



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 03:28 PM JST

PDB ID : 7E7O
EMDB ID : EMD-31001
Title : Cryo-EM structure of human ABCA4 in NRPE-bound state
Authors : Xie, T.; Zhang, Z.K.; Gong, X.
Deposited on : 2021-02-26
Resolution : 3.40 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

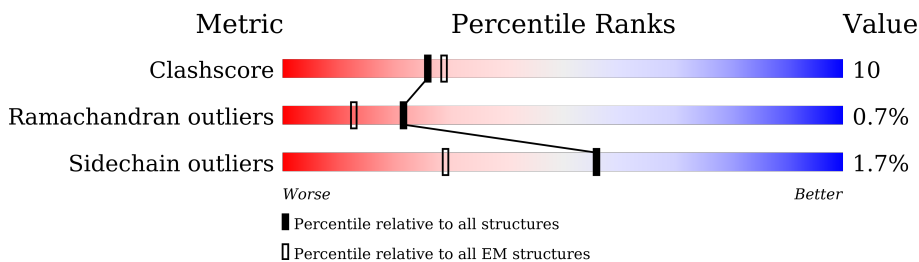
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	2317	<div> <div>9%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>14%</div> </div>
2	E	5	<div> <div>40%</div> <div>100%</div> </div>
2	N	5	<div> <div>40%</div> <div>20%</div> <div>40%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15816 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 Retinal-specific phospholipid-transporting ATPase ABCA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2003	Total	C	N	O	S	0	0
			15372	9917	2594	2775	86		

There are 44 discrepancies between the modelled and reference sequences:

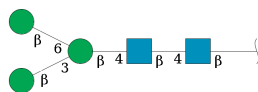
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P78363
A	-19	ALA	-	expression tag	UNP P78363
A	-18	ASP	-	expression tag	UNP P78363
A	-17	TYR	-	expression tag	UNP P78363
A	-16	LYS	-	expression tag	UNP P78363
A	-15	ASP	-	expression tag	UNP P78363
A	-14	ASP	-	expression tag	UNP P78363
A	-13	ASP	-	expression tag	UNP P78363
A	-12	ASP	-	expression tag	UNP P78363
A	-11	LYS	-	expression tag	UNP P78363
A	-10	SER	-	expression tag	UNP P78363
A	-9	GLY	-	expression tag	UNP P78363
A	-8	PRO	-	expression tag	UNP P78363
A	-7	ASP	-	expression tag	UNP P78363
A	-6	GLU	-	expression tag	UNP P78363
A	-5	VAL	-	expression tag	UNP P78363
A	-4	ASP	-	expression tag	UNP P78363
A	-3	ALA	-	expression tag	UNP P78363
A	-2	SER	-	expression tag	UNP P78363
A	-1	GLY	-	expression tag	UNP P78363
A	0	ARG	-	expression tag	UNP P78363
A	2274	LEU	-	expression tag	UNP P78363
A	2275	GLU	-	expression tag	UNP P78363
A	2276	GLY	-	expression tag	UNP P78363
A	2277	SER	-	expression tag	UNP P78363
A	2278	ASP	-	expression tag	UNP P78363
A	2279	GLU	-	expression tag	UNP P78363
A	2280	VAL	-	expression tag	UNP P78363

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2281	ASP	-	expression tag	UNP P78363
A	2282	ALA	-	expression tag	UNP P78363
A	2283	VAL	-	expression tag	UNP P78363
A	2284	GLU	-	expression tag	UNP P78363
A	2285	GLY	-	expression tag	UNP P78363
A	2286	SER	-	expression tag	UNP P78363
A	2287	HIS	-	expression tag	UNP P78363
A	2288	HIS	-	expression tag	UNP P78363
A	2289	HIS	-	expression tag	UNP P78363
A	2290	HIS	-	expression tag	UNP P78363
A	2291	HIS	-	expression tag	UNP P78363
A	2292	HIS	-	expression tag	UNP P78363
A	2293	HIS	-	expression tag	UNP P78363
A	2294	HIS	-	expression tag	UNP P78363
A	2295	HIS	-	expression tag	UNP P78363
A	2296	HIS	-	expression tag	UNP P78363

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



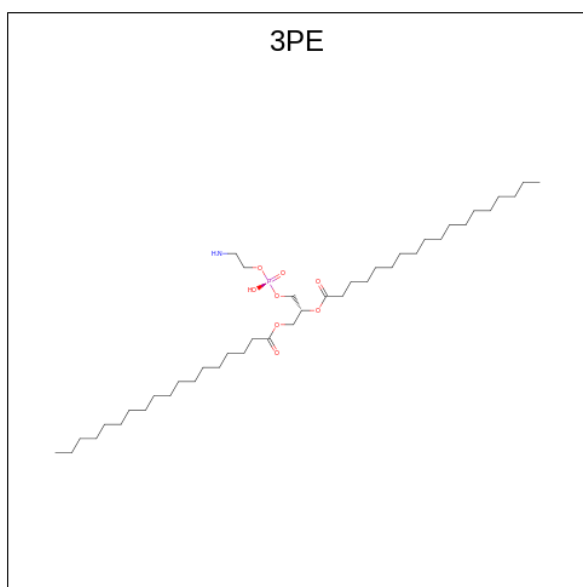
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	5	Total	C	N	O	0	0
			61	34	2	25		
2	N	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



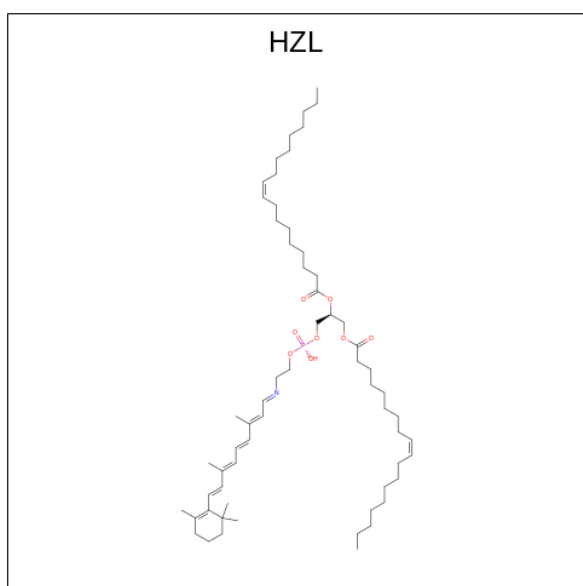
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is [(2S)-3-[2-[(E)-[(2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-tetraenylidene]amino]ethoxy-oxidanyl-phosphoryl]oxy-2-[(Z)-octadec-9-enoyl]oxy-propyl] (Z)-octadec-9-enoate (three-letter code: HZL) (formula: C₆₁H₁₀₄NO₈P) (labeled as "Ligand of Interest" by depositor).

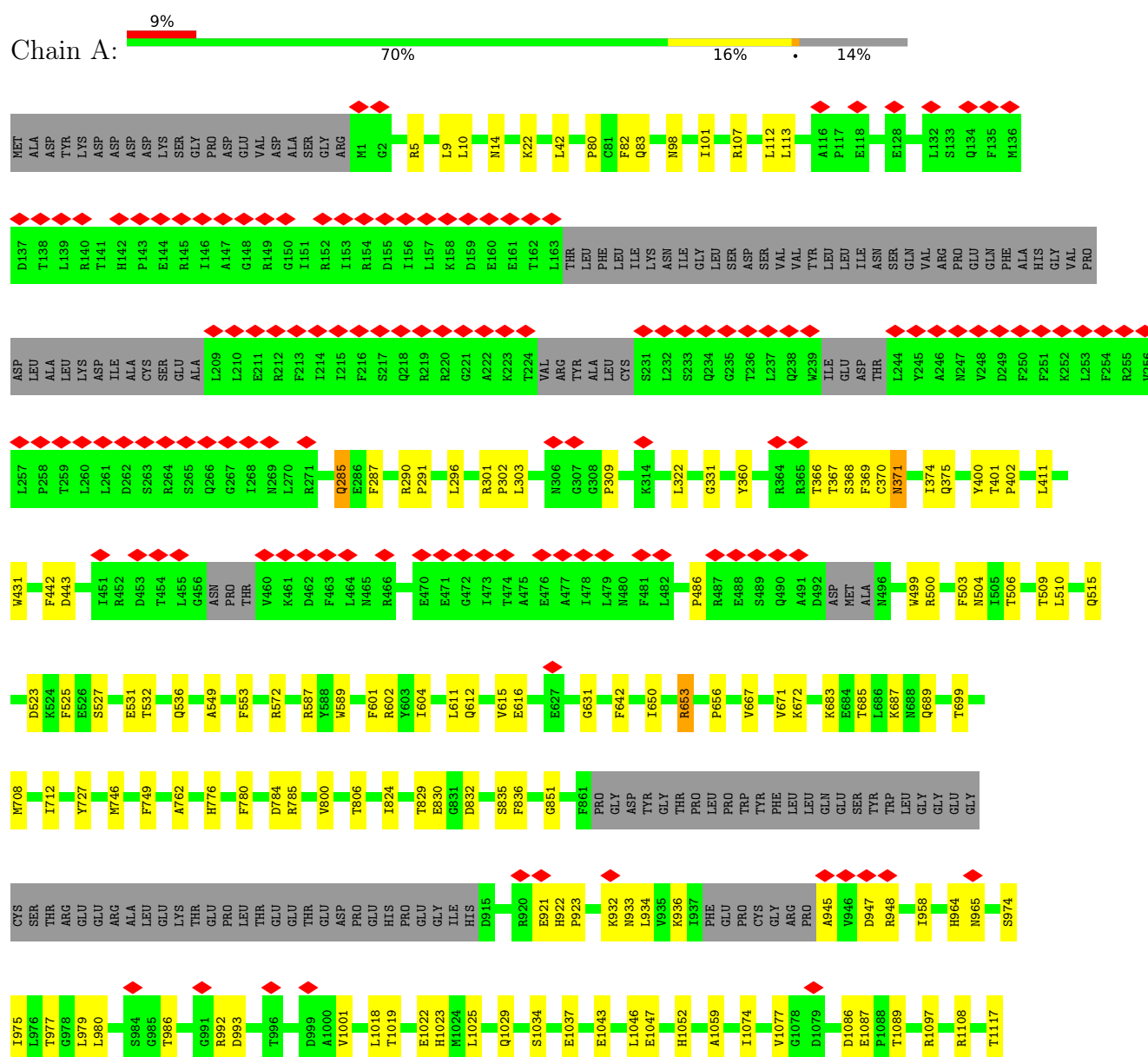


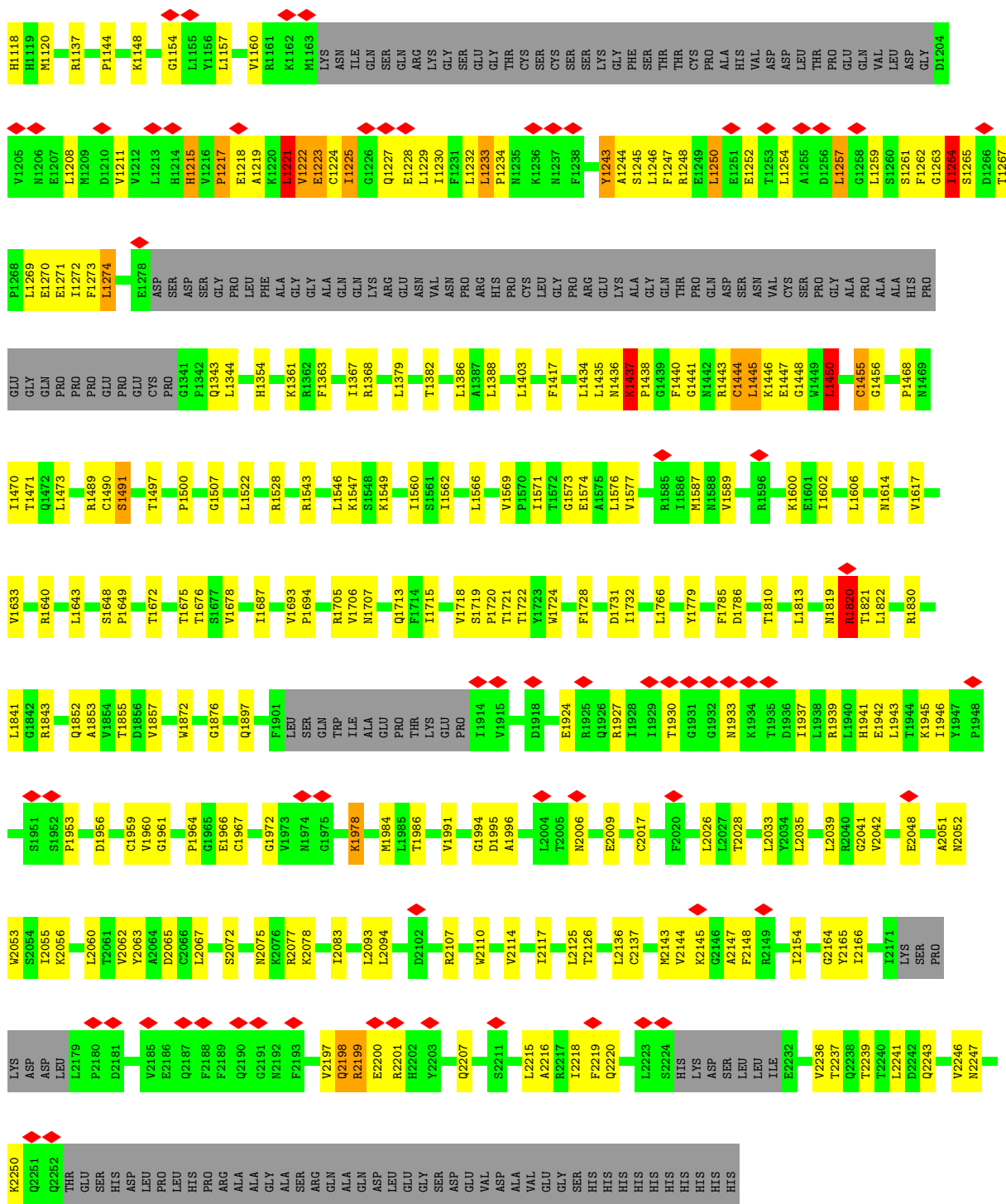
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	71	61	1	8	1	0

