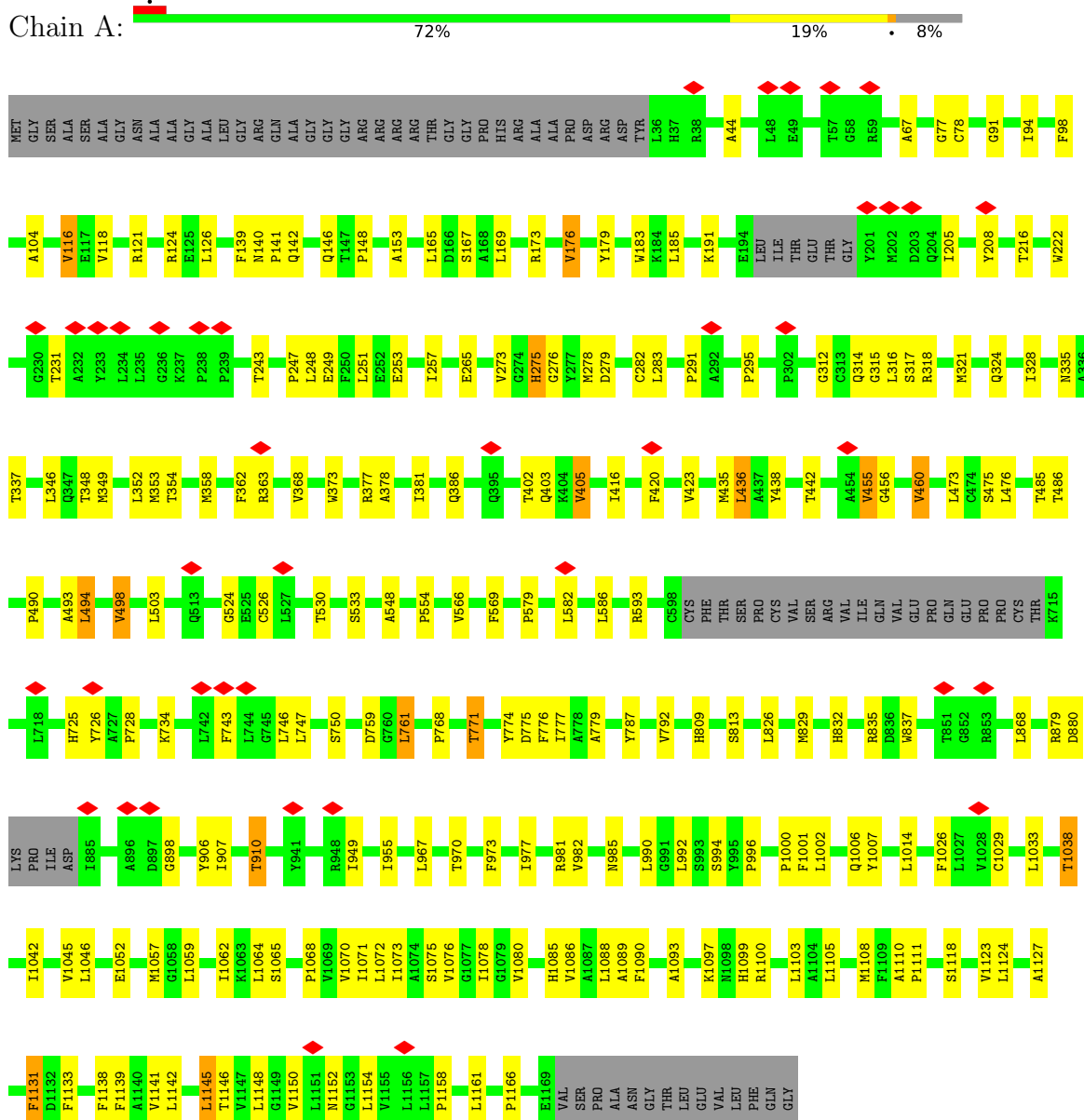


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	

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: Protein patched homolog 1, Protein patched homolog 1



