



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:18 AM JST

PDB ID : 6LCP / pdb_00006lcp
EMDB ID : EMD-0872
Title : Cryo-EM structure of Dnf1 from Chaetomium thermophilum in the E2P state
Authors : He, Y.; Xu, J.; Wu, X.; Li, L.
Deposited on : 2019-11-19
Resolution : 3.48 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:

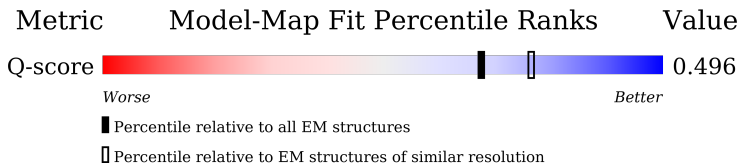
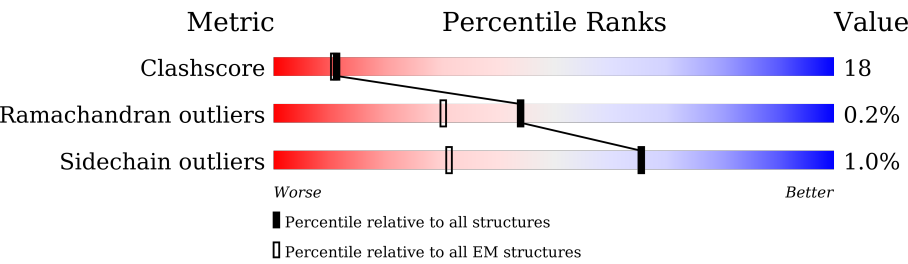
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.48 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.



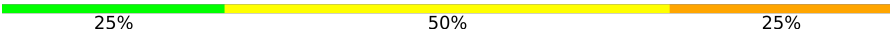
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13672 (2.98 - 3.98)

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	1555	6% 47% 26% • 27%
2	B	407	• 57% 33% •• 8%
3	C	2	100%
4	D	3	67% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	4	
6	F	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
8	BEF	A	2002	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 12421 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0
			9082	5832	1535	1664	51		

- Molecule 2 is a protein called Cdc50.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	376	Total	C	N	O	S	0	0
			3061	1979	512	558	12		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
3	C	2	Total	C	O	0	0
			22	12	10		

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



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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	4	Total	C	N	O	0	0
			50	28	2	20		

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

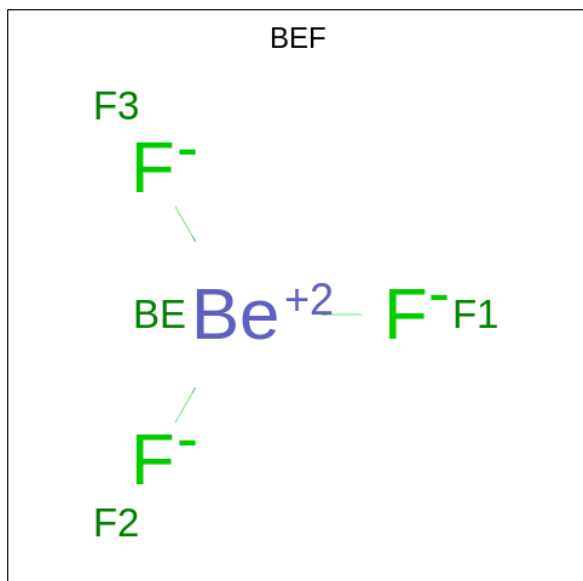


Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

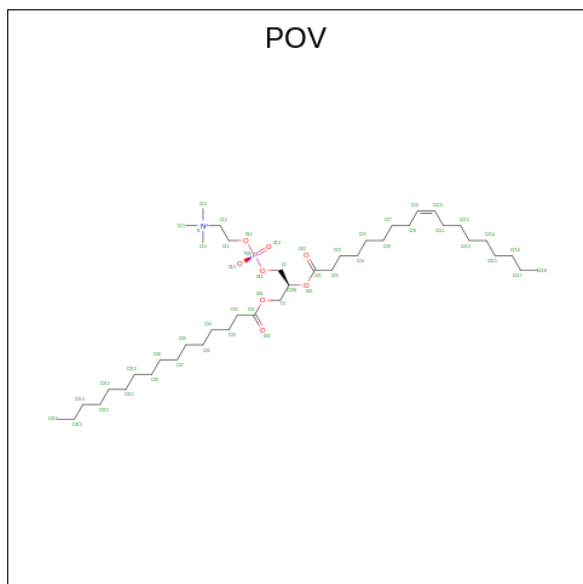
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	

- Molecule 8 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



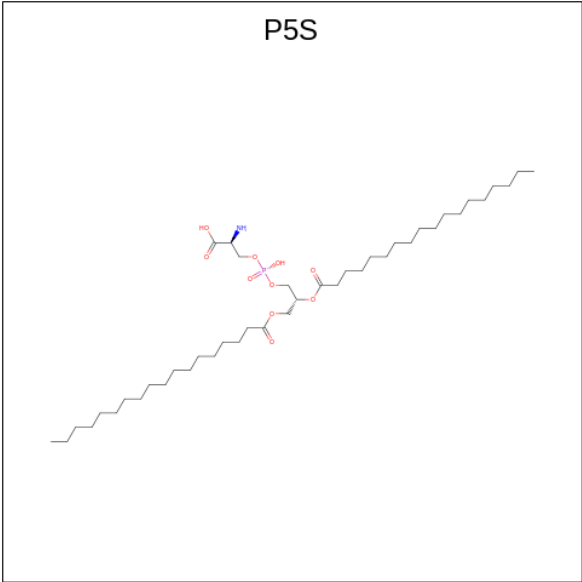
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	Be	F	0
			4	1	3	

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



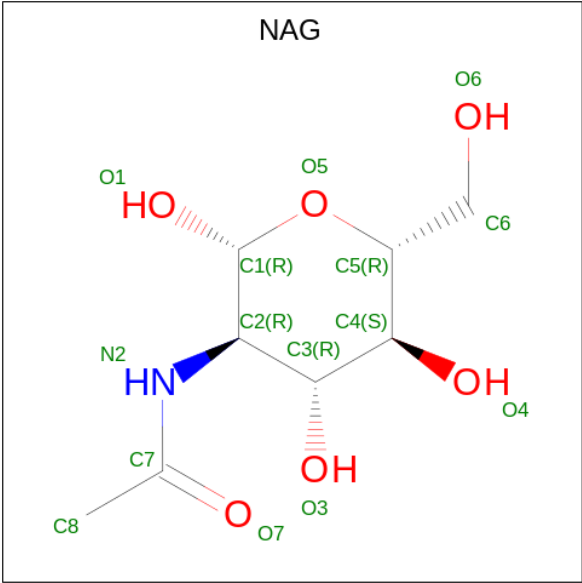
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
9	A	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 10 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).

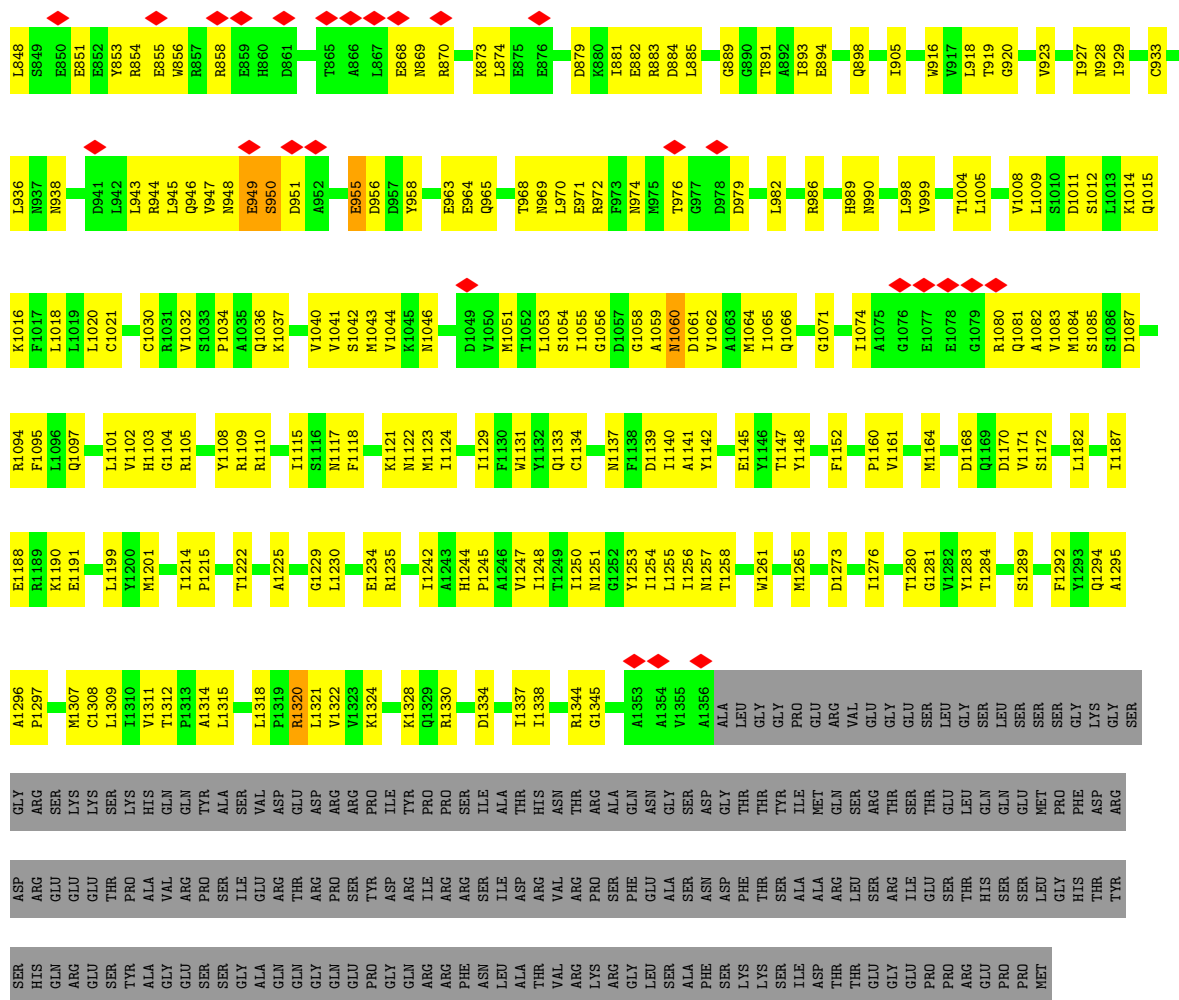


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	40	28	1	10	1	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

