Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 03:16 AM JST

PDB ID	:	7E1Z
EMDB ID	:	EMD-30947
Title	:	Cryo EM structure of a Na+-bound Na+,K+-ATPase in the E1 state
Authors	:	Guo, Y.Y.; Zhang, Y.Y.; Yan, R.H.; Huang, B.D.; Ye, F.F.; Wu, L.S.; Chi, X.M.; Zhou, Q.
Deposited on	:	2021-02-04
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 (i) 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 (1)) were used in the production of this report:

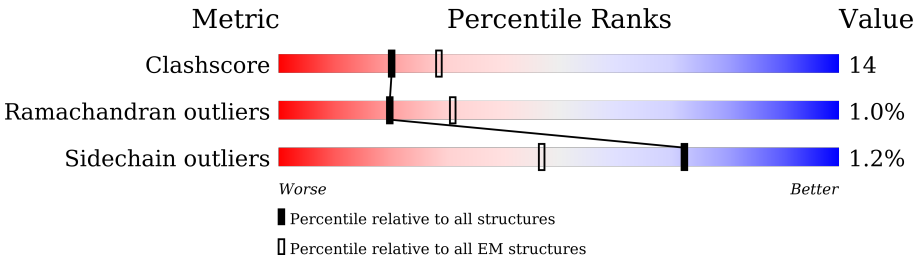
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1023	31% 78% 16% • 5%
2	B	303	12% 86% 9% • •
3	C	66	29% 42% 6% 52%
4	D	2	50% 100%

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	Y01	A	1106	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	Y01	A	1107	X	-	-	-
7	Y01	A	1108	X	-	-	-
7	Y01	A	1109	X	-	X	-
7	Y01	B	401	X	-	X	-
7	Y01	C	1501	X	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10550 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	976	7575	4833	1274	1422	46	0	0

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	294	2404	1557	397	439	11	0	0

- Molecule 3 is a protein called Sodium/potassium-transporting ATPase subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	32	256	173	39	44	0	0

- 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
			Total	C	N	O		
4	D	2	28	16	2	10	0	0

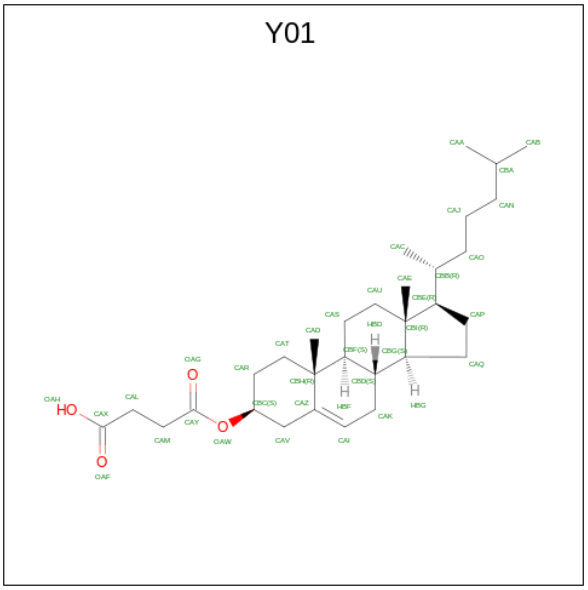
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
5	A	4	4	4	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

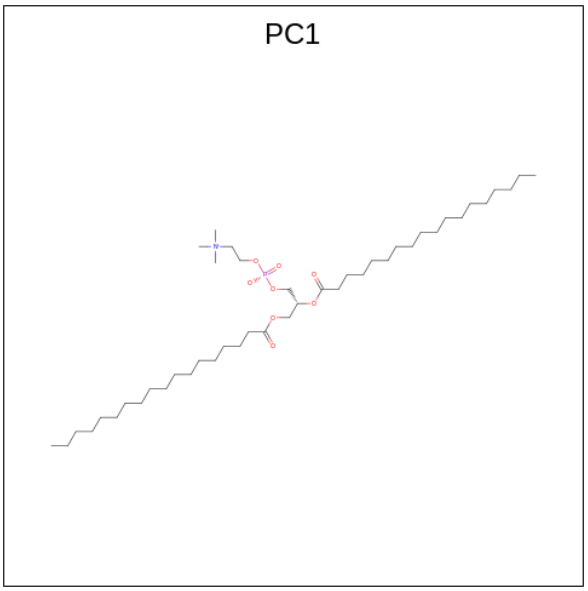
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



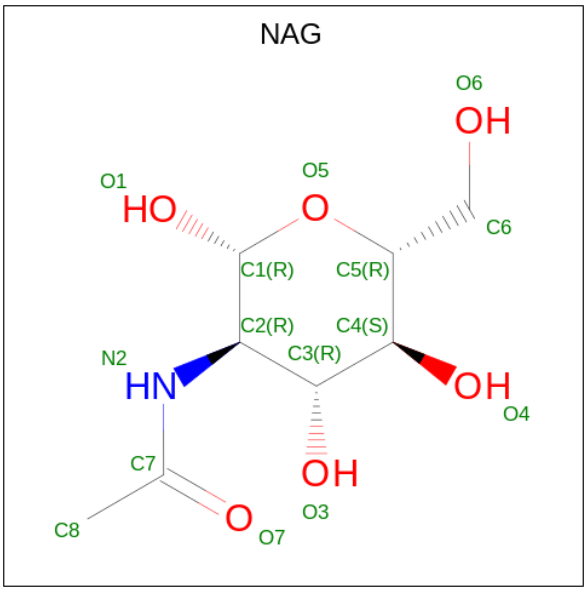
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	140	124	16	0
			Total	C	O	
7	A	1	140	124	16	0
			Total	C	O	
7	A	1	140	124	16	0
			Total	C	O	
7	A	1	140	124	16	0
			Total	C	O	
7	B	1	35	31	4	0
			Total	C	O	
7	C	1	35	31	4	0

- Molecule 8 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	54	44	1	8	1	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

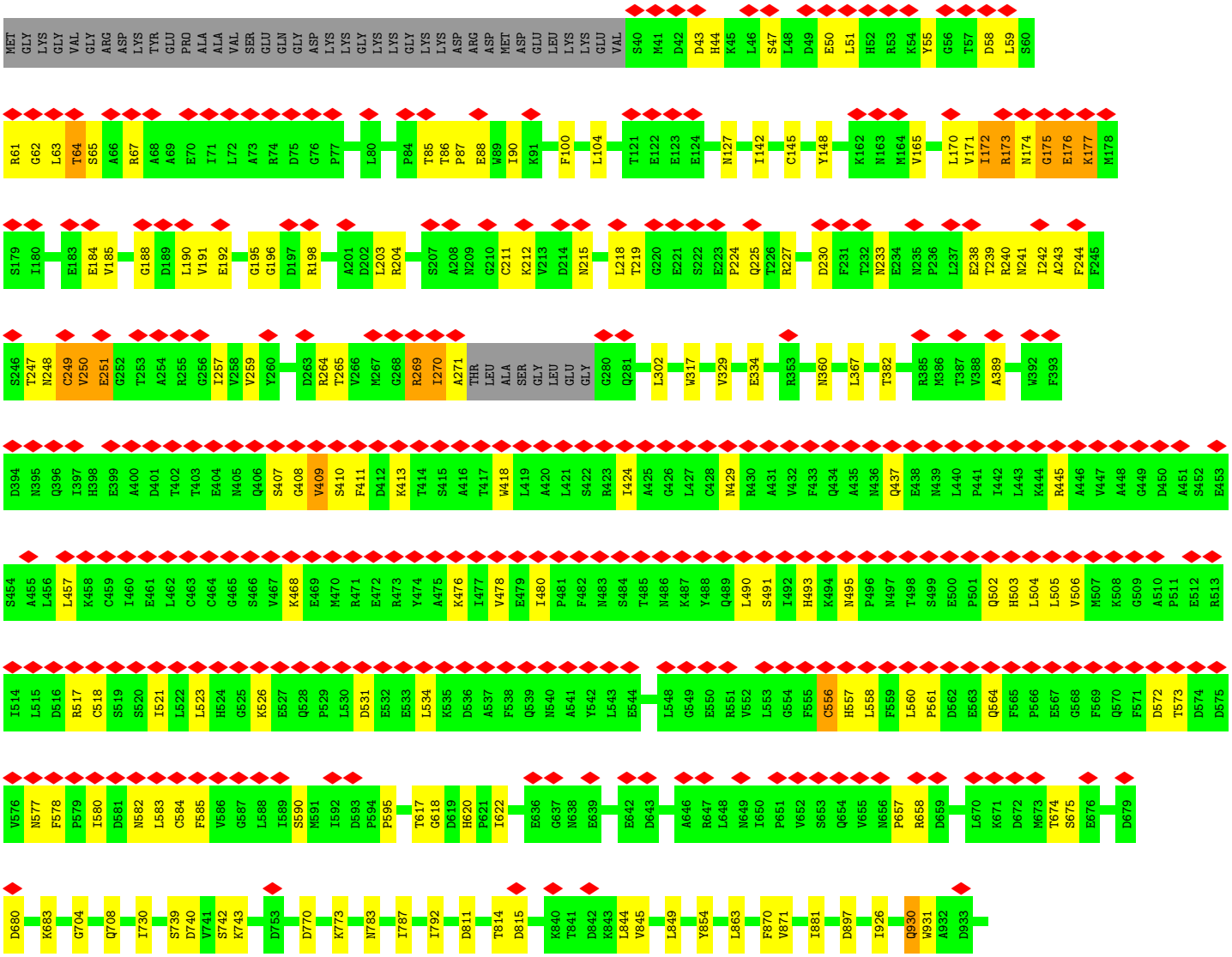
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
10	A	4	4	4	0

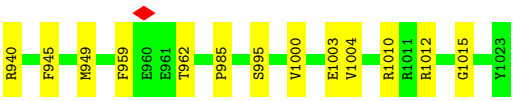
3 Residue-property plots (i)

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.

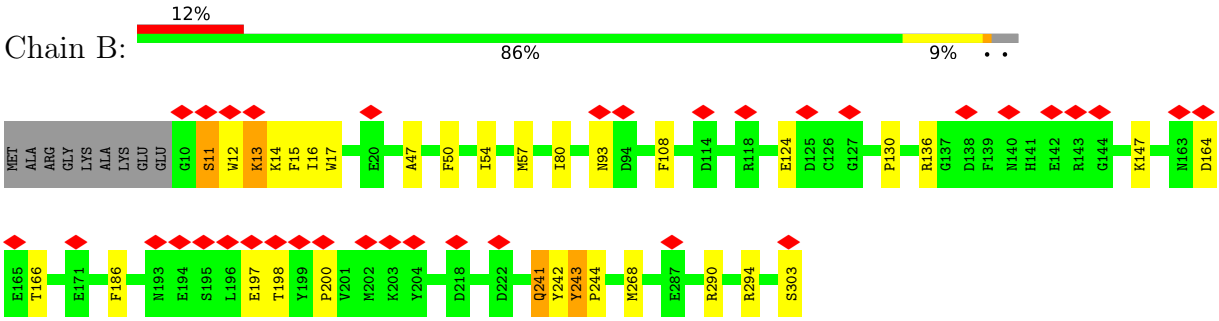
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:

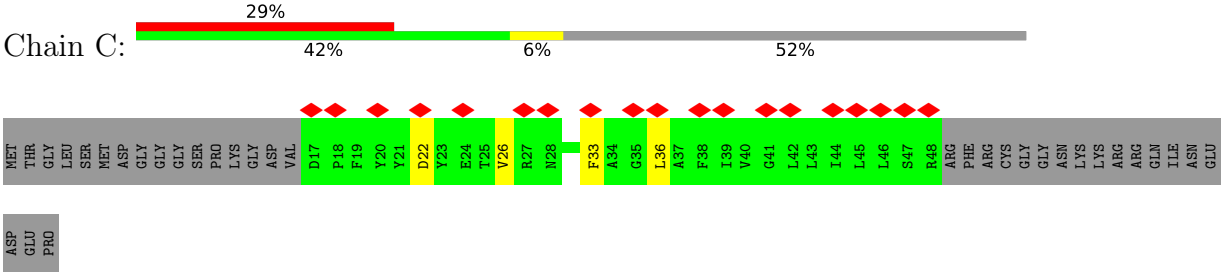




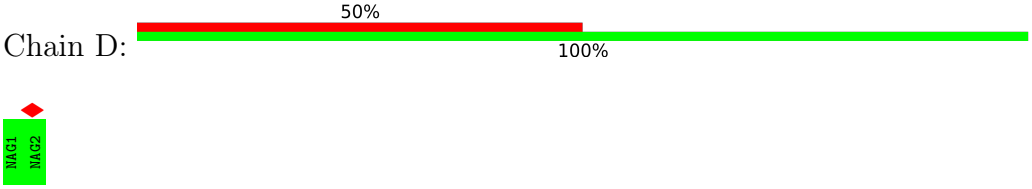
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Sodium/potassium-transporting ATPase subunit gamma



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	217.40001, 217.40001, 217.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NA, NAG, MG, PC1

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	0.38	0/7723	0.55	0/10482
2	B	0.47	0/2468	0.56	0/3330
3	C	0.33	0/262	0.50	0/355
All	All	0.40	0/10453	0.55	0/14167

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7575	0	7618	195	0
2	B	2404	0	2381	39	0
3	C	256	0	257	4	0
4	D	28	0	25	0	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	A	140	0	196	95	0
7	B	35	0	49	29	0
7	C	35	0	49	21	0
8	A	54	0	88	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	14	0	13	0	0
10	A	4	0	0	0	0
All	All	10550	0	10676	291	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 14.