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

Chain B:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	328720	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.899	Depositor
Minimum map value	-1.367	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.23	Depositor
Map size (\AA)	216.48, 216.48, 216.48	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/7147	0.75	0/9829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6984	0	6365	129	0
2	B	28	0	25	0	0
3	A	42	0	39	1	0
4	A	28	0	46	2	0
All	All	7082	0	6475	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (131) 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:141:PRO:HB3	1:A:349:MET:CE	1.60	1.30
1:A:141:PRO:CB	1:A:349:MET:HE2	1.88	1.02
1:A:141:PRO:HB3	1:A:349:MET:HE2	0.96	0.95
1:A:179:TYR:HB3	1:A:377:ARG:HH21	1.35	0.91
1:A:743:PHE:HZ	1:A:1152:ASN:HA	1.35	0.88
1:A:436:LEU:HA	1:A:460:VAL:HG11	1.56	0.86
1:A:176:VAL:HG23	1:A:183:TRP:HB2	1.60	0.84
1:A:276:GLY:HA2	1:A:318:ARG:HH22	1.47	0.80
1:A:248:LEU:HD12	1:A:275:HIS:HB2	1.68	0.74
1:A:743:PHE:CZ	1:A:1152:ASN:HA	2.22	0.73
1:A:1093:ALA:HB2	1:A:1103:LEU:HD22	1.71	0.71
1:A:141:PRO:CB	1:A:349:MET:CE	2.56	0.68
1:A:179:TYR:HB3	1:A:377:ARG:NH2	2.09	0.67
1:A:146:GLN:HE21	1:A:405:VAL:HG12	1.58	0.67
1:A:141:PRO:HB3	1:A:349:MET:HE3	1.71	0.66
1:A:1123:VAL:HG12	1:A:1139:PHE:HD1	1.60	0.66
1:A:139:PHE:CD2	1:A:349:MET:HE1	2.33	0.64
1:A:726:TYR:HD2	1:A:1105:LEU:HD21	1.63	0.63
1:A:126:LEU:HD11	1:A:1002:LEU:HD11	1.80	0.63
1:A:317:SER:HB2	1:A:321:MET:HE2	1.80	0.63
1:A:139:PHE:HD2	1:A:349:MET:HE1	1.64	0.61
1:A:77:GLY:HA3	1:A:524:GLY:HA2	1.83	0.61
1:A:116:VAL:O	1:A:554:PRO:HD3	2.01	0.60
1:A:1154:LEU:O	1:A:1158:PRO:HD2	2.01	0.60
1:A:1029:CYS:HB2	1:A:1033:LEU:HD12	1.84	0.60
1:A:222:TRP:HB3	1:A:282:CYS:HA	1.83	0.60
1:A:278:MET:HA	1:A:291:PRO:HG3	1.84	0.60
1:A:1057:MET:HG3	1:A:1062:ILE:HB	1.84	0.59
1:A:247:PRO:HD2	1:A:275:HIS:H	1.67	0.58
1:A:813:SER:HB2	1:A:826:LEU:HD11	1.86	0.58
1:A:1123:VAL:HG12	1:A:1139:PHE:CD1	2.38	0.58
1:A:835:ARG:HH21	1:A:898:GLY:HA3	1.69	0.57
1:A:455:VAL:HG11	1:A:582:LEU:HD23	1.86	0.56
1:A:420:PHE:HA	1:A:1131:PHE:CZ	2.41	0.56
1:A:208:TYR:O	1:A:231:THR:HG21	2.06	0.55
1:A:222:TRP:CD1	1:A:291:PRO:HD3	2.42	0.55
1:A:423:VAL:HB	1:A:486:THR:HB	1.88	0.55
1:A:169:LEU:HB2	1:A:173:ARG:HH12	1.71	0.55
1:A:317:SER:H	1:A:321:MET:HE3	1.72	0.55
1:A:1046:LEU:HD21	1:A:1080:VAL:HA	1.88	0.55
1:A:148:PRO:HG2	1:A:153:ALA:HB3	1.87	0.54
1:A:761:LEU:HB2	1:A:1007:TYR:OH	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:ILE:HG21	1:A:1141:VAL:HB	1.90	0.54
1:A:276:GLY:HA2	1:A:318:ARG:NH2	2.22	0.53
1:A:1038:THR:O	1:A:1042:ILE:HG23	2.09	0.52
1:A:279:ASP:O	1:A:295:PRO:HD2	2.10	0.52
1:A:98:PHE:HE1	1:A:473:LEU:HD13	1.75	0.52
1:A:315:GLY:HA3	1:A:321:MET:HG3	1.93	0.51
1:A:548:ALA:HB1	1:A:1070:VAL:HG13	1.93	0.51
1:A:967:LEU:HD22	1:A:973:PHE:HA	1.92	0.51
1:A:1007:TYR:HE1	1:A:1065:SER:HA	1.74	0.51
1:A:792:VAL:O	1:A:994:SER:HA	2.11	0.50
1:A:1076:VAL:O	1:A:1080:VAL:HG23	2.11	0.50
1:A:1090:PHE:HE1	1:A:1166:PRO:HD2	1.77	0.50
1:A:317:SER:H	1:A:321:MET:CE	2.25	0.50
1:A:378:ALA:HA	1:A:381:ILE:HD12	1.93	0.50
1:A:503:LEU:HD21	1:A:530:THR:HB	1.93	0.49
1:A:416:ILE:HD12	1:A:768:PRO:HD2	1.94	0.49
1:A:1033:LEU:HD23	1:A:1088:LEU:HD12	1.94	0.49
1:A:829:MET:HG3	1:A:832:HIS:H	1.76	0.49
1:A:273:VAL:HG23	1:A:316:LEU:O	2.13	0.49
1:A:335:ASN:HD21	3:A:1202:NAG:H83	1.77	0.49
1:A:1148:LEU:O	1:A:1152:ASN:HB3	2.13	0.49
1:A:498:VAL:HG12	1:A:1118:SER:HB2	1.94	0.48
1:A:314:GLN:HB3	1:A:318:ARG:HA	1.95	0.48
1:A:787:TYR:HB3	1:A:1000:PRO:HD3	1.96	0.48
1:A:104:ALA:HB3	1:A:475:SER:HB3	1.95	0.48
1:A:248:LEU:CD1	1:A:275:HIS:HB2	2.40	0.48
1:A:456:GLY:O	1:A:460:VAL:HG12	2.13	0.48
1:A:1065:SER:HB2	1:A:1068:PRO:HD2	1.95	0.47
1:A:98:PHE:CE1	1:A:473:LEU:HD13	2.49	0.47
1:A:44:ALA:HB1	1:A:67:ALA:HA	1.96	0.47
1:A:253:GLU:O	1:A:257:ILE:HG12	2.14	0.47
1:A:435:MET:SD	1:A:494:LEU:HG	2.55	0.47
1:A:879:ARG:O	1:A:880:ASP:C	2.53	0.47
1:A:981:ARG:NH1	1:A:996:PRO:HD2	2.29	0.47
1:A:216:THR:HG22	1:A:348:THR:HG22	1.95	0.47
1:A:358:MET:HE2	1:A:358:MET:HB2	1.87	0.46
1:A:1071:ILE:HD11	1:A:1138:PHE:CD2	2.50	0.46
1:A:548:ALA:HA	1:A:1073:ILE:HD12	1.98	0.46
1:A:282:CYS:O	1:A:283:LEU:HB3	2.16	0.45
1:A:485:THR:O	1:A:490:PRO:HD3	2.16	0.45
1:A:1089:ALA:HB2	1:A:1108:MET:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:MET:HG2	1:A:378:ALA:HB1	1.99	0.45
1:A:725:HIS:O	1:A:728:PRO:HD2	2.17	0.45
1:A:183:TRP:HA	1:A:183:TRP:CE3	2.51	0.45
1:A:1075:SER:HB2	1:A:1145:LEU:HD13	1.99	0.45
1:A:746:LEU:HD12	1:A:746:LEU:HA	1.80	0.45
1:A:1078:ILE:HB	1:A:1145:LEU:HD21	1.99	0.44
1:A:1110:ALA:HB3	1:A:1111:PRO:HD3	1.99	0.44
1:A:247:PRO:HD2	1:A:275:HIS:N	2.32	0.44
1:A:438:TYR:O	1:A:442:THR:HG23	2.17	0.44
1:A:579:PRO:HA	1:A:582:LEU:HD12	1.98	0.44
1:A:977:ILE:HG13	1:A:1001:PHE:HD1	1.82	0.44
1:A:1124:LEU:HA	1:A:1139:PHE:CE1	2.52	0.44
1:A:222:TRP:NE1	1:A:243:THR:OG1	2.50	0.44
1:A:142:GLN:NE2	1:A:386:GLN:HG2	2.32	0.44
1:A:363:ARG:HA	1:A:368:VAL:HG21	1.99	0.44
4:A:1204:CLR:H222	4:A:1204:CLR:H162	1.60	0.43
1:A:91:GLY:O	1:A:94:ILE:N	2.52	0.43
1:A:121:ARG:HA	1:A:124:ARG:HE	1.84	0.43
1:A:312:GLY:HA2	1:A:328:ILE:HD12	2.00	0.43
1:A:251:LEU:HD13	1:A:265:GLU:HA	2.01	0.43
1:A:759:ASP:HB3	1:A:1007:TYR:CD1	2.54	0.43
1:A:191:LYS:NZ	1:A:208:TYR:HA	2.34	0.42
1:A:747:LEU:HD12	1:A:750:SER:HB3	2.02	0.42
1:A:1014:LEU:HD13	1:A:1064:LEU:HD21	2.01	0.42
1:A:1146:THR:O	1:A:1150:VAL:HG13	2.19	0.42
1:A:906:TYR:O	1:A:910:THR:HG22	2.19	0.42
1:A:1064:LEU:HD12	1:A:1068:PRO:HB2	2.02	0.42
1:A:353:MET:HB2	1:A:358:MET:HE2	2.02	0.41
1:A:1046:LEU:HD13	1:A:1080:VAL:HG22	2.02	0.41
1:A:1064:LEU:HD12	1:A:1064:LEU:HA	1.96	0.41
1:A:1097:LYS:HA	1:A:1100:ARG:HD3	2.02	0.41
1:A:328:ILE:O	1:A:346:LEU:HA	2.21	0.41
1:A:771:THR:O	1:A:774:TYR:HB3	2.21	0.41
1:A:776:PHE:O	1:A:779:ALA:N	2.54	0.41
4:A:1204:CLR:H183	4:A:1204:CLR:H20	1.74	0.41
1:A:324:GLN:OE1	1:A:324:GLN:N	2.52	0.41
1:A:533:SER:HB3	1:A:1085:HIS:CE1	2.56	0.41
1:A:1026:PHE:HA	1:A:1029:CYS:SG	2.61	0.41
1:A:750:SER:OG	1:A:1052:GLU:HA	2.21	0.41
1:A:1161:LEU:HD23	1:A:1161:LEU:HA	1.77	0.41
1:A:1071:ILE:HG21	1:A:1071:ILE:HD12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:HB3	1:A:352:LEU:O	2.21	0.40
1:A:493:ALA:HB1	1:A:566:VAL:HG11	2.03	0.40
1:A:907:ILE:O	1:A:910:THR:HG23	2.21	0.40
1:A:970:THR:HA	1:A:973:PHE:HD2	1.86	0.40
1:A:982:VAL:HA	1:A:985:ASN:ND2	2.36	0.40
1:A:1071:ILE:HG23	1:A:1071:ILE:HD13	1.60	0.40
1:A:249:GLU:O	1:A:253:GLU:HG2	2.20	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	1000/1090 (92%)	965 (96%)	32 (3%)	3 (0%)	37 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1127	ALA
1	A	205	ILE
1	A	949	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	595/916 (65%)	547 (92%)	48 (8%)	9	32