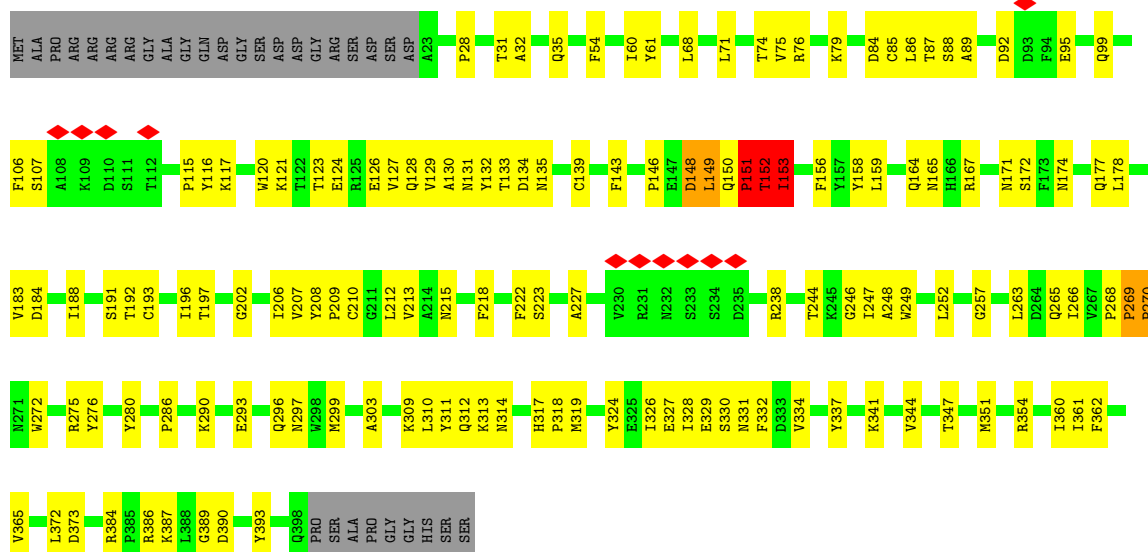


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	14	8	1	5	0
11	B	1	14	8	1	5	0

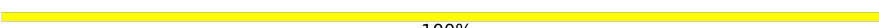


• Molecule 2: Cdc50

Chain B:



- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose

Chain C:  100%

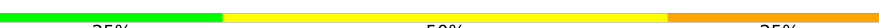
MAN1
MAN2

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

Chain D:  67% 33%

NAG1
NAG2
BNA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  25% 50% 25%

NAG1
NAG2
BNA3
MAN4

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249694	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	299.62, 299.62, 299.62	wwPDB
Map dimensions	284, 284, 284	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, NAG, MG, POV, BMA, MAN, BEF

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	0.37	4/9281 (0.0%)	0.52	4/12589 (0.0%)
2	B	0.38	2/3154 (0.1%)	0.56	4/4300 (0.1%)
All	All	0.37	6/12435 (0.0%)	0.53	8/16889 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1320	ARG	C-O	-7.36	1.14	1.24
1	A	526	TYR	CA-C	-6.34	1.44	1.52
1	A	949	GLU	CA-C	-5.77	1.46	1.53
2	B	153	ILE	C-O	-5.33	1.18	1.24
1	A	524	PHE	CA-C	-5.28	1.45	1.52
2	B	150	GLN	C-O	-5.07	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	GLY	N-CA-C	10.90	127.16	110.91
2	B	151	PRO	CA-C-N	7.23	135.35	121.54
2	B	151	PRO	C-N-CA	7.23	135.35	121.54
2	B	153	ILE	N-CA-CB	-6.79	103.29	110.82
1	A	1320	ARG	CB-CA-C	-6.06	99.03	110.67
1	A	949	GLU	N-CA-C	-6.05	97.56	108.58
1	A	524	PHE	N-CA-C	5.92	119.77	112.54
2	B	151	PRO	N-CA-C	5.61	124.02	112.47

There are no chirality outliers.

There are no planarity outliers.

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	9082	0	9056	338	0
2	B	3061	0	2980	124	0
3	C	22	0	19	5	0
4	D	39	0	34	1	0
5	E	50	0	43	6	0
6	F	28	0	25	1	0
7	A	1	0	0	0	0
8	A	4	0	0	2	0
9	A	66	0	80	2	0
10	A	40	0	46	5	0
11	B	28	0	26	3	0
All	All	12421	0	12309	447	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 18.