All (291) 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:195:GLY:HA2	1:A:250:VAL:O	1.40	1.18
2:B:47:ALA:CB	7:B:401:Y01:CAC	2.23	1.17
1:A:870:PHE:CE2	7:A:1109:Y01:CAE	2.30	1.15
1:A:51:LEU:HD21	1:A:257:ILE:CD1	1.77	1.14
1:A:1000:VAL:CG1	8:A:1110:PC1:H3F2	1.77	1.14
1:A:931:TRP:CH2	7:C:1501:Y01:HAU1	1.86	1.11
1:A:870:PHE:CE2	7:A:1109:Y01:HAE1	1.84	1.10
2:B:47:ALA:HB1	7:B:401:Y01:HAC1	1.28	1.10
1:A:870:PHE:HE2	7:A:1109:Y01:CAE	1.64	1.09
1:A:1003:GLU:HB3	7:A:1107:Y01:HAK2	1.35	1.08
1:A:1000:VAL:HG11	8:A:1110:PC1:C3H	1.85	1.07
2:B:47:ALA:CB	7:B:401:Y01:HAC1	1.83	1.06
1:A:100:PHE:HB2	1:A:334:GLU:OE2	1.52	1.05
1:A:51:LEU:CD2	1:A:257:ILE:HD13	1.85	1.05
7:A:1109:Y01:HAE3	7:A:1109:Y01:HAO2	1.32	1.05
1:A:1000:VAL:HG12	8:A:1110:PC1:H3F2	1.40	1.03
2:B:47:ALA:HB2	7:B:401:Y01:CAC	1.93	0.99
7:A:1109:Y01:HAU2	7:B:401:Y01:HAE1	1.43	0.98
7:B:401:Y01:HAE3	7:B:401:Y01:HAO1	1.45	0.97
1:A:792:ILE:CD1	7:A:1109:Y01:HAN2	1.95	0.96
2:B:11:SER:CB	2:B:14:LYS:HE2	1.94	0.96
7:C:1501:Y01:HAO1	7:C:1501:Y01:HAE3	1.44	0.96
1:A:863:LEU:CD2	7:A:1109:Y01:HAA1	1.97	0.93
1:A:250:VAL:HG23	1:A:251:GLU:H	1.30	0.92
2:B:47:ALA:HA	7:B:401:Y01:HAC2	1.48	0.92
1:A:212:LYS:HD3	1:A:251:GLU:OE2	1.70	0.91
7:B:401:Y01:HAN2	7:B:401:Y01:HAC3	1.51	0.91
2:B:47:ALA:CB	7:B:401:Y01:HAC2	2.01	0.90
1:A:51:LEU:HD21	1:A:257:ILE:HD13	0.91	0.90
1:A:881:ILE:HD13	7:A:1109:Y01:HAI	1.53	0.89
2:B:47:ALA:HB1	7:B:401:Y01:CAC	1.94	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:VAL:CG1	8:A:1110:PC1:C3F	2.51	0.89
1:A:44:HIS:HB2	1:A:241:ASN:CB	2.02	0.88
1:A:145:CYS:HB2	7:A:1108:Y01:HAE2	1.53	0.88
1:A:863:LEU:HD21	7:A:1109:Y01:HAA1	1.56	0.88
1:A:195:GLY:CA	1:A:250:VAL:O	2.21	0.87
1:A:870:PHE:CE2	7:A:1109:Y01:HAE2	2.10	0.87
2:B:47:ALA:CA	7:B:401:Y01:HAC2	2.04	0.86
1:A:931:TRP:HH2	7:C:1501:Y01:HAU1	1.38	0.86
1:A:407:SER:OG	1:A:409:VAL:HG13	1.76	0.85
1:A:930:GLN:NE2	1:A:930:GLN:HA	1.91	0.84
1:A:44:HIS:HB2	1:A:241:ASN:HB2	1.59	0.84
1:A:63:LEU:O	1:A:64:THR:OG1	1.93	0.84
1:A:881:ILE:HD11	7:A:1109:Y01:HAV1	1.57	0.84
1:A:881:ILE:HD11	7:A:1109:Y01:CAV	2.07	0.84
2:B:12:TRP:CE3	2:B:13:LYS:HB2	2.13	0.83
1:A:931:TRP:CH2	7:C:1501:Y01:CAU	2.62	0.83
1:A:1000:VAL:HG11	8:A:1110:PC1:H3F2	1.63	0.81
7:B:401:Y01:CAC	7:B:401:Y01:HAN2	2.10	0.81
7:A:1109:Y01:HAU2	7:B:401:Y01:CAE	2.10	0.81
7:A:1109:Y01:HBB	7:B:401:Y01:CAE	2.11	0.81
1:A:870:PHE:CZ	7:A:1109:Y01:HAE2	2.16	0.81
1:A:1000:VAL:HG12	8:A:1110:PC1:C3F	2.10	0.80
1:A:1000:VAL:HG11	8:A:1110:PC1:C3F	2.12	0.80
1:A:1000:VAL:HG11	8:A:1110:PC1:H3H1	1.64	0.80
1:A:171:VAL:HG12	1:A:191:VAL:HG12	1.63	0.79
1:A:863:LEU:HD21	7:A:1109:Y01:CAA	2.12	0.79
7:A:1107:Y01:HAC1	7:A:1107:Y01:HAU1	1.63	0.79
7:A:1107:Y01:HAC1	7:A:1107:Y01:CAU	2.13	0.78
1:A:870:PHE:CZ	7:A:1109:Y01:CAE	2.67	0.78
1:A:881:ILE:HD13	7:A:1109:Y01:CAI	2.14	0.77
7:A:1108:Y01:CAU	7:A:1108:Y01:HAC1	2.13	0.77
7:A:1106:Y01:HAN2	7:A:1106:Y01:CAC	2.15	0.77
2:B:12:TRP:CZ3	2:B:13:LYS:HB2	2.19	0.77
1:A:1000:VAL:HG11	8:A:1110:PC1:H3H2	1.64	0.76
7:A:1109:Y01:HAP1	7:B:401:Y01:HAE1	1.67	0.76
1:A:43:ASP:OD1	1:A:259:VAL:HG21	1.86	0.76
2:B:11:SER:OG	2:B:12:TRP:N	2.19	0.76
7:A:1106:Y01:CAE	7:C:1501:Y01:HAB3	2.16	0.75
1:A:863:LEU:HD23	7:A:1109:Y01:HAA1	1.69	0.75
1:A:930:GLN:HA	1:A:930:GLN:HE21	1.49	0.75
1:A:250:VAL:HG23	1:A:251:GLU:HG3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1106:Y01:HAE2	7:C:1501:Y01:HBA	1.70	0.74
1:A:792:ILE:HD13	7:A:1109:Y01:HAC3	1.70	0.73
1:A:51:LEU:HD11	1:A:257:ILE:HG21	1.70	0.72
1:A:269:ARG:O	1:A:270:ILE:HG12	1.90	0.71
1:A:61:ARG:O	1:A:174:ASN:HA	1.89	0.71
2:B:130:PRO:HA	2:B:241:GLN:OE1	1.91	0.70
7:A:1108:Y01:HAC1	7:A:1108:Y01:HAU1	1.71	0.70
1:A:142:ILE:HA	7:A:1108:Y01:CAE	2.22	0.70
7:A:1109:Y01:HAN1	7:A:1109:Y01:HAC2	1.72	0.70
1:A:250:VAL:HG23	1:A:251:GLU:N	2.07	0.69
1:A:142:ILE:HA	7:A:1108:Y01:HAE3	1.73	0.69
1:A:863:LEU:CD2	7:A:1109:Y01:CAA	2.67	0.69
7:B:401:Y01:HAC3	7:B:401:Y01:CAN	2.21	0.69
7:A:1109:Y01:HAD1	2:B:54:ILE:HG21	1.74	0.68
2:B:11:SER:HB2	2:B:14:LYS:HE2	1.73	0.68
7:A:1106:Y01:HAE3	7:A:1106:Y01:HAO2	1.75	0.68
1:A:100:PHE:HB2	1:A:334:GLU:CD	2.15	0.67
1:A:881:ILE:CD1	7:A:1109:Y01:CAV	2.74	0.66
1:A:1003:GLU:CB	7:A:1107:Y01:HAK2	2.20	0.65
1:A:145:CYS:HB3	7:A:1108:Y01:HBG	1.78	0.65
1:A:270:ILE:HG13	1:A:271:ALA:N	2.11	0.65
1:A:212:LYS:N	1:A:249:CYS:SG	2.70	0.65
1:A:265:THR:O	1:A:269:ARG:NH1	2.29	0.65
1:A:55:TYR:OH	1:A:259:VAL:HG23	1.97	0.64
1:A:408:GLY:O	1:A:410:SER:N	2.31	0.64
7:A:1109:Y01:HAC2	7:A:1109:Y01:CAN	2.27	0.64
1:A:792:ILE:HD13	7:A:1109:Y01:HAN2	1.81	0.63
7:A:1109:Y01:CAE	7:A:1109:Y01:HAO2	2.15	0.63
1:A:212:LYS:HB3	1:A:224:PRO:HB2	1.80	0.63
1:A:51:LEU:CD2	1:A:257:ILE:CD1	2.62	0.62
7:A:1106:Y01:HAN2	7:A:1106:Y01:HAC2	1.80	0.62
1:A:172:ILE:HD12	1:A:177:LYS:HG3	1.80	0.62
1:A:680:ASP:HA	1:A:683:LYS:HB2	1.82	0.62
7:B:401:Y01:HAO1	7:B:401:Y01:CAE	2.26	0.61
7:A:1106:Y01:HAE2	7:C:1501:Y01:CBA	2.31	0.61
7:A:1106:Y01:HAN2	7:A:1106:Y01:HAC3	1.82	0.61
1:A:170:LEU:HD23	1:A:192:GLU:O	2.01	0.61
7:A:1109:Y01:CAU	7:B:401:Y01:CAE	2.78	0.61
1:A:995:SER:OG	7:A:1106:Y01:HAA3	2.01	0.60
7:A:1106:Y01:CAE	7:C:1501:Y01:CAB	2.79	0.60
1:A:870:PHE:CZ	7:A:1109:Y01:HAE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HD12	1:A:506:VAL:HG23	1.82	0.60
1:A:959:PHE:CE1	7:C:1501:Y01:HAC1	2.36	0.60
7:A:1109:Y01:HAD1	7:A:1109:Y01:HBC	1.83	0.59
1:A:62:GLY:HA3	1:A:174:ASN:N	2.17	0.59
7:A:1108:Y01:HAC1	7:A:1108:Y01:HAU2	1.84	0.59
1:A:881:ILE:HD11	7:A:1109:Y01:HAV2	1.81	0.59
7:A:1106:Y01:HAE1	7:C:1501:Y01:HAB3	1.83	0.59
1:A:44:HIS:HB2	1:A:241:ASN:HB3	1.83	0.58
1:A:429:ASN:HD22	1:A:457:LEU:HG	1.66	0.58
7:A:1106:Y01:HAE2	7:C:1501:Y01:CAB	2.32	0.58
1:A:145:CYS:CB	7:A:1108:Y01:HAE2	2.30	0.58
1:A:165:VAL:HG13	1:A:165:VAL:O	2.02	0.58
1:A:1000:VAL:HG11	8:A:1110:PC1:C3G	2.34	0.58
1:A:63:LEU:C	1:A:64:THR:HG1	2.02	0.58
1:A:505:LEU:HB3	1:A:558:LEU:HD13	1.85	0.57
1:A:657:PRO:O	1:A:658:ARG:NH1	2.37	0.57
7:A:1106:Y01:CAE	7:C:1501:Y01:HBA	2.34	0.57
1:A:517:ARG:HH21	1:A:580:ILE:HB	1.70	0.57
2:B:12:TRP:CG	2:B:13:LYS:N	2.73	0.56
7:A:1109:Y01:HAE3	7:A:1109:Y01:CAO	2.23	0.56
7:A:1109:Y01:OAG	7:A:1109:Y01:HAR2	2.06	0.56
7:A:1109:Y01:HBF	7:B:401:Y01:HAD3	1.87	0.56
1:A:557:HIS:O	1:A:584:CYS:HB3	2.06	0.55
7:A:1106:Y01:CAE	7:C:1501:Y01:CBA	2.83	0.55
1:A:945:PHE:HA	7:A:1106:Y01:HAR1	1.88	0.55
7:B:401:Y01:HAE3	7:B:401:Y01:CAO	2.30	0.55
2:B:11:SER:OG	2:B:14:LYS:HE2	2.06	0.55
1:A:196:GLY:O	1:A:739:SER:HB3	2.07	0.54
1:A:1010:ARG:HH12	7:A:1107:Y01:HAM1	1.72	0.54
1:A:704:GLY:O	1:A:708:GLN:NE2	2.38	0.54
2:B:290:ARG:HE	2:B:294:ARG:HH22	1.56	0.53
1:A:881:ILE:CD1	7:A:1109:Y01:HAV1	2.34	0.53
1:A:211:CYS:C	1:A:249:CYS:SG	2.86	0.53
7:A:1109:Y01:HAQ1	7:B:401:Y01:HAD2	1.89	0.53
1:A:58:ASP:OD2	1:A:188:GLY:O	2.26	0.53
2:B:47:ALA:HB2	7:B:401:Y01:HAC3	1.88	0.53
1:A:1004:VAL:HG11	8:A:1110:PC1:H3B2	1.90	0.53
7:A:1108:Y01:CAU	7:A:1108:Y01:CAC	2.85	0.53
1:A:172:ILE:HG22	1:A:190:LEU:O	2.09	0.53
1:A:230:ASP:O	1:A:241:ASN:ND2	2.41	0.53
1:A:620:HIS:HD2	1:A:622:ILE:HG12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ASP:OD1	1:A:940:ARG:NH1	2.38	0.52
1:A:1012:ARG:HD3	8:A:1110:PC1:H12	1.92	0.52
2:B:186:PHE:O	2:B:244:PRO:HB3	2.09	0.52
1:A:174:ASN:OD1	1:A:175:GLY:N	2.42	0.52
1:A:504:LEU:HA	1:A:558:LEU:O	2.10	0.52
2:B:242:TYR:O	2:B:243:TYR:HB2	2.10	0.52
1:A:792:ILE:HD13	7:A:1109:Y01:CAC	2.39	0.51
1:A:949:MET:CG	7:A:1106:Y01:CAD	2.89	0.51
1:A:198:ARG:HA	1:A:248:ASN:HD22	1.75	0.51
1:A:239:THR:OG1	1:A:240:ARG:N	2.43	0.51
7:A:1106:Y01:HAO2	7:C:1501:Y01:CAA	2.40	0.51
7:A:1109:Y01:HAQ1	7:B:401:Y01:CAD	2.41	0.51
1:A:227:ARG:NH2	1:A:239:THR:O	2.43	0.51
1:A:792:ILE:HD11	7:A:1109:Y01:HAN2	1.90	0.51
1:A:870:PHE:HZ	7:A:1109:Y01:HAE2	1.74	0.51
1:A:203:LEU:HB2	1:A:243:ALA:HB3	1.93	0.51
1:A:495:ASN:H	1:A:503:HIS:HD2	1.57	0.50
3:C:33:PHE:CZ	7:C:1501:Y01:HBF	2.47	0.50
7:A:1106:Y01:HAE3	7:C:1501:Y01:HAA2	1.92	0.50
1:A:897:ASP:OD1	1:A:897:ASP:N	2.44	0.50
1:A:949:MET:HG2	7:A:1106:Y01:CAD	2.41	0.50
1:A:740:ASP:HA	1:A:743:LYS:HG2	1.94	0.50
1:A:792:ILE:HD12	7:A:1109:Y01:HAN2	1.90	0.50
1:A:881:ILE:CD1	7:A:1109:Y01:HAI	2.33	0.50
2:B:11:SER:HB3	2:B:14:LYS:HE2	1.88	0.50
1:A:413:LYS:H	1:A:418:TRP:HZ2	1.59	0.50
1:A:51:LEU:HD11	1:A:257:ILE:CG2	2.40	0.49
2:B:197:GLU:HG2	2:B:198:THR:HG23	1.94	0.49
1:A:945:PHE:HA	7:A:1106:Y01:CAR	2.43	0.49
1:A:523:LEU:HD23	1:A:526:LYS:HD3	1.95	0.49
1:A:531:ASP:HB3	1:A:534:LEU:HB2	1.93	0.49
1:A:871:VAL:HG22	2:B:57:MET:HG3	1.93	0.49
1:A:212:LYS:HA	1:A:225:GLN:O	2.12	0.49
1:A:170:LEU:HD23	1:A:192:GLU:HB3	1.93	0.49
1:A:170:LEU:HD21	1:A:192:GLU:OE2	2.13	0.49
2:B:136:ARG:NH1	2:B:147:LYS:O	2.46	0.49
1:A:521:ILE:HD13	1:A:534:LEU:HD21	1.95	0.49
1:A:881:ILE:CD1	7:A:1109:Y01:HAV2	2.39	0.49
7:A:1107:Y01:HAC1	7:A:1107:Y01:HAU2	1.93	0.49
7:A:1109:Y01:CAU	7:B:401:Y01:HAE3	2.43	0.49
1:A:145:CYS:HB2	7:A:1108:Y01:CAE	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:NZ	1:A:844:LEU:O	2.45	0.48
1:A:218:LEU:HD12	1:A:219:THR:HG23	1.94	0.48
1:A:62:GLY:HA3	1:A:173:ARG:C	2.34	0.48
1:A:573:THR:HA	1:A:578:PHE:HE2	1.78	0.48
1:A:215:ASN:O	1:A:219:THR:OG1	2.31	0.48
1:A:930:GLN:HE21	1:A:930:GLN:CA	2.23	0.48
1:A:556:CYS:HB3	1:A:585:PHE:HA	1.96	0.48
1:A:270:ILE:CG1	1:A:271:ALA:N	2.73	0.47
1:A:244:PHE:O	1:A:247:THR:OG1	2.31	0.47
1:A:502:GLN:HG2	1:A:561:PRO:HA	1.97	0.47
1:A:814:THR:HB	1:A:930:GLN:HG3	1.96	0.47
2:B:16:ILE:O	2:B:17:TRP:HB2	2.14	0.47
1:A:270:ILE:HG13	1:A:271:ALA:H	1.75	0.47
1:A:172:ILE:HG23	1:A:172:ILE:O	2.15	0.47
1:A:212:LYS:O	1:A:250:VAL:HG22	2.15	0.47
1:A:478:VAL:HG21	1:A:572:ASP:HA	1.96	0.46
7:A:1106:Y01:HAC2	7:A:1106:Y01:CAN	2.43	0.46
7:A:1109:Y01:CAN	7:A:1109:Y01:CAC	2.94	0.46
1:A:949:MET:CG	7:A:1106:Y01:HAD3	2.46	0.46
1:A:518:CYS:HA	1:A:583:LEU:H	1.81	0.46
1:A:558:LEU:HG	1:A:583:LEU:HG	1.98	0.46
1:A:564:GLN:NE2	1:A:577:ASN:O	2.48	0.46
7:A:1109:Y01:HAU1	7:B:401:Y01:HAE3	1.96	0.46
7:A:1109:Y01:HAD1	7:A:1109:Y01:CBC	2.44	0.45
1:A:985:PRO:HD3	3:C:26:VAL:HG11	1.99	0.45
1:A:476:LYS:HA	1:A:493:HIS:HD2	1.81	0.45
1:A:389:ALA:O	1:A:590:SER:OG	2.29	0.45
1:A:931:TRP:CZ2	7:C:1501:Y01:HAU2	2.51	0.45
1:A:88:GLU:OE2	1:A:148:TYR:OH	2.34	0.45
2:B:12:TRP:CD2	2:B:13:LYS:N	2.81	0.45
1:A:949:MET:HG3	7:A:1106:Y01:CAD	2.47	0.45
1:A:962:THR:HG21	7:C:1501:Y01:HAS2	1.98	0.45
2:B:16:ILE:O	2:B:16:ILE:HG22	2.15	0.45
1:A:382:THR:HA	1:A:595:PRO:HA	1.98	0.45
1:A:175:GLY:O	1:A:176:GLU:HB2	2.17	0.44
1:A:212:LYS:HD3	1:A:251:GLU:CD	2.37	0.44
2:B:268:MET:SD	2:B:303:SER:OG	2.75	0.44
1:A:63:LEU:HD21	1:A:67:ARG:HB3	2.00	0.44
1:A:127:ASN:OD1	1:A:127:ASN:N	2.50	0.44
2:B:12:TRP:CE3	2:B:13:LYS:CB	2.94	0.44
2:B:124:GLU:HB3	2:B:147:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HD12	2:B:80:ILE:HA	1.75	0.44
1:A:367:LEU:HD13	1:A:730:ILE:HD13	2.00	0.44
1:A:845:VAL:HA	1:A:849:LEU:HD23	2.00	0.44
1:A:739:SER:O	1:A:742:SER:OG	2.31	0.43
1:A:85:THR:OG1	1:A:86:THR:N	2.52	0.43
1:A:931:TRP:CZ2	7:C:1501:Y01:CAU	3.01	0.43
1:A:1003:GLU:HB3	7:A:1107:Y01:CAK	2.26	0.43
1:A:251:GLU:H	1:A:251:GLU:HG3	1.48	0.43
2:B:164:ASP:OD1	2:B:166:THR:OG1	2.33	0.43
2:B:241:GLN:H	2:B:241:GLN:HG2	1.51	0.43
1:A:51:LEU:HD22	1:A:59:LEU:HD21	2.01	0.43
1:A:233:ASN:ND2	1:A:238:GLU:O	2.47	0.43
1:A:480:ILE:HD12	1:A:490:LEU:HB2	2.00	0.43
1:A:63:LEU:HG	1:A:64:THR:N	2.34	0.43
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.91	0.43
1:A:437:GLN:HE21	1:A:445:ARG:HD3	1.83	0.43
1:A:674:THR:OG1	1:A:675:SER:N	2.52	0.43
1:A:959:PHE:HE1	7:C:1501:Y01:HAP2	1.84	0.43
7:B:401:Y01:HBE	7:B:401:Y01:HAJ1	1.59	0.43
2:B:80:ILE:HG12	2:B:108:PHE:CD2	2.54	0.43
7:A:1107:Y01:CAU	7:A:1107:Y01:CAC	2.85	0.42
7:B:401:Y01:CAE	7:B:401:Y01:CAO	2.93	0.42
2:B:15:PHE:CD1	2:B:15:PHE:O	2.72	0.42
1:A:410:SER:O	1:A:411:PHE:CD1	2.73	0.42
1:A:87:PRO:HD2	1:A:90:ILE:HD12	2.01	0.42
1:A:491:SER:H	1:A:506:VAL:HG12	1.85	0.42
1:A:949:MET:HG2	7:A:1106:Y01:HAD3	2.02	0.42
1:A:360:ASN:N	1:A:360:ASN:OD1	2.51	0.42
3:C:36:LEU:HD23	3:C:36:LEU:HA	1.92	0.42
1:A:409:VAL:HG23	1:A:411:PHE:CD2	2.55	0.41
1:A:44:HIS:HB3	1:A:242:ILE:HG23	2.02	0.41
1:A:783:ASN:ND2	1:A:854:TYR:OH	2.42	0.41
1:A:787:ILE:HD13	1:A:787:ILE:HA	1.90	0.41
1:A:792:ILE:HD11	7:A:1109:Y01:HAB1	2.02	0.41
1:A:1010:ARG:NH1	7:A:1107:Y01:CAX	2.83	0.41
1:A:104:LEU:HG	1:A:329:VAL:HG21	2.03	0.41
7:A:1106:Y01:CAE	7:A:1106:Y01:HAO2	2.48	0.41
1:A:145:CYS:CB	7:A:1108:Y01:HBG	2.49	0.41
1:A:1012:ARG:HD3	8:A:1110:PC1:C1	2.50	0.41
2:B:93:ASN:OD1	2:B:93:ASN:N	2.45	0.41
1:A:1015:GLY:HA2	8:A:1110:PC1:O14	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:CYS:O	1:A:250:VAL:C	2.59	0.41
1:A:926:ILE:O	1:A:930:GLN:HG2	2.21	0.41
7:A:1109:Y01:HBB	7:B:401:Y01:HAE3	1.94	0.41
7:A:1109:Y01:HAS1	2:B:50:PHE:HE2	1.86	0.41
7:B:401:Y01:HAC3	7:B:401:Y01:CAB	2.51	0.41
2:B:243:TYR:HA	2:B:244:PRO:HA	1.78	0.41
3:C:22:ASP:OD1	3:C:22:ASP:N	2.54	0.41
1:A:505:LEU:HD12	1:A:560:LEU:HD11	2.03	0.40
1:A:517:ARG:O	1:A:582:ASN:N	2.54	0.40
1:A:227:ARG:HE	1:A:240:ARG:HA	1.87	0.40
1:A:811:ASP:O	1:A:815:ASP:HB2	2.22	0.40
1:A:47:SER:N	1:A:50:GLU:OE1	2.54	0.40
1:A:617:THR:OG1	1:A:618:GLY:N	2.54	0.40
7:C:1501:Y01:HAO1	7:C:1501:Y01:CAE	2.25	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	972/1023 (95%)	902 (93%)	60 (6%)	10 (1%)	15	54
2	B	292/303 (96%)	267 (91%)	22 (8%)	3 (1%)	15	54
3	C	30/66 (46%)	25 (83%)	5 (17%)	0	100	100
All	All	1294/1392 (93%)	1194 (92%)	87 (7%)	13 (1%)	20	54