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	116	VAL
1	A	118	VAL
1	A	165	LEU
1	A	167	SER
1	A	176	VAL
1	A	185	LEU
1	A	275	HIS
1	A	337	THR
1	A	354	THR
1	A	362	PHE
1	A	373	TRP
1	A	402	THR
1	A	403	GLN
1	A	405	VAL
1	A	436	LEU
1	A	455	VAL
1	A	460	VAL
1	A	476	LEU
1	A	494	LEU
1	A	498	VAL
1	A	526	CYS
1	A	569	PHE
1	A	586	LEU
1	A	593	ARG
1	A	734	LYS
1	A	761	LEU
1	A	771	THR
1	A	775	ASP
1	A	777	ILE
1	A	809	HIS
1	A	837	TRP
1	A	868	LEU
1	A	910	THR
1	A	955	ILE
1	A	990	LEU
1	A	992	LEU
1	A	1006	GLN

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Mol	Chain	Res	Type
1	A	1038	THR
1	A	1045	VAL
1	A	1059	LEU
1	A	1072	LEU
1	A	1086	VAL
1	A	1099	HIS
1	A	1131	PHE
1	A	1133	PHE
1	A	1142	LEU
1	A	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	175	HIS
1	A	269	ASN
1	A	296	ASN
1	A	386	GLN
1	A	403	GLN
1	A	482	ASN
1	A	794	GLN
1	A	997	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 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	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.38	0	17,19,21	0.40	0
2	NAG	B	2	2	14,14,15	0.21	0	17,19,21	0.40	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
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

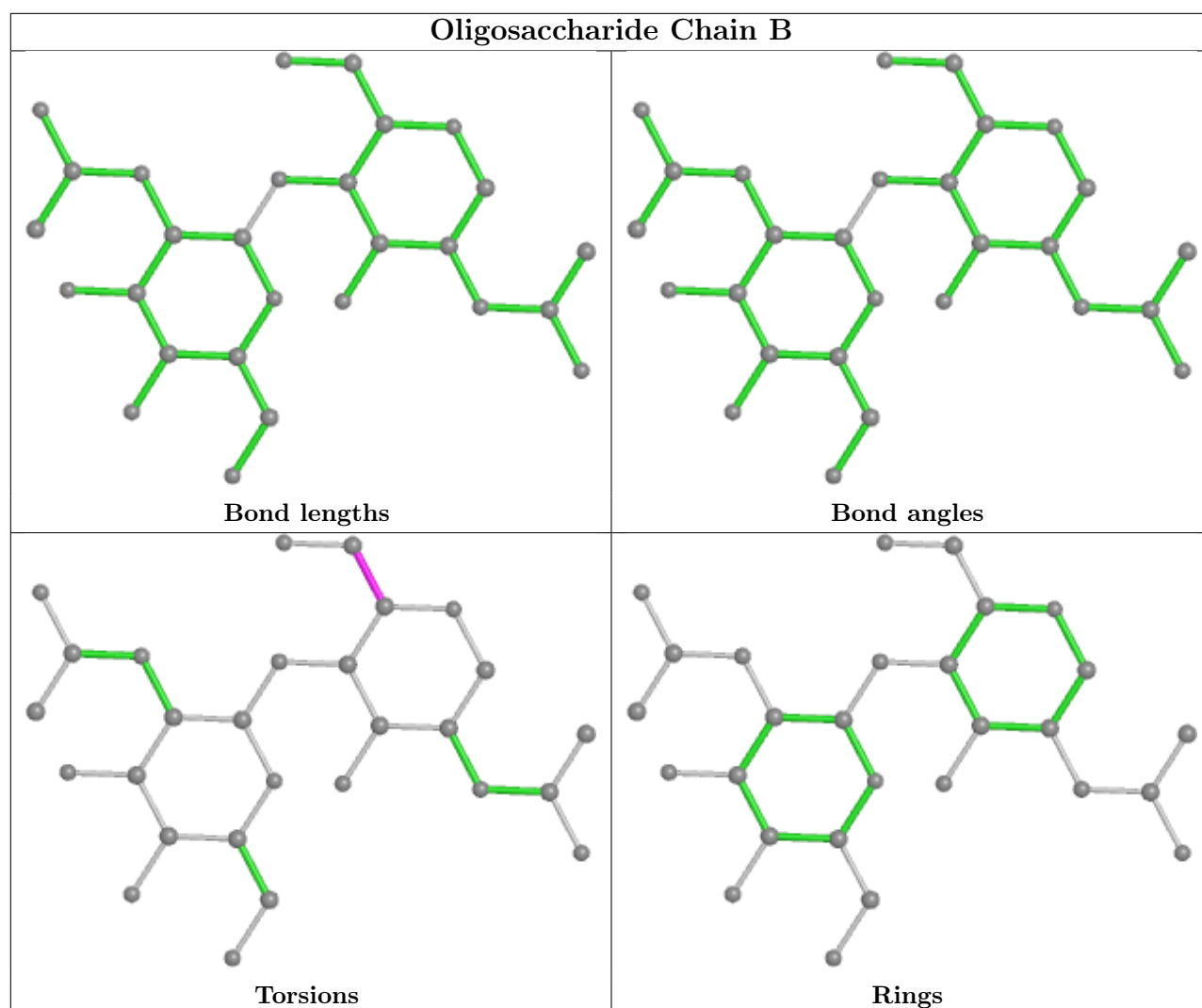
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

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](#)

4 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	$\# Z > 2$
4	CLR	A	1204	-	31,31,31	0.75	1 (3%)	48,48,48	1.35	7 (14%)
3	NAG	A	1201	1	14,14,15	0.24	0	17,19,21	0.38	0
3	NAG	A	1203	1	14,14,15	0.28	0	17,19,21	0.44	0
3	NAG	A	1202	1	14,14,15	0.30	0	17,19,21	0.41	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
4	CLR	A	1204	-	-	4/10/68/68	0/4/4/4
3	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1202	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1204	CLR	C10-C9	-2.01	1.52	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1204	CLR	C13-C17-C20	-3.79	113.55	119.49
4	A	1204	CLR	C13-C14-C8	-2.94	110.03	114.38
4	A	1204	CLR	C8-C7-C6	-2.87	108.61	112.73
4	A	1204	CLR	C17-C13-C14	2.79	103.38	100.07
4	A	1204	CLR	C19-C10-C9	-2.56	108.63	111.68
4	A	1204	CLR	C11-C9-C10	-2.54	109.74	113.08
4	A	1204	CLR	C3-C4-C5	-2.20	108.29	112.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

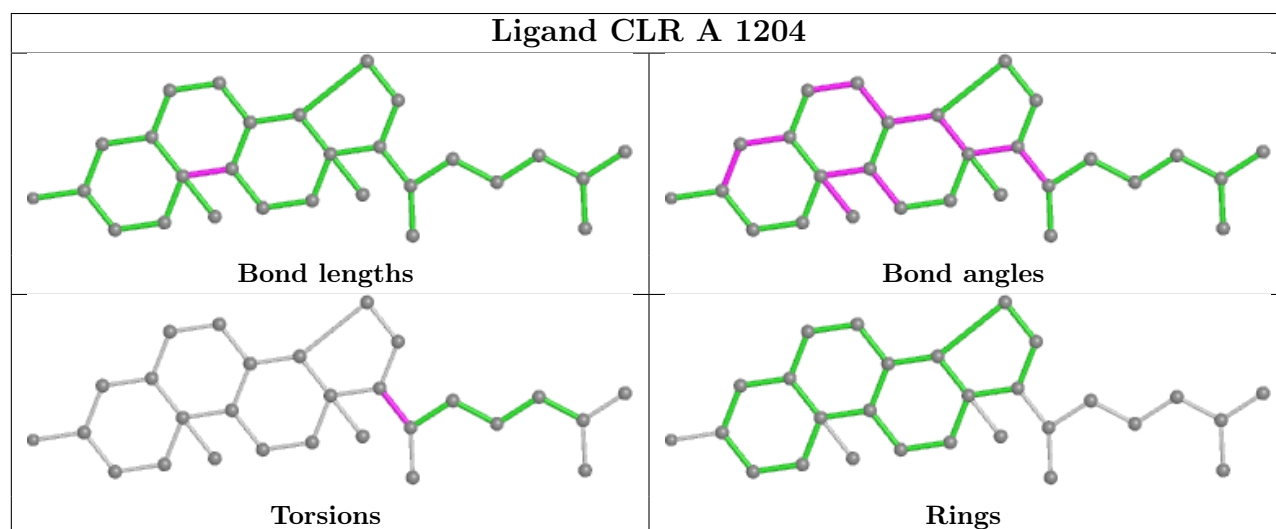
Mol	Chain	Res	Type	Atoms
4	A	1204	CLR	C13-C17-C20-C22
4	A	1204	CLR	C13-C17-C20-C21
3	A	1203	NAG	C4-C5-C6-O6
4	A	1204	CLR	C16-C17-C20-C21
3	A	1201	NAG	O5-C5-C6-O6
3	A	1203	NAG	O5-C5-C6-O6
3	A	1202	NAG	C8-C7-N2-C2
3	A	1202	NAG	O7-C7-N2-C2
4	A	1204	CLR	C16-C17-C20-C22
3	A	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

