



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 04:05 AM EDT

PDB ID : 7KYB / pdb_00007kyb
EMDB ID : EMD-23074
Title : Structure of the *S. cerevisiae* phosphatidylcholine flippase Dnf1-Lem3 complex in the E1-ADP state
Authors : Bai, L.; You, Q.; Jain, B.K.; Duan, H.D.; Kovach, A.; Graham, T.R.; Li, H.
Deposited on : 2020-12-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

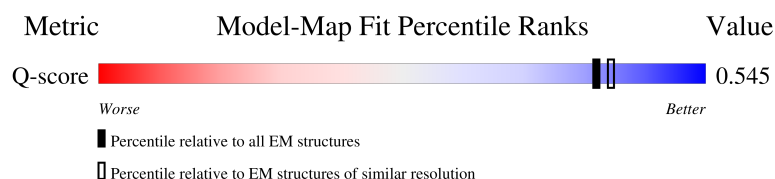
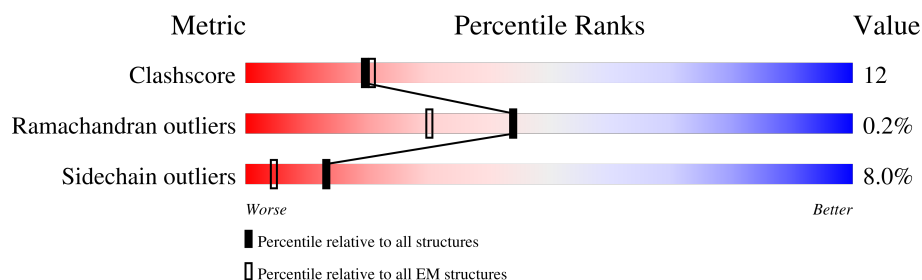
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1571	7% 42% 18% • 39%
2	B	414	64% 21% • 12%
3	C	3	100%
4	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
4	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ALF	A	1603	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10814 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.

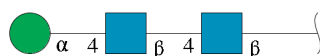
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	957	Total	C	N	O	S	0	0
			7646	4964	1250	1396	36		

- Molecule 2 is a protein called Alkylphosphocholine resistance protein LEM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	365	Total	C	N	O	S	0	0
			2959	1899	499	547	14		

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



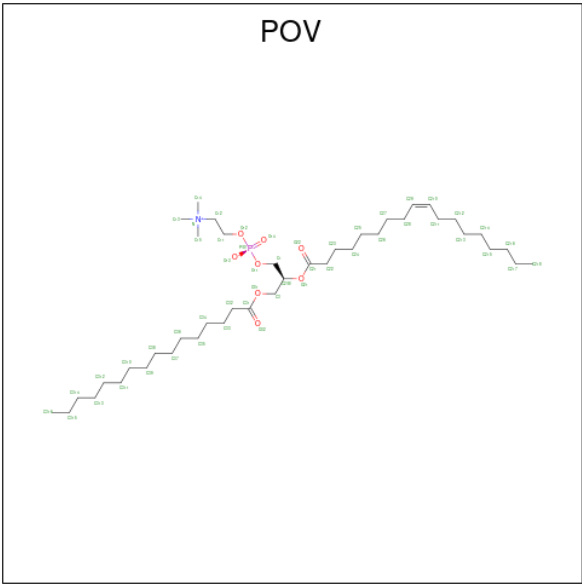
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

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



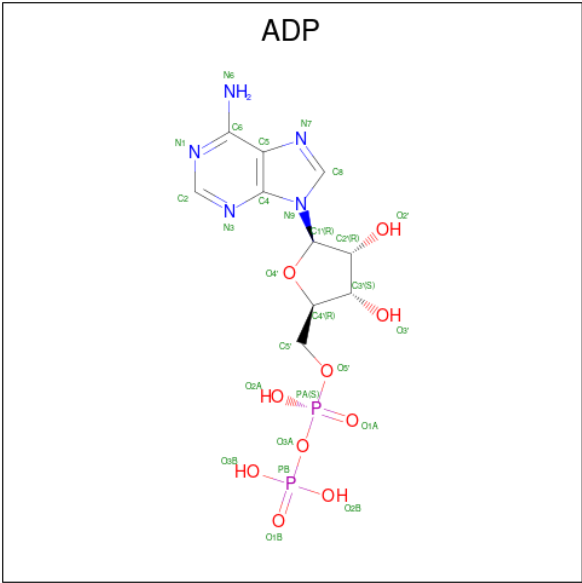
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



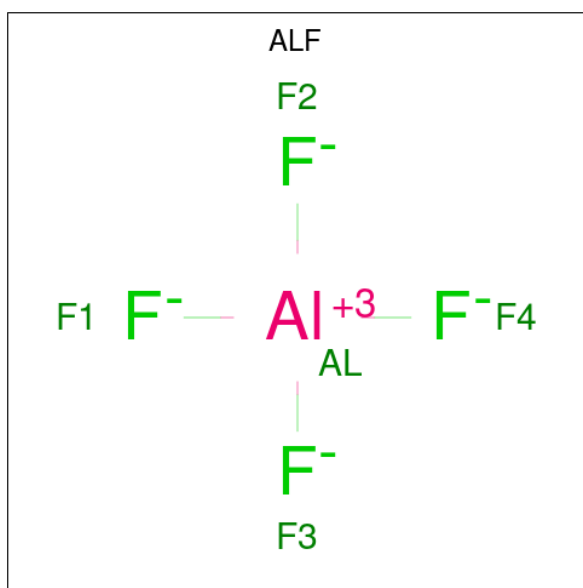
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	52	42	1	8	1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	27	10	5	10	2	0

- Molecule 7 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

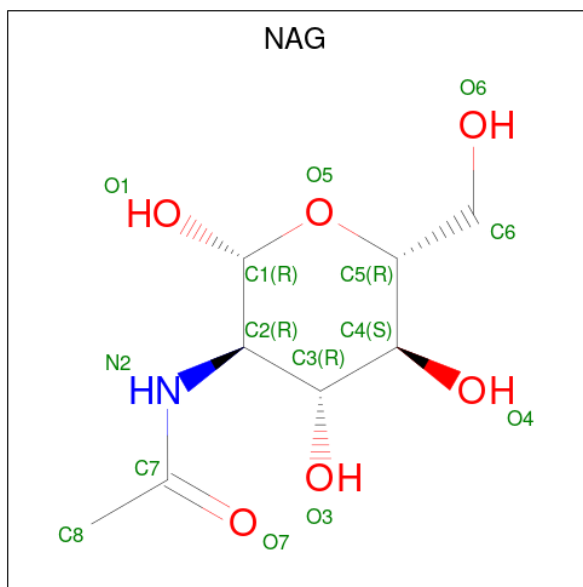


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Al	F	0
			5	1	4	

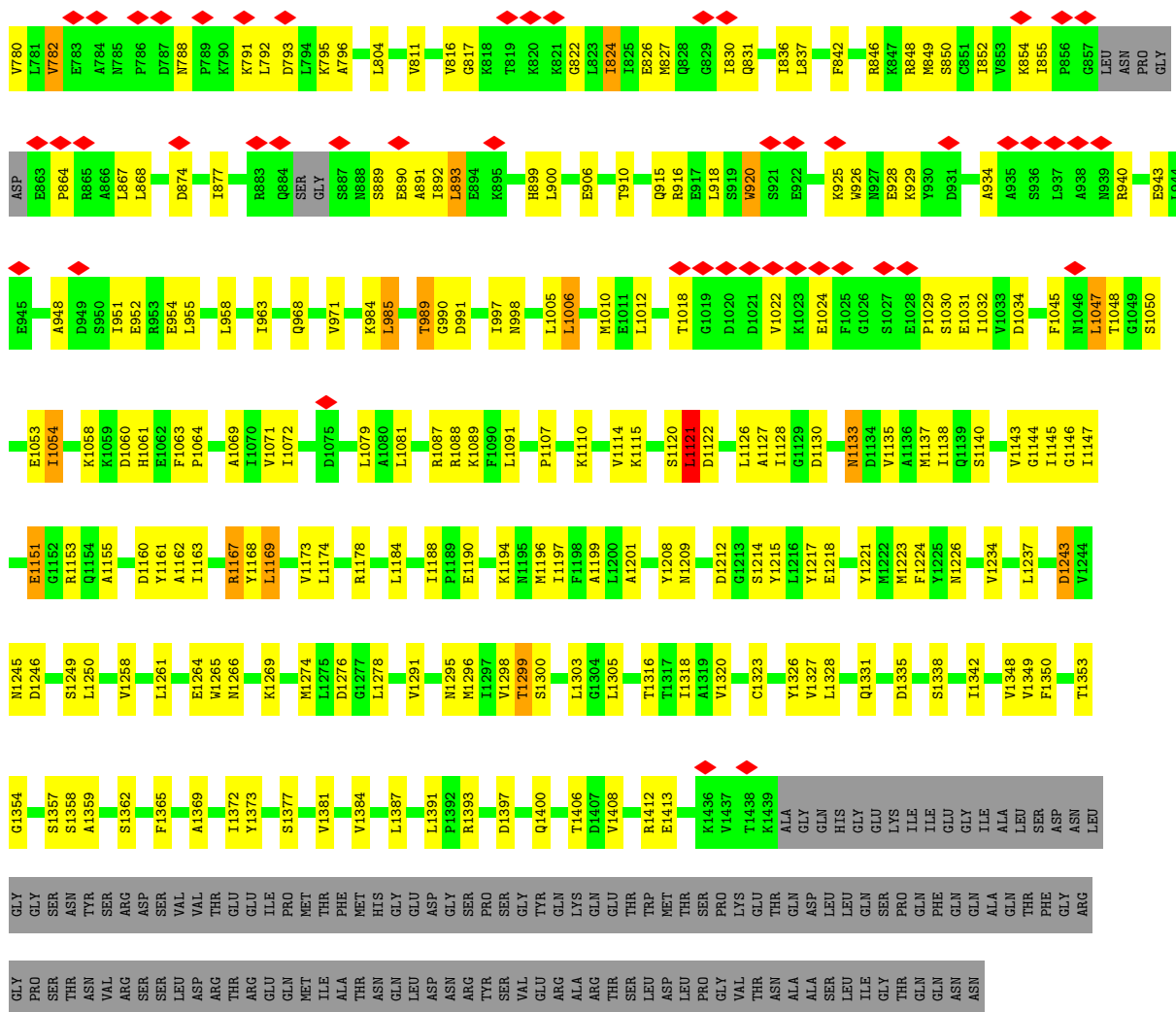
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Mg	0
			2	2	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).