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLU
1	A	250	VAL
1	A	409	VAL

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Mol	Chain	Res	Type
2	B	11	SER
1	A	175	GLY
1	A	270	ILE
1	A	317	TRP
1	A	64	THR
1	A	173	ARG
1	A	177	LYS
1	A	185	VAL
2	B	243	TYR
2	B	200	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	830/866 (96%)	819 (99%)	11 (1%)	69	87
2	B	263/269 (98%)	261 (99%)	2 (1%)	81	93
3	C	26/53 (49%)	26 (100%)	0	100	100
All	All	1119/1188 (94%)	1106 (99%)	13 (1%)	72	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	172	ILE
1	A	184	GLU
1	A	204	ARG
1	A	249	CYS
1	A	251	GLU
1	A	264	ARG
1	A	269	ARG
1	A	468	LYS
1	A	556	CYS
1	A	930	GLN
2	B	13	LYS

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Mol	Chain	Res	Type
2	B	241	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	225	GLN
1	A	241	ASN
1	A	248	ASN
1	A	406	GLN
1	A	429	ASN
1	A	437	GLN
1	A	503	HIS
1	A	528	GLN
1	A	540	ASN
1	A	570	GLN
1	A	744	GLN
1	A	896	ASN
1	A	942	ASN
1	A	946	GLN
2	B	18	ASN
2	B	104	ASN
2	B	140	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	2,4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.47	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

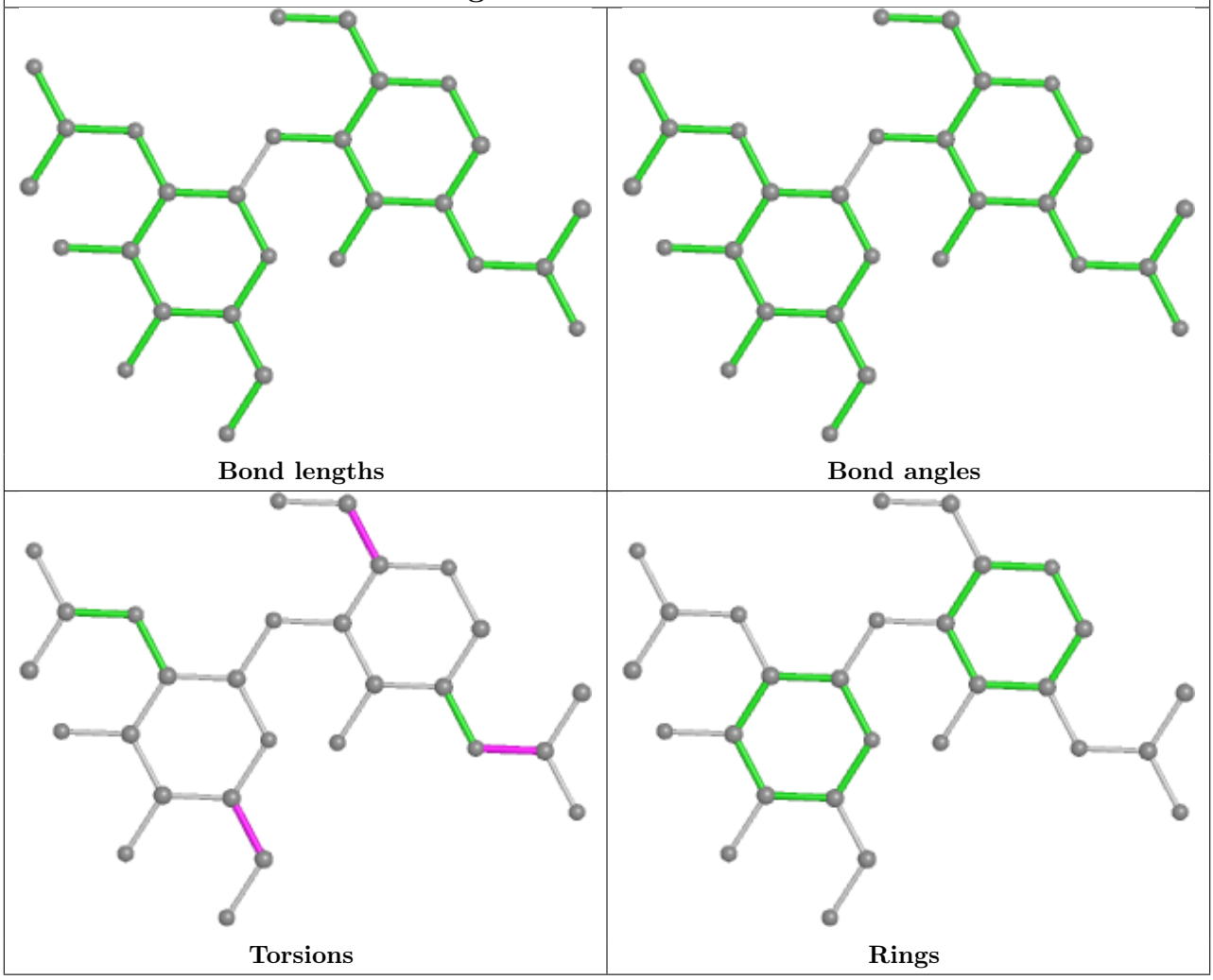
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
8	PC1	A	1110	-	53,53,53	0.98	4 (7%)	59,61,61	1.10	3 (5%)
7	Y01	A	1108	-	38,38,38	3.26	15 (39%)	57,57,57	2.42	17 (29%)
7	Y01	A	1107	-	38,38,38	3.26	15 (39%)	57,57,57	2.38	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	B	402	2	14,14,15	0.47	0	17,19,21	0.65	1 (5%)
7	Y01	A	1106	-	38,38,38	3.26	16 (42%)	57,57,57	2.49	16 (28%)
7	Y01	A	1109	-	38,38,38	3.28	15 (39%)	57,57,57	2.44	17 (29%)
7	Y01	C	1501	-	38,38,38	3.26	16 (42%)	57,57,57	2.59	19 (33%)
7	Y01	B	401	-	38,38,38	3.29	15 (39%)	57,57,57	2.58	20 (35%)