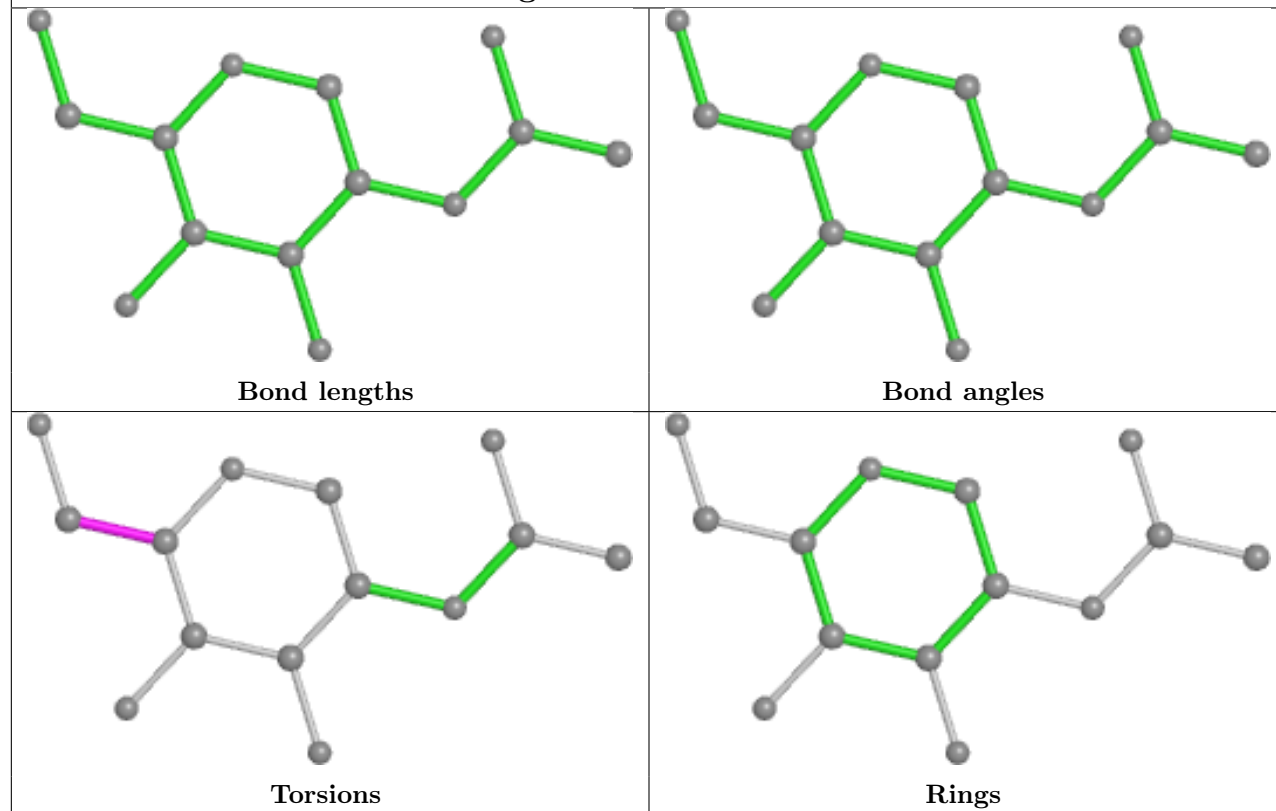
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1204	CLR	2	0
3	A	1202	NAG	1	0

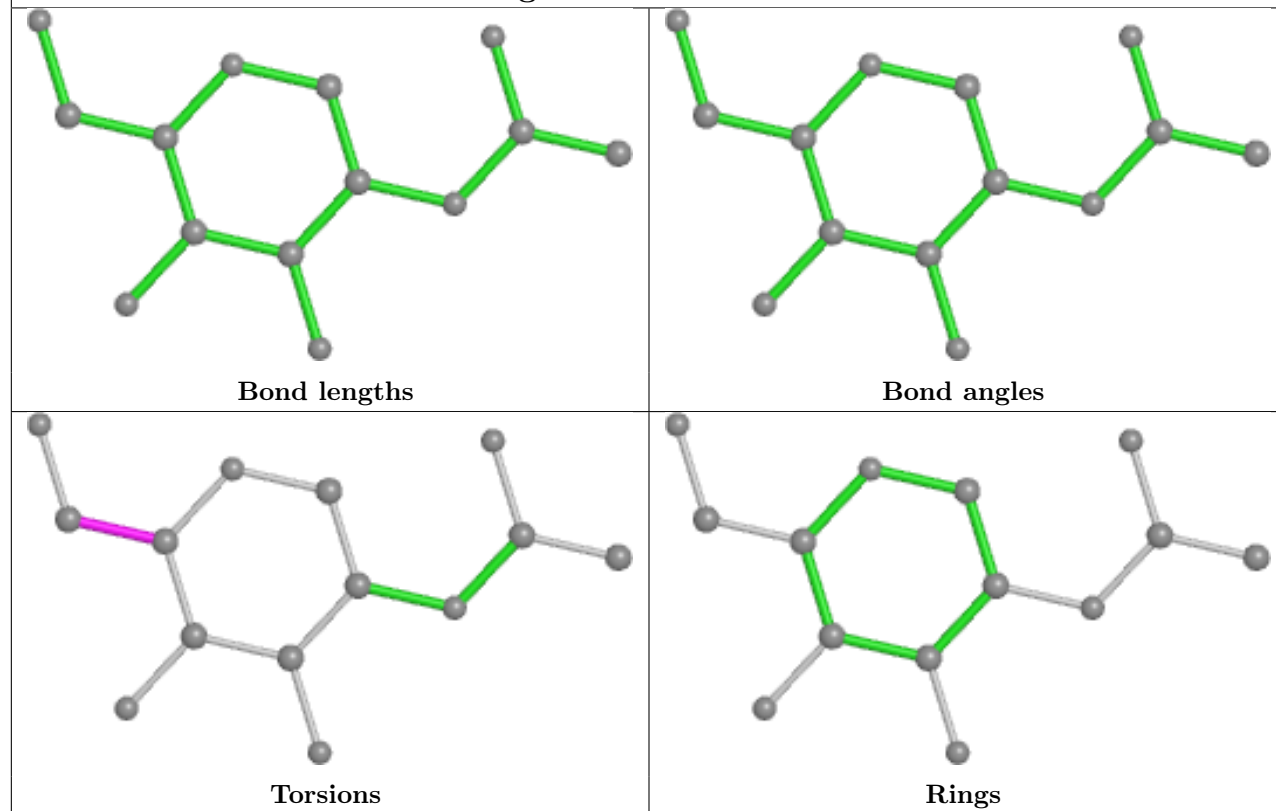
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