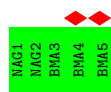
3 Residue-property plots

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: Retinal-specific phospholipid-transporting ATPase ABCA4

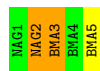






- Molecule 2: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 40% 20% 40%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184628	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.096	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (\AA)	302.40002, 302.40002, 302.40002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, HZL, 3PE, BMA

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	0.29	0/15730	0.49	1/21391 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1522	LEU	CA-CB-CG	5.10	127.04	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2197	VAL	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	15372	0	14897	299	0
2	E	61	0	52	0	0
2	N	61	0	52	2	0
3	A	98	0	91	1	0
4	A	153	0	246	7	0
5	A	71	0	0	7	0
All	All	15816	0	15338	311	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 (311) 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:1444:CYS:SG	1:A:1455:CYS:SG	1.37	1.37
1:A:1437:LYS:HB3	1:A:1438:PRO:CD	1.70	1.20
1:A:1244:ALA:HB1	1:A:2218:ILE:HG22	1.10	1.09
1:A:1217:PRO:HB2	1:A:1234:PRO:HD3	1.39	1.04
1:A:1437:LYS:CB	1:A:1438:PRO:HD3	1.88	1.04
1:A:1244:ALA:HB1	1:A:2218:ILE:CG2	1.90	1.02
1:A:1437:LYS:HB3	1:A:1438:PRO:HD3	1.02	1.01
1:A:1437:LYS:CB	1:A:1438:PRO:CD	2.36	1.01
1:A:1154:GLY:HA3	1:A:1233:LEU:O	1.67	0.95
1:A:653:ARG:HG3	1:A:653:ARG:HH11	1.35	0.91
1:A:653:ARG:NH2	1:A:780:PHE:CD2	2.39	0.91
1:A:1154:GLY:CA	1:A:1233:LEU:O	2.21	0.88
1:A:1489:ARG:HG3	1:A:1489:ARG:HH11	1.40	0.87
1:A:1233:LEU:HB2	1:A:1243:TYR:OH	1.75	0.86
1:A:1244:ALA:CB	1:A:2218:ILE:HG22	2.01	0.86
1:A:1217:PRO:CB	1:A:1234:PRO:HD3	2.06	0.85
1:A:587:ARG:NH1	5:A:2311:HZL:OAH	2.11	0.84
1:A:653:ARG:HE	1:A:780:PHE:HE2	1.22	0.83
1:A:653:ARG:NE	1:A:780:PHE:CE2	2.51	0.79
1:A:1019:THR:OG1	1:A:1022:GLU:OE1	2.01	0.79
1:A:1269:LEU:HD22	1:A:1269:LEU:O	1.83	0.79
1:A:587:ARG:HH22	5:A:2311:HZL:CCB	1.97	0.77
1:A:1160:VAL:HG11	1:A:1261:SER:OG	1.83	0.77
1:A:112:LEU:HD11	1:A:287:PHE:HB2	1.65	0.77
1:A:653:ARG:NH2	1:A:780:PHE:CE2	2.54	0.76
1:A:1160:VAL:CG1	1:A:1261:SER:OG	2.33	0.75
1:A:653:ARG:NH2	1:A:780:PHE:HD2	1.84	0.74
1:A:1034:SER:OG	1:A:1037:GLU:OE1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1546:LEU:O	1:A:1547:LYS:HG2	1.91	0.70
1:A:1344:LEU:HD22	1:A:2042:VAL:H	1.56	0.70
1:A:653:ARG:HG3	1:A:653:ARG:NH1	2.06	0.69
1:A:653:ARG:NE	1:A:780:PHE:HE2	1.90	0.69
1:A:1246:LEU:O	1:A:1246:LEU:HD23	1.93	0.69
1:A:1361:LYS:HG3	1:A:2035:LEU:HD22	1.73	0.68
1:A:2048:GLU:O	1:A:2052:ASN:ND2	2.28	0.67
1:A:1228:GLU:OE2	1:A:1228:GLU:HA	1.94	0.67
1:A:2199:ARG:HB3	1:A:2207:GLN:HB3	1.76	0.66
1:A:829:THR:HG22	1:A:830:GLU:H	1.60	0.66
1:A:1574:GLU:HA	1:A:1577:VAL:HG22	1.77	0.66
1:A:1946:ILE:HG13	1:A:1953:PRO:HB3	1.78	0.66
1:A:98:ASN:OD1	1:A:107:ARG:NH1	2.29	0.66
1:A:10:LEU:HB3	1:A:699:THR:HG21	1.78	0.66
1:A:1221:LEU:HD21	1:A:1229:LEU:HD11	1.78	0.66
1:A:776:HIS:HB2	1:A:800:VAL:HG12	1.78	0.65
1:A:1087:GLU:OE2	1:A:1118:HIS:ND1	2.26	0.65
1:A:1108:ARG:NH1	1:A:2200:GLU:OE1	2.30	0.65
1:A:1264:ILE:HD13	1:A:1264:ILE:O	1.96	0.65
1:A:1718:VAL:O	1:A:1722:THR:OG1	2.14	0.65
1:A:1154:GLY:HA2	1:A:1233:LEU:O	1.97	0.64
1:A:653:ARG:HH12	5:A:2311:HZL:CBQ	2.12	0.63
1:A:936:LYS:O	1:A:945:ALA:N	2.31	0.63
1:A:1705:ARG:NH1	1:A:1785:PHE:O	2.30	0.63
1:A:2107:ARG:HH21	1:A:2110:TRP:HE3	1.45	0.63
1:A:1813:LEU:HD22	1:A:1822:LEU:HD12	1.81	0.62
1:A:2198:GLN:O	1:A:2199:ARG:HB2	1.99	0.62
1:A:303:LEU:HA	1:A:309:PRO:HG3	1.81	0.62
1:A:1219:ALA:HB3	1:A:1232:LEU:O	1.99	0.62
1:A:1227:GLN:O	1:A:1227:GLN:HG2	1.99	0.61
1:A:486:PRO:O	1:A:500:ARG:NH2	2.34	0.61
1:A:2243:GLN:NE2	1:A:2247:ASN:OD1	2.34	0.61
1:A:1221:LEU:HD11	1:A:1229:LEU:HG	1.82	0.61
1:A:402:PRO:HG2	1:A:553:PHE:HB2	1.83	0.61
1:A:947:ASP:O	1:A:1137:ARG:NH1	2.34	0.61
1:A:112:LEU:HD12	1:A:113:LEU:HD22	1.83	0.60
1:A:977:THR:HG23	1:A:979:LEU:HD13	1.84	0.60
1:A:672:LYS:HB2	1:A:762:ALA:HB2	1.84	0.60
4:A:2309:3PE:H2A2	4:A:2309:3PE:H3A1	1.84	0.60
1:A:587:ARG:NH2	5:A:2311:HZL:CCB	2.64	0.60
1:A:936:LYS:HE3	1:A:980:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2302:NAG:H83	3:A:2302:NAG:H3	1.83	0.60
1:A:1144:PRO:O	1:A:1148:LYS:HG2	2.02	0.59
1:A:360:TYR:CE2	1:A:375:GLN:HB3	2.38	0.59
1:A:1223:GLU:OE1	1:A:1223:GLU:HA	2.03	0.59
1:A:2051:ALA:O	1:A:2055:ILE:HD12	2.01	0.59
1:A:1246:LEU:HD23	1:A:1246:LEU:C	2.22	0.59
1:A:1264:ILE:O	1:A:1264:ILE:HG23	2.03	0.59
1:A:1507:GLY:O	1:A:1528:ARG:NH1	2.37	0.58
1:A:2072:SER:OG	1:A:2075:ASN:OD1	2.20	0.58
1:A:1215:HIS:CD2	1:A:1215:HIS:H	2.21	0.58
1:A:1819:ASN:O	1:A:1821:THR:N	2.37	0.57
1:A:934:LEU:HD21	1:A:975:ILE:HG21	1.85	0.57
1:A:1719:SER:O	1:A:1721:THR:N	2.37	0.57
1:A:1215:HIS:CD2	1:A:1215:HIS:N	2.73	0.57
1:A:2165:TYR:HA	1:A:2237:THR:O	2.04	0.57
1:A:1018:LEU:O	1:A:1059:ALA:N	2.38	0.57
1:A:370:CYS:O	1:A:374:ILE:HG12	2.05	0.57
1:A:2125:LEU:HD23	1:A:2126:THR:N	2.20	0.57
1:A:531:GLU:OE2	1:A:572:ARG:NH1	2.39	0.56
1:A:1046:LEU:HD21	1:A:1052:HIS:HA	1.87	0.56
5:A:2311:HZL:CAT	5:A:2311:HZL:CAU	2.84	0.56
1:A:1943:LEU:HD11	1:A:1996:ALA:HB2	1.88	0.56
1:A:1573:GLY:O	1:A:1576:LEU:N	2.37	0.55
1:A:1489:ARG:HH11	1:A:1489:ARG:CG	2.14	0.55
1:A:2033:LEU:HD23	1:A:2083:ILE:HG22	1.88	0.55
1:A:1489:ARG:HG3	1:A:1489:ARG:NH1	2.14	0.54
1:A:1819:ASN:C	1:A:1820:ARG:HD3	2.27	0.54
1:A:653:ARG:CZ	1:A:780:PHE:CE2	2.90	0.54
1:A:2144:VAL:HG12	1:A:2145:LYS:H	1.72	0.54
1:A:2215:LEU:HD23	1:A:2218:ILE:HD11	1.89	0.54
1:A:653:ARG:CZ	1:A:780:PHE:CD2	2.91	0.54
1:A:1160:VAL:HG12	1:A:1261:SER:OG	2.06	0.54
1:A:1491:SER:HB3	1:A:1497:THR:H	1.73	0.54
1:A:1379:LEU:HD11	4:A:2309:3PE:H371	1.90	0.54
1:A:1560:ILE:HG12	1:A:1617:VAL:HG12	1.89	0.53
1:A:1705:ARG:NH1	1:A:1786:ASP:OD1	2.36	0.53
1:A:400:TYR:CZ	1:A:527:SER:HB3	2.43	0.53
1:A:964:HIS:CD2	1:A:965:ASN:H	2.26	0.53
1:A:992:ARG:HA	1:A:992:ARG:NE	2.23	0.53
1:A:1368:ARG:HH11	1:A:2067:LEU:HD11	1.74	0.53
5:A:2311:HZL:CCI	5:A:2311:HZL:CBD	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:SER:HA	1:A:977:THR:HG22	1.90	0.53
1:A:1648:SER:OG	1:A:1648:SER:O	2.27	0.53
1:A:1731:ASP:OD1	1:A:1779:TYR:OH	2.26	0.53
1:A:2136:LEU:HD12	1:A:2136:LEU:O	2.09	0.53
1:A:42:LEU:HD13	1:A:650:ILE:HD12	1.90	0.53
1:A:301:ARG:HB3	1:A:302:PRO:HD3	1.91	0.53
1:A:2201:ARG:HG2	1:A:2201:ARG:HH21	1.73	0.53
1:A:964:HIS:CG	1:A:965:ASN:H	2.26	0.52
1:A:2028:THR:HG22	1:A:2067:LEU:HD12	1.89	0.52
1:A:1225:ILE:HG22	1:A:1228:GLU:HB2	1.91	0.52
1:A:1724:TRP:HE1	1:A:1897:GLN:HG3	1.73	0.52
1:A:1368:ARG:HG3	1:A:2026:LEU:HD12	1.91	0.52
1:A:1250:LEU:HD13	1:A:1250:LEU:O	2.10	0.52
1:A:1972:GLY:HA2	1:A:2143:MET:H	1.74	0.52
1:A:80:PRO:HB2	1:A:331:GLY:HA3	1.91	0.52
1:A:602:ARG:HG3	1:A:602:ARG:HH11	1.74	0.52
1:A:1945:LYS:HB2	1:A:1984:MET:CE	2.40	0.52
1:A:824:ILE:O	1:A:835:SER:OG	2.28	0.51
1:A:1450:LEU:N	1:A:1450:LEU:CD1	2.73	0.51
1:A:932:LYS:HB2	1:A:986:THR:HB	1.92	0.51
1:A:653:ARG:NH1	1:A:653:ARG:CG	2.73	0.51
1:A:589:TRP:HB3	1:A:1549:LYS:HD3	1.92	0.51
1:A:933:ASN:HA	1:A:948:ARG:HA	1.92	0.51
1:A:1217:PRO:CB	1:A:1234:PRO:CD	2.85	0.51
2:N:2:NAG:H83	2:N:2:NAG:H3	1.91	0.51
1:A:1271:GLU:OE1	1:A:1271:GLU:HA	2.09	0.51
1:A:1967:CYS:SG	1:A:2137:CYS:HA	2.50	0.51
1:A:1927:ARG:HH21	1:A:1961:GLY:HA3	1.76	0.51
1:A:1991:VAL:HG22	1:A:1994:GLY:HA3	1.92	0.51
1:A:2216:ALA:O	1:A:2220:GLN:HG2	2.11	0.51
1:A:1437:LYS:CB	1:A:1438:PRO:HD2	2.36	0.50
1:A:2199:ARG:HG3	1:A:2200:GLU:H	1.76	0.50
1:A:366:THR:O	1:A:367:THR:OG1	2.22	0.50
1:A:366:THR:OG1	1:A:367:THR:N	2.43	0.50
1:A:1437:LYS:HB2	1:A:1438:PRO:CD	2.38	0.50
5:A:2311:HZL:NAJ	5:A:2311:HZL:CBY	2.72	0.50
1:A:1354:HIS:NE2	1:A:2039:LEU:O	2.44	0.50
1:A:602:ARG:HG3	1:A:602:ARG:NH1	2.27	0.50