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
8	PC1	A	1110	-	-	31/57/57/57	-
7	Y01	A	1108	-	5/5/12/13	6/19/77/77	0/4/4/4
7	Y01	A	1107	-	5/5/12/13	6/19/77/77	1/4/4/4
9	NAG	B	402	2	-	2/6/23/26	0/1/1/1
7	Y01	A	1106	-	5/5/12/13	10/19/77/77	0/4/4/4
7	Y01	A	1109	-	5/5/12/13	10/19/77/77	1/4/4/4
7	Y01	C	1501	-	5/5/12/13	12/19/77/77	0/4/4/4
7	Y01	B	401	-	5/5/12/13	11/19/77/77	0/4/4/4

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1501	Y01	CAI-CAZ	10.35	1.55	1.33
7	B	401	Y01	CAI-CAZ	10.26	1.55	1.33
7	A	1109	Y01	CAI-CAZ	10.25	1.55	1.33
7	A	1108	Y01	CAI-CAZ	10.21	1.55	1.33
7	A	1106	Y01	CAI-CAZ	10.21	1.55	1.33
7	A	1107	Y01	CAI-CAZ	10.20	1.55	1.33
7	B	401	Y01	CBI-CBG	-8.16	1.39	1.55
7	A	1106	Y01	CBI-CBG	-8.10	1.39	1.55
7	A	1108	Y01	CBI-CBG	-7.98	1.39	1.55
7	A	1107	Y01	CBI-CBG	-7.89	1.40	1.55
7	A	1109	Y01	CBI-CBG	-7.84	1.40	1.55
7	C	1501	Y01	CBI-CBG	-7.48	1.40	1.55
7	C	1501	Y01	CAK-CAI	6.51	1.64	1.50
7	A	1109	Y01	CBD-CBG	6.35	1.65	1.53
7	A	1107	Y01	CAK-CAI	6.33	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1109	Y01	CAK-CAI	6.30	1.63	1.50
7	B	401	Y01	CAK-CAI	6.25	1.63	1.50
7	A	1106	Y01	CAK-CAI	6.21	1.63	1.50
7	A	1108	Y01	CBD-CBG	6.18	1.65	1.53
7	A	1108	Y01	CAK-CAI	6.16	1.63	1.50
7	A	1107	Y01	CBD-CBG	6.14	1.65	1.53
7	B	401	Y01	CBD-CBG	6.01	1.65	1.53
7	C	1501	Y01	CBD-CBG	5.95	1.65	1.53
7	A	1106	Y01	CBD-CBG	5.86	1.64	1.53
7	C	1501	Y01	CAU-CBI	5.40	1.63	1.54
7	B	401	Y01	CBH-CBF	5.36	1.65	1.56
7	A	1108	Y01	CBH-CBF	5.34	1.65	1.56
7	A	1109	Y01	CBH-CBF	5.29	1.64	1.56
7	A	1106	Y01	CBH-CBF	5.24	1.64	1.56
7	A	1107	Y01	CBH-CBF	5.05	1.64	1.56
7	A	1106	Y01	CAU-CBI	4.82	1.62	1.54
7	A	1109	Y01	CAU-CBI	4.81	1.62	1.54
7	B	401	Y01	CAU-CBI	4.79	1.62	1.54
7	C	1501	Y01	CBH-CBF	4.72	1.63	1.56
7	A	1108	Y01	CAU-CBI	4.62	1.62	1.54
7	A	1107	Y01	CAU-CBI	4.56	1.62	1.54
7	A	1108	Y01	CAQ-CBG	4.05	1.62	1.54
7	A	1109	Y01	CAQ-CBG	4.04	1.62	1.54
7	A	1107	Y01	CAQ-CBG	4.04	1.62	1.54
7	C	1501	Y01	CAQ-CBG	4.02	1.62	1.54
7	A	1106	Y01	CAQ-CBG	4.00	1.62	1.54
7	B	401	Y01	CAQ-CBG	3.97	1.62	1.54
7	C	1501	Y01	CAP-CBE	-3.77	1.46	1.54
7	B	401	Y01	CAP-CBE	-3.64	1.46	1.54
7	A	1109	Y01	CAP-CBE	-3.61	1.46	1.54
7	A	1107	Y01	CAP-CBE	-3.59	1.46	1.54
7	A	1108	Y01	CAP-CBE	-3.50	1.47	1.54
7	A	1106	Y01	CAP-CBE	-3.43	1.47	1.54
7	A	1106	Y01	CAV-CAZ	3.43	1.59	1.51
7	B	401	Y01	CAV-CAZ	3.40	1.59	1.51
7	A	1107	Y01	CAV-CAZ	3.37	1.59	1.51
7	A	1109	Y01	CAV-CAZ	3.36	1.59	1.51
7	A	1108	Y01	CAV-CAZ	3.35	1.58	1.51
7	C	1501	Y01	CAV-CAZ	3.33	1.58	1.51
7	B	401	Y01	CAT-CBH	3.31	1.60	1.54
7	A	1106	Y01	CAT-CBH	3.24	1.60	1.54
7	A	1107	Y01	CAT-CBH	3.21	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1109	Y01	CAT-CBH	3.18	1.60	1.54
7	A	1108	Y01	OAW-CAY	3.18	1.43	1.34
7	C	1501	Y01	CAT-CBH	3.17	1.60	1.54
7	A	1108	Y01	CAT-CBH	3.16	1.60	1.54
7	A	1109	Y01	OAW-CAY	3.14	1.43	1.34
7	B	401	Y01	OAW-CAY	3.09	1.43	1.34
7	A	1107	Y01	OAW-CAY	3.02	1.42	1.34
7	A	1107	Y01	CAR-CBC	3.01	1.59	1.51
7	A	1106	Y01	OAW-CAY	2.99	1.42	1.34
7	A	1107	Y01	CAS-CBF	-2.93	1.48	1.53
7	A	1109	Y01	CAR-CBC	2.92	1.59	1.51
7	B	401	Y01	CAR-CBC	2.89	1.58	1.51
7	A	1108	Y01	CAR-CBC	2.86	1.58	1.51
7	C	1501	Y01	OAW-CAY	2.85	1.42	1.34
7	A	1106	Y01	CAR-CBC	2.84	1.58	1.51
7	C	1501	Y01	CAR-CBC	2.80	1.58	1.51
7	C	1501	Y01	OAW-CBC	-2.80	1.39	1.46
7	A	1106	Y01	CAS-CBF	-2.76	1.49	1.53
7	A	1109	Y01	CAS-CBF	-2.74	1.49	1.53
7	A	1108	Y01	CAS-CBF	-2.74	1.49	1.53
7	C	1501	Y01	CBI-CBE	2.70	1.60	1.55
7	A	1106	Y01	OAW-CBC	-2.67	1.39	1.46
7	B	401	Y01	CAS-CBF	-2.67	1.49	1.53
7	A	1107	Y01	OAW-CBC	-2.65	1.40	1.46
7	A	1108	Y01	OAW-CBC	-2.59	1.40	1.46
7	B	401	Y01	OAW-CBC	-2.58	1.40	1.46
7	A	1109	Y01	OAW-CBC	-2.48	1.40	1.46
8	A	1110	PC1	O21-C2	-2.48	1.40	1.46
7	C	1501	Y01	CAS-CBF	-2.47	1.49	1.53
8	A	1110	PC1	O31-C31	2.38	1.40	1.33
7	A	1107	Y01	CBI-CBE	2.33	1.59	1.55
7	A	1109	Y01	CBI-CBE	2.32	1.59	1.55
7	A	1108	Y01	CBI-CBE	2.32	1.59	1.55
7	A	1106	Y01	CBI-CBE	2.23	1.59	1.55
8	A	1110	PC1	O21-C21	2.15	1.40	1.34
7	C	1501	Y01	CBD-CBF	-2.11	1.49	1.53
8	A	1110	PC1	O31-C3	-2.09	1.40	1.45
7	B	401	Y01	CBI-CBE	2.02	1.58	1.55
7	A	1106	Y01	CBD-CBF	-2.01	1.49	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	401	Y01	CAU-CBI-CBE	-8.39	104.02	116.57
7	A	1109	Y01	CAU-CBI-CBE	-8.24	104.24	116.57
7	C	1501	Y01	CAU-CBI-CBE	-8.14	104.38	116.57
7	A	1106	Y01	CAU-CBI-CBE	-8.08	104.48	116.57
7	A	1108	Y01	CAU-CBI-CBE	-7.89	104.76	116.57
7	A	1107	Y01	CAU-CBI-CBE	-7.37	105.53	116.57
7	C	1501	Y01	CBH-CAZ-CAI	-7.21	111.87	122.90
7	A	1107	Y01	CBH-CAZ-CAI	-7.04	112.12	122.90
7	A	1108	Y01	CBH-CAZ-CAI	-6.94	112.28	122.90
7	A	1106	Y01	CBH-CAZ-CAI	-6.83	112.45	122.90
7	A	1109	Y01	CBH-CAZ-CAI	-6.73	112.61	122.90
7	A	1106	Y01	CAK-CAI-CAZ	-6.43	113.19	125.06
7	A	1109	Y01	CAK-CAI-CAZ	-6.39	113.27	125.06
7	B	401	Y01	CBH-CAZ-CAI	-6.30	113.26	122.90
7	A	1108	Y01	CAK-CAI-CAZ	-6.29	113.45	125.06
7	B	401	Y01	CAK-CAI-CAZ	-6.28	113.48	125.06
7	A	1107	Y01	CAK-CAI-CAZ	-5.99	114.00	125.06
7	C	1501	Y01	CAK-CAI-CAZ	-5.64	114.66	125.06
7	A	1107	Y01	CAD-CBH-CBF	-5.47	105.16	111.68
7	B	401	Y01	CBI-CBE-CBB	-5.41	111.02	119.49
7	C	1501	Y01	CAD-CBH-CBF	-5.40	105.24	111.68
7	B	401	Y01	CAD-CBH-CBF	-5.36	105.29	111.68
7	A	1108	Y01	CAV-CAZ-CAI	-5.26	113.03	120.61
7	A	1106	Y01	CAD-CBH-CBF	-5.22	105.46	111.68
7	B	401	Y01	CAV-CAZ-CAI	-5.07	113.30	120.61
7	A	1106	Y01	CBI-CBE-CBB	-4.85	111.89	119.49
7	A	1108	Y01	CAD-CBH-CBF	-4.80	105.96	111.68
7	A	1106	Y01	CAV-CAZ-CAI	-4.77	113.73	120.61
7	A	1109	Y01	CAD-CBH-CBF	-4.56	106.25	111.68
7	A	1109	Y01	CBI-CBE-CBB	-4.49	112.45	119.49
7	A	1107	Y01	CAV-CAZ-CAI	-4.32	114.38	120.61
7	B	401	Y01	CAV-CAZ-CBH	-4.16	110.89	116.42
7	A	1109	Y01	CAV-CAZ-CAI	-4.12	114.68	120.61
7	C	1501	Y01	CAV-CAZ-CAI	-4.10	114.70	120.61
7	A	1108	Y01	CBI-CBE-CBB	-4.07	113.11	119.49
7	A	1107	Y01	OAW-CAY-CAM	4.06	120.25	111.50
7	B	401	Y01	OAW-CAY-CAM	4.05	120.23	111.50
7	A	1107	Y01	CAT-CBH-CBF	4.00	114.32	108.73
7	A	1106	Y01	OAW-CAY-CAM	3.99	120.09	111.50
8	A	1110	PC1	O21-C21-C22	3.89	119.89	111.50
7	C	1501	Y01	CAU-CBI-CBG	3.89	113.31	107.27
7	C	1501	Y01	CAT-CBH-CBF	3.87	114.13	108.73
7	A	1109	Y01	OAW-CAY-CAM	3.85	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1501	Y01	CBG-CBI-CBE	3.82	104.60	100.07
7	C	1501	Y01	CAV-CAZ-CBH	-3.78	111.40	116.42
7	A	1108	Y01	OAW-CAY-CAM	3.63	119.33	111.50
7	C	1501	Y01	OAW-CAY-CAM	3.56	119.18	111.50
7	A	1107	Y01	CBI-CBE-CBB	-3.45	114.08	119.49
7	A	1106	Y01	CAK-CBD-CBF	3.36	113.78	109.71
7	B	401	Y01	CAT-CBH-CBF	3.34	113.40	108.73
7	C	1501	Y01	CBI-CBE-CBB	-3.34	114.25	119.49
7	A	1109	Y01	CAT-CBH-CBF	3.30	113.33	108.73
7	A	1109	Y01	CBG-CBI-CBE	3.29	103.97	100.07
7	A	1106	Y01	CAV-CAZ-CBH	-3.24	112.11	116.42
7	A	1106	Y01	CAT-CBH-CBF	3.15	113.13	108.73
7	C	1501	Y01	CAT-CBH-CAZ	3.09	114.42	108.75
7	A	1108	Y01	CAT-CBH-CBF	3.08	113.03	108.73
7	A	1109	Y01	CBF-CBD-CBG	3.08	113.21	109.09
7	A	1108	Y01	CBG-CBI-CBE	2.94	103.56	100.07
7	A	1107	Y01	CAT-CBH-CAZ	2.92	114.10	108.75
7	C	1501	Y01	CAU-CAS-CBF	2.92	118.17	113.11
7	A	1107	Y01	CAT-CAR-CBC	2.75	115.02	110.33
7	B	401	Y01	CAK-CBD-CBF	2.73	113.02	109.71
7	C	1501	Y01	CAR-CBC-CAV	2.72	115.04	110.99
7	C	1501	Y01	CAM-CAL-CAX	-2.68	107.85	113.60
7	A	1107	Y01	CBF-CBD-CBG	2.67	112.67	109.09
7	A	1108	Y01	CAK-CBD-CBF	2.64	112.91	109.71
8	A	1110	PC1	O31-C31-C32	2.63	120.17	111.91
7	B	401	Y01	CBF-CBH-CAZ	2.60	113.73	109.65
7	A	1109	Y01	CAV-CAZ-CBH	-2.58	112.99	116.42
7	B	401	Y01	CBG-CBI-CBE	2.57	103.11	100.07
7	A	1106	Y01	CAT-CBH-CAZ	2.56	113.43	108.75
7	B	401	Y01	CAD-CBH-CAT	-2.55	105.40	109.43
7	A	1106	Y01	CAD-CBH-CAT	-2.51	105.46	109.43
7	A	1109	Y01	CAD-CBH-CAT	-2.46	105.54	109.43
7	A	1108	Y01	CBF-CBD-CBG	2.46	112.39	109.09
7	A	1107	Y01	CAD-CBH-CAT	-2.44	105.57	109.43
7	A	1108	Y01	CAD-CBH-CAT	-2.42	105.60	109.43
7	A	1109	Y01	CAT-CBH-CAZ	2.38	113.11	108.75
7	C	1501	Y01	CAK-CBD-CBF	2.34	112.55	109.71
7	C	1501	Y01	CAC-CBB-CBE	-2.34	109.34	112.92
7	A	1108	Y01	CAT-CAR-CBC	2.33	114.30	110.33
7	A	1108	Y01	CAT-CBH-CAZ	2.33	113.01	108.75
7	A	1109	Y01	CAK-CBD-CBF	2.33	112.53	109.71
7	B	401	Y01	CAR-CBC-CAV	2.30	114.42	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1106	Y01	CAU-CBI-CBG	2.30	110.83	107.27
7	B	401	Y01	CBI-CBG-CBD	-2.27	111.02	114.38
7	A	1106	Y01	CBG-CBI-CBE	2.27	102.76	100.07
8	A	1110	PC1	O12-P-O14	-2.26	101.06	112.24
7	B	401	Y01	CAJ-CAO-CBB	-2.26	108.53	115.03
7	B	401	Y01	CAT-CBH-CAZ	2.26	112.88	108.75
7	B	401	Y01	CAU-CBI-CBG	2.24	110.75	107.27
7	A	1109	Y01	CAC-CBB-CBE	-2.24	109.49	112.92
7	A	1108	Y01	CAU-CBI-CBG	2.21	110.70	107.27
9	B	402	NAG	C1-O5-C5	2.21	115.19	112.19
7	A	1109	Y01	CAU-CBI-CBG	2.20	110.69	107.27
7	A	1106	Y01	CBC-CAV-CAZ	2.20	114.93	111.52
7	A	1107	Y01	CAR-CBC-CAV	2.17	114.22	110.99
7	C	1501	Y01	CAD-CBH-CAT	-2.15	106.03	109.43
7	A	1107	Y01	CBG-CBI-CBE	2.14	102.61	100.07
7	A	1108	Y01	CAV-CAZ-CBH	-2.12	113.60	116.42
7	C	1501	Y01	CAS-CAU-CBI	2.09	116.37	112.78
7	A	1108	Y01	CAM-CAL-CAX	-2.08	109.12	113.60
7	B	401	Y01	CBC-CAV-CAZ	2.07	114.73	111.52
7	A	1106	Y01	CBF-CBH-CAZ	2.04	112.84	109.65
7	B	401	Y01	CAD-CBH-CAZ	-2.02	105.08	108.34
7	A	1107	Y01	CAD-CBH-CAZ	-2.01	105.09	108.34
7	A	1109	Y01	CAS-CBF-CBH	-2.01	110.43	113.08