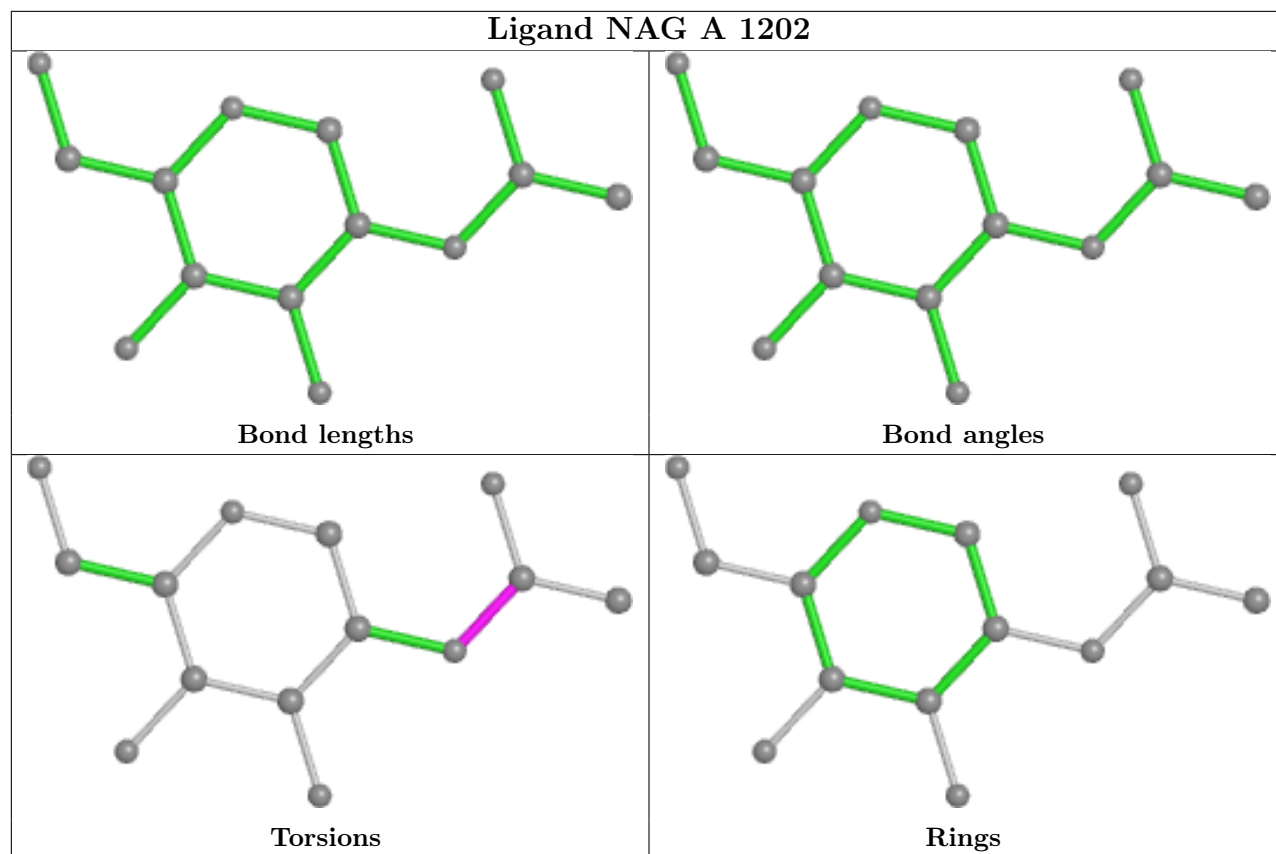


Ligand NAG A 1201



Ligand NAG A 1203





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.

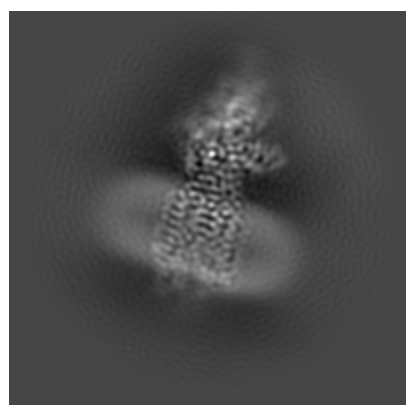
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31754. These allow visual inspection of the internal detail of the map and identification of artifacts.

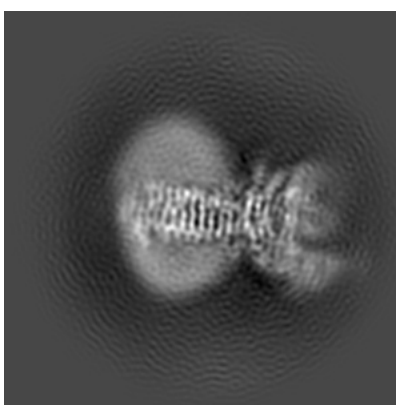
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

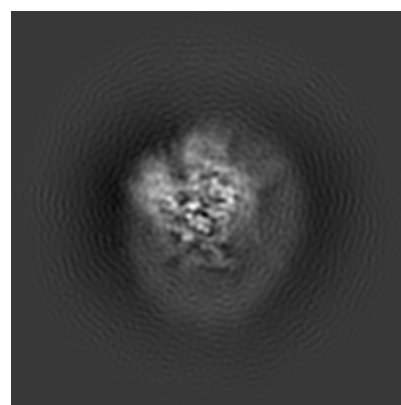
6.1.1 Primary map



X



Y

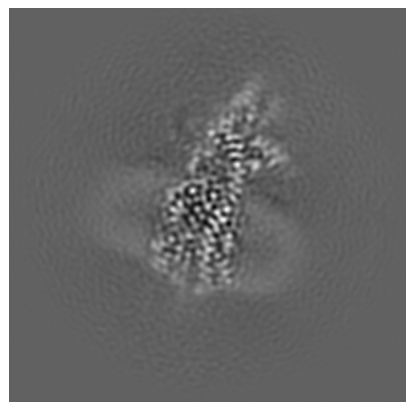


Z

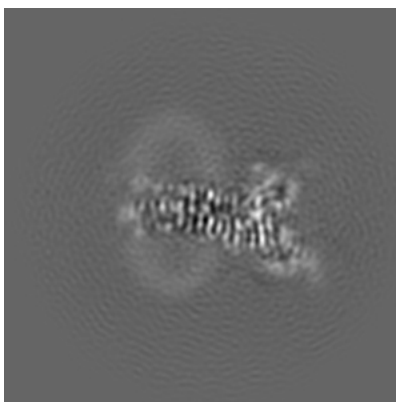
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

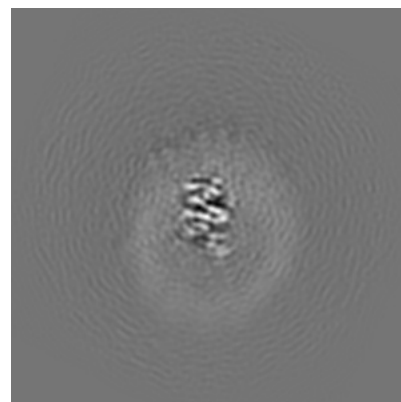
6.2.1 Primary map



X Index: 132



Y Index: 132

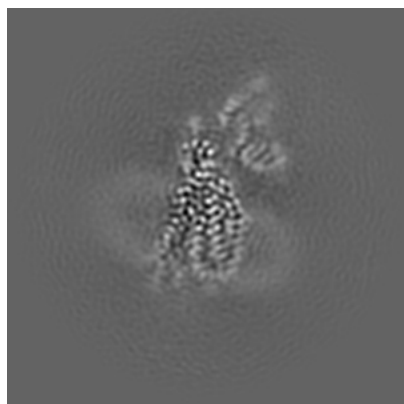


Z Index: 132

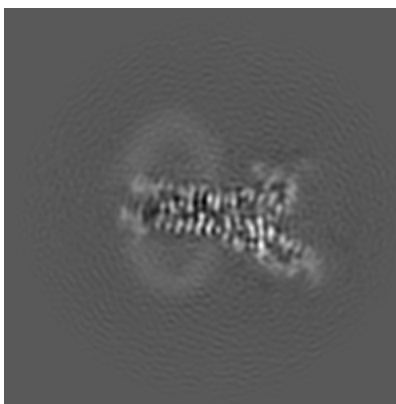
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