1:A:1943:LEU:HD23	1:A:1984:MET:SD	2.51	0.50
1:A:835:SER:OG	1:A:836:PHE:N	2.45	0.50
1:A:1941:HIS:ND1	1:A:1942:GLU:HG2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD12	1:A:296:LEU:HA	1.94	0.50
1:A:1157:LEU:HD12	1:A:1263:GLY:O	2.12	0.50
1:A:1960:VAL:HG11	1:A:2148:PHE:HE2	1.76	0.50
1:A:746:MET:HE1	1:A:749:PHE:HD2	1.77	0.49
1:A:2164:GLY:HA3	1:A:2239:THR:HG23	1.93	0.49
1:A:1500:PRO:O	1:A:1543:ARG:NH2	2.45	0.49
1:A:1273:PHE:C	1:A:1273:PHE:CD2	2.86	0.49
1:A:1937:ILE:HD11	1:A:1964:PRO:HB3	1.93	0.49
1:A:1872:TRP:H	1:A:1876:GLY:HA3	1.76	0.48
1:A:1810:THR:HG21	1:A:1830:ARG:HD3	1.94	0.48
1:A:921:GLU:N	1:A:921:GLU:OE1	2.46	0.48
1:A:1233:LEU:CB	1:A:1243:TYR:OH	2.55	0.48
1:A:1025:LEU:O	1:A:1029:GLN:HG3	2.14	0.48
1:A:1417:PHE:CE2	1:A:1435:LEU:HD11	2.48	0.48
1:A:499:TRP:CE3	1:A:500:ARG:HG2	2.49	0.48
1:A:549:ALA:HB3	1:A:611:LEU:HD23	1.96	0.47
1:A:290:ARG:CD	1:A:291:PRO:HD2	2.45	0.47
1:A:1245:SER:O	1:A:1248:ARG:CB	2.62	0.47
1:A:631:GLY:H	1:A:1614:ASN:HB3	1.78	0.47
1:A:1221:LEU:HD12	1:A:1221:LEU:HA	1.79	0.47
1:A:1232:LEU:HD23	1:A:1232:LEU:C	2.35	0.47
1:A:1447:GLU:HG3	1:A:1448:GLY:H	1.78	0.47
1:A:1924:GLU:HA	1:A:1959:CYS:SG	2.55	0.47
1:A:2055:ILE:HG23	1:A:2060:LEU:O	2.14	0.47
1:A:611:LEU:O	1:A:615:VAL:HG23	2.15	0.47
1:A:1675:THR:O	1:A:1678:VAL:HG12	2.15	0.47
1:A:1819:ASN:O	1:A:1820:ARG:HD3	2.15	0.47
1:A:2243:GLN:NE2	1:A:2243:GLN:O	2.48	0.47
1:A:1344:LEU:HB3	1:A:2041:GLY:HA3	1.97	0.46
1:A:1766:LEU:HG	1:A:1841:LEU:HD12	1.98	0.46
1:A:1643:LEU:HD21	1:A:1649:PRO:HB3	1.96	0.46
1:A:1468:PRO:HA	1:A:1471:THR:HG22	1.96	0.46
1:A:503:PHE:HA	1:A:506:THR:HG22	1.96	0.46
1:A:746:MET:CE	1:A:851:GLY:HA2	2.46	0.46
1:A:1363:PHE:CZ	1:A:1367:ILE:HD12	2.51	0.46
1:A:1687:ILE:HG12	1:A:1841:LEU:HD23	1.97	0.46
1:A:708:MET:O	1:A:712:ILE:HG12	2.16	0.46
1:A:1693:VAL:HB	1:A:1694:PRO:HD3	1.98	0.46
1:A:727:TYR:O	1:A:727:TYR:CD2	2.68	0.45
1:A:1254:LEU:HG	1:A:1259:LEU:HB2	1.97	0.45
1:A:2060:LEU:HD11	1:A:2078:LYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2246:VAL:O	1:A:2250:LYS:HB2	2.16	0.45
1:A:1569:VAL:HG22	1:A:1571:ILE:H	1.81	0.45
1:A:2006:ASN:HB3	1:A:2009:GLU:OE2	2.16	0.45
1:A:1489:ARG:CG	1:A:1489:ARG:NH1	2.73	0.45
1:A:5:ARG:O	1:A:9:LEU:HD23	2.17	0.45
2:N:3:BMA:H62	2:N:5:BMA:H2	1.49	0.45
1:A:14:ASN:HD22	1:A:699:THR:HG22	1.82	0.45
1:A:1087:GLU:HG2	1:A:1117:THR:HA	1.98	0.45
1:A:1843:ARG:HD2	1:A:1843:ARG:HA	1.71	0.45
1:A:431:TRP:CG	1:A:510:LEU:HD23	2.52	0.45
1:A:1089:THR:HB	1:A:1097:ARG:HG3	1.99	0.45
1:A:1577:VAL:CG1	1:A:1602:ILE:HG21	2.46	0.45
1:A:1941:HIS:HB3	1:A:1995:ASP:HB3	1.99	0.45
1:A:2065:ASP:N	1:A:2065:ASP:OD1	2.49	0.45
1:A:442:PHE:HB3	1:A:499:TRP:CZ2	2.50	0.45
1:A:523:ASP:N	1:A:523:ASP:OD1	2.50	0.45
1:A:1930:THR:HA	1:A:1933:ASN:OD1	2.17	0.45
1:A:1437:LYS:HB2	1:A:1438:PRO:HD2	1.99	0.45
1:A:922:HIS:ND1	1:A:923:PRO:HD2	2.32	0.45
1:A:653:ARG:HD2	1:A:653:ARG:HA	1.76	0.44
1:A:958:ILE:HG13	1:A:1108:ARG:HD3	1.99	0.44
1:A:993:ASP:O	1:A:1001:VAL:HG21	2.17	0.44
1:A:1438:PRO:HG3	1:A:1640:ARG:HD3	1.99	0.44
1:A:2053:TRP:HD1	1:A:2056:LYS:HZ1	1.63	0.44
1:A:506:THR:HA	1:A:509:THR:HG22	1.98	0.44
1:A:2218:ILE:HG13	1:A:2219:PHE:HD1	1.82	0.44
1:A:1930:THR:HG21	1:A:1939:ARG:HD3	1.98	0.44
1:A:1229:LEU:HD12	1:A:1229:LEU:HA	1.76	0.44
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.44
1:A:1074:ILE:O	1:A:1077:VAL:HG12	2.18	0.44
1:A:1232:LEU:HD23	1:A:1233:LEU:N	2.33	0.44
1:A:1382:THR:O	1:A:1386:LEU:HG	2.18	0.44
1:A:1956:ASP:HB2	1:A:2147:ALA:HB2	1.99	0.44
1:A:1434:LEU:HG	1:A:1440:PHE:HE1	1.82	0.44
1:A:1246:LEU:C	1:A:1246:LEU:CD2	2.86	0.44
1:A:1942:GLU:C	1:A:1943:LEU:HD12	2.39	0.43
1:A:2093:LEU:O	1:A:2094:LEU:HD23	2.18	0.43
1:A:667:VAL:O	1:A:671:VAL:HG23	2.18	0.43
1:A:1991:VAL:O	1:A:1991:VAL:HG13	2.19	0.43
1:A:685:THR:O	1:A:689:GLN:HG2	2.19	0.43
1:A:1445:LEU:HD23	1:A:1445:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:GLN:O	1:A:1718:VAL:HG23	2.18	0.43
1:A:1715:ILE:HD11	1:A:1986:THR:HB	1.99	0.43
1:A:285:GLN:HE21	1:A:285:GLN:HB3	1.70	0.43
1:A:1262:PHE:CG	1:A:1262:PHE:O	2.70	0.43
1:A:360:TYR:HE2	1:A:375:GLN:HB3	1.82	0.43
1:A:2236:VAL:O	1:A:2236:VAL:HG13	2.18	0.43
1:A:656:PRO:HD3	1:A:806:THR:HG21	2.01	0.43
1:A:829:THR:HG22	1:A:830:GLU:N	2.31	0.43
1:A:1447:GLU:HG3	1:A:1448:GLY:N	2.33	0.43
1:A:367:THR:HG22	1:A:368:SER:N	2.34	0.43
1:A:1222:VAL:HG13	1:A:1230:ILE:HG22	2.00	0.43
1:A:1470:ILE:HD13	1:A:1473:LEU:HD21	2.00	0.43
1:A:1852:GLN:HA	1:A:1855:THR:HG22	2.00	0.43
1:A:2017:CYS:SG	1:A:2077:ARG:NH1	2.91	0.43
1:A:401:THR:HB	1:A:402:PRO:HD3	2.00	0.43
1:A:1120:MET:HG3	1:A:1269:LEU:CD1	2.49	0.43
1:A:1257:LEU:HD22	1:A:1257:LEU:HA	1.81	0.43
1:A:1269:LEU:HD13	1:A:1269:LEU:C	2.39	0.43
1:A:1706:VAL:O	1:A:1707:ASN:OD1	2.36	0.43
1:A:1274:LEU:HA	1:A:1274:LEU:HD12	1.74	0.42
1:A:653:ARG:NH2	1:A:780:PHE:HE2	2.15	0.42
1:A:784:ASP:OD1	1:A:785:ARG:N	2.52	0.42
1:A:1600:LYS:HA	1:A:1600:LYS:HD3	1.71	0.42
1:A:1246:LEU:C	1:A:1248:ARG:H	2.23	0.42
1:A:1388:LEU:HD23	1:A:1388:LEU:HA	1.87	0.42
1:A:1441:GLY:HA2	1:A:1633:VAL:HG22	2.01	0.42
1:A:2144:VAL:HG12	1:A:2145:LYS:N	2.33	0.42
1:A:1566:LEU:HD23	1:A:1566:LEU:H	1.83	0.42
1:A:1343:GLN:CD	1:A:1343:GLN:H	2.23	0.42
1:A:22:LYS:HD2	1:A:22:LYS:HA	1.80	0.42
1:A:1434:LEU:HD22	1:A:1562:ILE:HD11	2.02	0.42
1:A:1247:PHE:CD2	1:A:1247:PHE:N	2.87	0.42
1:A:612:GLN:O	1:A:616:GLU:HG2	2.20	0.41
1:A:642:PHE:CD1	1:A:642:PHE:N	2.88	0.41
1:A:1853:ALA:O	1:A:1857:VAL:HG13	2.20	0.41
4:A:2310:3PE:H3A2	4:A:2310:3PE:H371	1.84	0.41
1:A:101:ILE:HG12	1:A:322:LEU:HA	2.02	0.41
1:A:1023:HIS:HE1	1:A:1059:ALA:HB2	1.85	0.41
1:A:1966:GLU:HA	1:A:2117:ILE:HD11	2.02	0.41
1:A:532:THR:O	1:A:536:GLN:HG3	2.20	0.41
1:A:1043:GLU:O	1:A:1047:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:LEU:HD12	1:A:1211:VAL:HG21	2.02	0.41
1:A:1587:MET:HG3	1:A:1589:VAL:HG23	2.02	0.41
1:A:2166:ILE:HD12	1:A:2166:ILE:H	1.85	0.41
1:A:290:ARG:HA	1:A:290:ARG:HD3	1.91	0.41
1:A:371:ASN:O	1:A:371:ASN:ND2	2.51	0.41
1:A:500:ARG:O	1:A:504:ASN:HB2	2.21	0.41
1:A:1250:LEU:HD22	1:A:1250:LEU:HA	1.94	0.41
1:A:1403:LEU:O	1:A:1403:LEU:HD23	2.20	0.41
1:A:1672:THR:O	1:A:1676:THR:HG23	2.21	0.41
4:A:2308:3PE:H352	4:A:2308:3PE:H321	1.81	0.41
1:A:601:PHE:CD1	1:A:604:ILE:HD12	2.56	0.41
1:A:1018:LEU:HD12	1:A:1018:LEU:HA	1.90	0.41
1:A:1217:PRO:HB2	1:A:1218:GLU:H	1.59	0.41
1:A:1728:PHE:CE2	1:A:1732:ILE:HD11	2.55	0.41
4:A:2308:3PE:H272	4:A:2308:3PE:H2A2	1.83	0.41
1:A:82:PHE:O	1:A:83:GLN:HB3	2.21	0.41
1:A:369:PHE:CD1	1:A:515:GLN:HG2	2.54	0.41
1:A:411:LEU:HD12	1:A:525:PHE:CE1	2.56	0.41
1:A:443:ASP:OD2	1:A:443:ASP:N	2.54	0.41
1:A:1606:LEU:HD23	1:A:1606:LEU:HA	1.95	0.41
1:A:2215:LEU:HD22	1:A:2219:PHE:CE1	2.56	0.41
4:A:2309:3PE:H382	4:A:2309:3PE:H252	2.03	0.41
1:A:1927:ARG:HA	1:A:1927:ARG:HH11	1.85	0.41
1:A:2114:VAL:O	1:A:2117:ILE:HG22	2.21	0.41
1:A:14:ASN:ND2	1:A:699:THR:HG22	2.37	0.41
1:A:1455:CYS:HB3	1:A:1456:GLY:H	1.65	0.41
1:A:683:LYS:HE2	1:A:687:LYS:NZ	2.36	0.40
1:A:1148:LYS:NZ	1:A:1267:THR:O	2.49	0.40
1:A:2039:LEU:HD23	1:A:2039:LEU:HA	1.88	0.40
1:A:2154:ILE:HG23	1:A:2241:LEU:HD12	2.03	0.40
1:A:653:ARG:NE	1:A:780:PHE:CD2	2.89	0.40
1:A:1978:LYS:HB3	1:A:1978:LYS:HE3	1.84	0.40
1:A:1264:ILE:CG2	1:A:2165:TYR:HE2	2.35	0.40
1:A:2062:VAL:HG13	1:A:2063:TYR:CD2	2.57	0.40
4:A:2308:3PE:H382	4:A:2308:3PE:H3B2	1.89	0.40
1:A:653:ARG:CZ	1:A:780:PHE:HE2	2.32	0.40
1:A:1086:ASP:OD1	1:A:1086:ASP:N	2.53	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	1977/2317 (85%)	1727 (87%)	237 (12%)	13 (1%)	19	47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1217	PRO
1	A	1437	LYS
1	A	2198	GLN
1	A	1221	LEU
1	A	1264	ILE
1	A	1443	ARG
1	A	1450	LEU
1	A	2199	ARG
1	A	1436	ASN
1	A	1445	LEU
1	A	1252	GLU
1	A	1820	ARG
1	A	1720	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1593/2027 (79%)	1566 (98%)	27 (2%)	56	74