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1106	Y01	CBB
7	A	1106	Y01	CBD
7	A	1106	Y01	CBF
7	A	1106	Y01	CBI
7	A	1106	Y01	CBH
7	A	1107	Y01	CBB
7	A	1107	Y01	CBD
7	A	1107	Y01	CBF
7	A	1107	Y01	CBI
7	A	1107	Y01	CBH
7	A	1108	Y01	CBB
7	A	1108	Y01	CBD
7	A	1108	Y01	CBF
7	A	1108	Y01	CBI
7	A	1108	Y01	CBH

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Mol	Chain	Res	Type	Atom
7	A	1109	Y01	CBB
7	A	1109	Y01	CBD
7	A	1109	Y01	CBF
7	A	1109	Y01	CBI
7	A	1109	Y01	CBH
7	B	401	Y01	CBB
7	B	401	Y01	CBD
7	B	401	Y01	CBF
7	B	401	Y01	CBI
7	B	401	Y01	CBH
7	C	1501	Y01	CBB
7	C	1501	Y01	CBD
7	C	1501	Y01	CBF
7	C	1501	Y01	CBI
7	C	1501	Y01	CBH

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1107	Y01	OAG-CAY-OAW-CBC
7	A	1107	Y01	CAM-CAY-OAW-CBC
7	B	401	Y01	OAG-CAY-OAW-CBC
7	C	1501	Y01	CAM-CAY-OAW-CBC
8	A	1110	PC1	C11-O13-P-O12
8	A	1110	PC1	C11-O13-P-O14
8	A	1110	PC1	C1-O11-P-O12
8	A	1110	PC1	C22-C21-O21-C2
7	C	1501	Y01	OAG-CAY-OAW-CBC
7	A	1109	Y01	CAV-CBC-OAW-CAY
7	B	401	Y01	CAM-CAY-OAW-CBC
7	A	1106	Y01	CAO-CBB-CBE-CAP
8	A	1110	PC1	O22-C21-O21-C2
9	B	402	NAG	O5-C5-C6-O6
7	A	1108	Y01	CAO-CBB-CBE-CAP
7	B	401	Y01	CAO-CBB-CBE-CBI
7	A	1106	Y01	CAO-CBB-CBE-CBI
7	A	1106	Y01	CAC-CBB-CBE-CAP
7	A	1107	Y01	CAC-CBB-CBE-CAP
7	A	1108	Y01	CAC-CBB-CBE-CAP
7	C	1501	Y01	CAC-CBB-CBE-CBI
9	B	402	NAG	C4-C5-C6-O6
7	A	1109	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
7	A	1109	Y01	CAO-CBB-CBE-CAP
7	C	1501	Y01	CAO-CBB-CBE-CAP
8	A	1110	PC1	C2-C1-O11-P
7	B	401	Y01	CAC-CBB-CBE-CBI
7	B	401	Y01	CAO-CBB-CBE-CAP
7	A	1109	Y01	CAO-CBB-CBE-CBI
7	C	1501	Y01	CAO-CBB-CBE-CBI
8	A	1110	PC1	C32-C31-O31-C3
7	A	1106	Y01	CAC-CBB-CBE-CBI
7	A	1107	Y01	CAO-CAJ-CAN-CBA
8	A	1110	PC1	C11-O13-P-O11
8	A	1110	PC1	C1-O11-P-O13
7	A	1109	Y01	CAC-CBB-CBE-CAP
7	C	1501	Y01	CAC-CBB-CBE-CAP
8	A	1110	PC1	C27-C28-C29-C2A
7	B	401	Y01	CAC-CBB-CBE-CAP
7	A	1106	Y01	CAM-CAY-OAW-CBC
8	A	1110	PC1	C38-C39-C3A-C3B
8	A	1110	PC1	C37-C38-C39-C3A
8	A	1110	PC1	O32-C31-O31-C3
7	A	1106	Y01	OAG-CAY-OAW-CBC
8	A	1110	PC1	C2D-C2E-C2F-C2G
8	A	1110	PC1	C3A-C3B-C3C-C3D
7	A	1107	Y01	CAO-CBB-CBE-CAP
8	A	1110	PC1	C2C-C2D-C2E-C2F
8	A	1110	PC1	C21-C22-C23-C24
7	C	1501	Y01	CAN-CAJ-CAO-CBB
8	A	1110	PC1	C33-C34-C35-C36
7	A	1109	Y01	CAM-CAY-OAW-CBC
8	A	1110	PC1	O11-C1-C2-C3
8	A	1110	PC1	C2F-C2G-C2H-C2I
8	A	1110	PC1	C2A-C2B-C2C-C2D
7	C	1501	Y01	CAO-CAJ-CAN-CBA
7	A	1109	Y01	OAG-CAY-OAW-CBC
8	A	1110	PC1	C2B-C2C-C2D-C2E
7	A	1108	Y01	CAC-CBB-CBE-CBI
7	C	1501	Y01	CAJ-CAO-CBB-CBE
8	A	1110	PC1	C1-O11-P-O14
8	A	1110	PC1	O11-C1-C2-O21
8	A	1110	PC1	C3B-C3C-C3D-C3E
7	A	1106	Y01	CAJ-CAN-CBA-CAB
7	A	1109	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
8	A	1110	PC1	O13-C11-C12-N
7	A	1106	Y01	CAJ-CAN-CBA-CAA
7	B	401	Y01	CAJ-CAN-CBA-CAA
7	B	401	Y01	CAJ-CAN-CBA-CAB
7	A	1108	Y01	CAO-CBB-CBE-CBI
8	A	1110	PC1	C2E-C2F-C2G-C2H
8	A	1110	PC1	C25-C26-C27-C28
8	A	1110	PC1	C39-C3A-C3B-C3C
7	A	1106	Y01	CAN-CAJ-CAO-CBB
7	A	1107	Y01	CAC-CBB-CBE-CBI
7	B	401	Y01	CAN-CAJ-CAO-CBB
7	B	401	Y01	CAM-CAL-CAX-OAF
7	A	1109	Y01	CAR-CBC-OAW-CAY
7	B	401	Y01	CAM-CAL-CAX-OAH
8	A	1110	PC1	O21-C21-C22-C23
7	A	1109	Y01	CAN-CAJ-CAO-CBB
7	A	1106	Y01	CAJ-CAO-CBB-CAC
7	A	1108	Y01	CAL-CAM-CAY-OAW
8	A	1110	PC1	C35-C36-C37-C38
7	C	1501	Y01	CAJ-CAO-CBB-CAC
7	C	1501	Y01	CAM-CAL-CAX-OAH
7	C	1501	Y01	CAM-CAL-CAX-OAF
7	A	1108	Y01	CAL-CAM-CAY-OAG

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1107	Y01	CAR-CAT-CAV-CAZ-CBC-CBH
7	A	1109	Y01	CAR-CAT-CAV-CAZ-CBC-CBH

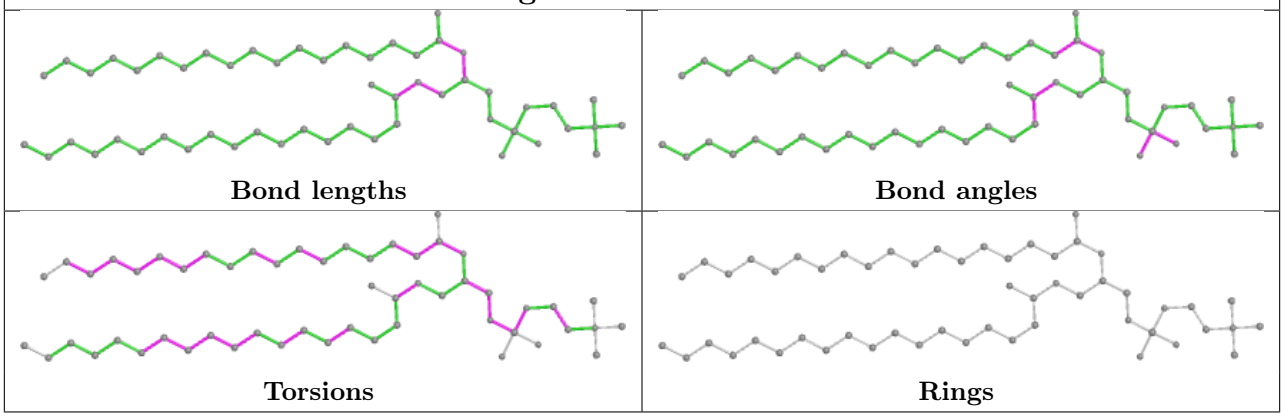
7 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1110	PC1	14	0
7	A	1108	Y01	11	0
7	A	1107	Y01	9	0
7	A	1106	Y01	24	0
7	A	1109	Y01	51	0
7	C	1501	Y01	21	0
7	B	401	Y01	29	0

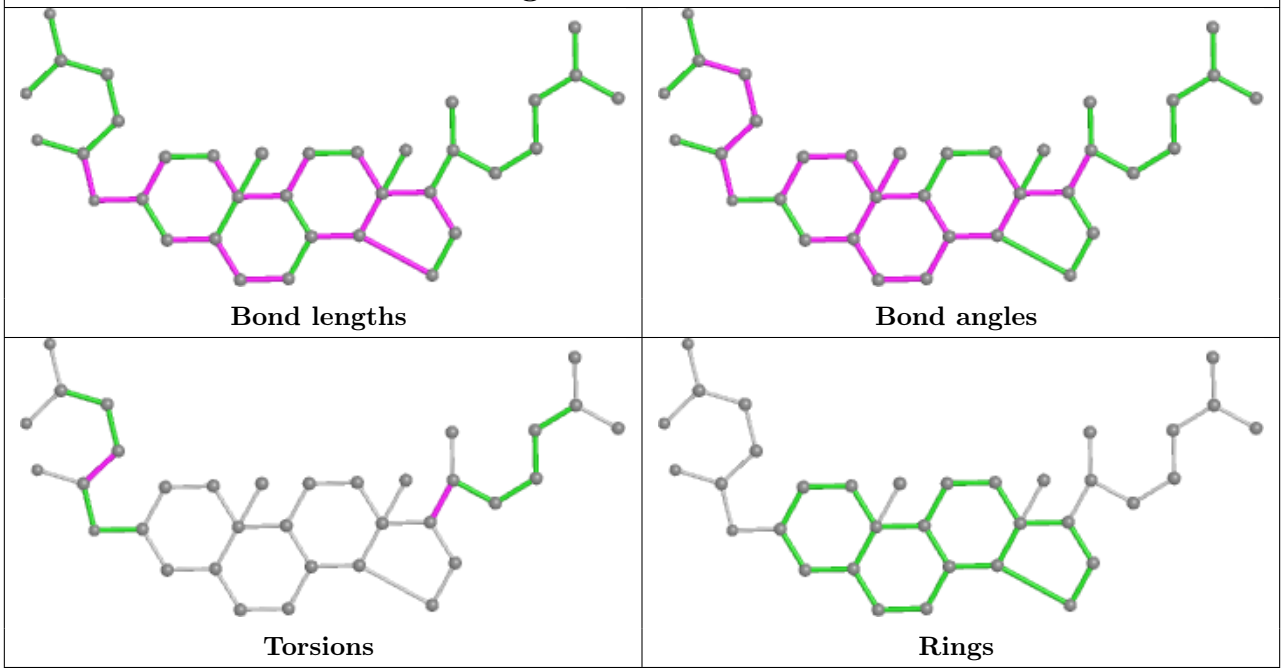
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