All (447) 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:114:ARG:NH2	1:A:476:ILE:CD1	1.79	1.44
1:A:114:ARG:NH2	1:A:476:ILE:HD11	1.45	1.20
3:C:1:MAN:H5	5:E:3:BMA:O6	1.51	1.11
1:A:114:ARG:NH2	1:A:476:ILE:HD12	1.49	1.05
1:A:114:ARG:HH22	1:A:476:ILE:CD1	1.68	1.02
1:A:529:ILE:HG22	1:A:539:ILE:HD13	1.39	0.98
1:A:948:ASN:O	1:A:950:SER:N	2.04	0.90
1:A:114:ARG:HH21	1:A:476:ILE:HD12	1.11	0.90
1:A:1320:ARG:NH2	10:A:2005:P5S:O47	2.03	0.90
1:A:606:ASP:OD1	8:A:2002:BEF:F1	1.81	0.89
1:A:196:ARG:O	1:A:326:PHE:HA	1.74	0.88
1:A:114:ARG:HH22	1:A:476:ILE:HD11	1.27	0.85
2:B:84:ASP:HA	2:B:87:THR:HB	1.58	0.85
2:B:148:ASP:OD1	2:B:148:ASP:N	2.07	0.84
1:A:971:GLU:O	1:A:974:ASN:N	2.10	0.84
1:A:351:ASP:HB2	1:A:463:PHE:HB2	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:GLU:OE1	1:A:956:ASP:N	2.09	0.84
2:B:149:LEU:HB2	2:B:153:ILE:HD11	1.60	0.84
1:A:114:ARG:CZ	1:A:476:ILE:HD11	2.09	0.83
1:A:115:THR:O	1:A:477:THR:HG21	1.78	0.82
1:A:600:ILE:HD12	1:A:1053:LEU:HB2	1.63	0.79
1:A:1248:ILE:HD12	1:A:1309:LEU:HD11	1.65	0.77
1:A:529:ILE:CG2	1:A:539:ILE:HD13	2.15	0.76
1:A:375:THR:HG22	1:A:614:ASN:HD21	1.52	0.75
1:A:1105:ARG:NH2	1:A:1170:ASP:OD2	2.18	0.75
2:B:84:ASP:HB2	2:B:120:TRP:HH2	1.52	0.74
2:B:244:THR:HG22	2:B:312:GLN:HG2	1.69	0.73
2:B:152:THR:HG23	2:B:152:THR:O	1.87	0.73
2:B:269:PRO:HB2	2:B:270:PRO:HD3	1.70	0.73
1:A:846:ARG:NH2	1:A:881:ILE:O	2.23	0.72
1:A:846:ARG:HB2	1:A:885:LEU:HD23	1.72	0.72
1:A:1058:GLY:H	1:A:1061:ASP:HB2	1.55	0.71
2:B:248:ALA:HB1	2:B:252:LEU:HD12	1.72	0.71
3:C:1:MAN:H5	5:E:3:BMA:C6	2.20	0.71
1:A:1256:ILE:O	1:A:1324:LYS:NZ	2.23	0.70
1:A:963:GLU:OE2	1:A:1016:LYS:NZ	2.23	0.70
1:A:1307:MET:HG3	2:B:68:LEU:HD11	1.73	0.70
1:A:597:VAL:HG23	1:A:1104:GLY:HA2	1.72	0.70
1:A:1320:ARG:O	1:A:1320:ARG:HG2	1.92	0.70
2:B:128:GLN:HA	2:B:133:THR:HA	1.72	0.70
1:A:1215:PRO:HB2	1:A:1242:ILE:HG22	1.73	0.70
1:A:753:THR:HG23	1:A:765:ASN:HB3	1.74	0.70
2:B:131:ASN:HB3	11:B:501:NAG:HN2	1.57	0.69
1:A:715:LEU:HD22	1:A:792:VAL:HG11	1.73	0.69
1:A:1289:SER:OG	1:A:1292:PHE:O	2.07	0.69
1:A:854:ARG:HH11	1:A:858:ARG:HH21	1.41	0.68
2:B:314:ASN:OD1	6:F:1:NAG:C7	2.41	0.68
1:A:98:LYS:HB3	1:A:103:HIS:HA	1.74	0.68
1:A:355:LEU:HD21	1:A:389:LEU:HD12	1.74	0.68
1:A:115:THR:OG1	1:A:477:THR:CG2	2.41	0.68
2:B:207:VAL:HG11	2:B:269:PRO:HB3	1.75	0.68
1:A:344:ASN:HD21	1:A:455:GLU:HA	1.59	0.68
1:A:115:THR:O	1:A:477:THR:CG2	2.43	0.67
2:B:115:PRO:HD3	2:B:146:PRO:HG3	1.76	0.67
1:A:345:ASP:OD1	1:A:452:ARG:NH1	2.28	0.67
1:A:1139:ASP:OD2	2:B:167:ARG:NH1	2.26	0.67
1:A:800:LEU:HD11	1:A:845:GLU:HB2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:OG1	1:A:477:THR:HG21	1.94	0.67
1:A:1055:ILE:HD11	1:A:1074:ILE:HD11	1.75	0.66
1:A:193:PRO:HA	1:A:329:ASP:O	1.95	0.66
2:B:223:SER:HB2	2:B:327:GLU:HB2	1.78	0.66
1:A:369:LYS:HD3	1:A:614:ASN:HD22	1.58	0.66
2:B:149:LEU:HB3	2:B:347:THR:HG21	1.77	0.66
1:A:341:ARG:HH21	1:A:458:LEU:HD12	1.61	0.66
1:A:529:ILE:HG22	1:A:539:ILE:CD1	2.20	0.66
3:C:1:MAN:C5	5:E:3:BMA:O6	2.37	0.65
2:B:196:ILE:HD11	2:B:270:PRO:HD3	1.78	0.65
2:B:332:PHE:O	2:B:341:LYS:NZ	2.29	0.65
1:A:1133:GLN:HE22	1:A:1141:ALA:H	1.45	0.65
2:B:165:ASN:ND2	2:B:303:ALA:O	2.30	0.64
2:B:208:TYR:HB3	2:B:209:PRO:HD3	1.78	0.64
1:A:1065:ILE:HG23	1:A:1071:GLY:HA3	1.80	0.64
1:A:342:ILE:HD13	1:A:348:LEU:HD22	1.80	0.63
2:B:387:LYS:HE3	2:B:390:ASP:HB3	1.81	0.63
2:B:202:GLY:O	4:D:2:NAG:O3	2.16	0.63
2:B:132:TYR:OH	2:B:275:ARG:O	2.17	0.62
1:A:945:LEU:HG	1:A:998:LEU:HD11	1.79	0.62
1:A:1059:ALA:O	1:A:1062:VAL:HG12	1.98	0.62
2:B:297:ASN:O	2:B:309:LYS:NZ	2.32	0.62
2:B:164:GLN:HE22	2:B:309:LYS:HE3	1.63	0.62
1:A:1280:THR:O	1:A:1284:THR:HG22	2.00	0.62
1:A:403:GLU:OE1	1:A:419:ARG:NH2	2.33	0.62
1:A:526:TYR:OH	2:B:215:ASN:ND2	2.32	0.62
1:A:1171:VAL:HG23	1:A:1172:SER:H	1.64	0.62
1:A:948:ASN:C	1:A:950:SER:N	2.57	0.62
1:A:607:LYS:HD3	1:A:929:ILE:HG13	1.80	0.62
1:A:1284:THR:OG1	1:A:1295:ALA:N	2.26	0.61
2:B:246:GLY:N	2:B:293:GLU:OE2	2.30	0.61
1:A:85:ARG:HH21	1:A:407:PRO:HD3	1.66	0.61
1:A:557:TYR:O	1:A:561:GLU:HG2	2.00	0.61
1:A:918:LEU:HD13	1:A:1037:LYS:HG2	1.82	0.61
1:A:955:GLU:O	1:A:958:TYR:HB2	2.01	0.60
2:B:268:PRO:HG3	2:B:276:TYR:HB2	1.82	0.60
2:B:76:ARG:NH1	2:B:107:SER:OG	2.35	0.60
1:A:1011:ASP:OD1	1:A:1012:SER:N	2.34	0.60
1:A:593:ILE:HG22	1:A:596:ASP:HB2	1.83	0.60
1:A:543:ALA:HB1	1:A:1140:ILE:HD11	1.82	0.60
1:A:1080:ARG:HB3	1:A:1083:VAL:HB	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:ASN:ND2	1:A:1164:MET:SD	2.75	0.60
1:A:99:ASP:O	1:A:103:HIS:N	2.34	0.60
1:A:658:ILE:HG23	1:A:686:ILE:HD11	1.84	0.60
1:A:186:ASP:OD1	1:A:190:ASN:ND2	2.35	0.60
2:B:129:VAL:HG13	2:B:130:ALA:H	1.67	0.59
1:A:1109:ARG:NH1	1:A:1168:ASP:OD2	2.28	0.59
1:A:507:ALA:HB2	1:A:541:PHE:HB2	1.84	0.59
1:A:1320:ARG:NH1	10:A:2005:P5S:HB	2.18	0.58
2:B:151:PRO:HG3	2:B:317:HIS:O	2.02	0.58
1:A:780:GLU:O	1:A:785:ARG:NH1	2.31	0.58
1:A:971:GLU:O	1:A:974:ASN:CA	2.51	0.58
2:B:183:VAL:HG23	2:B:184:ASP:H	1.67	0.58
2:B:177:GLN:NE2	2:B:208:TYR:O	2.36	0.58
2:B:191:SER:HG	2:B:193:CYS:HG	1.50	0.58
1:A:113:ILE:HG12	1:A:447:ARG:HH22	1.68	0.58
2:B:227:ALA:HB3	2:B:238:ARG:HB2	1.84	0.58
1:A:719:VAL:HG22	1:A:735:ALA:HB2	1.86	0.57
1:A:1009:LEU:HA	1:A:1014:LYS:HG3	1.86	0.57
2:B:247:ILE:HG22	2:B:293:GLU:HB3	1.86	0.57
1:A:600:ILE:HA	1:A:1051:MET:HB2	1.87	0.57
1:A:868:GLU:O	1:A:873:LYS:NZ	2.37	0.57
1:A:1108:TYR:CE2	1:A:1191:GLU:HB2	2.39	0.57
1:A:779:ILE:O	1:A:788:MET:HG2	2.05	0.57
2:B:139:CYS:HB3	2:B:328:ILE:HG13	1.87	0.57
1:A:408:GLN:HG2	1:A:410:ASN:H	1.70	0.57
1:A:617:GLU:HB3	1:A:684:THR:HG21	1.86	0.57
2:B:92:ASP:HA	2:B:121:LYS:HE2	1.87	0.56
1:A:555:SER:HG	1:A:1118:PHE:HZ	1.52	0.56
2:B:331:ASN:ND2	5:E:1:NAG:H82	2.20	0.56
2:B:191:SER:OG	2:B:193:CYS:SG	2.63	0.56
2:B:121:LYS:NZ	2:B:123:THR:OG1	2.38	0.56
1:A:1315:LEU:HD13	2:B:365:VAL:HG22	1.86	0.56
1:A:529:ILE:CD1	2:B:167:ARG:NH2	2.69	0.56
1:A:955:GLU:OE1	1:A:956:ASP:CA	2.53	0.56
2:B:329:GLU:OE2	2:B:331:ASN:ND2	2.37	0.56
1:A:1071:GLY:O	1:A:1087:ASP:N	2.39	0.56
1:A:1170:ASP:OD1	1:A:1170:ASP:N	2.39	0.56
1:A:662:LYS:O	1:A:666:ILE:HG13	2.06	0.56
2:B:131:ASN:HB3	11:B:501:NAG:N2	2.21	0.56
1:A:529:ILE:HG21	1:A:539:ILE:HG21	1.86	0.55
1:A:338:ASP:O	1:A:461:VAL:HG12	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:HA	1:A:486:ARG:HE	1.70	0.55
1:A:514:TRP:HZ3	1:A:527:GLY:O	1.89	0.55
1:A:1337:ILE:HG23	2:B:389:GLY:HA2	1.88	0.55
1:A:90:ASN:O	1:A:93:LEU:N	2.40	0.55
1:A:182:ARG:NH2	1:A:589:LYS:O	2.39	0.55
1:A:476:ILE:HG12	1:A:476:ILE:O	2.06	0.55
1:A:1032:VAL:HG22	1:A:1036:GLN:HB2	1.89	0.55
1:A:369:LYS:HD3	1:A:614:ASN:ND2	2.22	0.55
1:A:821:ASP:OD1	1:A:821:ASP:N	2.39	0.55
1:A:1041:VAL:HG21	1:A:1064:MET:HG3	1.88	0.55
1:A:1308:CYS:HA	1:A:1311:VAL:HG12	1.88	0.55
2:B:266:ILE:HG13	2:B:280:TYR:HD2	1.73	0.54
2:B:269:PRO:HB2	2:B:270:PRO:CD	2.38	0.54