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	371	ASN
1	A	653	ARG
1	A	1215	HIS
1	A	1221	LEU
1	A	1222	VAL
1	A	1223	GLU
1	A	1224	CYS
1	A	1225	ILE
1	A	1233	LEU
1	A	1243	TYR
1	A	1250	LEU
1	A	1257	LEU
1	A	1264	ILE
1	A	1265	SER
1	A	1270	GLU
1	A	1272	ILE
1	A	1274	LEU
1	A	1437	LYS
1	A	1444	CYS
1	A	1446	LYS
1	A	1450	LEU
1	A	1455	CYS
1	A	1490	CYS
1	A	1491	SER
1	A	1820	ARG
1	A	1978	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	964	HIS
1	A	1215	HIS
1	A	2052	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 ⓘ

10 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	E	1	2,1	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	BMA	E	3	2	11,11,12	0.79	0	15,15,17	0.95	0
2	BMA	E	4	2	11,11,12	0.52	0	15,15,17	0.85	0
2	BMA	E	5	2	11,11,12	0.64	0	15,15,17	1.01	0
2	NAG	N	1	2,1	14,14,15	0.41	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.34	0	17,19,21	1.42	3 (17%)
2	BMA	N	3	2	11,11,12	0.76	0	15,15,17	1.73	3 (20%)
2	BMA	N	4	2	11,11,12	0.67	0	15,15,17	1.01	0
2	BMA	N	5	2	11,11,12	0.84	0	15,15,17	0.83	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	BMA	E	4	2	-	2/2/19/22	0/1/1/1
2	BMA	E	5	2	-	1/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	5/6/23/26	0/1/1/1
2	BMA	N	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	N	4	2	-	0/2/19/22	0/1/1/1
2	BMA	N	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	NAG	C2-N2-C7	4.42	129.19	122.90
2	N	3	BMA	C1-C2-C3	-3.69	105.13	109.67
2	N	3	BMA	O3-C3-C2	3.69	117.06	109.99
2	N	3	BMA	C1-O5-C5	2.97	116.21	112.19
2	N	2	NAG	C1-C2-N2	2.37	114.53	110.49
2	N	2	NAG	C1-O5-C5	2.16	115.11	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

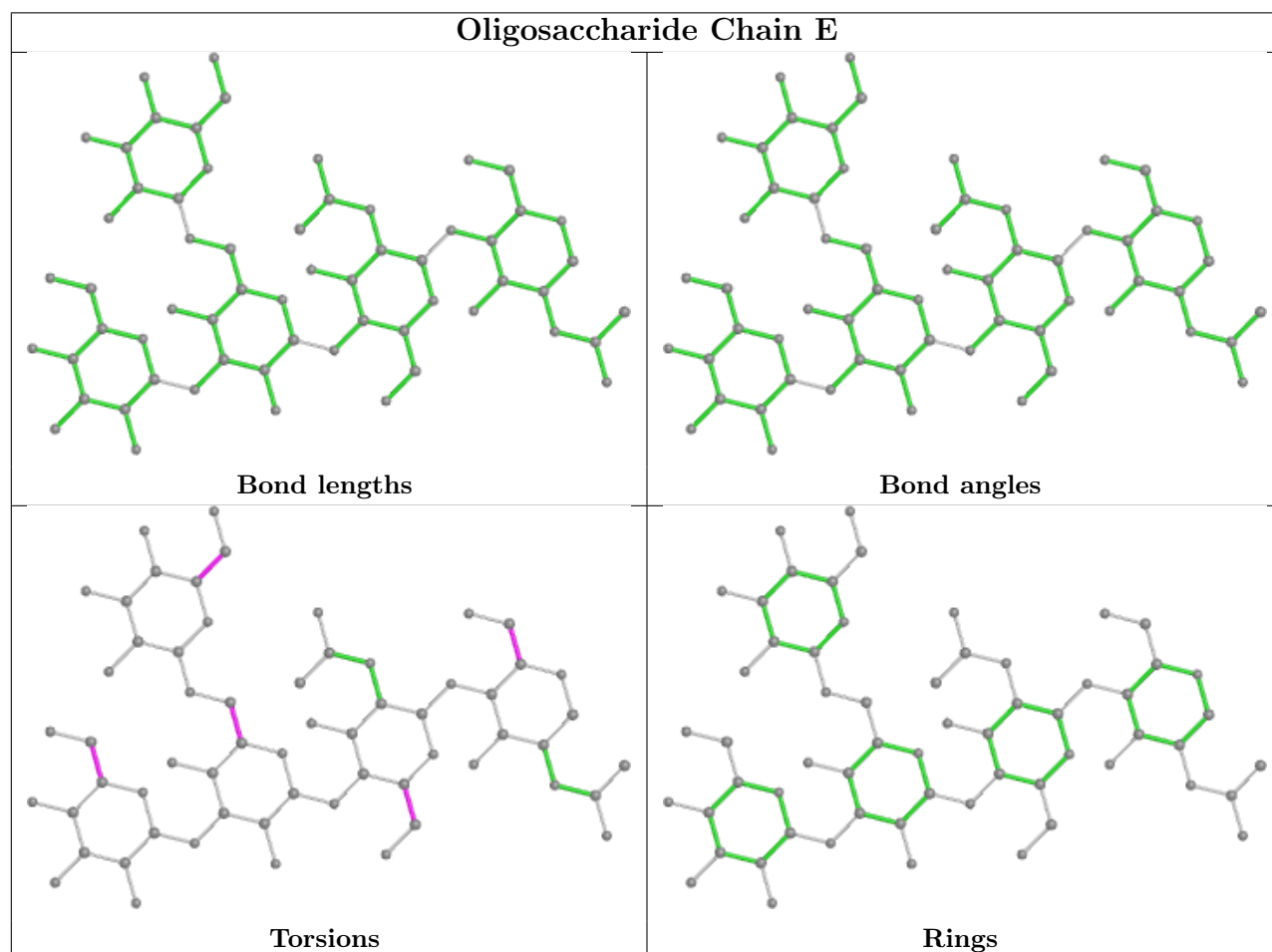
Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	4	BMA	C4-C5-C6-O6
2	E	4	BMA	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	E	5	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	N	2	NAG	C3-C2-N2-C7

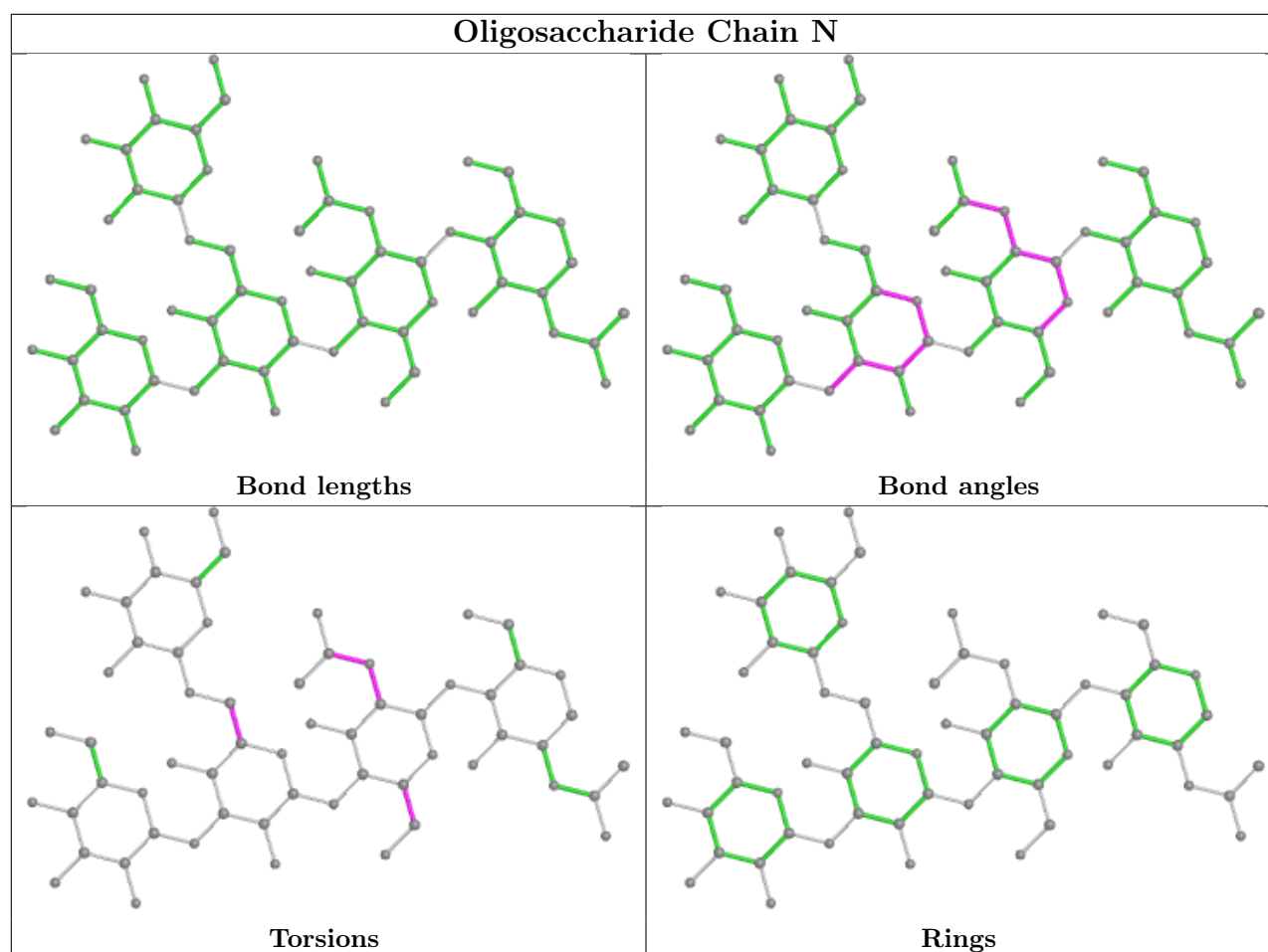
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	3	BMA	1	0
2	N	2	NAG	1	0
2	N	5	BMA	1	0