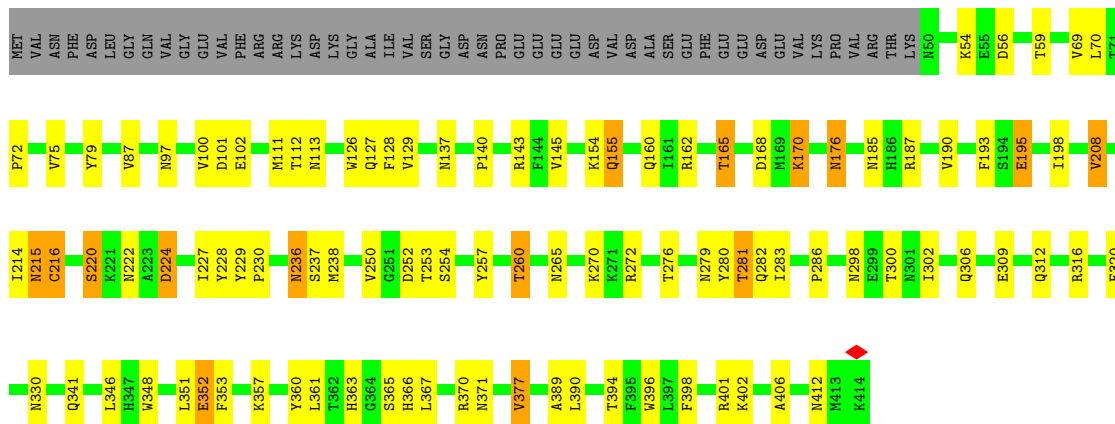


Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	



• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B: 64% 21% 12%



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2
MAN3

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

Chain D:  50%
 100%

MAG1
MAG2

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

Chain E:  50%
 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	716510	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	231.28, 231.28, 231.28	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, NAG, ALF, MAN, POV, MG

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	0.45	0/7820	0.47	1/10592 (0.0%)
2	B	0.58	0/3042	0.49	0/4136
All	All	0.49	0/10862	0.48	1/14728 (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
2	B	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	1121	LEU	N-CA-C	-5.49	104.49	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	LYS	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	7646	0	7644	209	0
2	B	2959	0	2866	61	0
3	C	39	0	34	0	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	52	0	82	4	0
6	A	27	0	12	1	0
7	A	5	0	0	4	0
8	A	2	0	0	0	0
9	B	28	0	26	0	0
All	All	10814	0	10714	268	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 12.