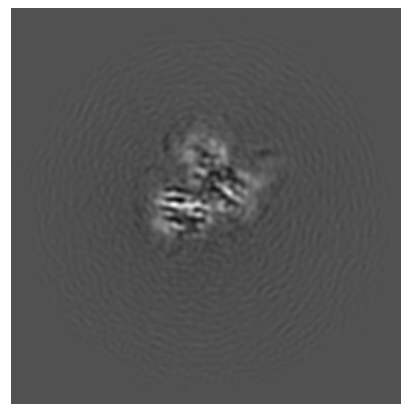
6.3.1 Primary map



X Index: 122



Y Index: 134

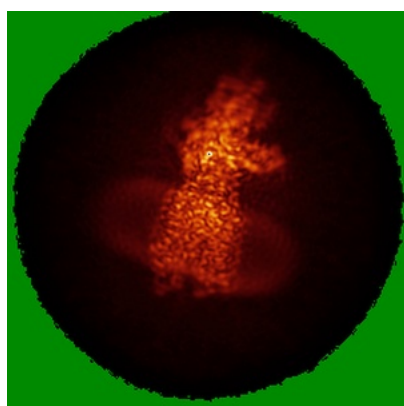


Z Index: 169

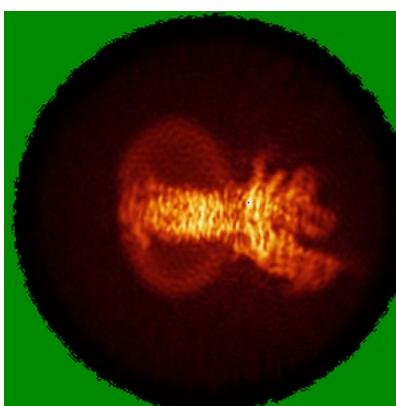
The images above show the largest variance slices of the map in three orthogonal directions.

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

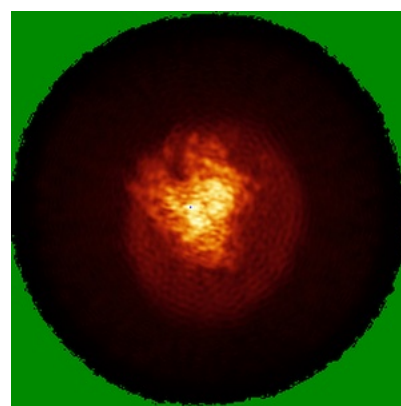
6.4.1 Primary map



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

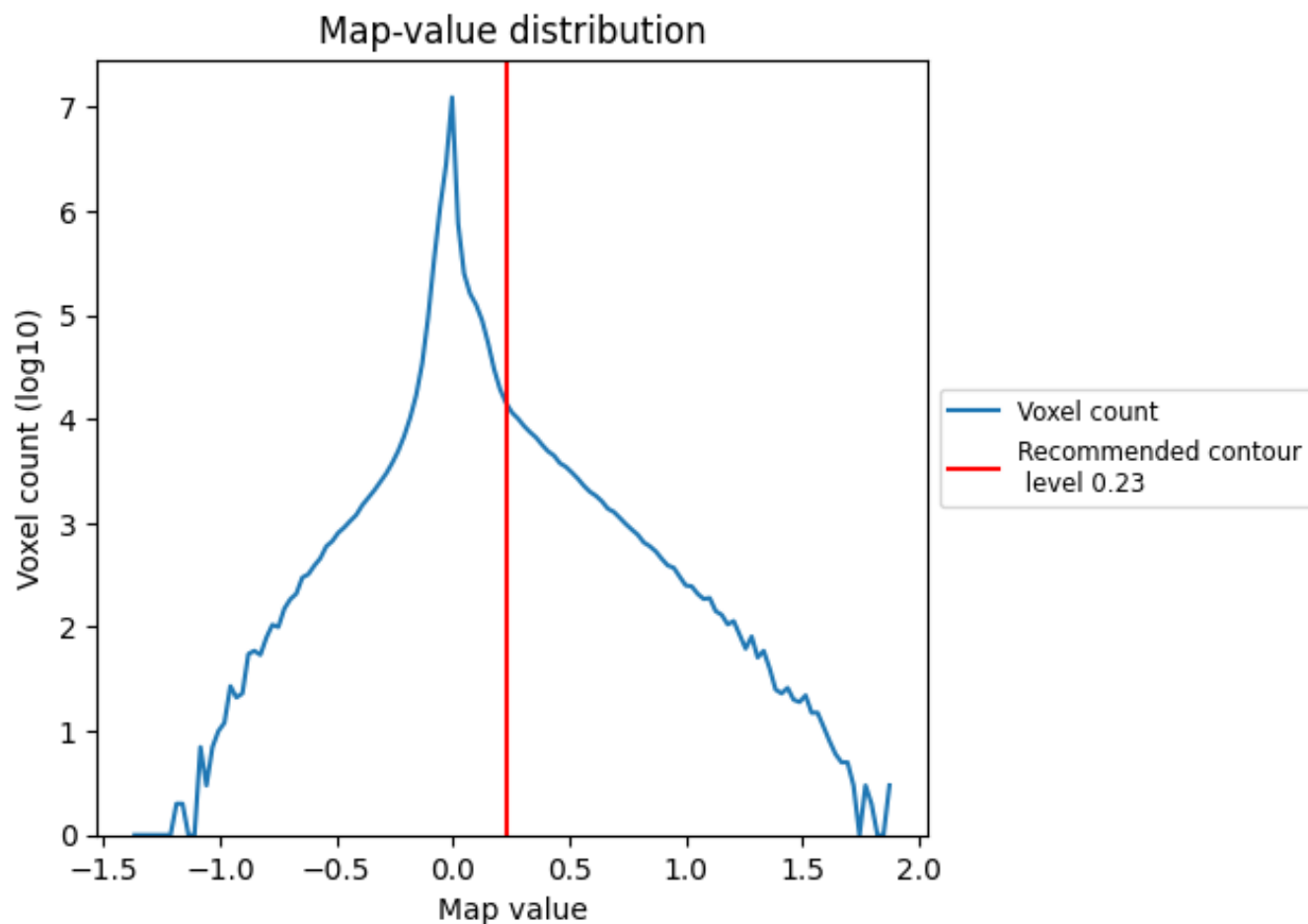
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