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





5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	NAG	A	2306	1	14,14,15	0.87	1 (7%)	17,19,21	1.32	1 (5%)
5	HZL	A	2311	-	71,71,71	3.16	14 (19%)	81,84,84	1.56	13 (16%)
3	NAG	A	2307	1	14,14,15	0.25	0	17,19,21	0.34	0
3	NAG	A	2301	1	14,14,15	0.15	0	17,19,21	0.48	0
3	NAG	A	2302	1	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
4	3PE	A	2309	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2303	1	14,14,15	0.34	0	17,19,21	0.61	0
4	3PE	A	2310	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	3 (5%)
4	3PE	A	2308	-	50,50,50	0.94	2 (4%)	53,55,55	1.04	2 (3%)
3	NAG	A	2305	1	14,14,15	0.90	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	A	2304	1	14,14,15	0.95	1 (7%)	17,19,21	1.21	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
3	NAG	A	2306	1	-	2/6/23/26	0/1/1/1
5	HZL	A	2311	-	-	33/70/87/87	0/1/1/1
3	NAG	A	2307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2302	1	-	3/6/23/26	0/1/1/1
4	3PE	A	2309	-	-	15/54/54/54	-
3	NAG	A	2303	1	-	3/6/23/26	0/1/1/1
4	3PE	A	2310	-	-	14/54/54/54	-
4	3PE	A	2308	-	-	19/54/54/54	-
3	NAG	A	2305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2304	1	-	3/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2311	HZL	CBZ-CBV	13.75	1.54	1.35
5	A	2311	HZL	CAX-CAV	12.70	1.52	1.35
5	A	2311	HZL	CAK-CAN	-9.88	1.40	1.53
5	A	2311	HZL	CBM-CBR	7.18	1.53	1.34
5	A	2311	HZL	CAU-CAS	6.51	1.52	1.33
5	A	2311	HZL	CAO-CAP	-5.50	1.40	1.51
5	A	2311	HZL	CAP-CAN	4.48	1.42	1.34
5	A	2311	HZL	CBZ-CCA	4.44	1.53	1.44
4	A	2308	3PE	O31-C31	4.38	1.46	1.33
4	A	2310	3PE	O31-C31	4.22	1.45	1.33
4	A	2308	3PE	O21-C21	4.16	1.46	1.34
4	A	2309	3PE	O31-C31	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2310	3PE	O21-C21	4.10	1.45	1.34
4	A	2309	3PE	O21-C21	4.10	1.45	1.34
5	A	2311	HZL	CBE-CBA	3.74	1.53	1.31
5	A	2311	HZL	CBD-CAZ	3.74	1.53	1.31
5	A	2311	HZL	CAU-CAV	3.39	1.53	1.45
3	A	2304	NAG	O5-C1	3.20	1.48	1.43
3	A	2306	NAG	O5-C1	3.14	1.48	1.43
5	A	2311	HZL	CBR-CBV	3.07	1.52	1.45
5	A	2311	HZL	CBM-CAX	3.06	1.52	1.43
5	A	2311	HZL	PAA-OAH	3.00	1.61	1.50
3	A	2305	NAG	O5-C1	2.61	1.47	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2311	HZL	CAS-CAU-CAV	-5.27	118.27	126.23
3	A	2306	NAG	C1-O5-C5	4.97	118.92	112.19
5	A	2311	HZL	CBM-CAX-CAV	-4.89	120.33	127.31
5	A	2311	HZL	CCA-CBZ-CBV	-4.75	120.81	126.25
5	A	2311	HZL	CAX-CBM-CBR	-4.66	108.68	123.22
3	A	2304	NAG	C1-O5-C5	4.59	118.41	112.19
3	A	2302	NAG	C2-N2-C7	4.33	129.07	122.90
4	A	2309	3PE	O21-C21-C22	4.01	120.14	111.50
4	A	2308	3PE	O21-C21-C22	3.94	119.99	111.50
4	A	2310	3PE	O21-C21-C22	3.88	119.86	111.50
3	A	2305	NAG	C1-O5-C5	3.30	116.66	112.19
4	A	2308	3PE	O31-C31-C32	2.92	121.08	111.91
4	A	2309	3PE	C2-O21-C21	-2.89	110.68	117.79
5	A	2311	HZL	CBU-OAB-CBS	-2.88	110.69	117.79
4	A	2310	3PE	C2-O21-C21	-2.64	111.29	117.79
4	A	2310	3PE	O31-C31-C32	2.47	119.66	111.91
4	A	2309	3PE	O31-C31-C32	2.40	119.43	111.91
5	A	2311	HZL	CBZ-CCA-NAJ	-2.38	117.89	122.53
5	A	2311	HZL	CAW-CAV-CAU	2.32	121.73	118.08
5	A	2311	HZL	CBM-CBR-CBV	-2.31	119.92	126.42
5	A	2311	HZL	CAU-CAS-CAN	-2.25	120.88	127.20
5	A	2311	HZL	CAM-CAL-CAK	-2.23	106.62	114.60
5	A	2311	HZL	CAK-CAN-CAP	-2.11	119.64	122.61
5	A	2311	HZL	CAS-CAN-CAP	2.06	126.45	121.46
5	A	2311	HZL	CBW-OAC-CBT	-2.01	109.68	117.12

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2308	3PE	C11-O13-P-O11
4	A	2309	3PE	C11-O13-P-O11
4	A	2309	3PE	C11-O13-P-O14
4	A	2310	3PE	C1-O11-P-O14
5	A	2311	HZL	CAK-CAN-CAS-CAU
5	A	2311	HZL	CAP-CAN-CAS-CAU
5	A	2311	HZL	CBP-CBS-OAB-CBU
5	A	2311	HZL	OAE-CBT-OAC-CBW
5	A	2311	HZL	NAJ-CCB-CCC-OAG
5	A	2311	HZL	CCC-CCB-NAJ-CCA
5	A	2311	HZL	CCC-OAG-PAA-OAF
5	A	2311	HZL	CBQ-CBT-OAC-CBW
5	A	2311	HZL	OAD-CBS-OAB-CBU
3	A	2305	NAG	C4-C5-C6-O6
3	A	2303	NAG	O5-C5-C6-O6
3	A	2304	NAG	O5-C5-C6-O6
3	A	2305	NAG	O5-C5-C6-O6
5	A	2311	HZL	CAY-CBC-CBG-CBI
3	A	2303	NAG	C4-C5-C6-O6
3	A	2304	NAG	C4-C5-C6-O6
3	A	2307	NAG	O5-C5-C6-O6
3	A	2302	NAG	C8-C7-N2-C2
3	A	2302	NAG	O7-C7-N2-C2
3	A	2301	NAG	O5-C5-C6-O6
3	A	2301	NAG	C4-C5-C6-O6
4	A	2309	3PE	C34-C35-C36-C37
4	A	2309	3PE	C3B-C3C-C3D-C3E
4	A	2309	3PE	C3C-C3D-C3E-C3F
4	A	2309	3PE	C2C-C2D-C2E-C2F
5	A	2311	HZL	CBH-CBJ-CBL-CBO
4	A	2308	3PE	C2B-C2C-C2D-C2E
5	A	2311	HZL	CBD-CCF-CCG-CCH
5	A	2311	HZL	CBK-CBN-CBP-CBS
4	A	2308	3PE	C29-C2A-C2B-C2C
5	A	2311	HZL	CBC-CBG-CBI-CBK
5	A	2311	HZL	CCN-CCO-CCP-CCQ
5	A	2311	HZL	CCO-CCP-CCQ-CCR
4	A	2310	3PE	C29-C2A-C2B-C2C
5	A	2311	HZL	CBB-CBF-CBH-CBJ
4	A	2310	3PE	C23-C24-C25-C26
4	A	2310	3PE	C2B-C2C-C2D-C2E
5	A	2311	HZL	CBG-CBI-CBK-CBN

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Mol	Chain	Res	Type	Atoms
5	A	2311	HZL	CAZ-CAY-CBC-CBG
5	A	2311	HZL	CBA-CBB-CBF-CBH
4	A	2308	3PE	C22-C23-C24-C25
4	A	2308	3PE	C2E-C2F-C2G-C2H
4	A	2310	3PE	C22-C21-O21-C2
5	A	2311	HZL	CCE-CCN-CCO-CCP
4	A	2309	3PE	C37-C38-C39-C3A
4	A	2310	3PE	O22-C21-O21-C2
5	A	2311	HZL	CBX-OAF-PAA-OAG
5	A	2311	HZL	CBL-CBO-CBQ-CBT
3	A	2307	NAG	C4-C5-C6-O6
5	A	2311	HZL	CCP-CCQ-CCR-CCS
4	A	2308	3PE	C3A-C3B-C3C-C3D
4	A	2308	3PE	C28-C29-C2A-C2B
4	A	2308	3PE	C33-C34-C35-C36
5	A	2311	HZL	CBF-CBH-CBJ-CBL
4	A	2309	3PE	C24-C25-C26-C27
5	A	2311	HZL	CCI-CCJ-CCK-CCL
5	A	2311	HZL	CBX-CBU-OAB-CBS
3	A	2306	NAG	O5-C5-C6-O6
4	A	2309	3PE	C1-C2-C3-O31
4	A	2310	3PE	O11-C1-C2-O21
4	A	2309	3PE	O21-C2-C3-O31
4	A	2310	3PE	C1-O11-P-O13
4	A	2308	3PE	C11-O13-P-O12
5	A	2311	HZL	CBX-OAF-PAA-OAH
5	A	2311	HZL	CBX-OAF-PAA-OAI
5	A	2311	HZL	CCB-CCC-OAG-PAA
4	A	2308	3PE	C34-C35-C36-C37
4	A	2308	3PE	O11-C1-C2-O21
4	A	2308	3PE	C1-O11-P-O13
4	A	2309	3PE	C1-O11-P-O13
4	A	2310	3PE	C11-O13-P-O11
5	A	2311	HZL	CBX-CBU-CBW-OAC
5	A	2311	HZL	CBI-CBK-CBN-CBP
4	A	2308	3PE	C2C-C2D-C2E-C2F
3	A	2302	NAG	C3-C2-N2-C7
3	A	2303	NAG	C3-C2-N2-C7
3	A	2304	NAG	C3-C2-N2-C7
3	A	2306	NAG	C3-C2-N2-C7
4	A	2309	3PE	O13-C11-C12-N
4	A	2308	3PE	O21-C21-C22-C23