All (268) 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:1047:LEU:HB2	1:A:1053:GLU:OE1	1.25	1.36
1:A:1091:LEU:HD21	1:A:1121:LEU:CD2	1.55	1.34
1:A:1120:SER:O	1:A:1121:LEU:HG	1.31	1.26
1:A:1091:LEU:HD11	1:A:1121:LEU:HD21	1.36	1.06
1:A:1091:LEU:CD2	1:A:1121:LEU:HD23	1.86	1.04
1:A:1091:LEU:CD2	1:A:1121:LEU:CD2	2.40	0.97
1:A:1091:LEU:HD21	1:A:1121:LEU:HD23	0.99	0.97
1:A:1047:LEU:HB2	1:A:1053:GLU:CD	1.90	0.95
1:A:1353:THR:HG21	1:A:1373:TYR:CE2	2.02	0.94
1:A:1350:PHE:O	1:A:1353:THR:HG22	1.69	0.91
1:A:1048:THR:H	1:A:1053:GLU:CD	1.79	0.91
1:A:1091:LEU:HD21	1:A:1121:LEU:HD21	1.54	0.87
1:A:1091:LEU:CD1	1:A:1121:LEU:HD21	2.06	0.85
1:A:852:ILE:HG12	1:A:868:LEU:HD23	1.63	0.81
1:A:1353:THR:CG2	1:A:1373:TYR:HE2	1.94	0.81
1:A:667:ASP:OD1	7:A:1603:ALF:F2	1.92	0.78
1:A:1120:SER:C	1:A:1121:LEU:HG	2.07	0.78
5:A:1601:POV:H38A	5:A:1601:POV:H25A	1.66	0.77
1:A:1353:THR:HG21	1:A:1373:TYR:CZ	2.20	0.77
1:A:1353:THR:HG21	1:A:1373:TYR:OH	1.86	0.76
1:A:918:LEU:HD11	1:A:951:ILE:HD11	1.68	0.76
1:A:667:ASP:OD1	7:A:1603:ALF:F3	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:SER:O	1:A:1121:LEU:CG	2.26	0.74
1:A:1320:VAL:HG11	1:A:1349:VAL:HG21	1.67	0.74
1:A:1209:ASN:ND2	1:A:1214:SER:OG	2.21	0.74
1:A:696:ALA:HB1	1:A:998:ASN:HD21	1.53	0.72
1:A:671:THR:O	1:A:968:GLN:NE2	2.23	0.72
1:A:1353:THR:CG2	1:A:1373:TYR:CE2	2.72	0.71
1:A:1237:LEU:HD12	1:A:1327:VAL:HG13	1.72	0.71
1:A:1178:ARG:NH1	1:A:1249:SER:OG	2.25	0.70
1:A:1393:ARG:NH1	1:A:1397:ASP:OD1	2.24	0.70
1:A:837:LEU:HD11	1:A:854:LYS:HG3	1.75	0.69
1:A:848:ARG:NH2	1:A:952:GLU:OE1	2.27	0.68
1:A:864:PRO:HG2	1:A:920:TRP:HE1	1.57	0.68
1:A:1048:THR:N	1:A:1053:GLU:OE2	2.26	0.68
1:A:1243:ASP:OD2	1:A:1243:ASP:N	2.27	0.67
1:A:842:PHE:HB2	1:A:849:MET:HB2	1.77	0.67
1:A:1121:LEU:HD12	1:A:1121:LEU:O	1.94	0.67
1:A:752:VAL:HA	1:A:755:LEU:HD12	1.77	0.67
1:A:1091:LEU:HD11	1:A:1121:LEU:CD2	2.22	0.67
1:A:824:ILE:HD11	1:A:831:GLN:HB3	1.78	0.66
1:A:683:THR:HG22	1:A:688:SER:HA	1.77	0.66
1:A:571:ASN:HD22	1:A:601:SER:HB2	1.59	0.66
1:A:1058:LYS:HG2	1:A:1121:LEU:HA	1.79	0.64
1:A:549:LEU:HD11	1:A:617:LEU:HD21	1.79	0.63
1:A:1115:LYS:HE3	1:A:1140:SER:HB3	1.79	0.63
1:A:1133:ASN:OD1	1:A:1133:ASN:N	2.32	0.63
1:A:1091:LEU:CG	1:A:1121:LEU:CD2	2.77	0.63
1:A:1331:GLN:HE22	1:A:1338:SER:HB3	1.63	0.62
1:A:1091:LEU:CD2	1:A:1121:LEU:HD21	2.18	0.62
1:A:207:LEU:O	1:A:211:ILE:HG12	1.99	0.62
1:A:549:LEU:HD13	1:A:1188:ILE:HD13	1.83	0.61
2:B:100:VAL:O	2:B:370:ARG:NH1	2.33	0.61
2:B:79:TYR:HB3	2:B:389:ALA:HB2	1.83	0.61
1:A:264:ARG:HH12	5:A:1601:POV:H34	1.65	0.61
1:A:1030:SER:H	1:A:1079:LEU:HD13	1.66	0.60
1:A:719:ILE:HG23	1:A:747:VAL:HG11	1.84	0.60
1:A:237:VAL:O	1:A:238:THR:OG1	2.16	0.59
1:A:1047:LEU:CB	1:A:1053:GLU:CD	2.72	0.59
1:A:1022:VAL:HG13	1:A:1032:ILE:HG13	1.83	0.59
1:A:685:ASN:ND2	1:A:766:CYS:SG	2.77	0.58
1:A:762:VAL:HA	1:A:765:ARG:HH11	1.67	0.58
1:A:691:ARG:HB3	1:A:719:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:LEU:CG	1:A:1121:LEU:HD21	2.33	0.58
2:B:237:SER:O	2:B:237:SER:OG	2.16	0.58
1:A:618:TYR:O	1:A:622:GLU:HG2	2.04	0.58
1:A:771:MET:HG3	1:A:811:VAL:HG21	1.85	0.58
1:A:934:ALA:O	1:A:940:ARG:NH1	2.36	0.58
1:A:780:VAL:HG22	1:A:796:ALA:HB2	1.84	0.57
2:B:154:LYS:NZ	2:B:352:GLU:OE2	2.37	0.57
1:A:846:ARG:HH11	1:A:848:ARG:HH21	1.52	0.57
1:A:1061:HIS:HB2	1:A:1261:LEU:HD23	1.85	0.57
2:B:265:ASN:OD1	2:B:316:ARG:NH2	2.33	0.57
1:A:1350:PHE:O	1:A:1353:THR:CG2	2.48	0.56
2:B:195:GLU:OE2	2:B:272:ARG:NE	2.35	0.56
1:A:543:SER:OG	1:A:654:ILE:HA	2.06	0.56
1:A:712:GLY:O	1:A:716:LYS:HG3	2.06	0.55
1:A:916:ARG:HH11	1:A:954:GLU:HB3	1.71	0.55
1:A:568:GLY:HA2	1:A:601:SER:OG	2.07	0.55
1:A:229:LEU:HD23	1:A:607:ILE:HD11	1.89	0.54
1:A:926:TRP:CD1	1:A:951:ILE:HB	2.42	0.54
1:A:943:GLU:N	1:A:943:GLU:OE1	2.41	0.54
1:A:846:ARG:HH11	1:A:848:ARG:NH2	2.06	0.54
1:A:571:ASN:HD22	1:A:601:SER:CB	2.21	0.54
6:A:1602:ADP:O1B	7:A:1603:ALF:F2	2.16	0.54
2:B:348:TRP:O	2:B:357:LYS:NZ	2.41	0.54
1:A:1223:MET:HG3	1:A:1224:PHE:HD1	1.72	0.54
1:A:690:GLY:H	1:A:748:SER:HB2	1.73	0.53
1:A:1353:THR:HG23	1:A:1354:GLY:N	2.21	0.53
1:A:925:LYS:O	1:A:929:LYS:HG3	2.08	0.53
2:B:363:HIS:O	2:B:363:HIS:ND1	2.41	0.53
1:A:1194:LYS:NZ	1:A:1226:ASN:OD1	2.42	0.53
2:B:222:ASN:HB3	2:B:228:TYR:CE1	2.44	0.53
1:A:985:LEU:HB3	1:A:1005:LEU:HD11	1.91	0.52
1:A:1320:VAL:HG11	1:A:1349:VAL:CG2	2.36	0.52
1:A:585:TYR:HE2	2:B:353:PHE:HE1	1.56	0.52
1:A:721:LYS:O	1:A:725:THR:HG23	2.10	0.52
1:A:1299:THR:OG1	1:A:1303:LEU:O	2.23	0.52
2:B:214:ILE:HG13	2:B:214:ILE:O	2.08	0.52
1:A:601:SER:HA	1:A:604:VAL:HG12	1.91	0.52
2:B:238:MET:O	2:B:348:TRP:NE1	2.42	0.52
2:B:279:ASN:C	2:B:281:THR:H	2.18	0.52
1:A:697:LEU:HD13	1:A:906:GLU:HG3	1.92	0.51
2:B:306:GLN:O	2:B:312:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:PHE:CD2	1:A:1064:PRO:HD2	2.45	0.51
1:A:726:MET:O	1:A:730:LEU:HG	2.10	0.51
1:A:1201:ALA:HB3	1:A:1217:TYR:OH	2.10	0.51
1:A:1048:THR:N	1:A:1053:GLU:CD	2.59	0.51
1:A:1296:MET:HE1	2:B:320:PHE:HD2	1.75	0.51
1:A:1050:SER:OG	1:A:1053:GLU:HG3	2.11	0.50
2:B:102:GLU:HG2	2:B:129:VAL:HB	1.93	0.50
1:A:685:ASN:HB3	1:A:763:GLN:NE2	2.26	0.50
1:A:1048:THR:O	1:A:1053:GLU:CD	2.53	0.50
1:A:816:VAL:O	1:A:824:ILE:HG23	2.11	0.50
2:B:270:LYS:NZ	2:B:309:GLU:OE2	2.34	0.50
1:A:849:MET:HG2	1:A:850:SER:N	2.25	0.50
1:A:1126:LEU:HD21	1:A:1145:ILE:HD12	1.93	0.50
2:B:229:TYR:HB2	2:B:283:ILE:HB	1.93	0.50
1:A:989:THR:HG22	1:A:990:GLY:H	1.77	0.50
2:B:128:PHE:CZ	2:B:140:PRO:HG3	2.47	0.49
1:A:685:ASN:HB3	1:A:763:GLN:HE22	1.77	0.49
1:A:1328:LEU:HB2	1:A:1342:ILE:HD13	1.94	0.49
1:A:1006:LEU:HD13	1:A:1012:LEU:HD21	1.93	0.49
1:A:948:ALA:HA	1:A:951:ILE:HG22	1.93	0.49
1:A:989:THR:HG22	1:A:991:ASP:H	1.78	0.49
1:A:1048:THR:N	1:A:1053:GLU:OE1	2.46	0.49
1:A:1054:ILE:HG13	1:A:1088:ARG:HG2	1.94	0.49
1:A:889:SER:C	1:A:891:ALA:H	2.21	0.49
1:A:1276:ASP:OD1	1:A:1326:TYR:OH	2.29	0.49
1:A:1151:GLU:OE2	7:A:1603:ALF:F1	2.20	0.49
1:A:1034:ASP:OD2	1:A:1089:LYS:HE3	2.13	0.49
1:A:1081:LEU:HA	1:A:1087:ARG:HG2	1.96	0.48
1:A:1413:GLU:OE1	2:B:401:ARG:NH1	2.39	0.48
1:A:779:SER:O	1:A:779:SER:OG	2.27	0.48
1:A:769:HIS:NE2	1:A:915:GLN:OE1	2.45	0.48
1:A:1029:PRO:C	1:A:1031:GLU:H	2.22	0.48
1:A:1110:LYS:O	1:A:1114:VAL:HG23	2.14	0.48
1:A:1138:ILE:HG23	1:A:1144:GLY:HA3	1.96	0.48
1:A:684:ILE:HG21	1:A:767:CYS:HA	1.96	0.48
2:B:111:MET:SD	2:B:155:GLN:HA	2.54	0.47
2:B:126:TRP:O	2:B:127:GLN:HG3	2.14	0.47
1:A:916:ARG:HB2	1:A:955:LEU:HD23	1.95	0.47
2:B:224:ASP:OD1	2:B:224:ASP:N	2.46	0.47
2:B:257:TYR:CZ	2:B:330:ASN:ND2	2.83	0.47
1:A:782:VAL:HG13	1:A:792:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:ILE:HD11	1:A:867:LEU:HD22	1.96	0.47
1:A:889:SER:HG	1:A:892:ILE:H	1.62	0.47
1:A:984:LYS:HE2	1:A:1064:PRO:HD3	1.97	0.47
1:A:1127:ALA:HB1	1:A:1137:MET:HG2	1.97	0.47
1:A:1130:ASP:HA	1:A:1155:ALA:HB3	1.97	0.47
1:A:1174:LEU:HD12	1:A:1250:LEU:HD23	1.96	0.47
2:B:215:ASN:HD22	2:B:215:ASN:N	2.13	0.47
1:A:1010:MET:HE2	1:A:1069:ALA:HB2	1.97	0.47
1:A:1018:THR:O	1:A:1022:VAL:HG23	2.14	0.47
1:A:237:VAL:HG11	2:B:187:ARG:HD2	1.95	0.47
1:A:889:SER:OG	1:A:892:ILE:HG22	2.15	0.47
1:A:1353:THR:HG21	1:A:1373:TYR:HH	1.76	0.46
1:A:650:LYS:N	1:A:1160:ASP:O	2.46	0.46
1:A:1335:ASP:OD2	1:A:1335:ASP:N	2.31	0.46
1:A:1357:SER:O	1:A:1359:ALA:N	2.49	0.46
2:B:252:ASP:OD2	2:B:254:SER:OG	2.26	0.46
1:A:900:LEU:HD22	1:A:910:THR:HB	1.96	0.46
1:A:1353:THR:HG23	1:A:1373:TYR:HE2	1.75	0.46
1:A:782:VAL:HG11	1:A:817:GLY:H	1.81	0.46
2:B:230:PRO:HD2	2:B:286:PRO:HD3	1.97	0.46
1:A:754:ASP:HA	1:A:758:ALA:HB3	1.97	0.46
1:A:1114:VAL:HG21	1:A:1137:MET:HG3	1.98	0.46
1:A:1353:THR:CG2	1:A:1354:GLY:N	2.79	0.46
1:A:1354:GLY:HA2	1:A:1369:ALA:HB2	1.98	0.46
2:B:193:PHE:HE1	2:B:195:GLU:HG2	1.80	0.46
1:A:611:SER:HB2	1:A:1199:ALA:HB2	1.98	0.45
1:A:822:GLY:HA2	1:A:836:ILE:H	1.81	0.45
1:A:1047:LEU:HA	1:A:1053:GLU:OE2	2.17	0.45
1:A:638:LEU:HD23	1:A:1168:TYR:HB3	1.98	0.45
2:B:406:ALA:O	2:B:412:ASN:ND2	2.44	0.45
1:A:1237:LEU:HG	1:A:1331:GLN:HG2	1.99	0.45
1:A:625:LYS:HE3	1:A:1184:LEU:HD11	1.98	0.45
2:B:229:TYR:HB3	2:B:230:PRO:HD3	1.97	0.45
1:A:925:LYS:O	1:A:928:GLU:HG2	2.16	0.45
2:B:72:PRO:HG2	2:B:396:TRP:CE2	2.51	0.45
1:A:671:THR:HG23	1:A:1147:ILE:HD12	1.99	0.45
2:B:222:ASN:HB3	2:B:228:TYR:CZ	2.51	0.45
5:A:1601:POV:H39	5:A:1601:POV:H36	1.57	0.45
2:B:215:ASN:HD22	2:B:215:ASN:H	1.64	0.45
2:B:155:GLN:NE2	2:B:346:LEU:HB3	2.33	0.44
2:B:279:ASN:O	2:B:281:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:GLY:N	1:A:748:SER:HB2	2.33	0.44
1:A:1362:SER:HB2	1:A:1365:PHE:HB3	1.98	0.44
1:A:608:LEU:HD12	1:A:1215:TYR:CE1	2.52	0.44
2:B:101:ASP:OD2	2:B:101:ASP:N	2.50	0.44
2:B:162:ARG:HE	2:B:341:GLN:HE21	1.65	0.44
1:A:1047:LEU:CA	1:A:1053:GLU:OE2	2.66	0.44
1:A:1146:GLY:O	1:A:1162:ALA:HA	2.18	0.44
2:B:168:ASP:OD1	2:B:168:ASP:N	2.51	0.44
2:B:215:ASN:O	2:B:215:ASN:ND2	2.51	0.44
1:A:649:PRO:HB3	1:A:1161:TYR:CE1	2.52	0.44
2:B:97:ASN:HD21	2:B:371:ASN:H	1.66	0.44
1:A:548:GLU:HB2	1:A:1265:TRP:HE1	1.83	0.43
1:A:701:ARG:HA	1:A:701:ARG:HD3	1.85	0.43
2:B:236:ASN:HB2	2:B:286:PRO:HB3	2.01	0.43
1:A:224:LEU:O	1:A:228:ILE:HG12	2.17	0.43
2:B:165:THR:O	2:B:165:THR:OG1	2.37	0.43
2:B:260:THR:OG1	4:E:1:NAG:H83	2.19	0.43
1:A:743:GLU:N	1:A:743:GLU:OE1	2.51	0.43
1:A:788:ASN:HB3	1:A:791:LYS:HB2	2.00	0.43
2:B:126:TRP:H	2:B:126:TRP:CD1	2.36	0.43
1:A:1110:LYS:NZ	1:A:1133:ASN:HD22	2.16	0.43
1:A:1350:PHE:C	1:A:1353:THR:HG22	2.42	0.43
1:A:1408:VAL:O	1:A:1412:ARG:HG3	2.18	0.43
2:B:401:ARG:NH2	2:B:402:LYS:O	2.52	0.43
1:A:212:LEU:O	1:A:216:HIS:ND1	2.50	0.43
1:A:795:LYS:HE2	1:A:795:LYS:HB3	1.70	0.43
1:A:867:LEU:HD11	1:A:915:GLN:HB2	2.00	0.43
1:A:874:ASP:OD2	1:A:874:ASP:N	2.44	0.43
1:A:997:ILE:HD11	1:A:1071:VAL:HG11	2.00	0.43
1:A:1167:ARG:HE	1:A:1167:ARG:HB2	1.70	0.43
2:B:208:VAL:HG13	2:B:216:CYS:SG	2.59	0.43
1:A:754:ASP:OD2	1:A:759:SER:OG	2.31	0.42
1:A:1012:LEU:HD23	1:A:1069:ALA:HB3	2.00	0.42
2:B:253:THR:HG22	2:B:253:THR:O	2.19	0.42
1:A:774:LEU:HD22	1:A:804:LEU:HD22	2.01	0.42
1:A:916:ARG:HE	1:A:954:GLU:HB3	1.85	0.42
1:A:1169:LEU:HD22	1:A:1173:VAL:HG23	2.02	0.42
2:B:143:ARG:NH2	2:B:160:GLN:OE1	2.52	0.42
1:A:1107:PRO:HB3	1:A:1133:ASN:HA	2.02	0.42
1:A:1274:MET:HE3	1:A:1274:MET:HB3	1.79	0.42
2:B:137:ASN:OD1	2:B:137:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:ARG:NH1	1:A:954:GLU:HB3	2.35	0.42
1:A:926:TRP:NE1	1:A:951:ILE:HB	2.35	0.42
1:A:968:GLN:HB2	1:A:971:VAL:HG23	2.01	0.42
1:A:793:ASP:OD1	1:A:795:LYS:HG3	2.19	0.42
1:A:827:MET:HB3	1:A:827:MET:HE2	1.80	0.42
5:A:1601:POV:H11	5:A:1601:POV:H13B	1.84	0.41
2:B:176:ASN:HD22	2:B:360:TYR:HD2	1.67	0.41
2:B:229:TYR:CD1	2:B:229:TYR:C	2.95	0.41
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.92	0.41
1:A:1221:TYR:CD1	1:A:1316:THR:HG21	2.54	0.41
1:A:646:PRO:O	1:A:648:THR:HG23	2.21	0.41
1:A:738:GLN:HE22	1:A:792:LEU:HD13	1.85	0.41
1:A:741:PRO:HA	1:A:744:VAL:HG23	2.01	0.41
1:A:1128:ILE:HA	1:A:1145:ILE:O	2.20	0.41
1:A:1354:GLY:HA2	1:A:1369:ALA:CB	2.50	0.41
2:B:54:LYS:NZ	2:B:56:ASP:HB2	2.35	0.41
2:B:365:SER:OG	2:B:366:HIS:N	2.54	0.41
1:A:548:GLU:CB	1:A:1265:TRP:HE1	2.33	0.41
2:B:394:THR:O	2:B:398:PHE:HD2	2.04	0.41
1:A:244:ALA:O	1:A:248:VAL:HG23	2.19	0.41
1:A:612:LEU:HG	1:A:1199:ALA:HB3	2.03	0.41
1:A:877:ILE:HD13	1:A:877:ILE:HA	1.85	0.41
1:A:1298:VAL:HG23	1:A:1305:LEU:HD12	2.02	0.41
1:A:1318:ILE:HD11	1:A:1381:VAL:HG12	2.03	0.41
1:A:1372:ILE:HD13	1:A:1372:ILE:HG21	1.83	0.41
1:A:1163:ILE:H	1:A:1163:ILE:HG12	1.73	0.41
1:A:1196:MET:HE2	1:A:1278:LEU:HB2	2.02	0.41
1:A:1264:GLU:O	1:A:1269:LYS:HD3	2.20	0.41
2:B:216:CYS:O	2:B:220:SER:HB3	2.21	0.41
1:A:683:THR:HG21	1:A:899:HIS:HB3	2.03	0.41
1:A:1245:ASN:OD1	1:A:1245:ASN:N	2.54	0.41
1:A:1384:VAL:HG21	2:B:377:VAL:HG13	2.02	0.41
1:A:226:LEU:HG	1:A:607:ILE:HG23	2.02	0.41
1:A:1174:LEU:O	1:A:1178:ARG:HB2	2.20	0.41
1:A:738:GLN:HE21	1:A:792:LEU:HD22	1.86	0.40
1:A:1208:TYR:O	2:B:185:ASN:ND2	2.54	0.40
1:A:1359:ALA:O	1:A:1362:SER:OG	2.37	0.40
2:B:283:ILE:HD11	2:B:302:ILE:HD13	2.02	0.40
1:A:890:GLU:HA	1:A:893:LEU:HB2	2.02	0.40
2:B:128:PHE:HZ	2:B:140:PRO:HG3	1.85	0.40
2:B:170:LYS:HB2	2:B:170:LYS:HE2	1.80	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	951/1571 (60%)	876 (92%)	73 (8%)	2 (0%)	43	73
2	B	363/414 (88%)	332 (92%)	31 (8%)	0	100	100
All	All	1314/1985 (66%)	1208 (92%)	104 (8%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	ALA
1	A	1358	SER