2:B:293:GLU:HA	2:B:296:GLN:HG3	1.89	0.54
1:A:1097:GLN:O	1:A:1101:LEU:HB2	2.07	0.54
1:A:1320:ARG:O	1:A:1320:ARG:CG	2.56	0.54
1:A:95:PRO:HG2	1:A:98:LYS:HE3	1.88	0.54
1:A:788:MET:HE1	1:A:804:LYS:HE2	1.89	0.54
2:B:149:LEU:HD12	2:B:153:ILE:HD13	1.88	0.54
1:A:623:ILE:HG22	1:A:889:GLY:HA3	1.90	0.54
1:A:680:ASP:N	1:A:680:ASP:OD1	2.38	0.54
1:A:949:GLU:O	1:A:949:GLU:HG3	2.08	0.54
2:B:158:TYR:O	2:B:341:LYS:HA	2.07	0.54
1:A:119:THR:OG1	1:A:122:SER:OG	2.25	0.53
1:A:1164:MET:HE1	1:A:1257:ASN:HB3	1.90	0.53
1:A:529:ILE:HG22	1:A:529:ILE:O	2.09	0.53
2:B:188:ILE:HD11	2:B:210:CYS:HB3	1.90	0.53
1:A:647:VAL:HG13	1:A:648:GLU:H	1.73	0.53
1:A:488:LEU:HD11	1:A:556:LEU:HD21	1.91	0.53
1:A:325:ARG:HD2	1:A:326:PHE:H	1.74	0.53
1:A:1281:GLY:HA2	1:A:1296:ALA:HB2	1.89	0.53
1:A:477:THR:O	1:A:477:THR:OG1	2.21	0.53
1:A:579:TYR:HB2	1:A:1095:PHE:HE1	1.74	0.53
1:A:469:LYS:O	1:A:473:ASN:ND2	2.42	0.52
1:A:195:HIS:HB3	1:A:326:PHE:HB3	1.90	0.52
2:B:31:THR:HG22	2:B:32:ALA:H	1.73	0.52
1:A:1037:LYS:O	1:A:1041:VAL:HG23	2.08	0.52
1:A:1060:ASN:N	1:A:1060:ASN:OD1	2.40	0.52
2:B:174:ASN:HB2	2:B:210:CYS:SG	2.49	0.52
2:B:152:THR:O	2:B:152:THR:CG2	2.55	0.52
1:A:1320:ARG:HH22	10:A:2005:P5S:C38	2.14	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:GLU:HG3	1:A:1190:LYS:HG3	1.92	0.52
1:A:607:LYS:HA	1:A:611:LEU:HD12	1.92	0.52
1:A:1042:SER:OG	1:A:1046:ASN:ND2	2.43	0.52
2:B:127:VAL:O	2:B:133:THR:HA	2.10	0.52
1:A:571:ILE:HG12	1:A:1103:HIS:CD2	2.45	0.52
1:A:1182:LEU:HD21	1:A:1338:ILE:HG13	1.93	0.51
1:A:1320:ARG:HH11	10:A:2005:P5S:HB	1.75	0.51
2:B:134:ASP:OD2	2:B:135:ASN:N	2.44	0.51
1:A:148:ILE:HG12	1:A:156:ASN:HD22	1.76	0.51
2:B:153:ILE:HD12	2:B:319:MET:HE3	1.92	0.51
1:A:370:ASN:HD21	1:A:1081:GLN:HG3	1.76	0.51
2:B:86:LEU:HD13	2:B:330:SER:HB2	1.92	0.51
2:B:206:ILE:O	2:B:266:ILE:HA	2.11	0.51
1:A:393:ARG:NH1	1:A:394:ASP:OD2	2.44	0.50
1:A:582:ILE:HG13	1:A:584:GLN:HG3	1.93	0.50
1:A:971:GLU:O	1:A:974:ASN:HA	2.11	0.50
2:B:84:ASP:HB2	2:B:120:TRP:CH2	2.40	0.50
1:A:1056:GLY:HA3	1:A:1061:ASP:HB3	1.93	0.50
1:A:111:ASN:HD22	1:A:334:LEU:HB2	1.76	0.50
1:A:604:PHE:HD1	1:A:918:LEU:HD21	1.75	0.50
1:A:1244:HIS:HB2	1:A:1245:PRO:HD3	1.92	0.50
2:B:263:LEU:HD13	2:B:286:PRO:HD3	1.93	0.50
1:A:856:TRP:CG	1:A:881:ILE:HD12	2.46	0.50
1:A:1133:GLN:NE2	1:A:1140:ILE:HA	2.26	0.50
1:A:197:LEU:HD23	1:A:339:PHE:HB2	1.94	0.50
1:A:944:ARG:HD2	1:A:999:VAL:O	2.11	0.50
2:B:275:ARG:HH21	2:B:276:TYR:HE1	1.59	0.50
1:A:623:ILE:HG21	1:A:709:PHE:CG	2.47	0.50
1:A:1330:ARG:HG2	2:B:384:ARG:HH22	1.77	0.50
1:A:1102:VAL:HG12	1:A:1103:HIS:ND1	2.27	0.49
1:A:727:ASP:O	1:A:728:PRO:C	2.55	0.49
1:A:1054:SER:HB2	1:A:1064:MET:HG2	1.94	0.49
1:A:114:ARG:NH1	1:A:116:ALA:O	2.44	0.49
1:A:776:LEU:HB3	1:A:853:TYR:CZ	2.46	0.49
1:A:646:ASN:ND2	1:A:650:GLU:HG2	2.28	0.49
1:A:666:ILE:O	1:A:670:ARG:HG2	2.12	0.49
1:A:715:LEU:HD21	1:A:773:PHE:CD2	2.47	0.49
1:A:1253:TYR:CZ	1:A:1320:ARG:HD2	2.47	0.49
1:A:1320:ARG:NH2	10:A:2005:P5S:C38	2.74	0.49
2:B:85:CYS:HA	2:B:89:ALA:HB2	1.95	0.49
1:A:618:PHE:HE1	1:A:891:THR:HB	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:PRO:HG3	2:B:317:HIS:C	2.37	0.49
2:B:222:PHE:CD1	2:B:328:ILE:HG22	2.47	0.49
1:A:606:ASP:HB3	1:A:610:THR:HG23	1.95	0.49
1:A:618:PHE:HD2	1:A:685:PHE:HB2	1.77	0.49
1:A:650:GLU:HA	1:A:653:VAL:HG12	1.93	0.49
1:A:344:ASN:ND2	1:A:455:GLU:HA	2.27	0.49
1:A:813:ARG:NE	1:A:882:GLU:OE2	2.46	0.49
1:A:951:ASP:OD2	1:A:951:ASP:N	2.45	0.49
2:B:171:ASN:O	2:B:192:THR:OG1	2.28	0.49
1:A:578:TYR:OH	1:A:583:ASP:OD1	2.28	0.48
2:B:151:PRO:HD3	2:B:318:PRO:HB3	1.94	0.48
2:B:265:GLN:N	2:B:265:GLN:OE1	2.46	0.48
1:A:562:ILE:HG12	9:A:2004:POV:H38A	1.95	0.48
2:B:386:ARG:O	2:B:386:ARG:HD3	2.13	0.48
1:A:1094:ARG:O	1:A:1097:GLN:HG2	2.13	0.48
1:A:510:ASN:ND2	1:A:540:THR:OG1	2.47	0.48
1:A:919:THR:OG1	1:A:920:GLY:N	2.46	0.48
9:A:2003:POV:H25	9:A:2003:POV:H32	1.95	0.48
1:A:136:ALA:HB2	1:A:492:VAL:HG11	1.95	0.48
1:A:851:GLU:CD	1:A:851:GLU:H	2.22	0.48
2:B:71:LEU:HD13	2:B:351:MET:HB2	1.95	0.48
1:A:807:ASP:OD1	1:A:807:ASP:N	2.47	0.48
1:A:869:ASN:HB3	1:A:873:LYS:HE3	1.95	0.48
1:A:447:ARG:HB3	1:A:470:ILE:HG21	1.96	0.48
1:A:602:TYR:HB3	1:A:604:PHE:CE2	2.49	0.48
1:A:623:ILE:HG21	1:A:709:PHE:CD2	2.48	0.48
1:A:821:ASP:HA	1:A:824:ARG:HG2	1.96	0.48
1:A:1344:ARG:HG3	1:A:1345:GLY:H	1.78	0.48
1:A:156:ASN:OD1	1:A:156:ASN:N	2.40	0.48
1:A:613:GLN:HE21	1:A:898:GLN:HA	1.78	0.48
1:A:1054:SER:OG	1:A:1065:ILE:HA	2.13	0.48
2:B:257:GLY:HA2	2:B:290:LYS:HE3	1.95	0.48
1:A:480:LYS:HB2	1:A:593:ILE:HD11	1.96	0.47
1:A:548:PHE:HE1	1:A:1129:ILE:HG22	1.79	0.47
1:A:119:THR:HG1	1:A:122:SER:HG	1.62	0.47
1:A:352:ILE:HG12	1:A:461:VAL:HA	1.97	0.47
2:B:31:THR:HG22	2:B:32:ALA:N	2.29	0.47
1:A:342:ILE:O	1:A:456:TRP:HA	2.15	0.47
1:A:969:ASN:O	1:A:972:ARG:HG2	2.15	0.47
1:A:1123:MET:HE3	1:A:1201:MET:HG2	1.96	0.47
1:A:1255:LEU:O	1:A:1258:THR:HG22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:LYS:O	1:A:1328:LYS:HG2	2.14	0.47
1:A:155:VAL:HG23	1:A:157:PRO:HD2	1.96	0.47
1:A:617:GLU:O	1:A:893:ILE:HG23	2.14	0.47
1:A:1034:PRO:HB3	1:A:1060:ASN:HA	1.95	0.47
1:A:1148:TYR:O	1:A:1152:PHE:HB2	2.14	0.47
1:A:1214:ILE:HD12	2:B:361:ILE:HD13	1.97	0.47
2:B:60:ILE:HG23	2:B:61:TYR:CD1	2.48	0.47
2:B:71:LEU:O	2:B:74:THR:HG22	2.14	0.47
2:B:149:LEU:HD13	2:B:347:THR:CG2	2.44	0.47
1:A:1018:LEU:HD21	1:A:1043:MET:HG2	1.96	0.47
1:A:1230:LEU:HD22	2:B:249:TRP:CD2	2.49	0.47
1:A:1321:LEU:HD22	2:B:54:PHE:HE2	1.80	0.47
1:A:1160:PRO:HG2	1:A:1251:ASN:ND2	2.30	0.47
1:A:1247:VAL:HG21	1:A:1276:ILE:HD12	1.96	0.47
2:B:268:PRO:HB2	2:B:272:TRP:HB2	1.96	0.47
1:A:618:PHE:CD2	1:A:746:THR:HG21	2.50	0.46
1:A:943:LEU:O	1:A:998:LEU:HD12	2.16	0.46
1:A:525:GLU:HG3	2:B:212:LEU:HD11	1.96	0.46
1:A:607:LYS:HB3	1:A:919:THR:HB	1.97	0.46
1:A:905:ILE:HD12	1:A:933:CYS:HB3	1.97	0.46
1:A:982:LEU:O	1:A:986:ARG:HG2	2.16	0.46
1:A:326:PHE:HD2	1:A:392:ALA:HB1	1.80	0.46
1:A:989:HIS:O	1:A:990:ASN:ND2	2.49	0.46
1:A:1257:ASN:OD1	1:A:1320:ARG:NE	2.49	0.46
1:A:111:ASN:ND2	1:A:334:LEU:HB2	2.31	0.46
1:A:1222:THR:HG21	1:A:1225:ALA:HB2	1.98	0.46
1:A:159:LEU:HD12	1:A:159:LEU:H	1.80	0.46
1:A:474:ALA:HB1	1:A:1066:GLN:OE1	2.16	0.46
1:A:348:LEU:HG	1:A:449:CYS:O	2.16	0.46
1:A:1152:PHE:HZ	1:A:1250:ILE:HD12	1.80	0.46
1:A:136:ALA:HB3	1:A:557:TYR:CE2	2.51	0.45
1:A:1133:GLN:NE2	1:A:1141:ALA:H	2.12	0.45
2:B:183:VAL:HG23	2:B:184:ASP:N	2.30	0.45
1:A:947:VAL:HG23	1:A:947:VAL:O	2.17	0.45
1:A:1258:THR:HG21	1:A:1265:MET:SD	2.57	0.45
1:A:1062:VAL:HG23	1:A:1085:SER:HB2	1.98	0.45
1:A:1308:CYS:O	1:A:1312:THR:HG23	2.15	0.45
1:A:848:LEU:HD23	1:A:853:TYR:HB2	1.98	0.45
2:B:143:PHE:HE1	2:B:326:ILE:HG13	1.81	0.45
1:A:870:ARG:HG2	1:A:874:LEU:HD13	1.99	0.45
1:A:1322:VAL:HG21	2:B:372:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:GLU:OE1	2:B:135:ASN:HB3	2.17	0.45