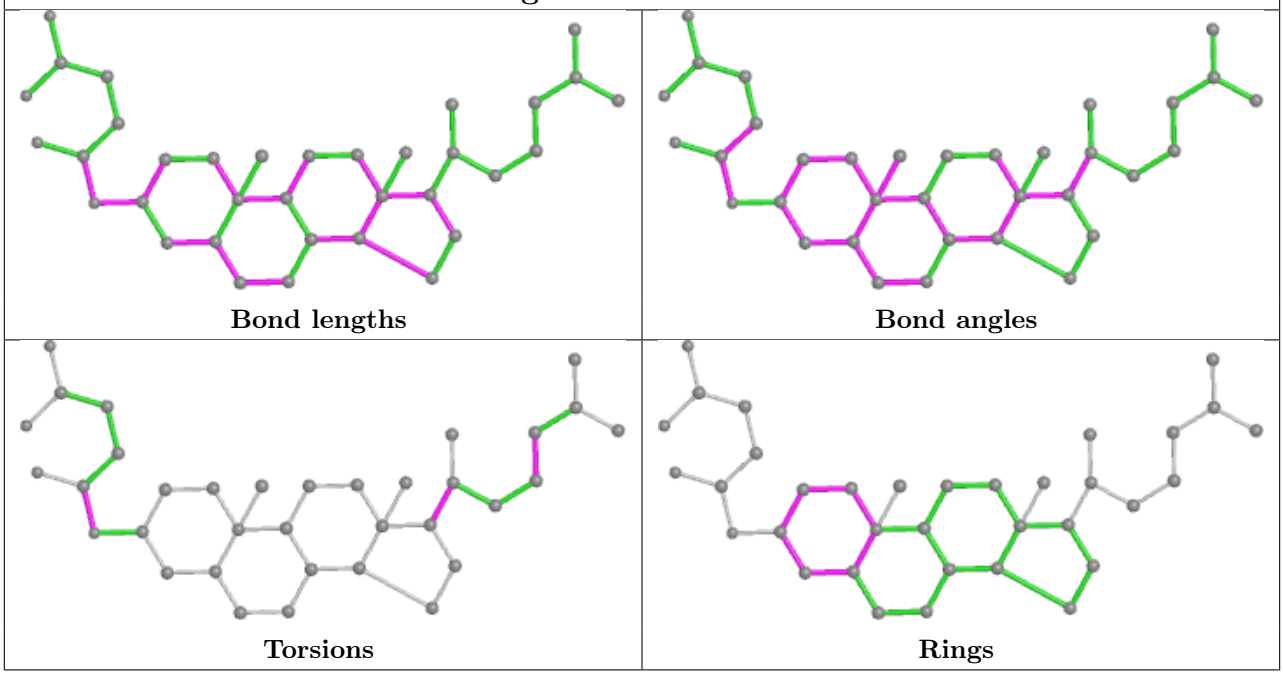
Ligand PC1 A 1110



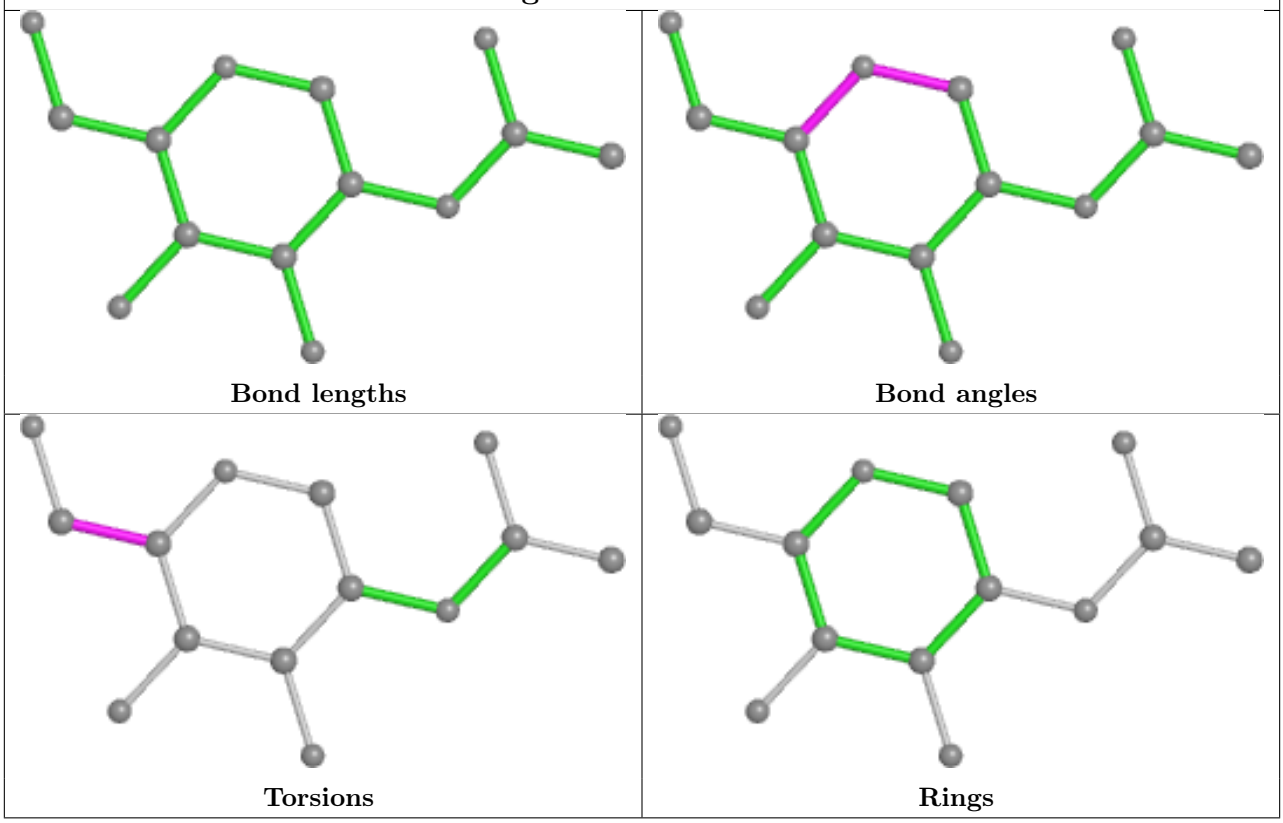
Ligand Y01 A 1108



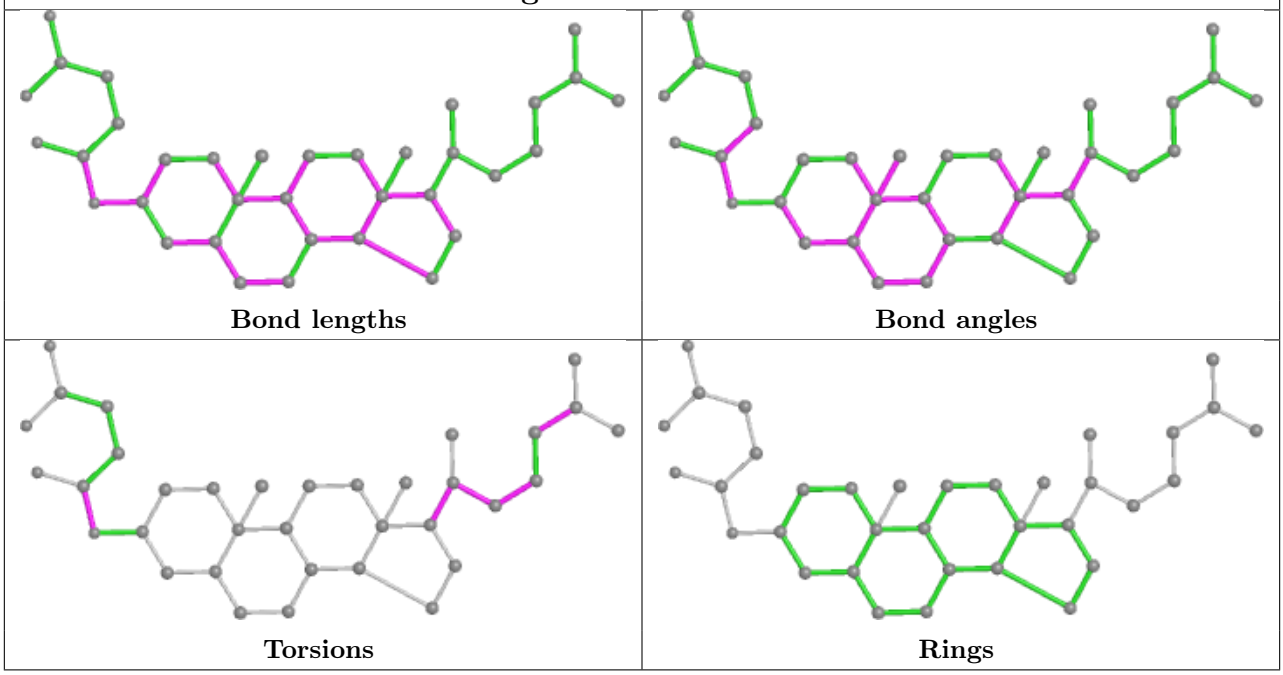
Ligand Y01 A 1107



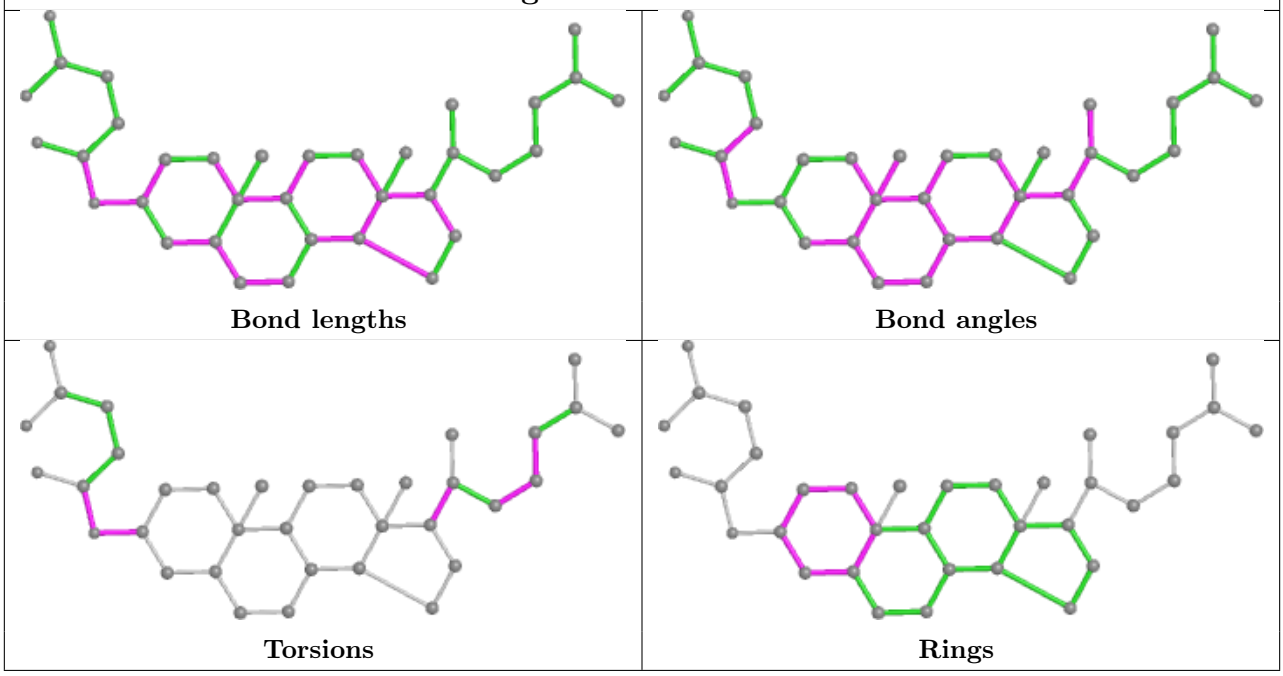
Ligand NAG B 402



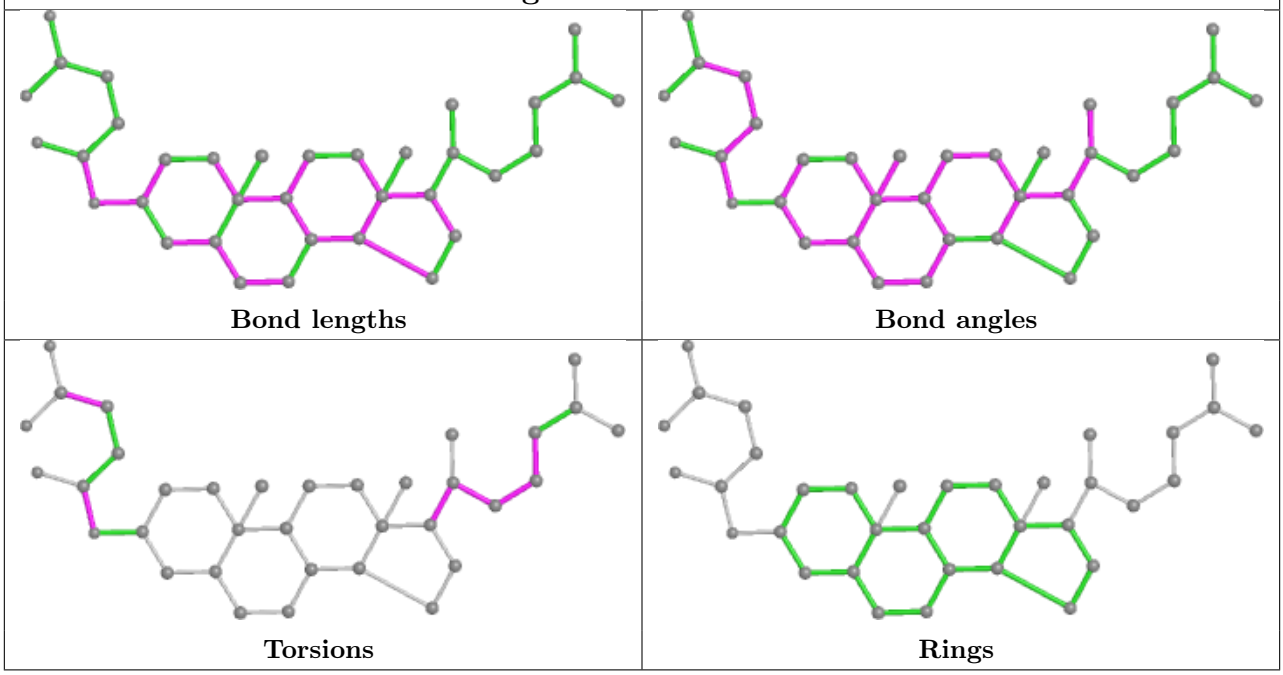
Ligand Y01 A 1106



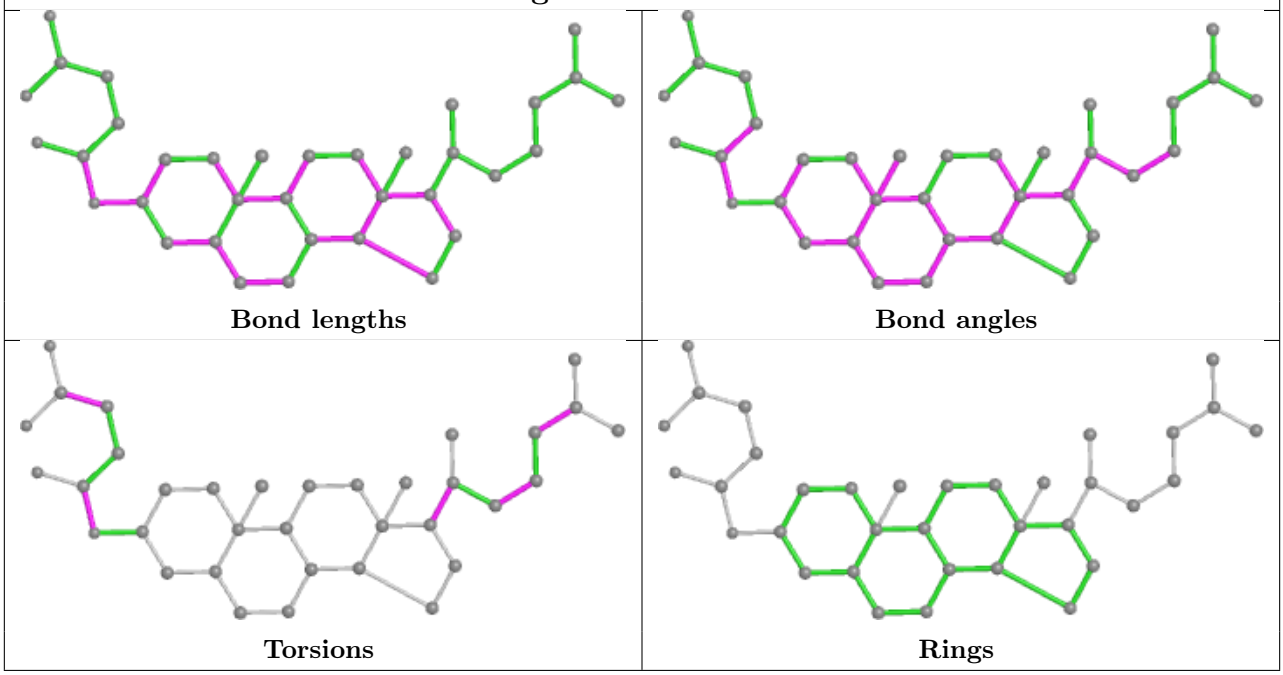
Ligand Y01 A 1109



Ligand Y01 C 1501



Ligand Y01 B 401



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.

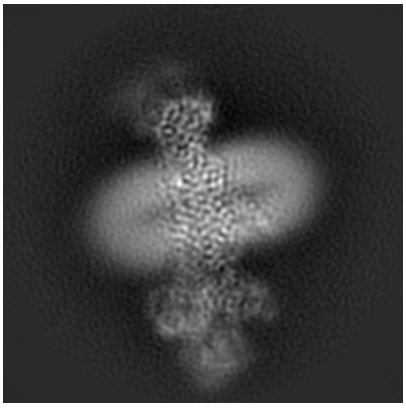
6 Map visualisation (i)

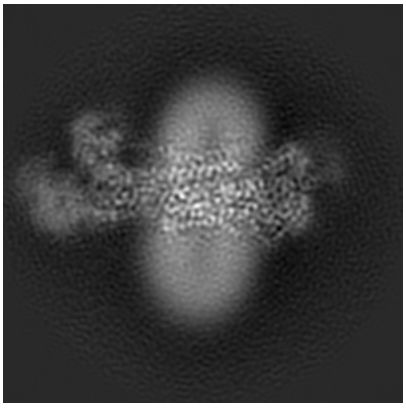
This section contains visualisations of the EMDB entry EMD-30947. These allow visual inspection of the internal detail of the map and identification of artifacts.

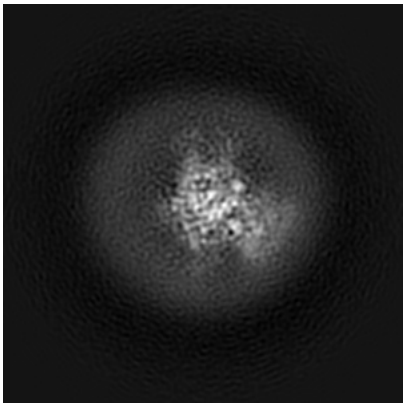