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	823/1367 (60%)	766 (93%)	57 (7%)	14	45
2	B	321/364 (88%)	286 (89%)	35 (11%)	6	26
All	All	1144/1731 (66%)	1052 (92%)	92 (8%)	13	40

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	VAL

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Mol	Chain	Res	Type
1	A	260	ILE
1	A	267	VAL
1	A	540	THR
1	A	574	TYR
1	A	581	SER
1	A	615	ILE
1	A	651	SER
1	A	747	VAL
1	A	749	LYS
1	A	772	LEU
1	A	782	VAL
1	A	824	ILE
1	A	826	GLU
1	A	830	ILE
1	A	893	LEU
1	A	920	TRP
1	A	958	LEU
1	A	963	ILE
1	A	985	LEU
1	A	989	THR
1	A	1006	LEU
1	A	1024	GLU
1	A	1045	PHE
1	A	1047	LEU
1	A	1054	ILE
1	A	1060	ASP
1	A	1072	ILE
1	A	1121	LEU
1	A	1122	ASP
1	A	1133	ASN
1	A	1135	VAL
1	A	1143	VAL
1	A	1151	GLU
1	A	1153	ARG
1	A	1167	ARG
1	A	1169	LEU
1	A	1190	GLU
1	A	1197	ILE
1	A	1212	ASP
1	A	1218	GLU
1	A	1234	VAL
1	A	1243	ASP

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Mol	Chain	Res	Type
1	A	1246	ASP
1	A	1258	VAL
1	A	1266	ASN
1	A	1291	VAL
1	A	1295	ASN
1	A	1299	THR
1	A	1300	SER
1	A	1323	CYS
1	A	1348	VAL
1	A	1377	SER
1	A	1387	LEU
1	A	1391	LEU
1	A	1400	GLN
1	A	1406	THR
2	B	59	THR
2	B	69	VAL
2	B	70	LEU
2	B	75	VAL
2	B	87	VAL
2	B	112	THR
2	B	113	ASN
2	B	145	VAL
2	B	155	GLN
2	B	165	THR
2	B	176	ASN
2	B	190	VAL
2	B	195	GLU
2	B	198	ILE
2	B	208	VAL
2	B	215	ASN
2	B	216	CYS
2	B	220	SER
2	B	224	ASP
2	B	227	ILE
2	B	236	ASN
2	B	250	VAL
2	B	260	THR
2	B	276	THR
2	B	280	TYR
2	B	281	THR
2	B	282	GLN
2	B	298	ASN

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Mol	Chain	Res	Type
2	B	300	THR
2	B	351	LEU
2	B	352	GLU
2	B	361	LEU
2	B	367	LEU
2	B	377	VAL
2	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	220	ASN
1	A	550	ASN
1	A	571	ASN
1	A	653	ASN
1	A	660	GLN
1	A	685	ASN
1	A	738	GLN
1	A	797	GLN
1	A	902	GLN
1	A	939	ASN
1	A	998	ASN
1	A	1061	HIS
1	A	1139	GLN
1	A	1331	GLN
2	B	60	GLN
2	B	96	GLN
2	B	131	HIS
2	B	155	GLN
2	B	172	ASN
2	B	176	ASN
2	B	209	HIS
2	B	215	ASN
2	B	246	GLN
2	B	341	GLN

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 ⓘ

7 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	$\# Z > 2$
3	NAG	C	1	2,3	14,14,15	0.47	0	17,19,21	0.74	1 (5%)
3	NAG	C	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.54	0
3	MAN	C	3	3	11,11,12	0.94	0	15,15,17	1.10	2 (13%)
4	NAG	D	1	4,2	14,14,15	0.49	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	E	1	4,2	14,14,15	0.50	0	17,19,21	0.39	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.46	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
3	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	1/2/19/22	1/1/1/1
4	NAG	D	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	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)
3	C	2	NAG	O5-C1	-3.22	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	O2-C2-C3	-2.92	104.11	110.15
3	C	3	MAN	C1-O5-C5	2.48	115.51	112.19
3	C	1	NAG	C1-O5-C5	2.40	115.41	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7

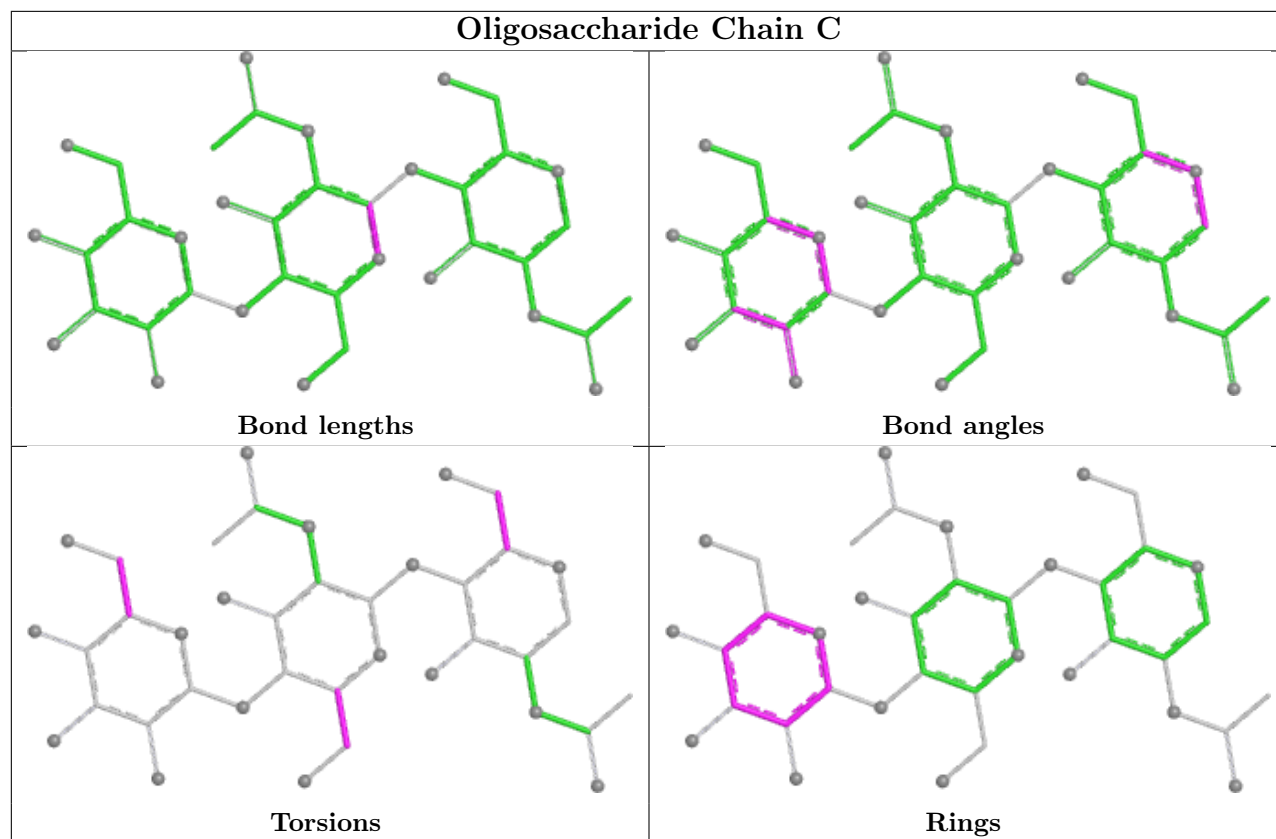
All (1) ring outliers are listed below:

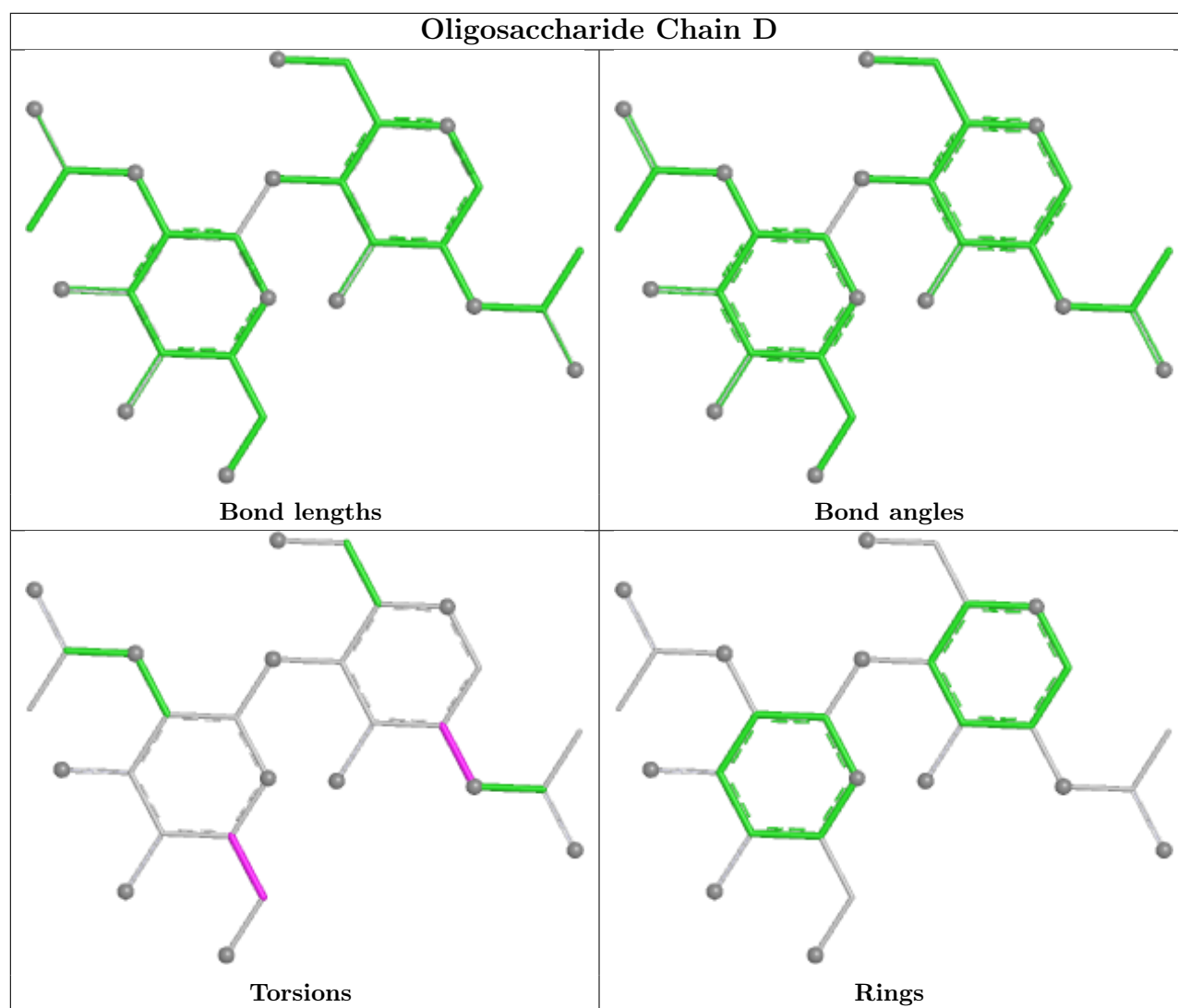
Mol	Chain	Res	Type	Atoms
3	C	3	MAN	C1-C2-C3-C4-C5-O5

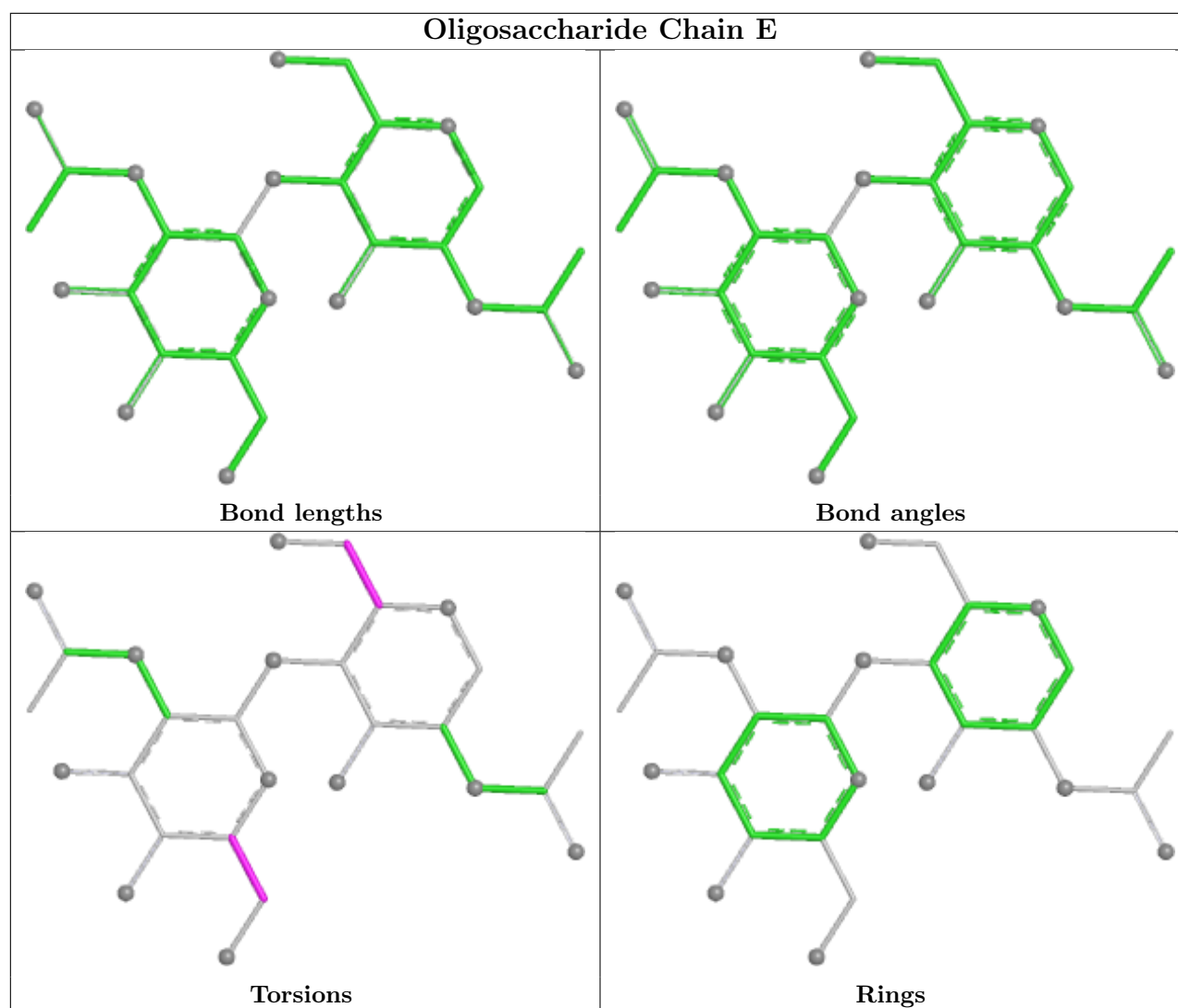
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
6	ADP	A	1602	8	28,29,29	1.37	5 (17%)	43,45,45	1.84	9 (20%)
9	NAG	B	1001	2	14,14,15	0.23	0	17,19,21	0.52	0
7	ALF	A	1603	1	4,4,4	1.33	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	1002	2	14,14,15	0.32	0	17,19,21	0.42	0
5	POV	A	1601	-	51,51,51	1.25	5 (9%)	57,59,59	1.05	2 (3%)

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
9	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
6	ADP	A	1602	8	-	7/16/32/32	0/3/3/3
5	POV	A	1601	-	-	26/55/55/55	-
9	NAG	B	1002	2	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1602	ADP	C5-C4	4.15	1.46	1.39
5	A	1601	POV	O31-C31	3.17	1.42	1.33
5	A	1601	POV	O21-C21	2.89	1.42	1.34
5	A	1601	POV	O21-C2	-2.67	1.40	1.46
6	A	1602	ADP	C5-N7	-2.56	1.34	1.39
5	A	1601	POV	C14-N	-2.32	1.43	1.50
6	A	1602	ADP	C5-C6	2.30	1.47	1.41
6	A	1602	ADP	C8-N7	2.12	1.35	1.31
5	A	1601	POV	C13-N	-2.10	1.43	1.50
6	A	1602	ADP	C4-N9	-2.05	1.33	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1602	ADP	C5-C4-N3	-5.87	118.64	126.72
6	A	1602	ADP	N3-C4-N9	4.77	135.27	127.17
5	A	1601	POV	O21-C21-C22	4.22	120.60	111.48
6	A	1602	ADP	C2-N3-C4	3.66	120.78	111.83
6	A	1602	ADP	N3-C2-N1	-3.17	123.79	128.58
6	A	1602	ADP	C4-C5-N7	-3.09	107.05	110.58
6	A	1602	ADP	C4-N9-C8	2.71	108.58	105.74
5	A	1601	POV	O31-C31-C32	2.54	119.58	111.83
6	A	1602	ADP	C5-N7-C8	2.29	107.05	103.45
6	A	1602	ADP	C3'-C2'-C1'	2.17	105.57	101.46

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1602	ADP	O2A-PA-O1A	2.02	121.86	112.44

There are no chirality outliers.

All (36) torsion outliers are listed below:

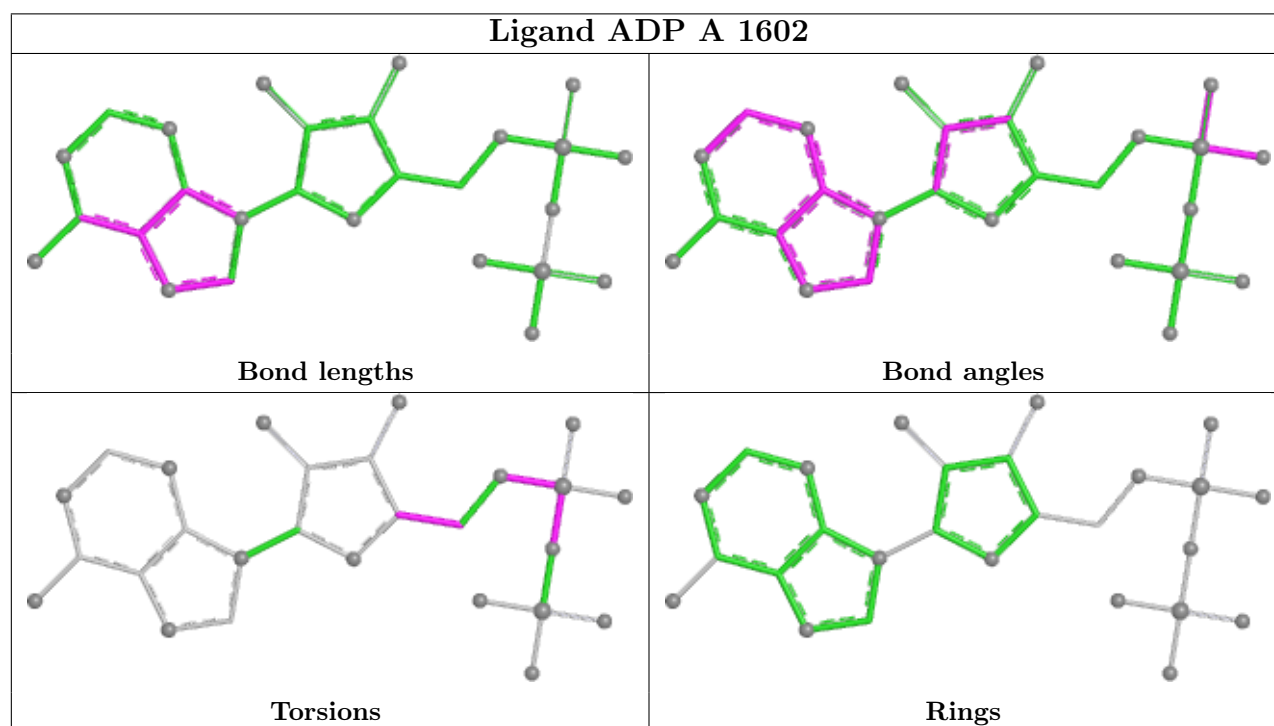
Mol	Chain	Res	Type	Atoms
5	A	1601	POV	C1-O11-P-O13
5	A	1601	POV	C11-O12-P-O11
5	A	1601	POV	C11-O12-P-O13
5	A	1601	POV	C11-O12-P-O14
5	A	1601	POV	O12-C11-C12-N
6	A	1602	ADP	C5'-O5'-PA-O1A
6	A	1602	ADP	C5'-O5'-PA-O2A
6	A	1602	ADP	C5'-O5'-PA-O3A
9	B	1001	NAG	O5-C5-C6-O6
9	B	1001	NAG	C4-C5-C6-O6
6	A	1602	ADP	O4'-C4'-C5'-O5'
6	A	1602	ADP	C3'-C4'-C5'-O5'
5	A	1601	POV	C213-C214-C215-C216
5	A	1601	POV	C310-C311-C312-C313
5	A	1601	POV	C39-C310-C311-C312
5	A	1601	POV	C36-C37-C38-C39
5	A	1601	POV	C210-C211-C212-C213
5	A	1601	POV	C33-C34-C35-C36
5	A	1601	POV	C32-C33-C34-C35
5	A	1601	POV	C311-C310-C39-C38
5	A	1601	POV	C23-C24-C25-C26
5	A	1601	POV	C211-C212-C213-C214
5	A	1601	POV	O21-C2-C3-O31
5	A	1601	POV	C24-C25-C26-C27
5	A	1601	POV	C1-O11-P-O12
5	A	1601	POV	C1-O11-P-O14
6	A	1602	ADP	PB-O3A-PA-O2A
5	A	1601	POV	C32-C31-O31-C3
5	A	1601	POV	O32-C31-O31-C3
9	B	1002	NAG	C4-C5-C6-O6
5	A	1601	POV	C215-C216-C217-C218
5	A	1601	POV	C27-C28-C29-C210
5	A	1601	POV	C1-C2-C3-O31
6	A	1602	ADP	PB-O3A-PA-O1A
5	A	1601	POV	O21-C21-C22-C23
5	A	1601	POV	O22-C21-C22-C23

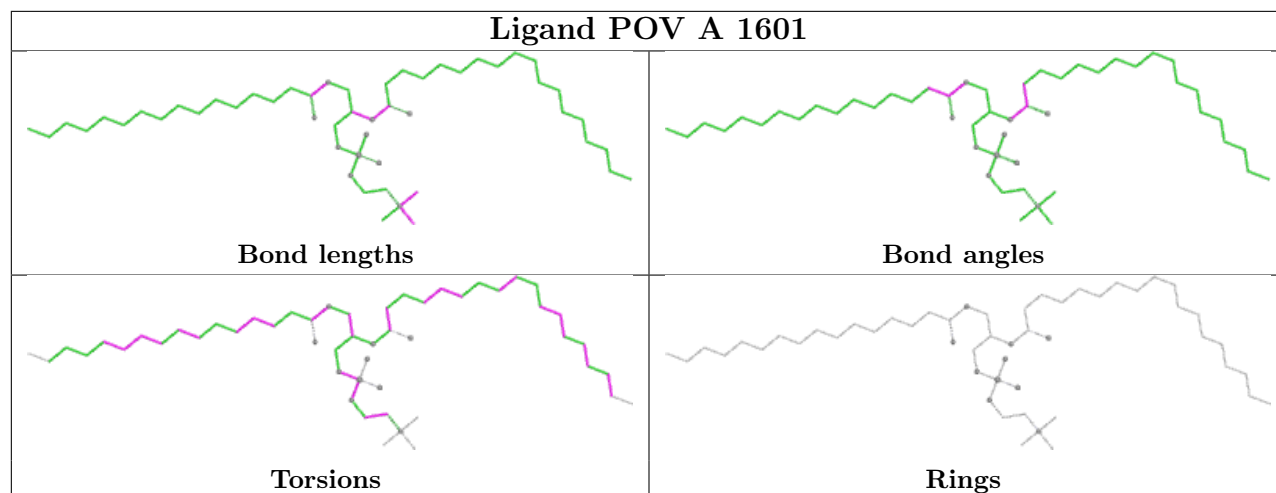
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1602	ADP	1	0
7	A	1603	ALF	4	0
5	A	1601	POV	4	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.

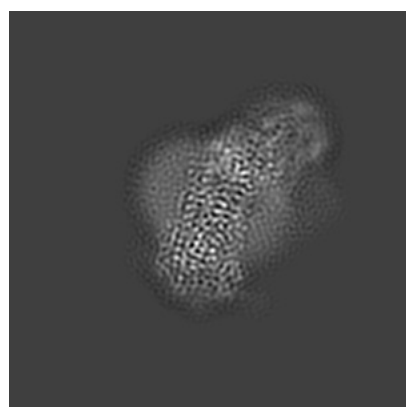
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23074. These allow visual inspection of the internal detail of the map and identification of artifacts.

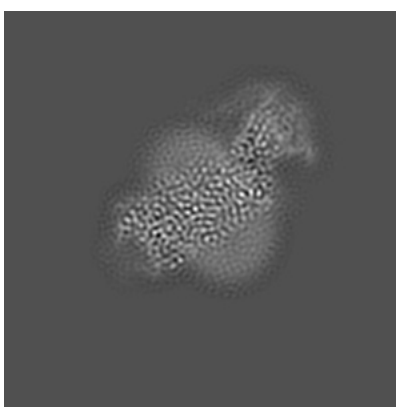
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

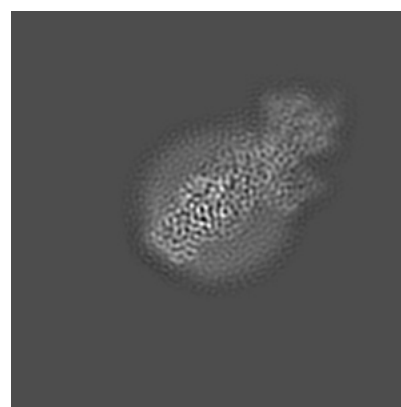
6.1.1 Primary map



X



Y

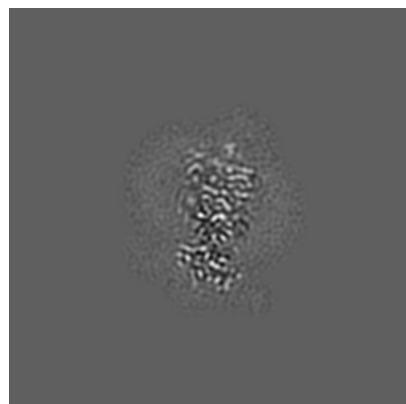


Z

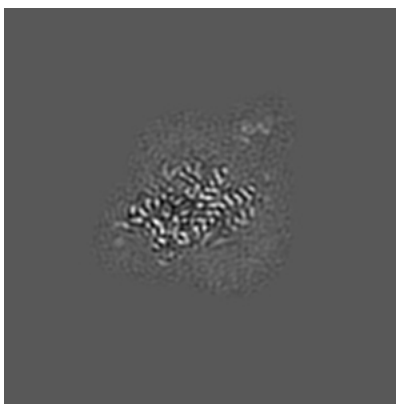
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

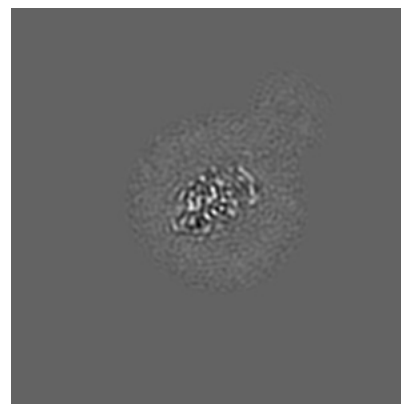
6.2.1 Primary map



X Index: 140



Y Index: 140

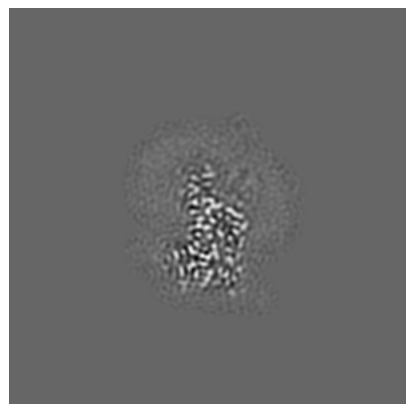


Z Index: 140

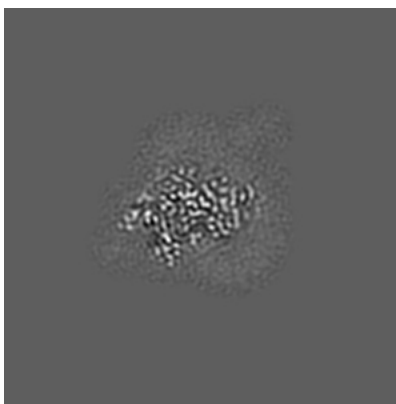
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

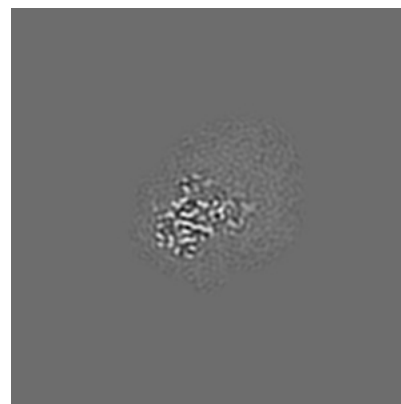
6.3.1 Primary map



X Index: 131



Y Index: 136

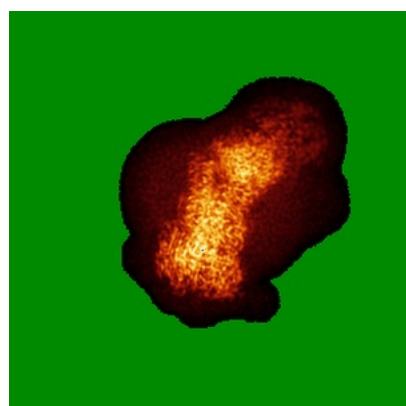


Z Index: 112

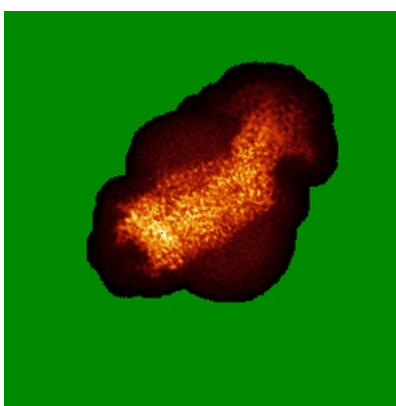
The images above show the largest variance slices of the map in three orthogonal directions.