1:A:526:TYR:HD1	3:C:2:MAN:HO3	1.58	0.45
1:A:955:GLU:CD	1:A:955:GLU:C	2.85	0.45
1:A:788:MET:HE3	1:A:788:MET:HB3	1.68	0.45
2:B:99:GLN:HE22	2:B:116:TYR:HB3	1.82	0.45
1:A:603:ILE:HG23	1:A:1053:LEU:HD22	1.98	0.45
1:A:856:TRP:CD1	1:A:881:ILE:HB	2.52	0.45
1:A:100:GLU:HG2	1:A:101:GLU:OE2	2.16	0.45
1:A:786:LYS:HB2	1:A:809:VAL:HG21	1.98	0.45
2:B:246:GLY:O	2:B:313:LYS:NZ	2.41	0.45
1:A:499:LEU:O	1:A:502:MET:HG2	2.17	0.44
1:A:1337:ILE:CD1	2:B:393:TYR:HB2	2.47	0.44
1:A:405:GLU:HB3	1:A:406:PRO:HD2	1.99	0.44
1:A:405:GLU:HG3	1:A:415:ASN:OD1	2.17	0.44
1:A:846:ARG:HG3	1:A:884:ASP:O	2.18	0.44
1:A:855:GLU:O	1:A:858:ARG:HG2	2.17	0.44
1:A:1273:ASP:O	1:A:1276:ILE:HG22	2.17	0.44
2:B:156:PHE:HB2	2:B:344:VAL:HG22	1.99	0.44
2:B:311:TYR:CD2	2:B:312:GLN:HG3	2.52	0.44
1:A:1142:TYR:O	1:A:1235:ARG:NH1	2.50	0.44
1:A:686:ILE:HG13	1:A:686:ILE:O	2.16	0.44
1:A:1139:ASP:OD1	2:B:167:ARG:N	2.29	0.44
1:A:365:TYR:HB3	1:A:377:LEU:HB3	1.98	0.44
1:A:1161:VAL:HB	1:A:1254:ILE:HD13	1.98	0.44
5:E:1:NAG:H61	5:E:2:NAG:HN2	1.82	0.44
1:A:127:ASN:HD21	1:A:172:ALA:HA	1.82	0.44
1:A:601:GLU:HB3	1:A:1187:ILE:HD12	2.00	0.44
1:A:1131:TRP:O	1:A:1134:CYS:HB3	2.17	0.44
1:A:1234:GLU:HG2	1:A:1235:ARG:N	2.33	0.44
1:A:787:ARG:NH2	1:A:882:GLU:OE1	2.51	0.44
1:A:181:ARG:O	1:A:184:ILE:HG22	2.18	0.44
1:A:560:LEU:HD21	1:A:1115:ILE:HG22	2.00	0.44
2:B:331:ASN:HD21	5:E:1:NAG:H82	1.81	0.44
2:B:79:LYS:HB2	2:B:344:VAL:HG12	2.00	0.43
2:B:172:SER:O	2:B:172:SER:OG	2.32	0.43
1:A:524:PHE:HE2	2:B:337:TYR:CE1	2.35	0.43
2:B:227:ALA:HB2	2:B:324:TYR:CE1	2.53	0.43
1:A:103:HIS:CG	1:A:104:PRO:HD3	2.53	0.43
1:A:1005:LEU:HD21	1:A:1040:VAL:HG21	2.01	0.43
2:B:76:ARG:HH12	2:B:107:SER:CB	2.32	0.43
1:A:553:PRO:HB3	1:A:1122:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLU:OE1	1:A:650:GLU:N	2.50	0.43
1:A:970:LEU:HB3	1:A:976:THR:HA	2.01	0.43
2:B:124:GLU:OE2	2:B:135:ASN:HB2	2.18	0.43
1:A:482:ALA:C	1:A:484:ILE:H	2.27	0.43
1:A:1133:GLN:NE2	1:A:1133:GLN:HA	2.34	0.43
2:B:129:VAL:HG13	2:B:130:ALA:N	2.32	0.43
2:B:149:LEU:HD13	2:B:347:THR:HG23	2.00	0.43
1:A:608:THR:N	8:A:2002:BEF:F2	2.38	0.43
1:A:1145:GLU:O	1:A:1147:THR:N	2.52	0.43
1:A:103:HIS:ND1	1:A:104:PRO:HD3	2.34	0.43
1:A:835:VAL:HG11	1:A:938:ASN:HD21	1.84	0.43
1:A:923:VAL:HA	1:A:1030:CYS:SG	2.59	0.43
2:B:75:VAL:HG23	2:B:354:ARG:HB2	2.01	0.43
2:B:95:GLU:O	2:B:120:TRP:HD1	2.02	0.43
1:A:946:GLN:O	1:A:965:GLN:NE2	2.38	0.43
2:B:131:ASN:CB	11:B:501:NAG:HN2	2.30	0.43
1:A:415:ASN:OD1	1:A:415:ASN:N	2.52	0.43
1:A:1214:ILE:HB	1:A:1215:PRO:HD3	2.01	0.43
1:A:610:THR:OG1	1:A:611:LEU:N	2.51	0.42
1:A:1296:ALA:HB3	1:A:1297:PRO:HD3	2.00	0.42
2:B:334:VAL:HG23	2:B:337:TYR:OH	2.19	0.42
1:A:462:VAL:HG12	1:A:463:PHE:CD2	2.55	0.42
1:A:919:THR:O	1:A:1032:VAL:HG12	2.19	0.42
1:A:1004:THR:O	1:A:1008:VAL:HG22	2.20	0.42
1:A:1337:ILE:HD11	2:B:393:TYR:HB2	2.02	0.42
1:A:916:TRP:CH2	1:A:1021:CYS:HB3	2.54	0.42
1:A:1311:VAL:HB	2:B:362:PHE:CZ	2.54	0.42
2:B:84:ASP:O	2:B:88:SER:N	2.40	0.42
2:B:159:LEU:HD21	2:B:218:PHE:CE1	2.54	0.42
1:A:945:LEU:HD11	1:A:1020:LEU:HD23	2.01	0.42
2:B:268:PRO:CB	2:B:272:TRP:HB2	2.48	0.42
1:A:374:GLU:HB2	1:A:378:LYS:NZ	2.34	0.42
1:A:702:GLN:O	1:A:706:THR:HG23	2.20	0.42
1:A:462:VAL:HG12	1:A:463:PHE:HD2	1.83	0.42
1:A:192:ALA:HA	1:A:193:PRO:HD3	1.91	0.42
1:A:353:ILE:HG12	1:A:462:VAL:HG21	2.00	0.42
1:A:533:PRO:HA	1:A:536:THR:HG22	2.02	0.42
1:A:1080:ARG:O	1:A:1084:MET:HG3	2.20	0.42
2:B:106:PHE:HE1	2:B:149:LEU:HD21	1.85	0.42
1:A:1121:LYS:O	1:A:1124:ILE:HG22	2.19	0.42
1:A:364:CYS:HA	1:A:454:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ILE:HG23	1:A:686:ILE:CD1	2.49	0.42
1:A:839:ARG:HG2	1:A:928:ASN:ND2	2.33	0.42
1:A:1261:TRP:CD1	1:A:1261:TRP:N	2.88	0.42
1:A:1314:ALA:O	1:A:1318:LEU:HB2	2.20	0.42
1:A:93:LEU:HA	1:A:94:PRO:HD3	1.90	0.42
2:B:178:LEU:HD11	2:B:299:MET:HE1	2.02	0.42
1:A:927:ILE:HG23	1:A:936:LEU:HD13	2.02	0.41
1:A:1199:LEU:HD23	1:A:1199:LEU:HA	1.86	0.41
1:A:1253:TYR:HA	1:A:1256:ILE:HG22	2.00	0.41
1:A:1148:TYR:OH	1:A:1280:THR:OG1	2.35	0.41
1:A:979:ASP:HA	1:A:1015:GLN:NE2	2.35	0.41
1:A:529:ILE:CG2	1:A:529:ILE:O	2.68	0.41
1:A:786:LYS:HE2	1:A:786:LYS:HB3	1.92	0.41
1:A:814:LEU:HD23	1:A:814:LEU:HA	1.92	0.41
1:A:851:GLU:HA	1:A:854:ARG:HE	1.85	0.41
1:A:1229:GLY:O	1:A:1230:LEU:HD12	2.20	0.41
1:A:1253:TYR:OH	1:A:1320:ARG:HD2	2.21	0.41
1:A:358:SER:OG	1:A:359:ASP:N	2.54	0.41
1:A:575:VAL:HG12	2:B:28:PRO:HG2	2.03	0.41
1:A:838:LEU:HD22	1:A:894:GLU:HB2	2.03	0.41
2:B:54:PHE:HB3	2:B:373:ASP:HB2	2.01	0.41
1:A:555:SER:OG	1:A:1118:PHE:HZ	2.02	0.41
1:A:1334:ASP:O	1:A:1338:ILE:HG12	2.20	0.41
3:C:1:MAN:H3	3:C:2:MAN:H2	1.90	0.41
1:A:357:THR:OG1	1:A:358:SER:N	2.54	0.41
1:A:647:VAL:HG13	1:A:648:GLU:N	2.34	0.41
1:A:147:VAL:HG23	1:A:156:ASN:HB3	2.03	0.41
1:A:185:LEU:HD21	1:A:589:LYS:HE3	2.03	0.41
1:A:413:LYS:HA	1:A:413:LYS:HD2	1.89	0.41
1:A:683:MET:HE2	1:A:683:MET:HB3	1.94	0.41
1:A:715:LEU:HD13	1:A:802:PHE:CE2	2.56	0.41
1:A:1040:VAL:O	1:A:1044:VAL:HG23	2.21	0.41
1:A:1283:TYR:CZ	1:A:1289:SER:HB3	2.55	0.41
1:A:1284:THR:O	1:A:1294:GLN:HA	2.21	0.41
2:B:188:ILE:O	2:B:197:THR:OG1	2.18	0.41
1:A:84:PRO:HB3	1:A:406:PRO:HD3	2.03	0.41
1:A:529:ILE:CD1	2:B:167:ARG:HH21	2.33	0.41
1:A:879:ASP:HB3	1:A:883:ARG:HH21	1.86	0.41
1:A:1034:PRO:HG3	1:A:1060:ASN:HB3	2.02	0.41
2:B:117:LYS:HE2	2:B:117:LYS:HB3	1.87	0.41
1:A:480:LYS:HB2	1:A:593:ILE:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:VAL:HG22	2:B:35:GLN:OE1	2.21	0.40
1:A:476:ILE:O	1:A:476:ILE:CG1	2.69	0.40
1:A:529:ILE:HD13	2:B:167:ARG:HH21	1.86	0.40
1:A:785:ARG:HD3	1:A:787:ARG:NH1	2.37	0.40
1:A:1110:ARG:NE	1:A:1168:ASP:O	2.37	0.40
1:A:547:VAL:HG22	1:A:1142:TYR:CE1	2.57	0.40
1:A:591:TRP:CD1	1:A:591:TRP:N	2.88	0.40
1:A:964:GLU:O	1:A:968:THR:HG22	2.22	0.40
2:B:172:SER:O	2:B:213:VAL:HG12	2.21	0.40
1:A:477:THR:N	1:A:478:PRO:CD	2.85	0.40
1:A:719:VAL:HG11	1:A:733:PHE:HB3	2.03	0.40
1:A:918:LEU:O	1:A:918:LEU:HD12	2.22	0.40
1:A:1137:ASN:C	1:A:1139:ASP:H	2.30	0.40
1:A:1171:VAL:HG23	1:A:1172:SER:N	2.32	0.40
2:B:156:PHE:CE1	2:B:310:LEU:HD13	2.56	0.40
1:A:618:PHE:CE1	1:A:891:THR:HB	2.53	0.40
1:A:683:MET:HE3	1:A:686:ILE:HG22	2.03	0.40
1:A:743:LEU:HG	1:A:893:ILE:HD11	2.03	0.40
1:A:1058:GLY:O	1:A:1082:ALA:HB2	2.21	0.40
2:B:326:ILE:HG22	2:B:328:ILE:HG23	2.03	0.40
2:B:360:ILE:HD13	2:B:360:ILE:HA	1.93	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	1132/1555 (73%)	1026 (91%)	106 (9%)	0	100	100
2	B	374/407 (92%)	329 (88%)	42 (11%)	3 (1%)	16	49
All	All	1506/1962 (77%)	1355 (90%)	148 (10%)	3 (0%)	44	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	PRO
2	B	152	THR
2	B	269	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	973/1329 (73%)	965 (99%)	8 (1%)	73	76
2	B	335/357 (94%)	330 (98%)	5 (2%)	57	71
All	All	1308/1686 (78%)	1295 (99%)	13 (1%)	65	75