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

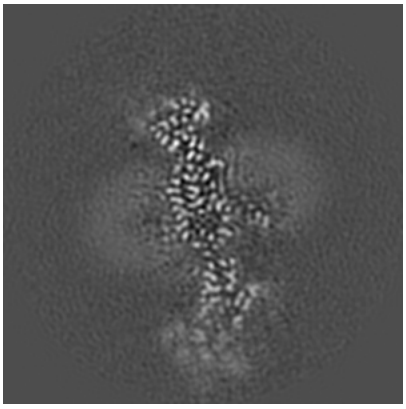

Y

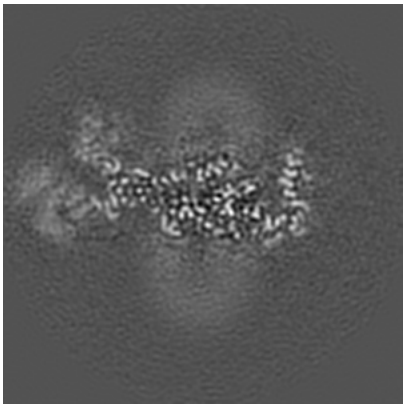

Z

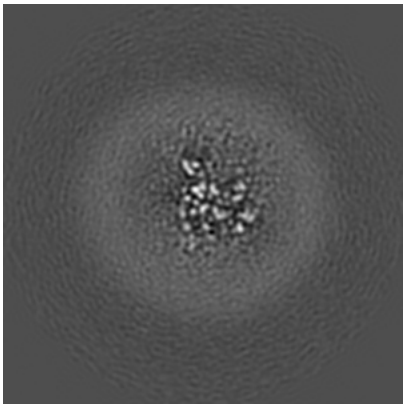
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 100

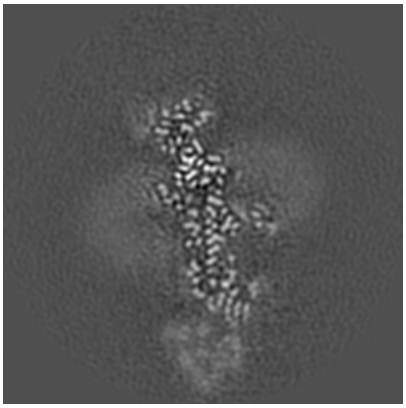

Y Index: 100


Z Index: 100

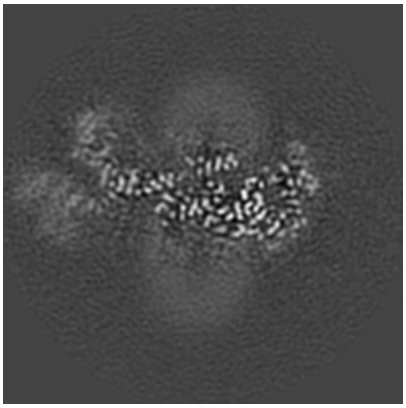
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

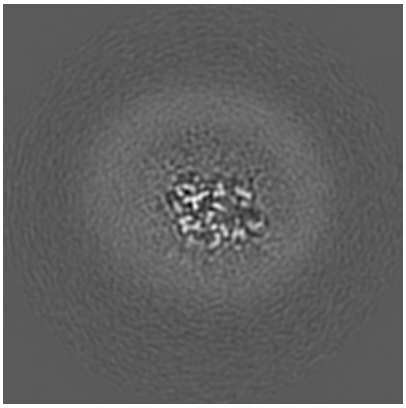
6.3.1 Primary map



X Index: 104



Y Index: 98



Z Index: 109

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

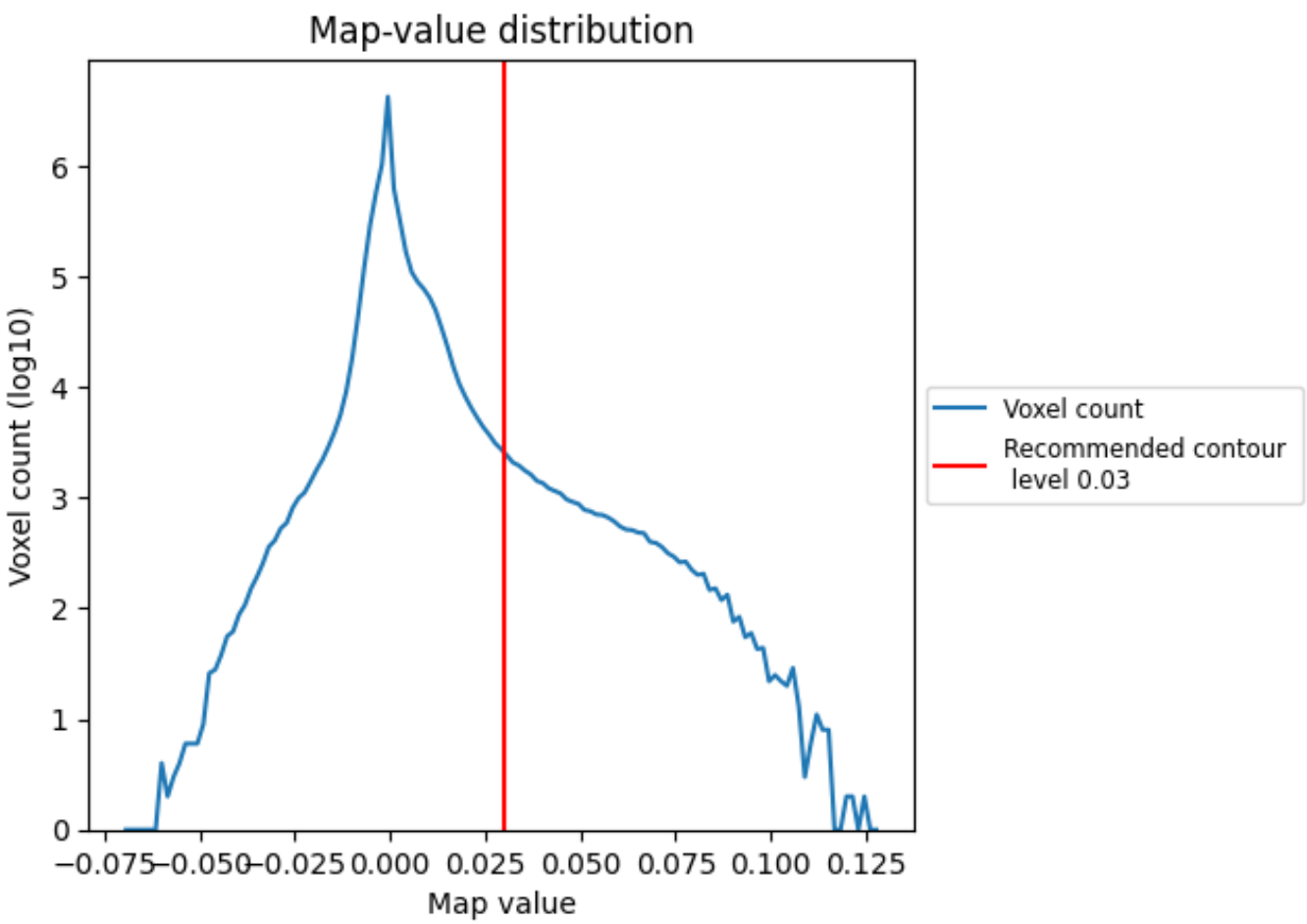
6.5 Mask visualisation (i)

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

7 Map analysis (i)

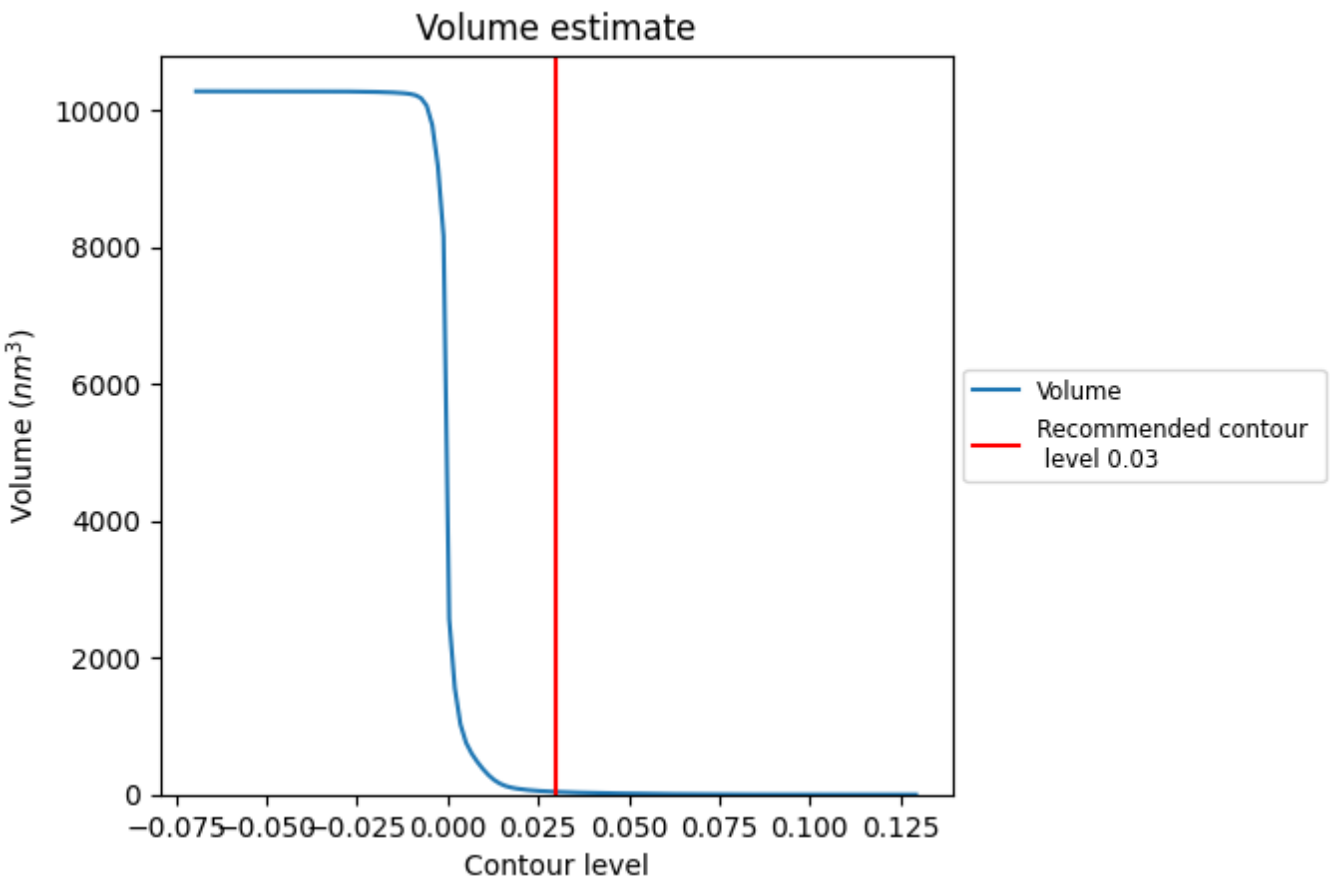
This section contains the results of statistical analysis of the map.