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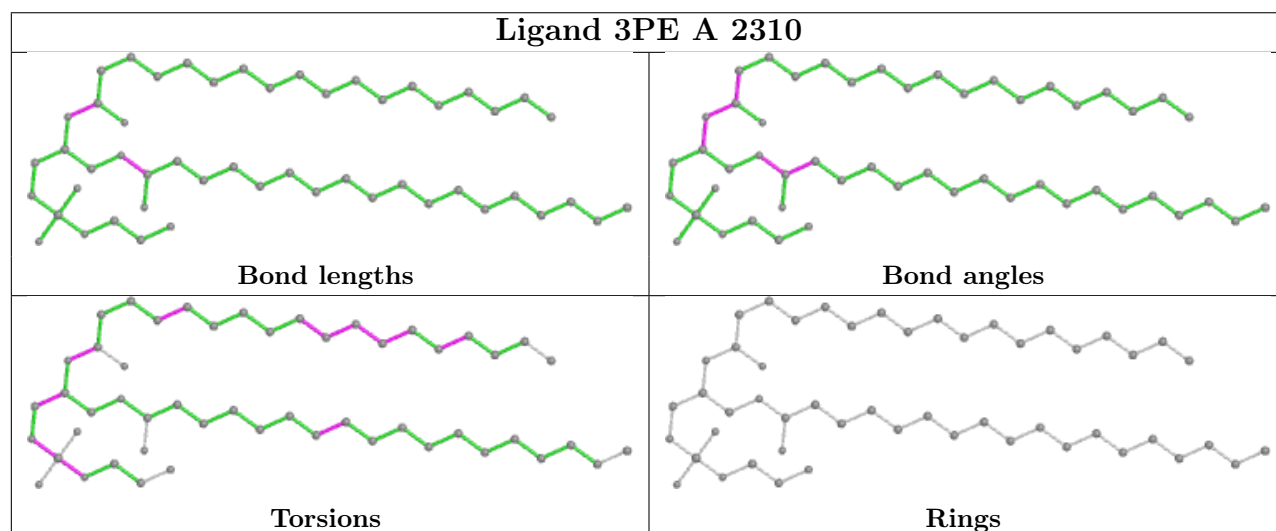
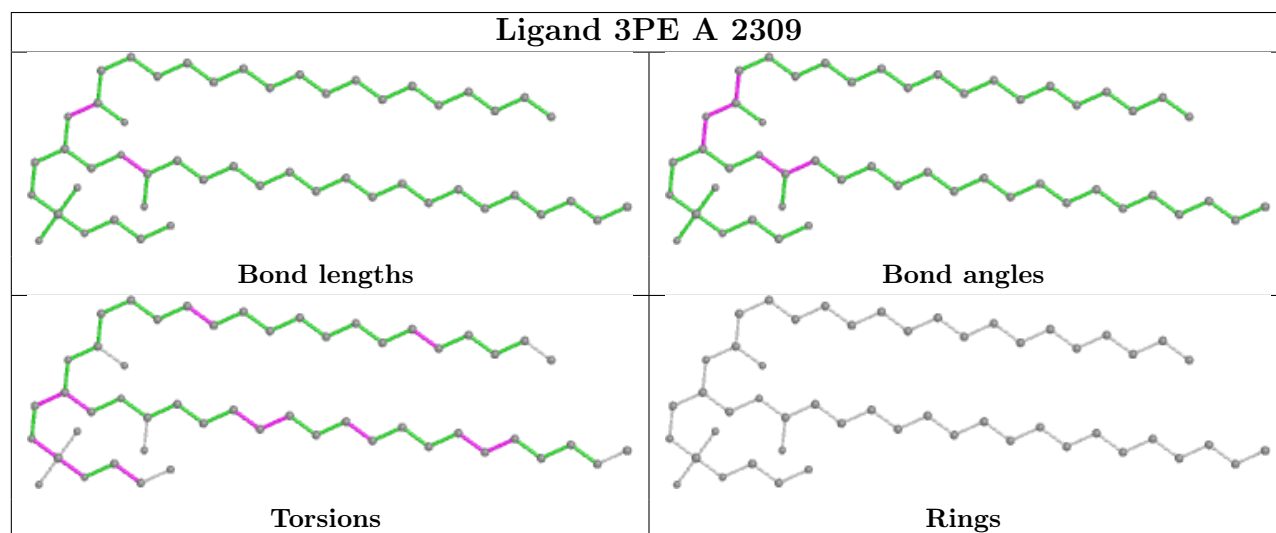
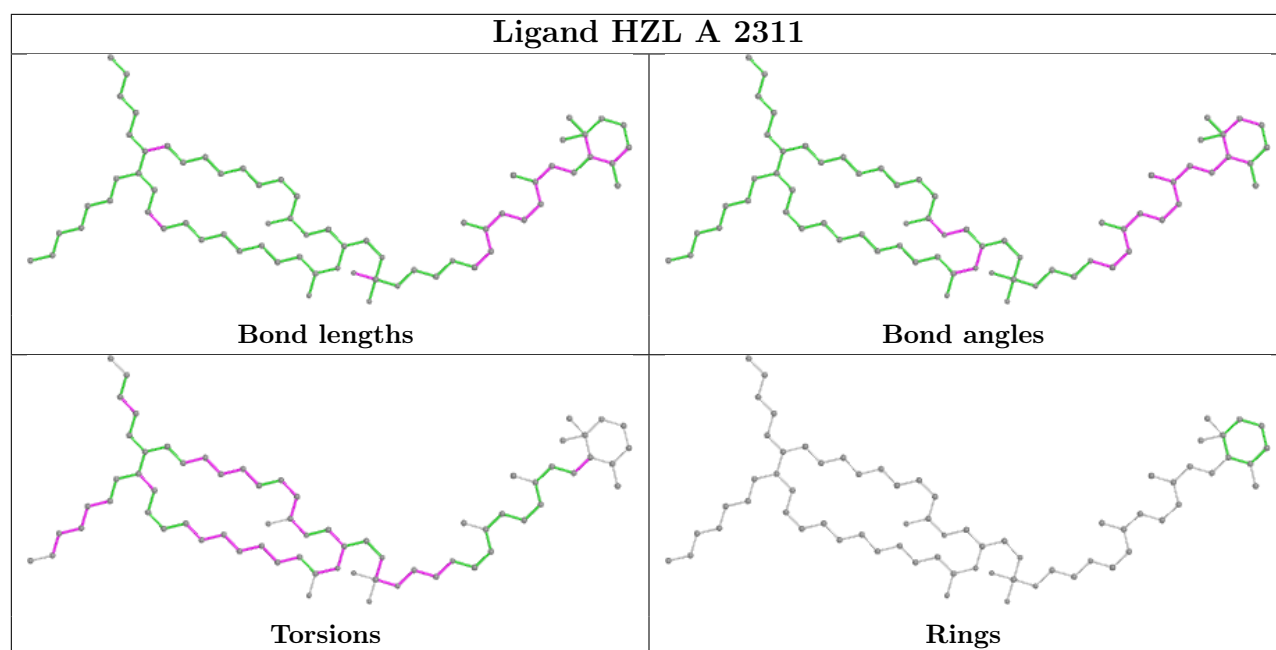
Mol	Chain	Res	Type	Atoms
4	A	2310	3PE	C28-C29-C2A-C2B
4	A	2310	3PE	C2A-C2B-C2C-C2D
4	A	2308	3PE	C35-C36-C37-C38
4	A	2308	3PE	C3C-C3D-C3E-C3F
4	A	2308	3PE	C2D-C2E-C2F-C2G
4	A	2310	3PE	C36-C37-C38-C39
4	A	2308	3PE	C2F-C2G-C2H-C2I
4	A	2309	3PE	O11-C1-C2-C3
4	A	2310	3PE	O11-C1-C2-C3
4	A	2309	3PE	C33-C34-C35-C36
4	A	2309	3PE	C1-O11-P-O14
5	A	2311	HZL	CBO-CBQ-CBT-OAC
4	A	2310	3PE	C2D-C2E-C2F-C2G
4	A	2308	3PE	O31-C31-C32-C33

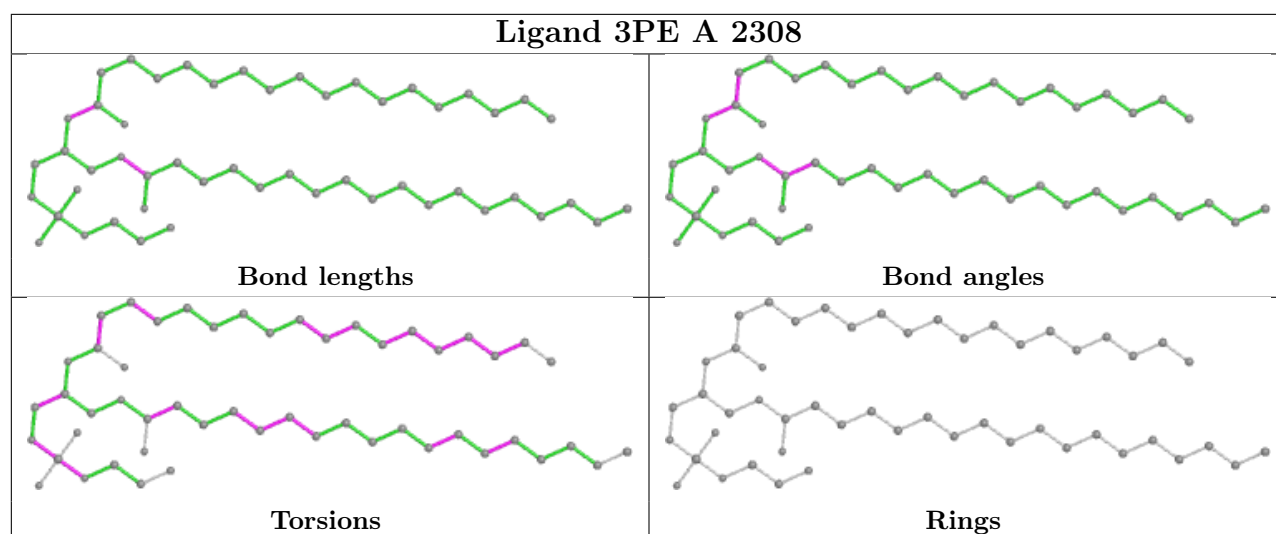
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2311	HZL	7	0
3	A	2302	NAG	1	0
4	A	2309	3PE	3	0
4	A	2310	3PE	1	0
4	A	2308	3PE	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

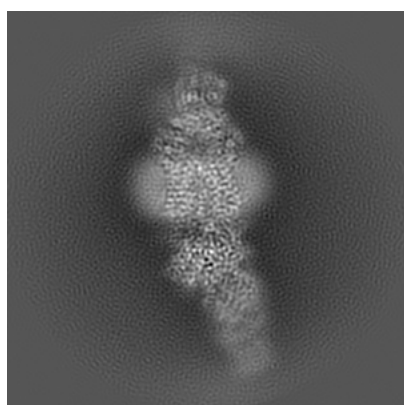
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31001. These allow visual inspection of the internal detail of the map and identification of artifacts.

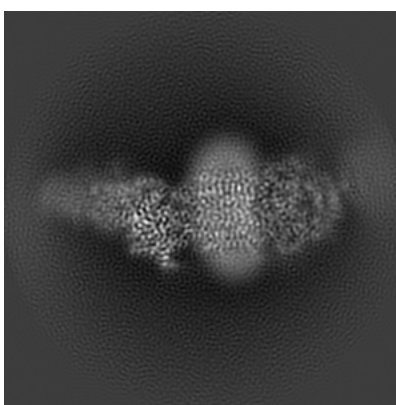
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

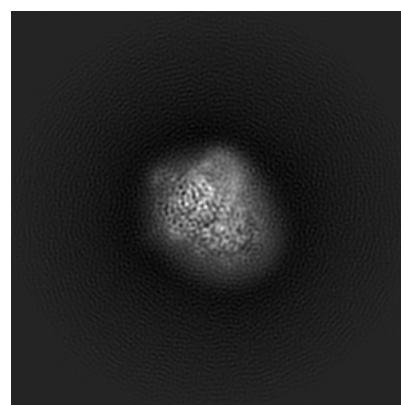
6.1.1 Primary map



X



Y

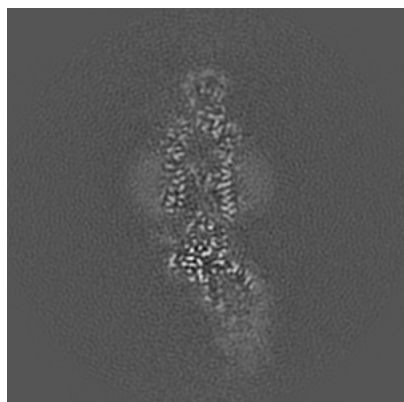


Z

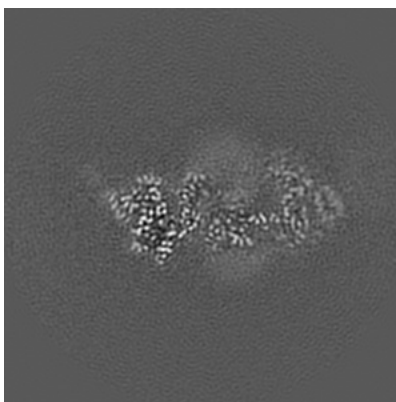
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