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

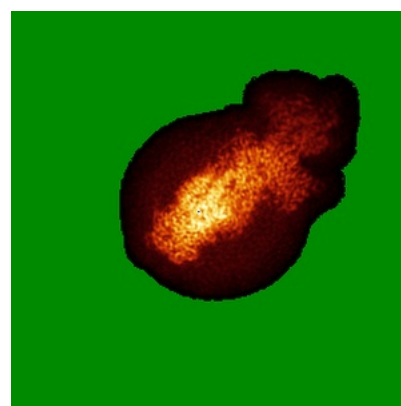
6.4.1 Primary map



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

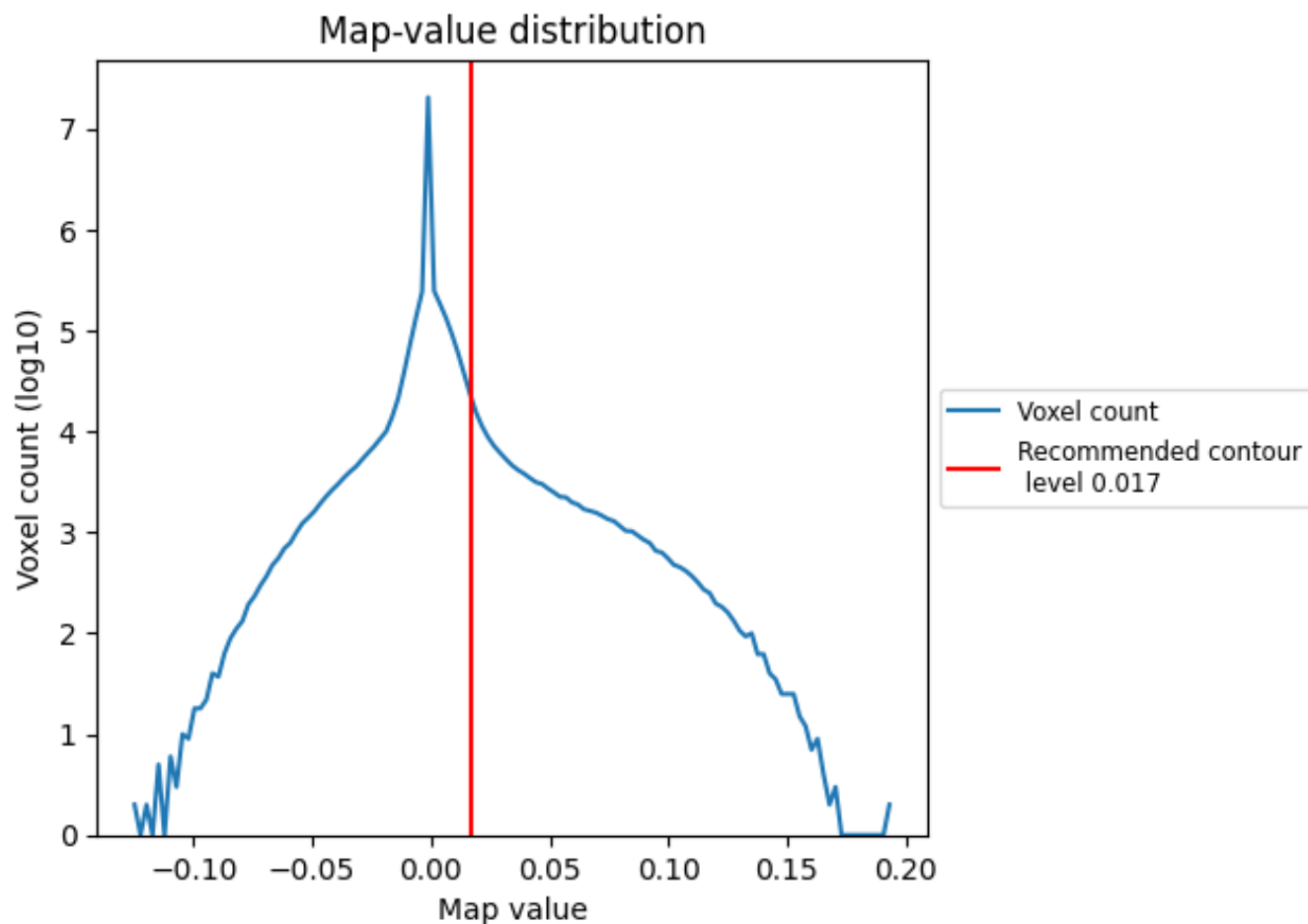
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

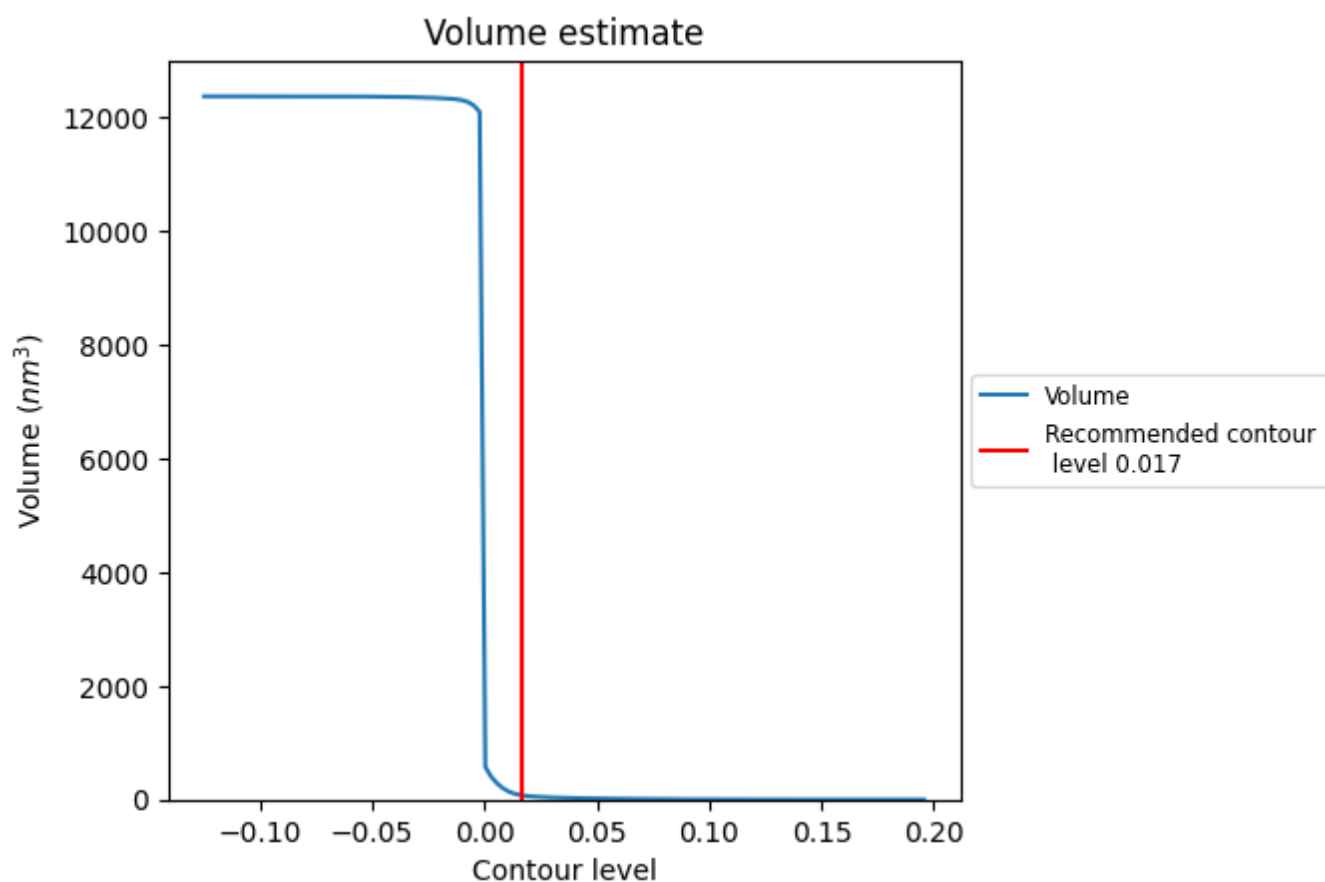
This section contains the results of statistical analysis of the map.

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.

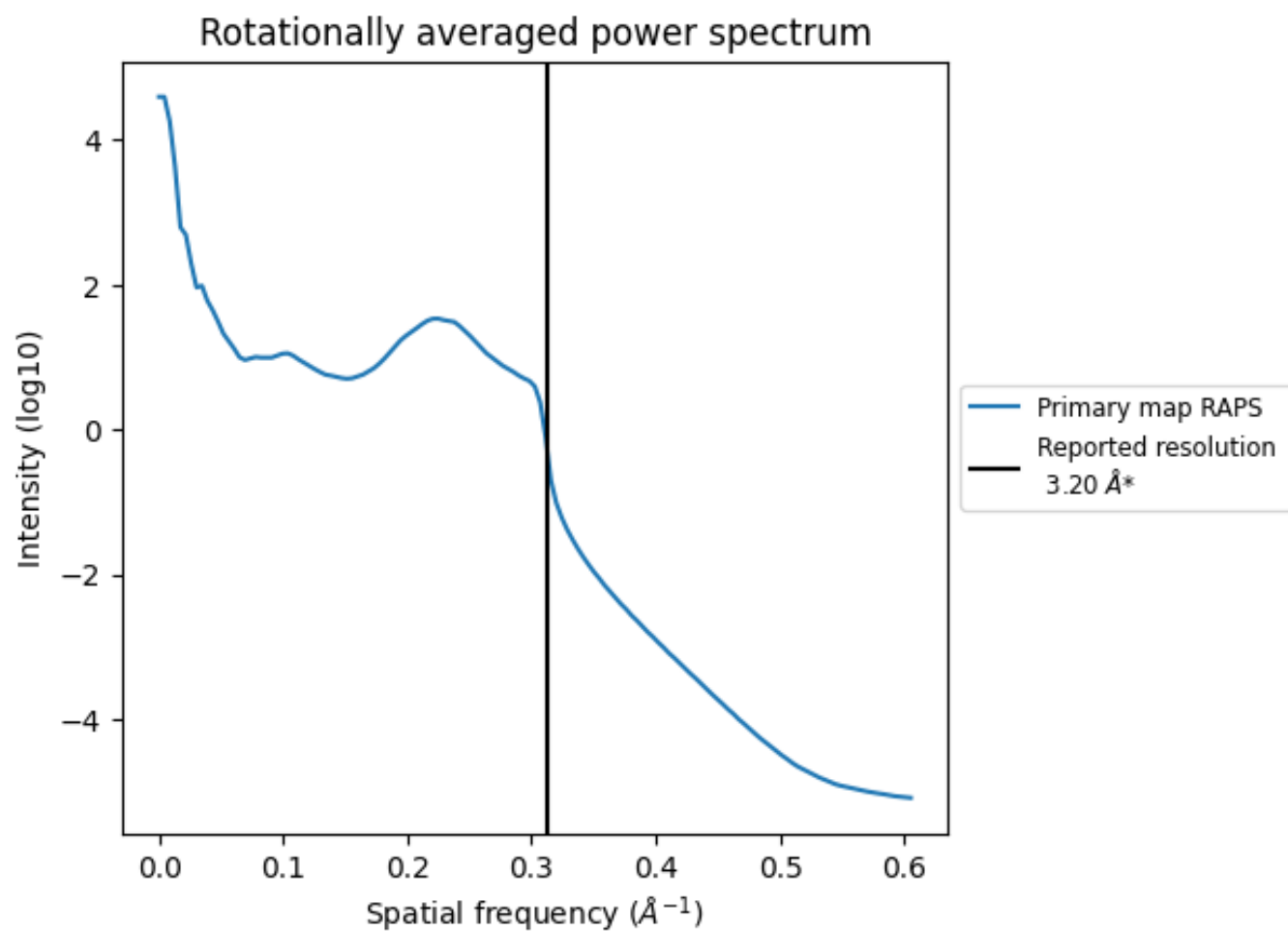
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 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 0.312 Å⁻¹