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.

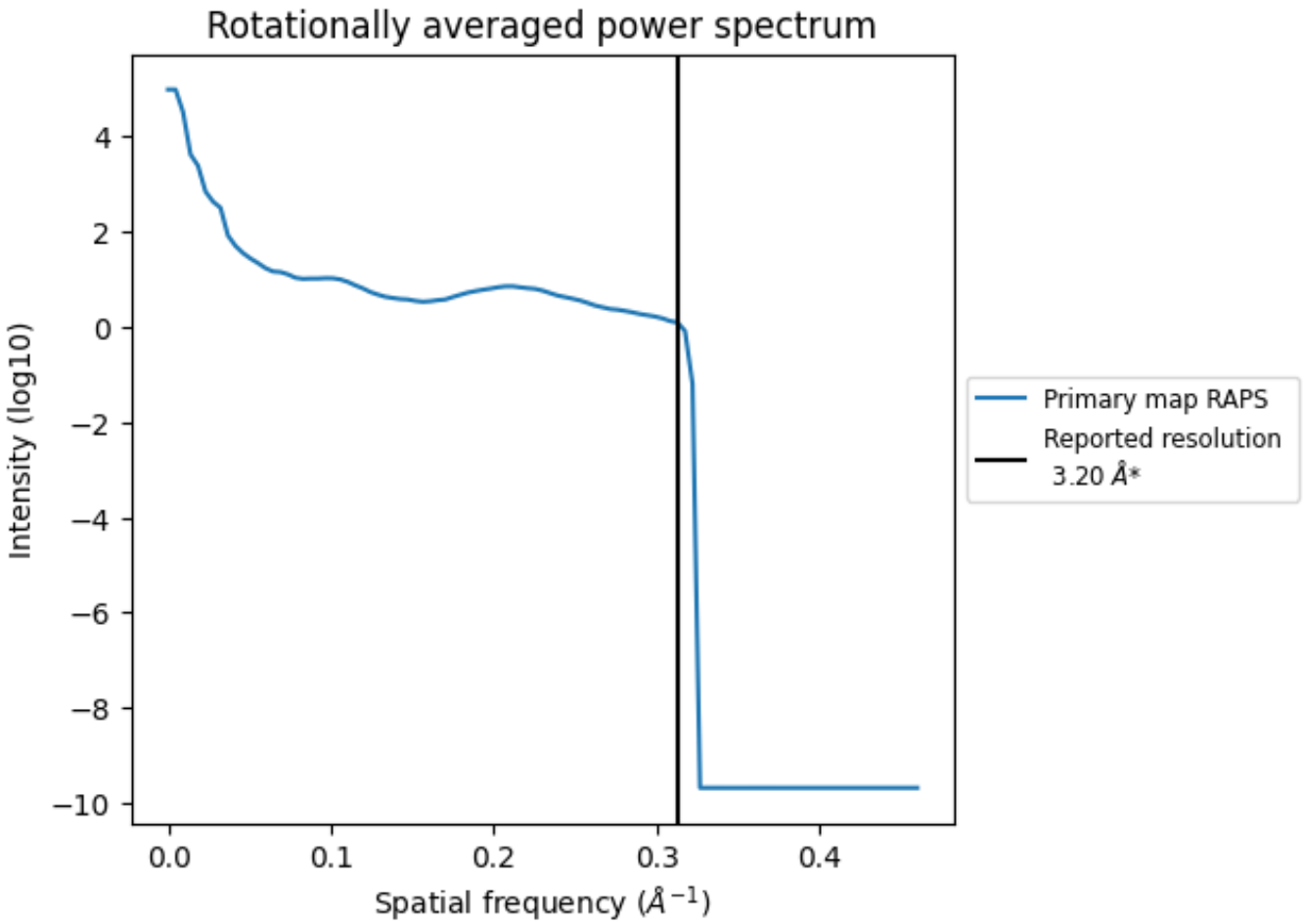
7.2 Volume estimate (i)



The volume at the recommended contour level is 40 nm^3; this corresponds to an approximate mass of 36 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

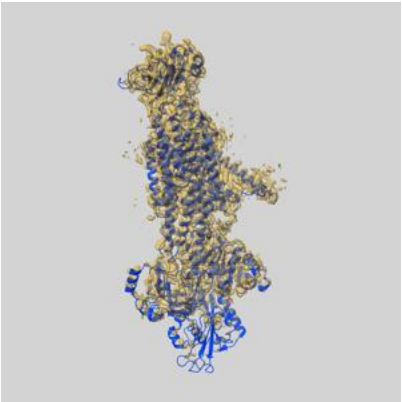
8 Fourier-Shell correlation (i)

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

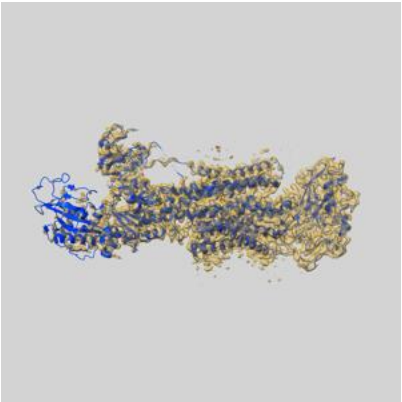
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30947 and PDB model 7E1Z. Per-residue inclusion information can be found in section 3 on page 8.

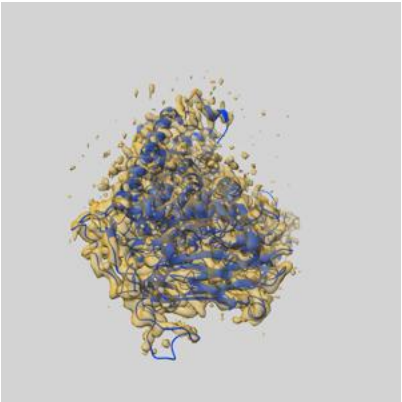
9.1 Map-model overlay (i)



X



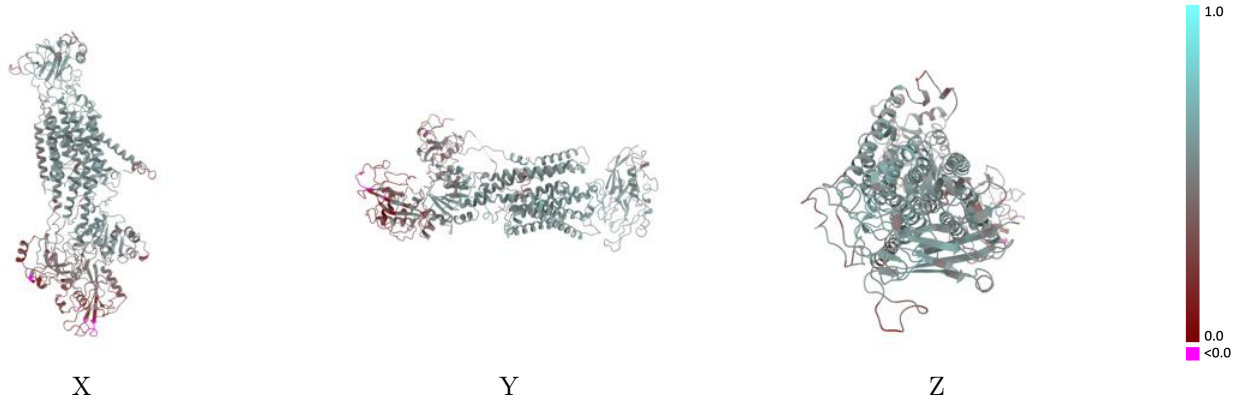
Y



Z

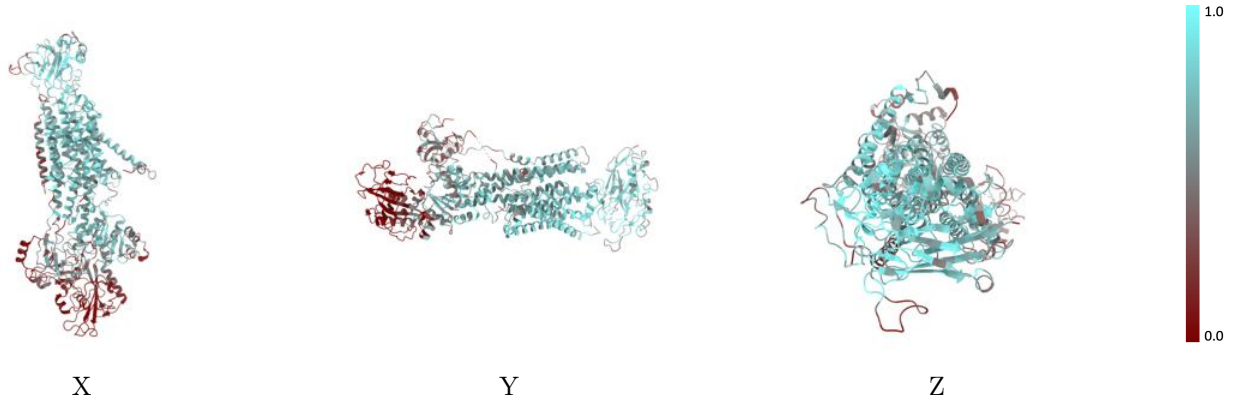
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



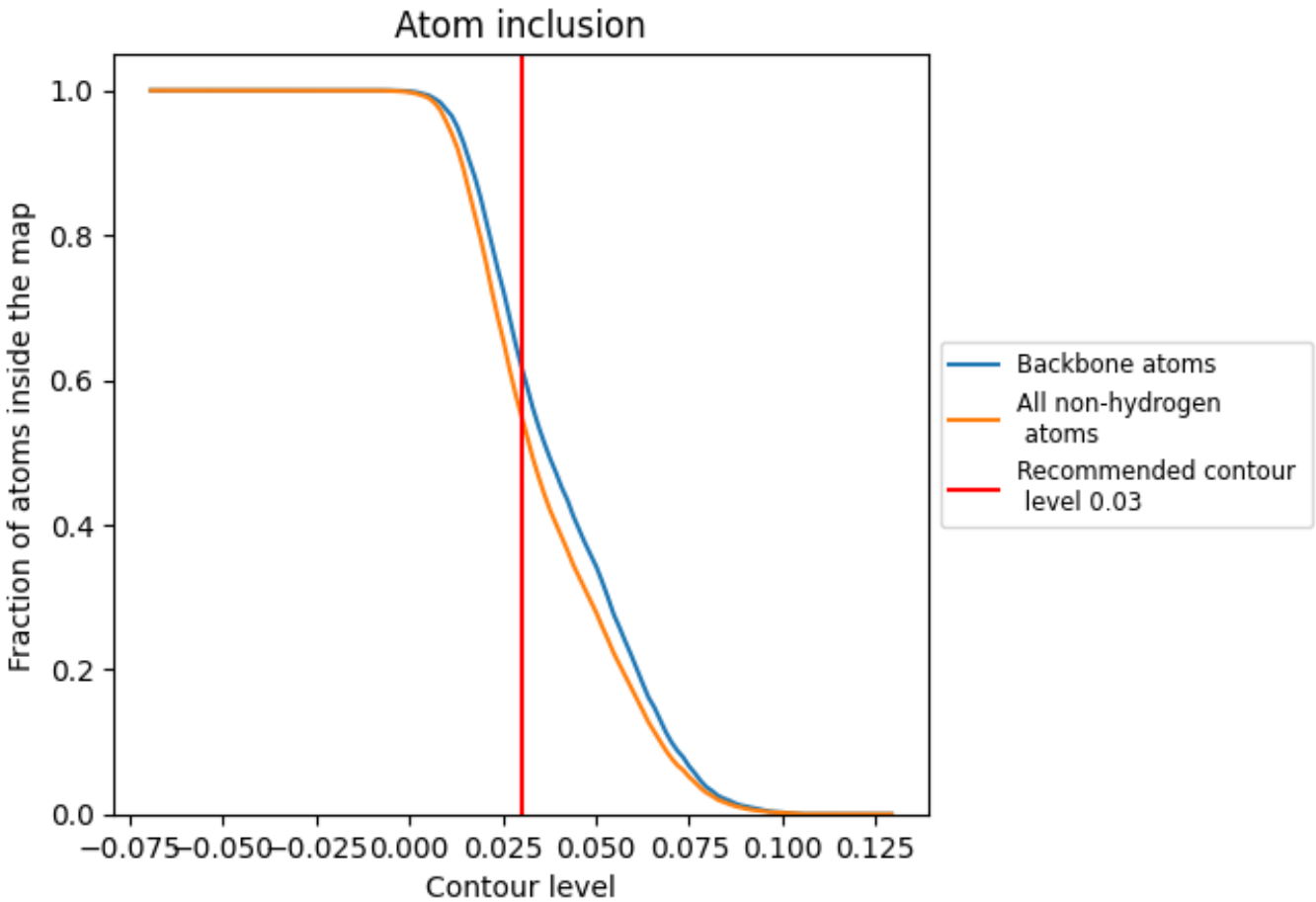
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5501	0.4790
A	0.5173	0.4690
B	0.6830	0.5120
C	0.3688	0.4550
D	0.3214	0.3420