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

Mol	Chain	Res	Type
1	A	156	ASN
1	A	476	ILE
1	A	478	PRO
1	A	592	ASN
1	A	658	ILE
1	A	950	SER
1	A	955	GLU
1	A	1060	ASN
2	B	148	ASP
2	B	149	LEU
2	B	151	PRO
2	B	152	THR
2	B	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	ASN
1	A	344	ASN
1	A	370	ASN
1	A	408	GLN
1	A	450	HIS
1	A	473	ASN
1	A	510	ASN
1	A	613	GLN
1	A	614	ASN
1	A	646	ASN
1	A	698	ASN
1	A	704	GLN
1	A	717	HIS
1	A	724	GLN
1	A	928	ASN
1	A	938	ASN
1	A	974	ASN
1	A	990	ASN
1	A	1023	GLN
1	A	1046	ASN
1	A	1133	GLN
1	A	1251	ASN
2	B	164	GLN
2	B	171	ASN
2	B	271	ASN
2	B	296	GLN
2	B	397	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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	MAN	C	1	3	11,11,12	0.24	0	15,15,17	0.57	0
3	MAN	C	2	3	11,11,12	0.24	0	15,15,17	0.58	0
4	NAG	D	1	2,4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.56	0
4	BMA	D	3	4	11,11,12	0.55	0	15,15,17	0.92	0
5	NAG	E	1	2,5	14,14,15	0.22	0	17,19,21	0.94	1 (5%)
5	NAG	E	2	5	14,14,15	0.26	0	17,19,21	0.42	0
5	BMA	E	3	5	11,11,12	0.22	0	15,15,17	0.63	0
5	MAN	E	4	5	11,11,12	0.24	0	15,15,17	0.59	0
6	NAG	F	1	6,2	14,14,15	0.28	0	17,19,21	0.57	0
6	NAG	F	2	6	14,14,15	0.28	0	17,19,21	0.59	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	MAN	C	1	3	-	0/2/19/22	0/1/1/1
3	MAN	C	2	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	3.20	116.53	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