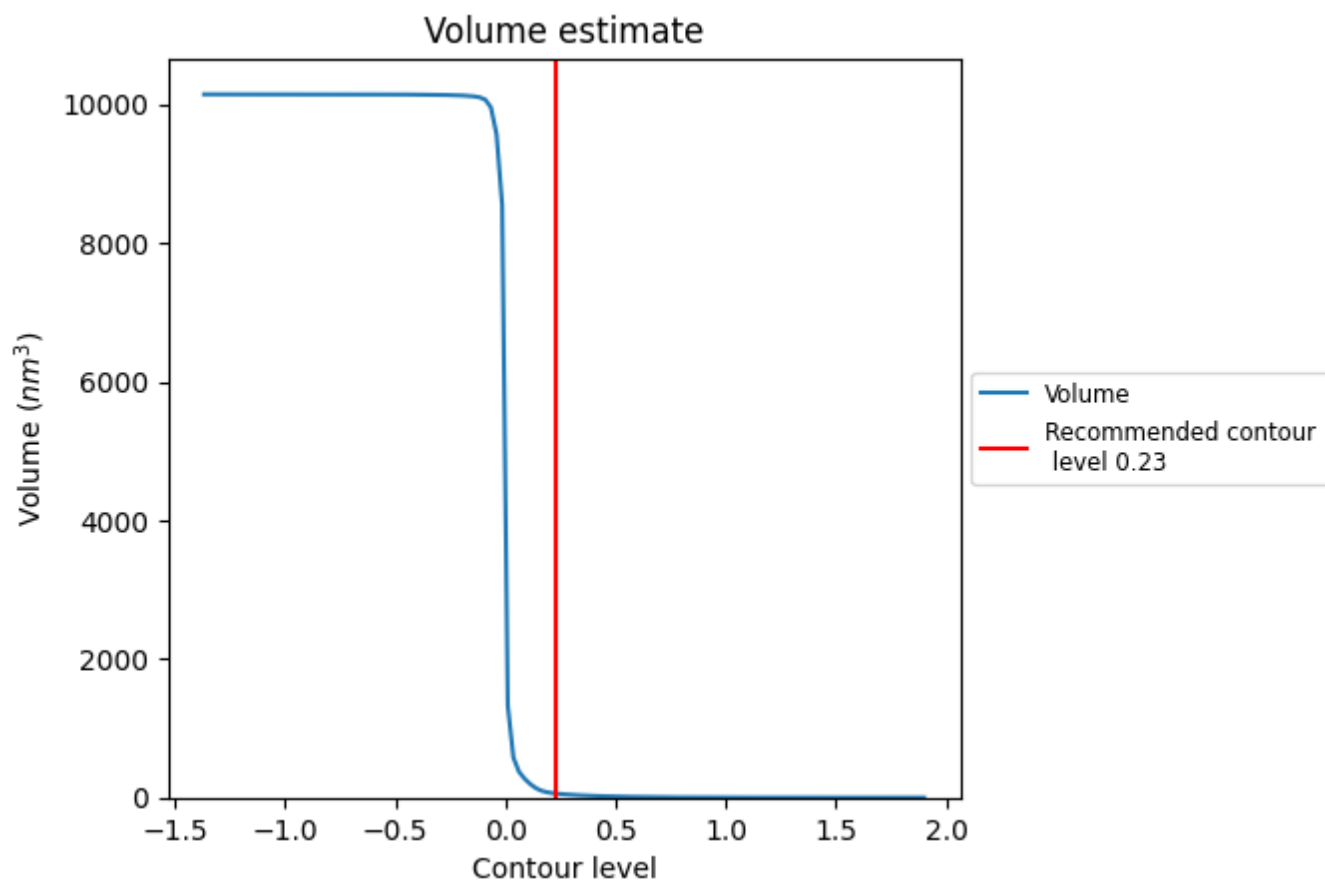
This section contains the results of statistical analysis of the map.

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.

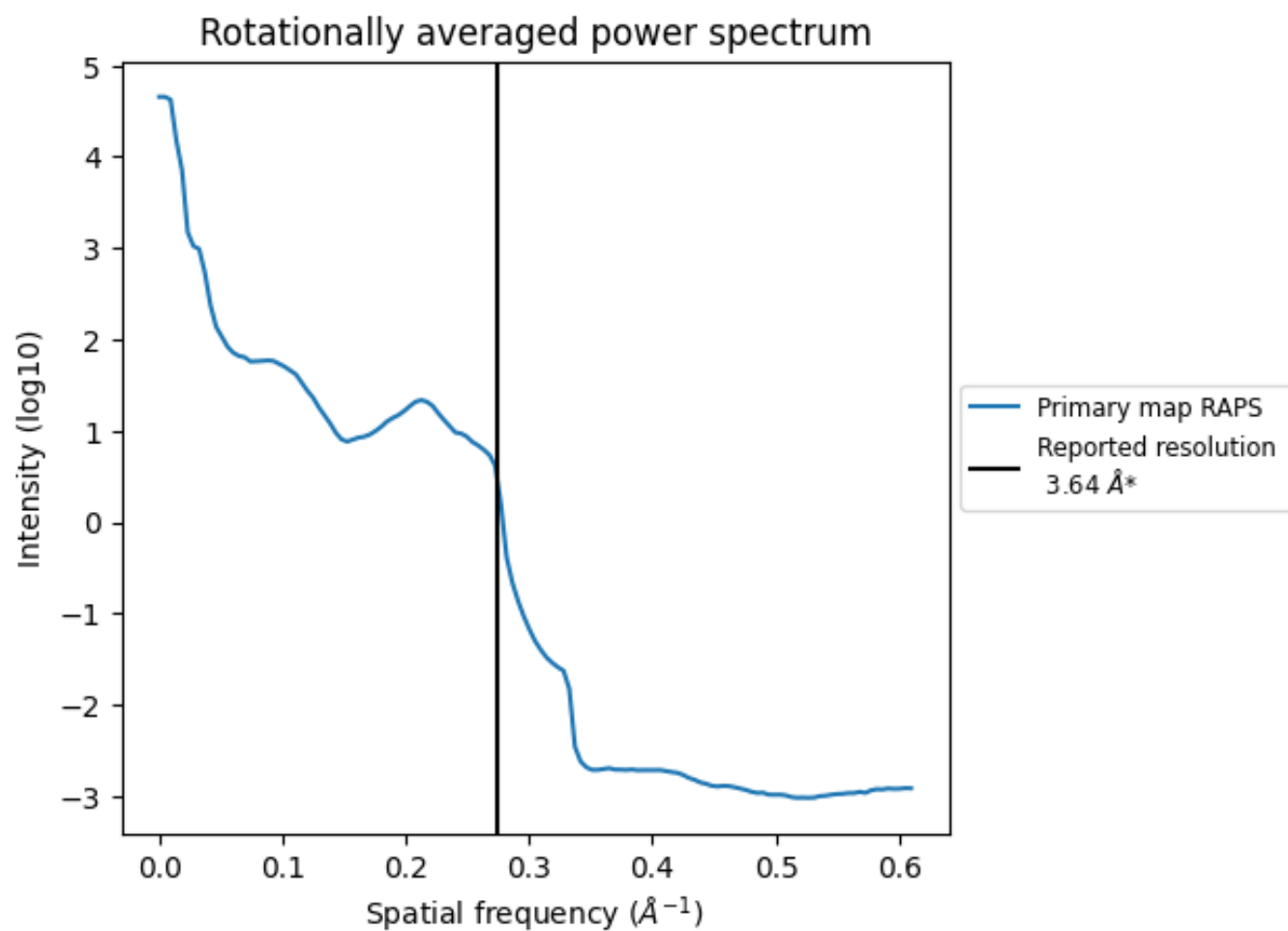
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 52 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 0.275 Å⁻¹

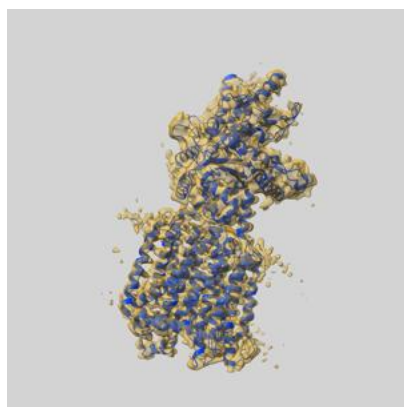
8 Fourier-Shell correlation ⓘ

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

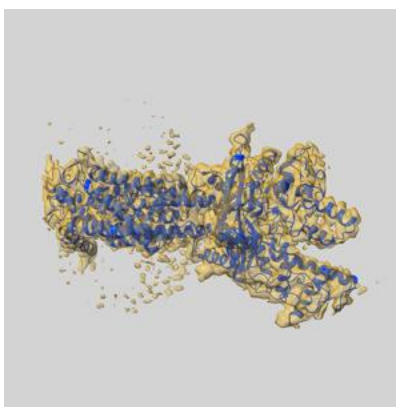
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31754 and PDB model 7V6Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