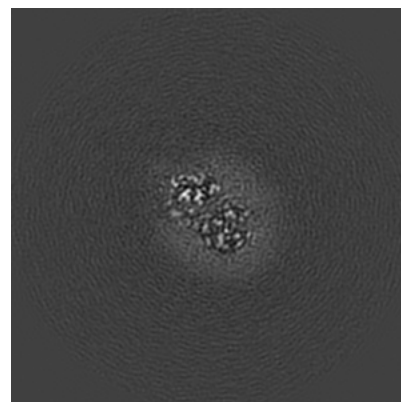
6.2.1 Primary map



X Index: 140



Y Index: 140

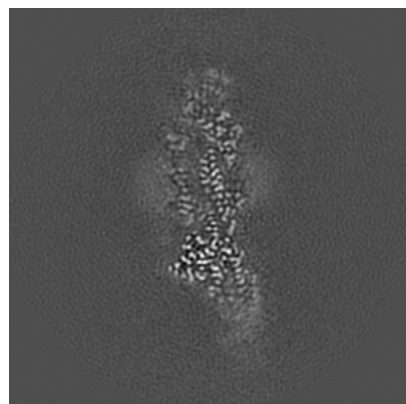


Z Index: 140

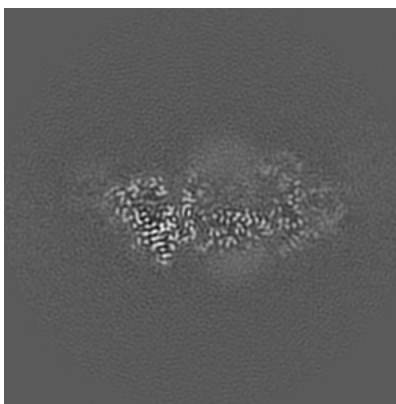
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

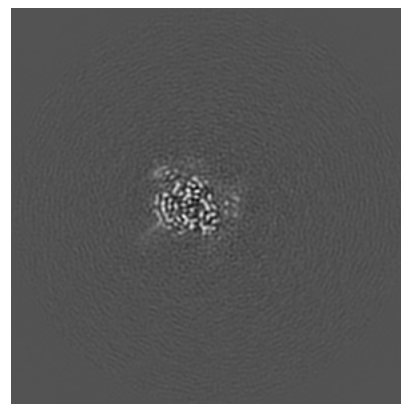
6.3.1 Primary map



X Index: 135



Y Index: 143

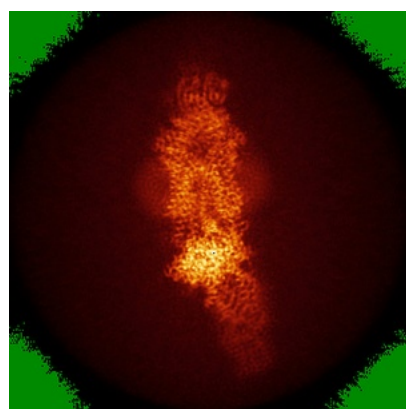


Z Index: 112

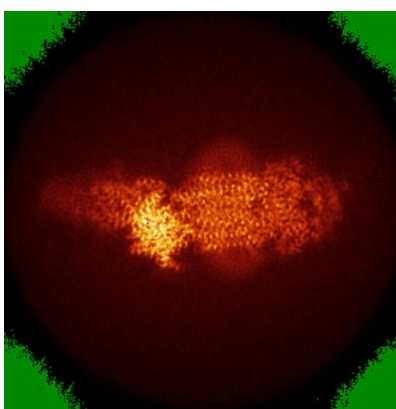
The images above show the largest variance slices of the map in three orthogonal directions.

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

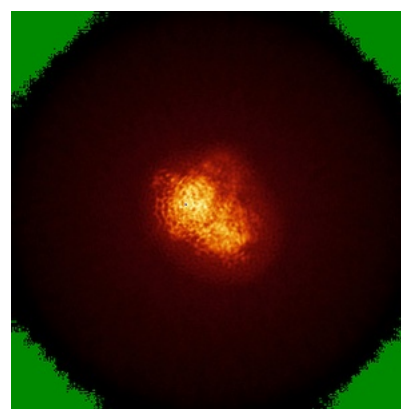
6.4.1 Primary map



X



Y

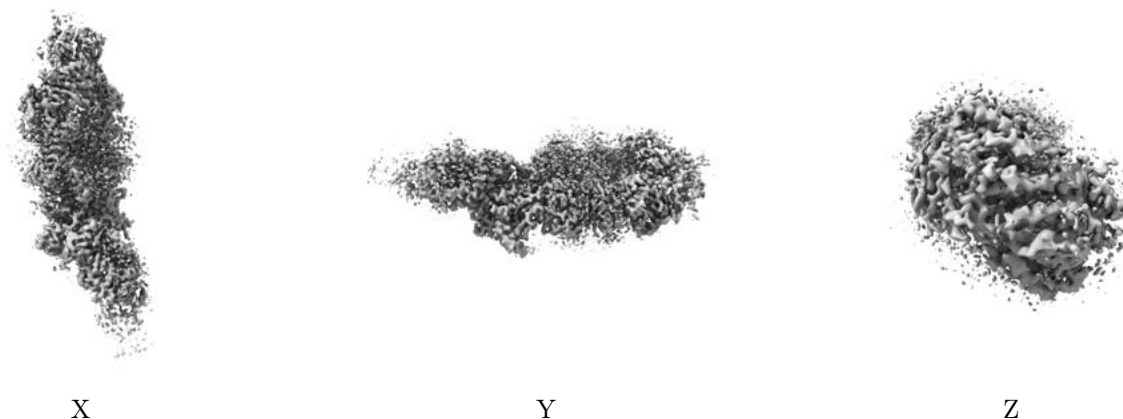


Z

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

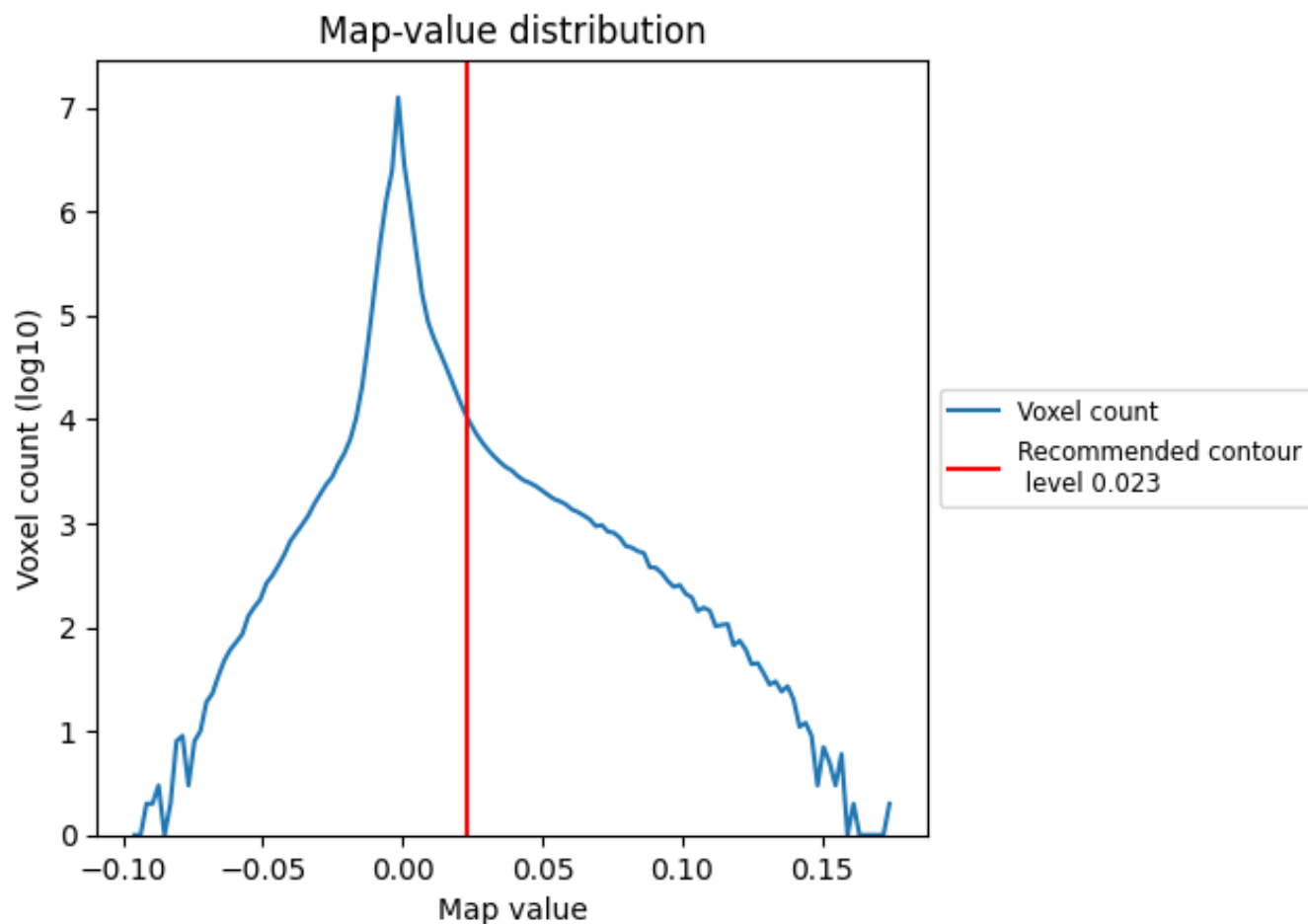
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

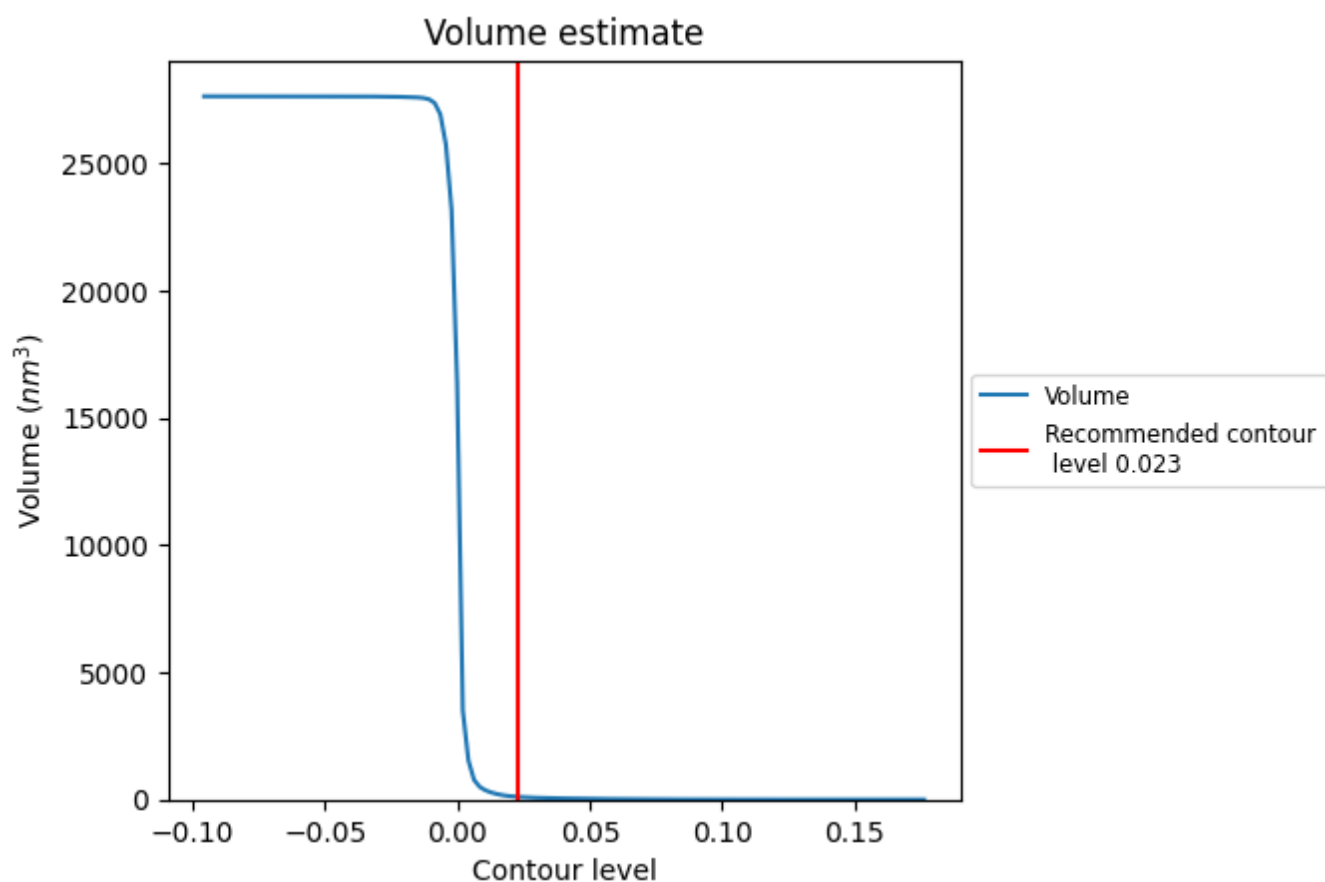
This section contains the results of statistical analysis of the map.

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.