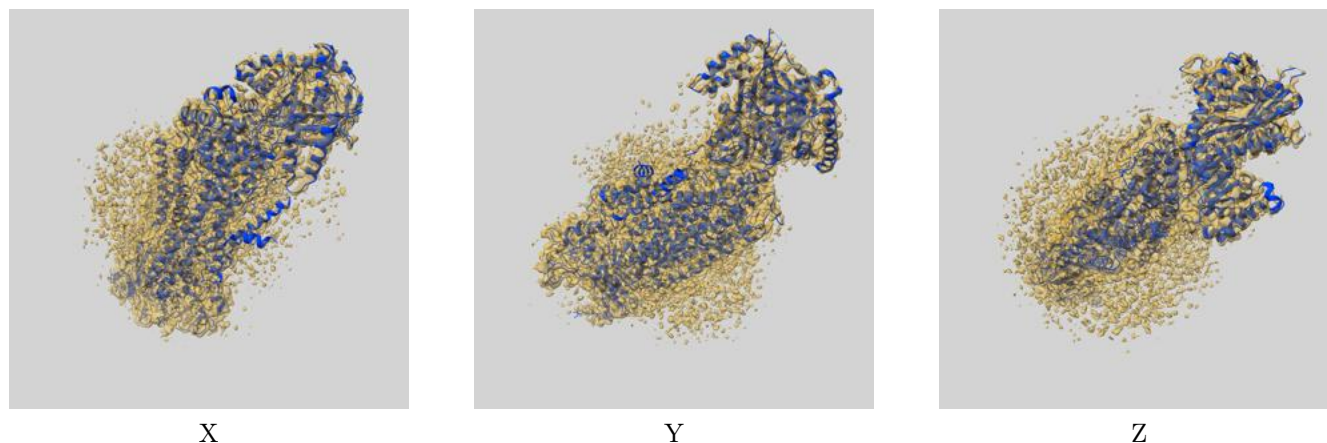
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

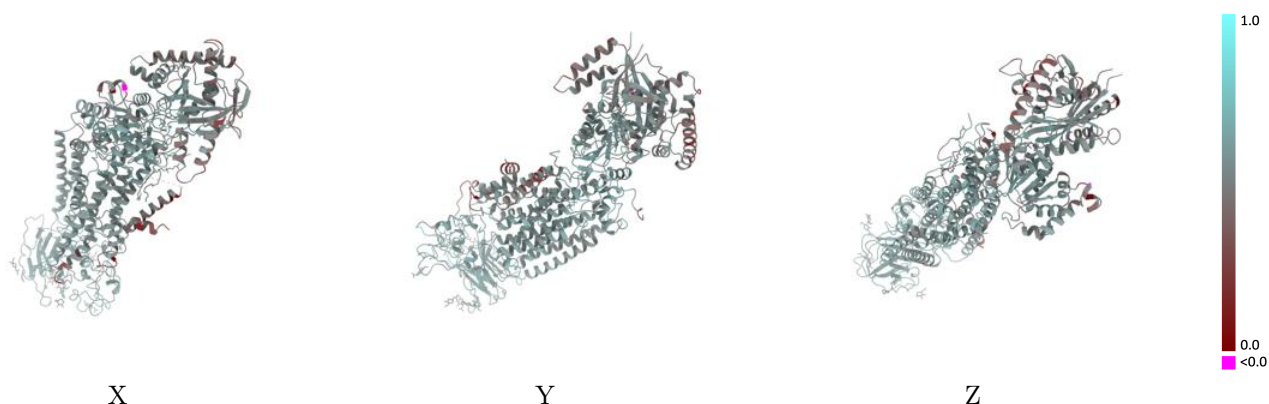
This section contains information regarding the fit between EMDB map EMD-23074 and PDB model 7KYB. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



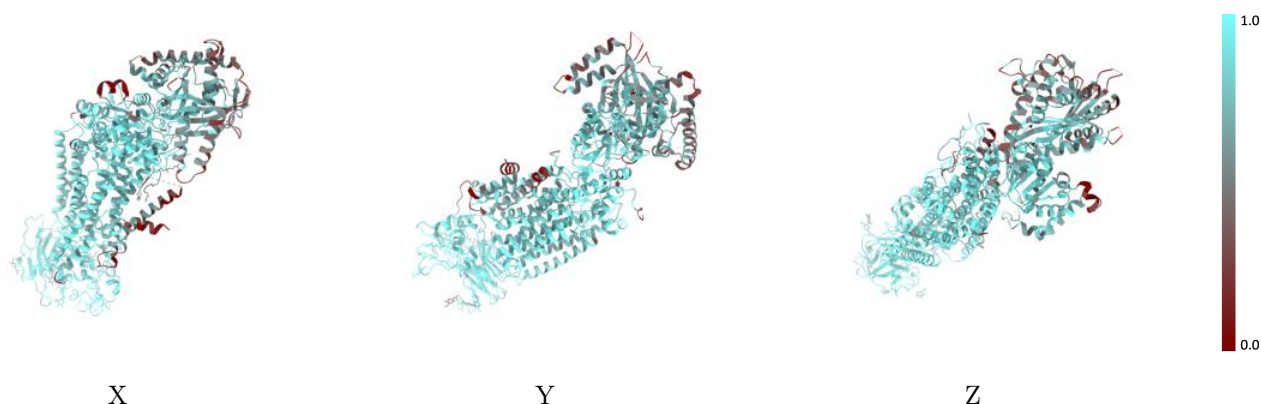
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



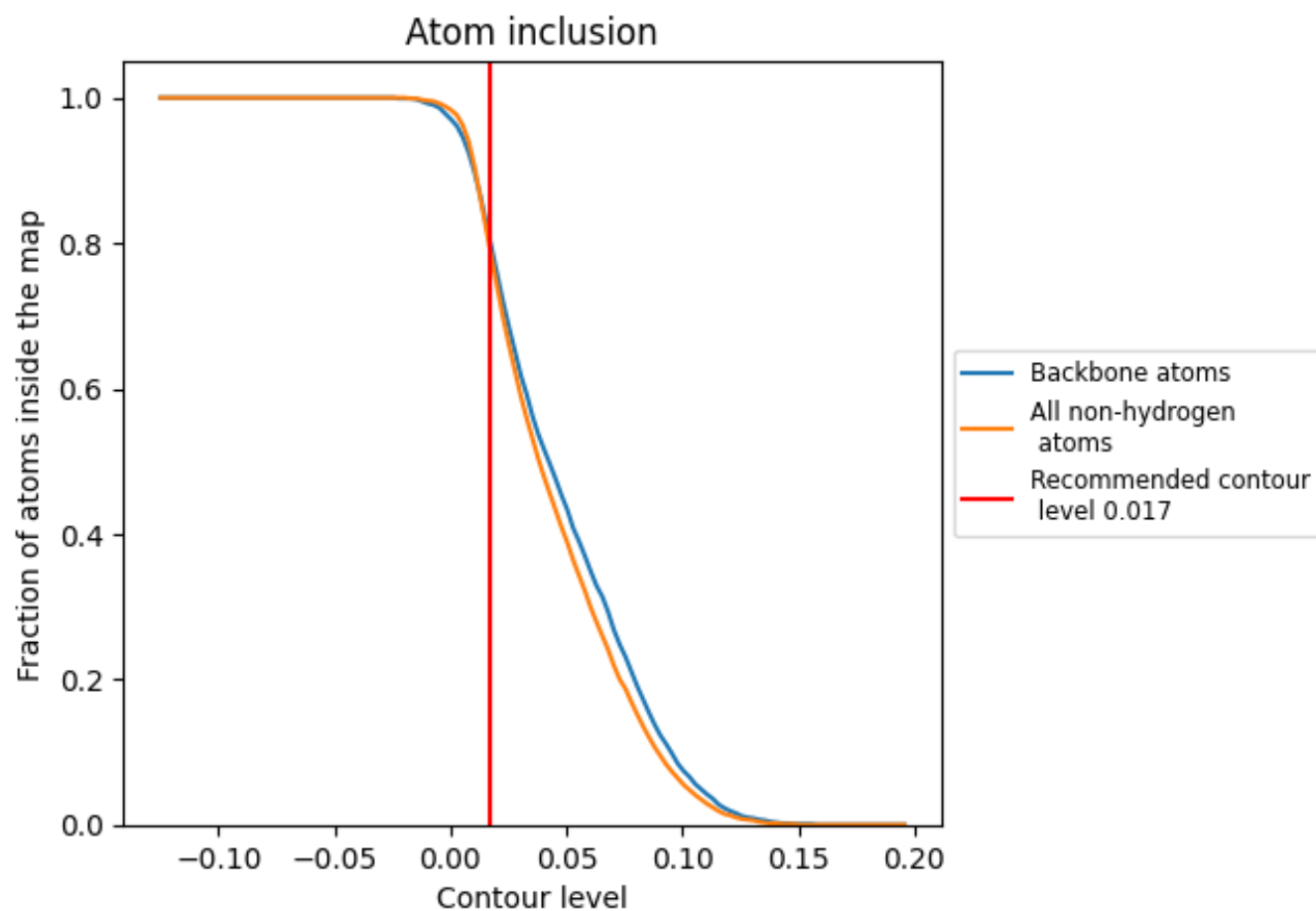
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.5450
A	0.7540	0.5330
B	0.8940	0.5780
C	0.9490	0.5830
D	0.5710	0.4490
E	0.6790	0.5300