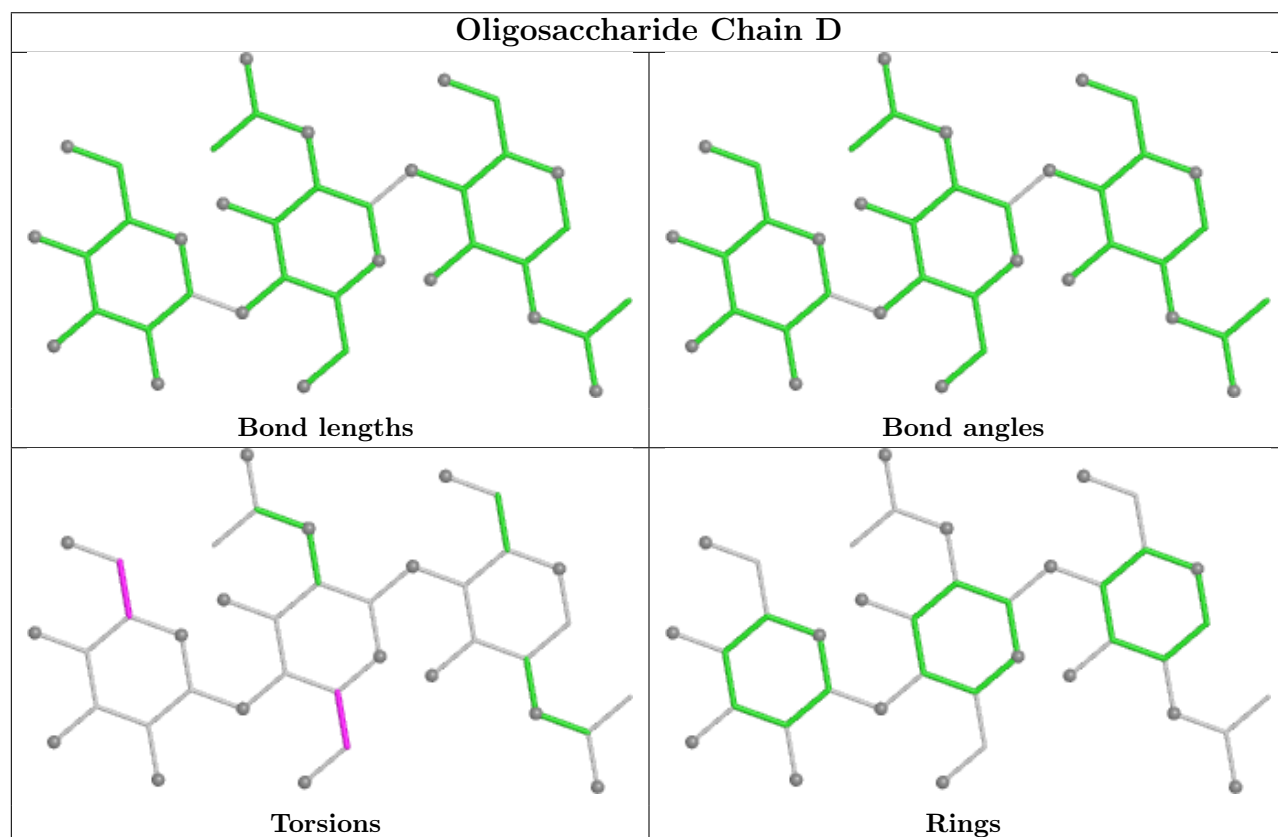
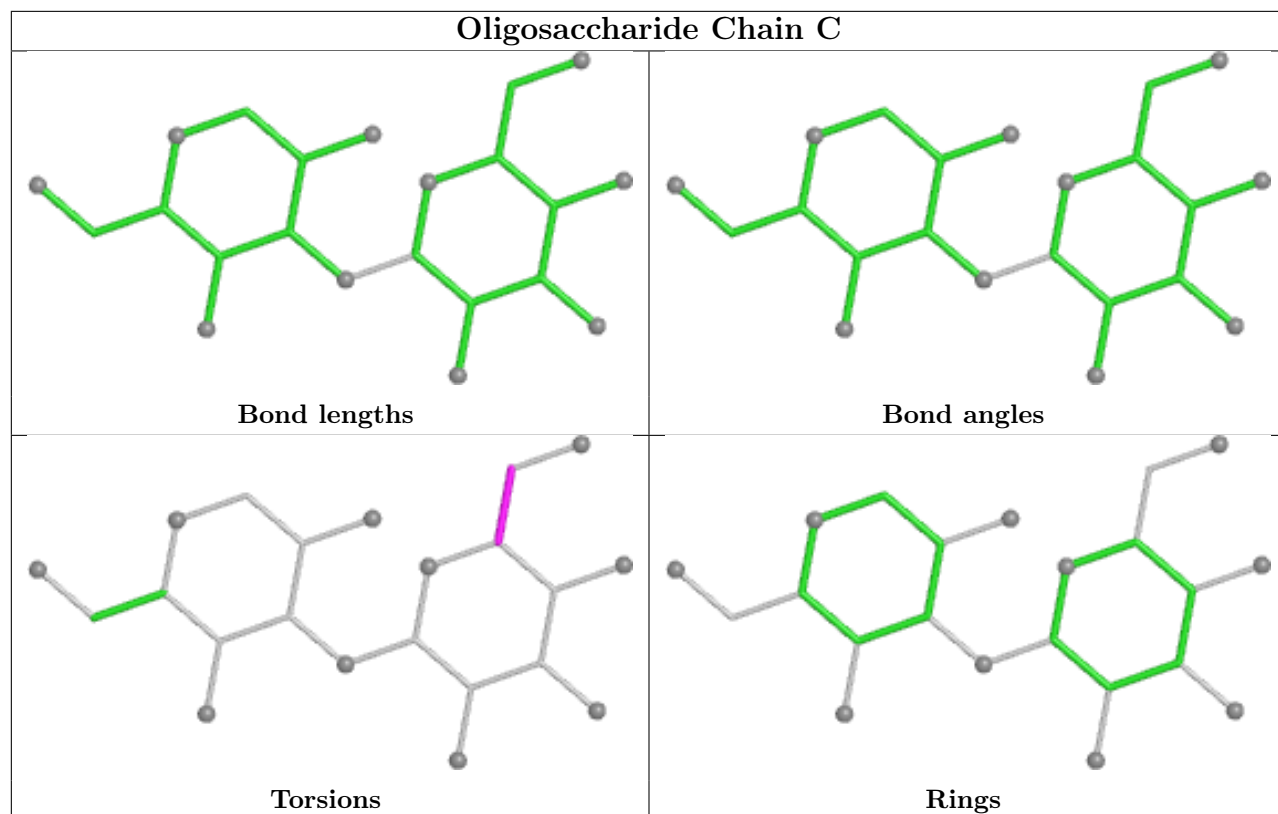
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
3	C	2	MAN	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

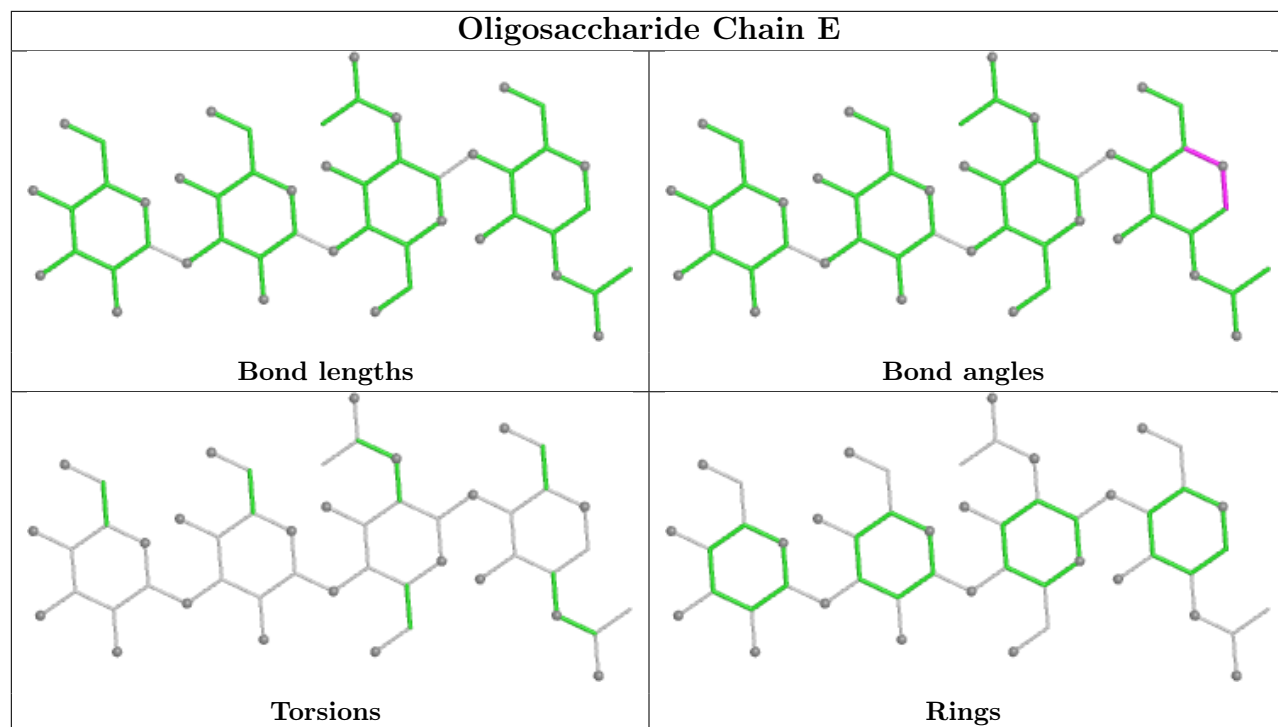
There are no ring outliers.