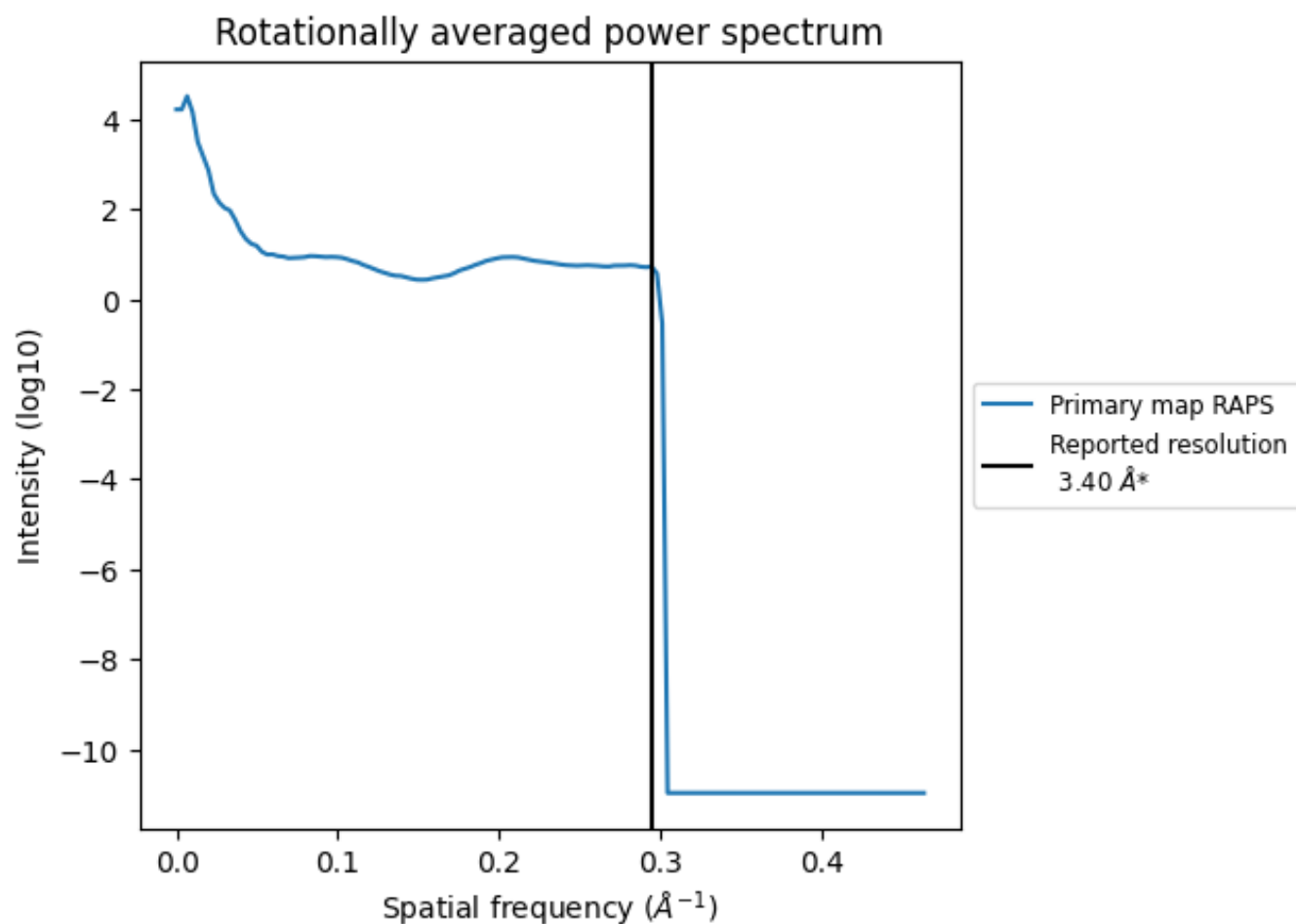
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm³; this corresponds to an approximate mass of 94 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 0.294 Å⁻¹

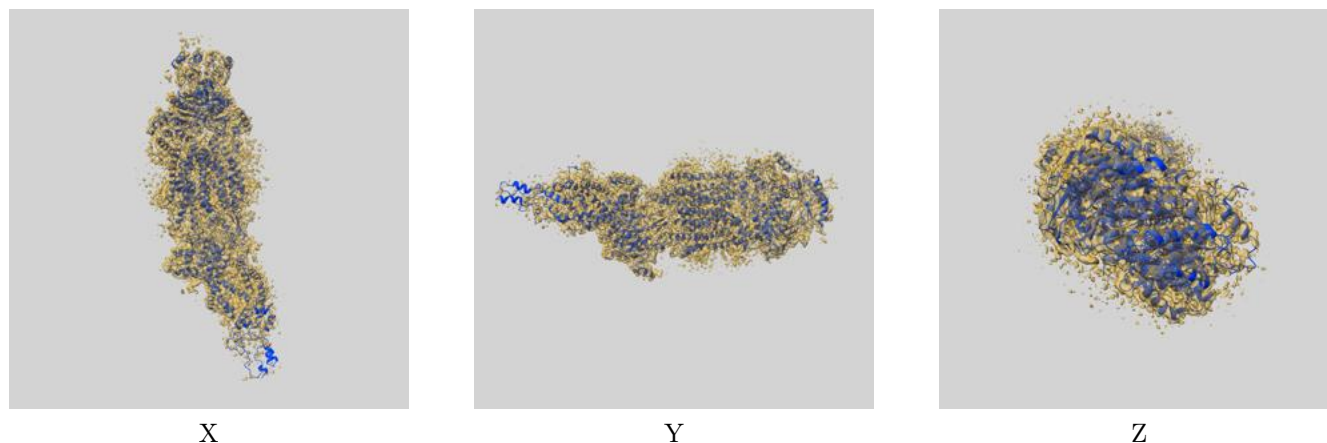
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

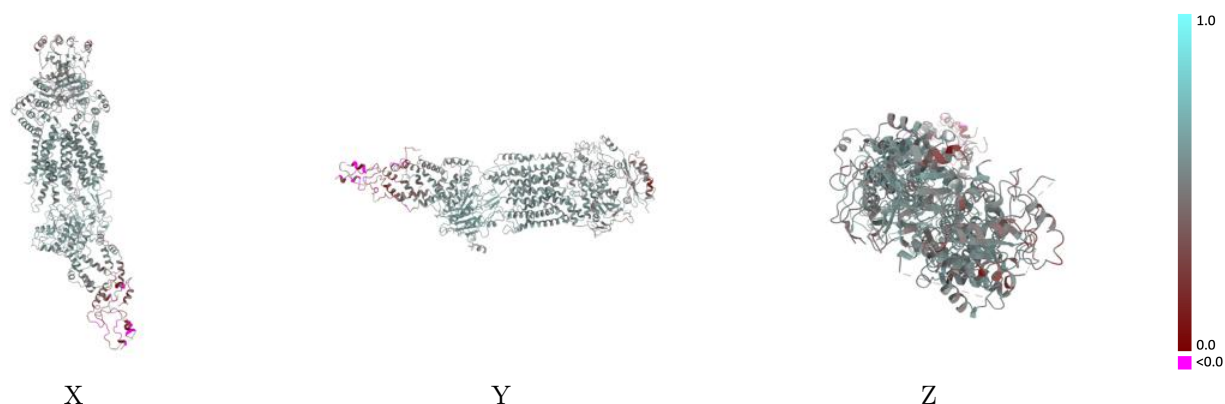
This section contains information regarding the fit between EMDB map EMD-31001 and PDB model 7E7O. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



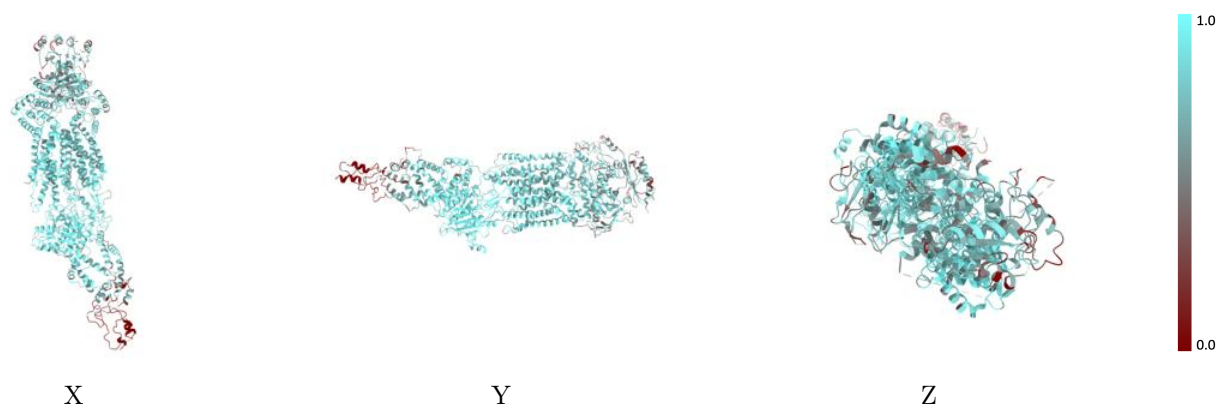
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



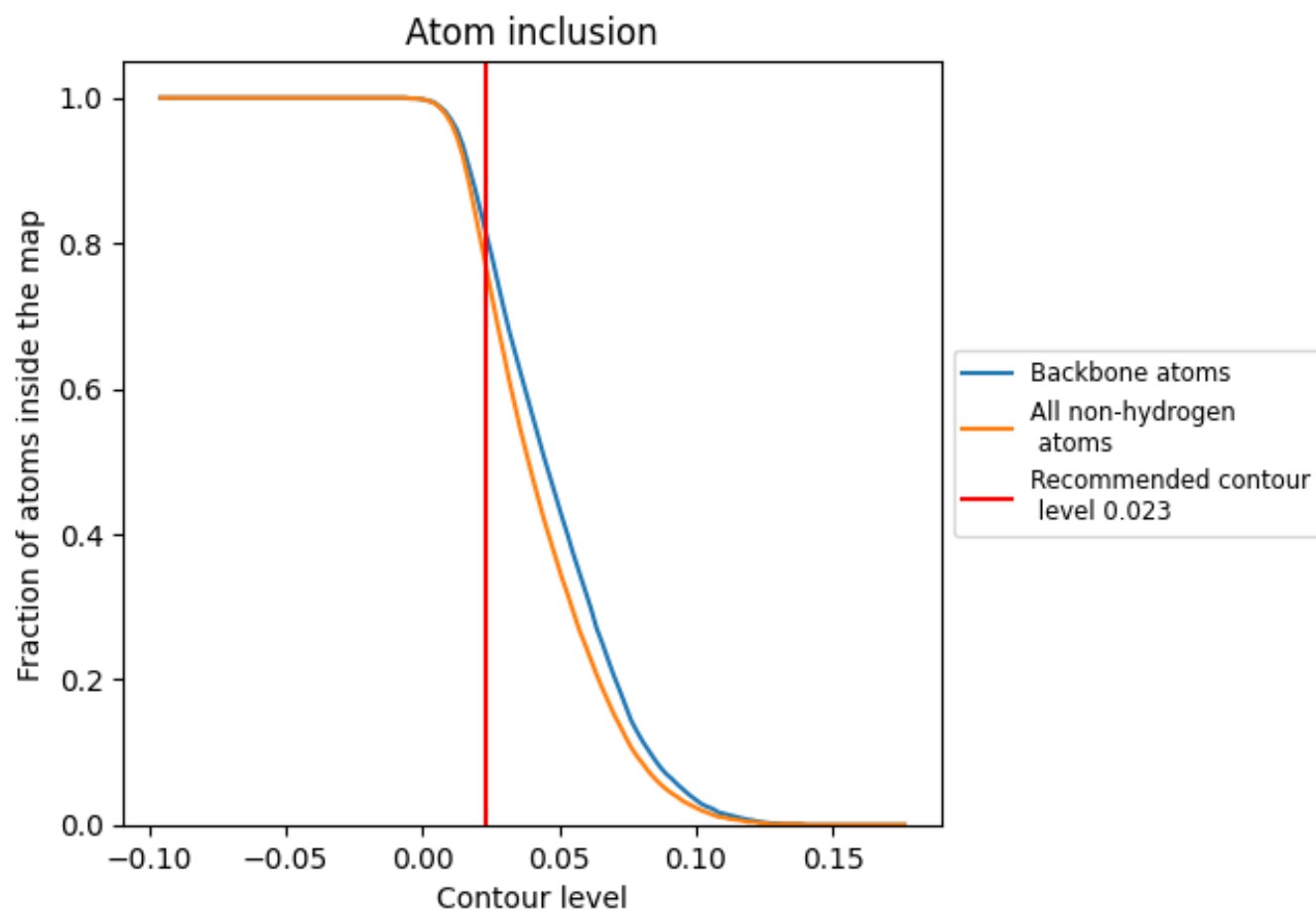
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7720	<div></div> 0.5180
A	<div></div> 0.7720	<div></div> 0.5180
E	<div></div> 0.6720	<div></div> 0.4790
N	<div></div> 0.8530	<div></div> 0.5080