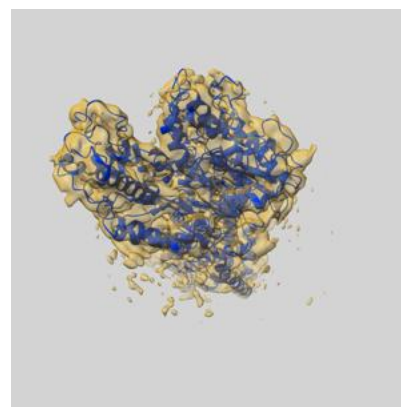
9.1 Map-model overlay [i](#)



X



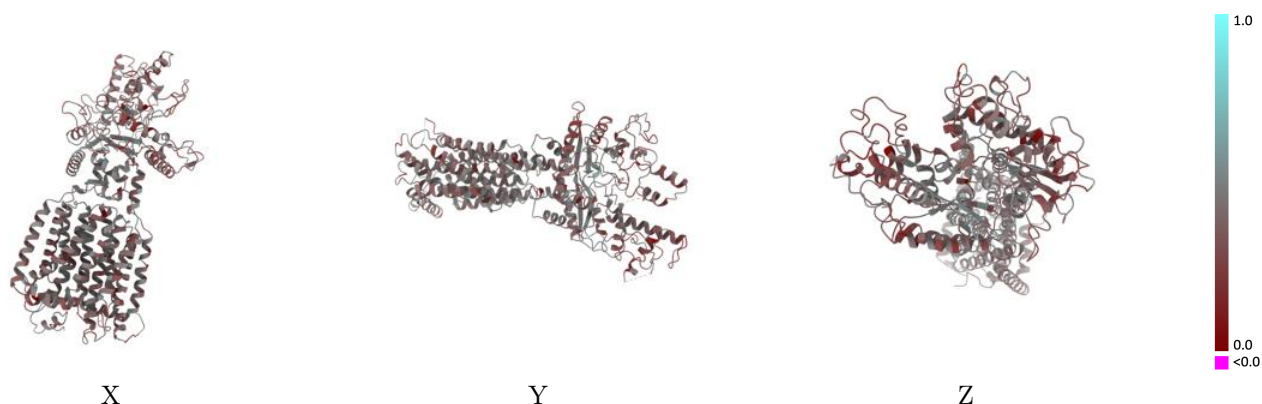
Y



Z

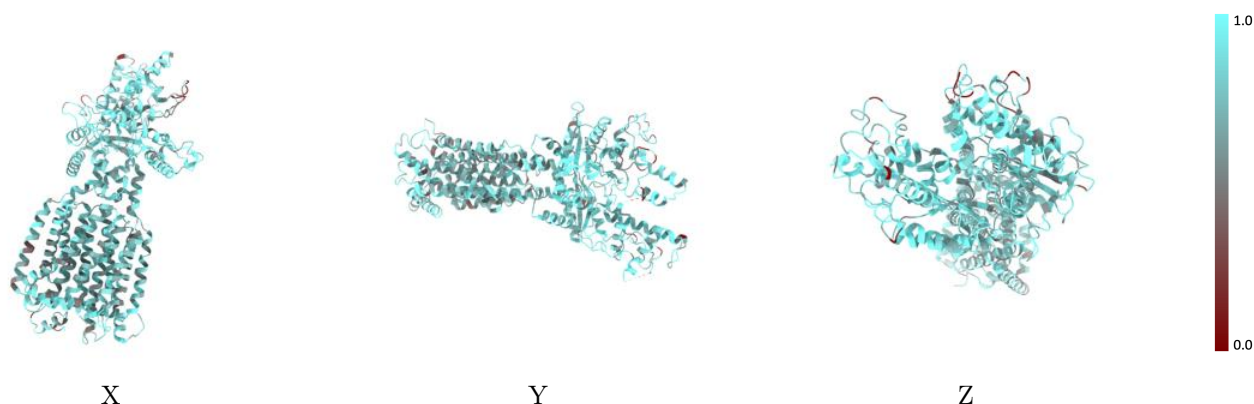
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



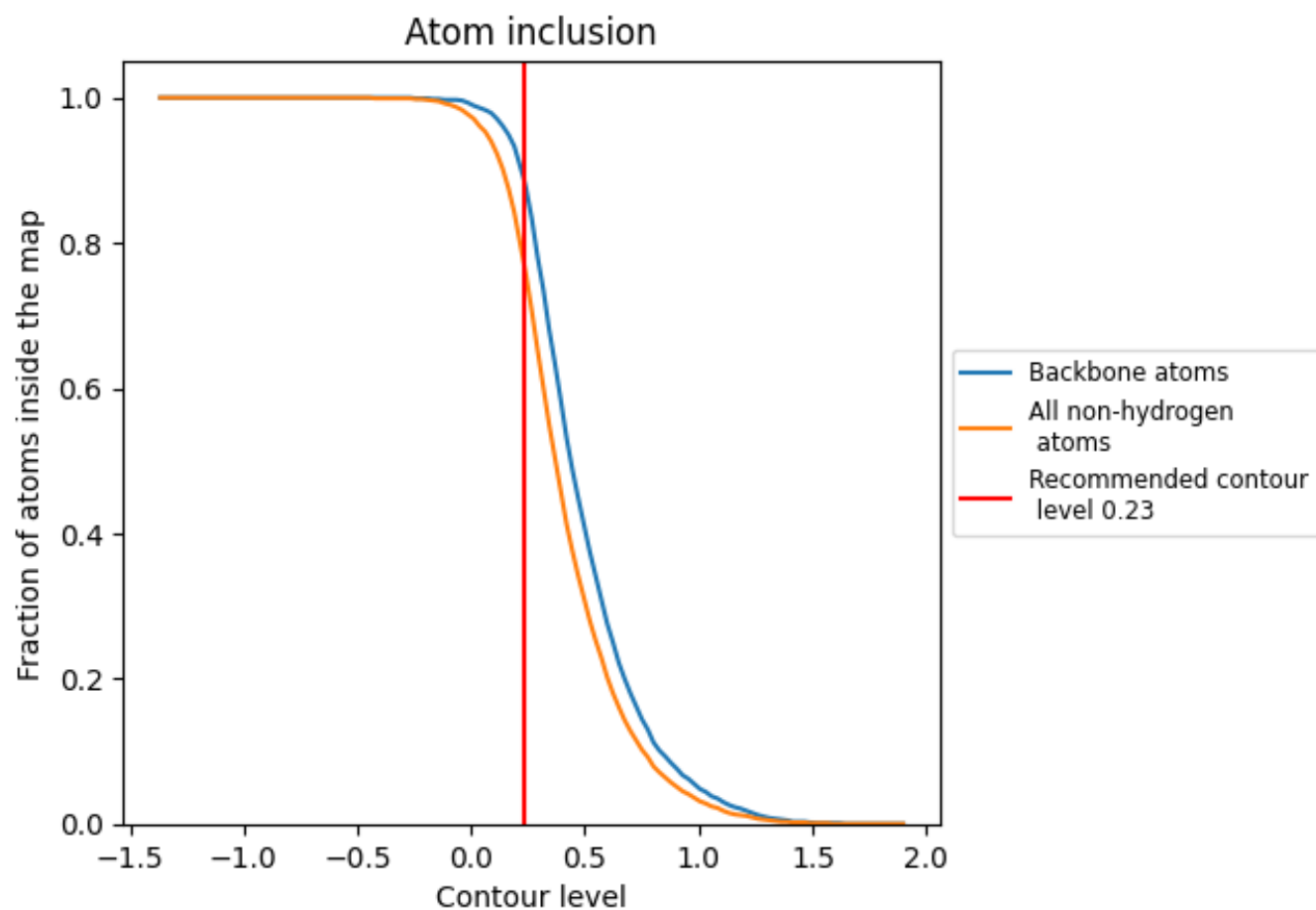
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7760	<div></div> 0.3920
A	<div></div> 0.7770	<div></div> 0.3920
B	<div></div> 0.4640	<div></div> 0.4150