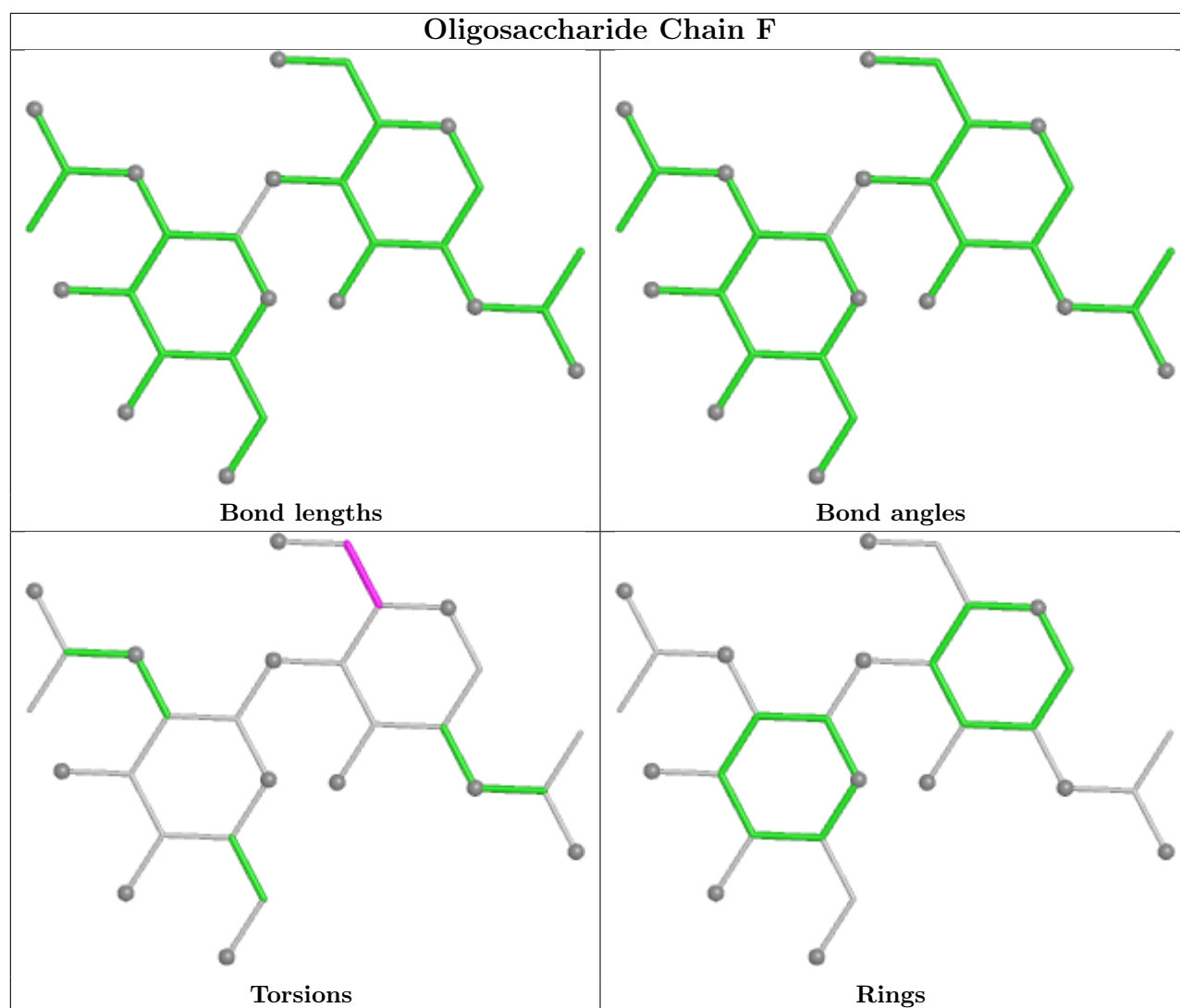
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	MAN	4	0
6	F	1	NAG	1	0
5	E	1	NAG	3	0
5	E	2	NAG	1	0
4	D	2	NAG	1	0
5	E	3	BMA	3	0
3	C	2	MAN	2	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, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	BEF	A	2002	-	0,3,3	-	-	-		
11	NAG	B	509	2	14,14,15	0.24	0	17,19,21	0.36	0
9	POV	A	2003	-	32,32,51	1.18	2 (6%)	38,40,59	1.20	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	B	501	2	14,14,15	0.58	0	17,19,21	0.67	1 (5%)
10	P5S	A	2005	-	38,39,53	1.06	2 (5%)	42,46,60	1.24	5 (11%)
9	POV	A	2004	-	32,32,51	1.18	2 (6%)	38,40,59	1.10	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	509	2	-	0/6/23/26	0/1/1/1
9	POV	A	2003	-	-	12/36/36/55	-
11	NAG	B	501	2	-	3/6/23/26	0/1/1/1
10	P5S	A	2005	-	-	13/45/45/59	-
9	POV	A	2004	-	-	9/36/36/55	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2003	POV	O31-C31	4.28	1.45	1.33
10	A	2005	P5S	O19-C17	4.17	1.45	1.33
10	A	2005	P5S	O37-C38	4.14	1.46	1.34
9	A	2004	POV	O31-C31	4.12	1.45	1.33
9	A	2004	POV	O21-C21	4.02	1.45	1.34
9	A	2003	POV	O21-C21	3.84	1.45	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2005	P5S	O37-C38-C39	4.11	120.37	111.50
9	A	2004	POV	O21-C21-C22	3.91	119.93	111.50
9	A	2003	POV	O21-C21-C22	3.65	119.37	111.50
9	A	2003	POV	O31-C31-C32	2.78	120.64	111.91
10	A	2005	P5S	OG-CB-CA	2.56	110.29	108.06
10	A	2005	P5S	O19-C17-C20	2.52	119.81	111.91
9	A	2003	POV	C2-O21-C21	-2.42	111.82	117.79
9	A	2004	POV	O31-C31-C32	2.39	119.42	111.91
11	B	501	NAG	C1-O5-C5	2.28	115.28	112.19
10	A	2005	P5S	OXT-C-O	-2.22	119.06	124.09
10	A	2005	P5S	OXT-C-CA	2.08	120.47	113.38

There are no chirality outliers.

All (37) torsion outliers are listed below:

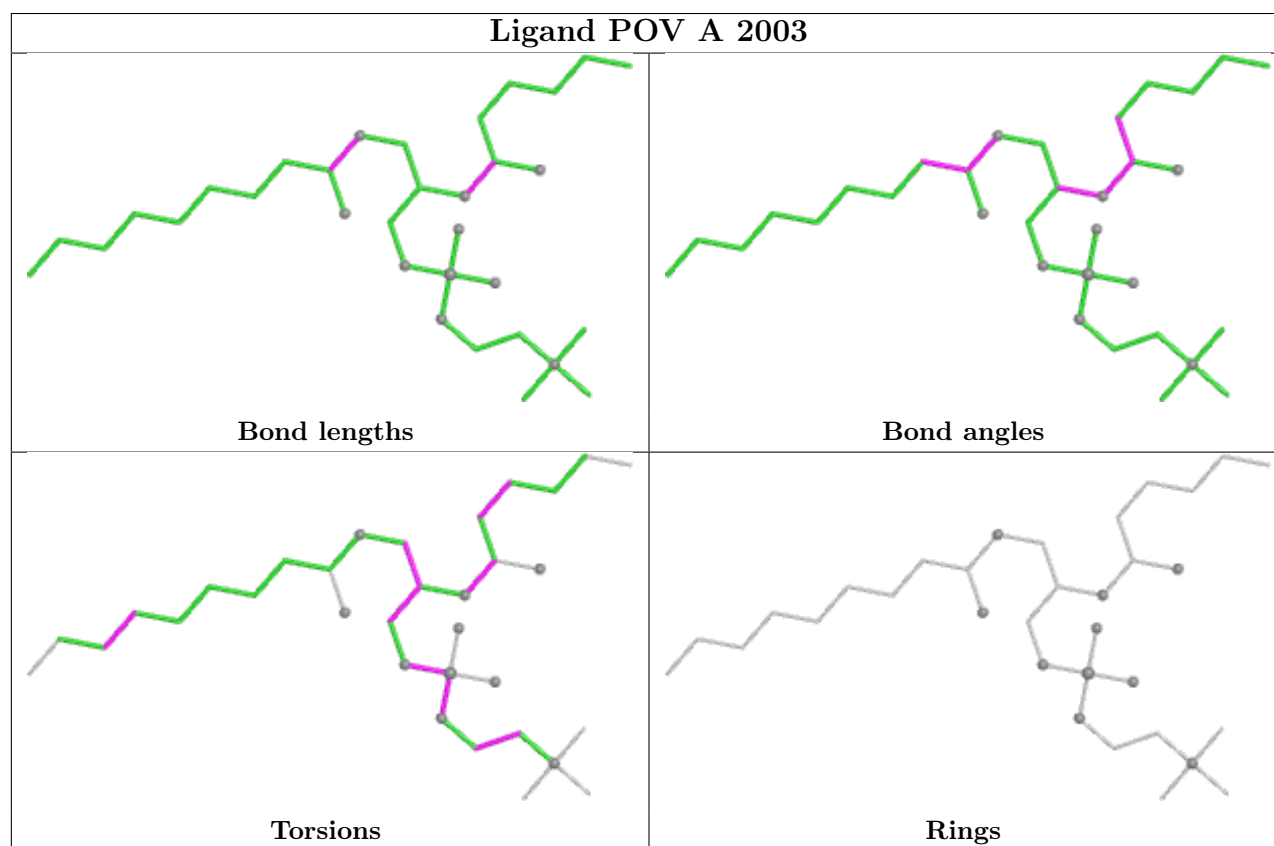
Mol	Chain	Res	Type	Atoms
9	A	2003	POV	C11-O12-P-O14
9	A	2003	POV	C22-C21-O21-C2
9	A	2004	POV	C1-O11-P-O12
9	A	2004	POV	C11-O12-P-O13
9	A	2004	POV	O12-C11-C12-N
9	A	2003	POV	O22-C21-O21-C2
11	B	501	NAG	O5-C5-C6-O6
11	B	501	NAG	C4-C5-C6-O6
10	A	2005	P5S	OXT-C-CA-N
9	A	2004	POV	C11-O12-P-O11
9	A	2003	POV	O21-C2-C3-O31
10	A	2005	P5S	C39-C40-C41-C42
10	A	2005	P5S	C38-C39-C40-C41
9	A	2003	POV	C1-C2-C3-O31
9	A	2003	POV	C21-C22-C23-C24
9	A	2003	POV	O11-C1-C2-O21
9	A	2003	POV	O11-C1-C2-C3
10	A	2005	P5S	O37-C38-C39-C40
9	A	2003	POV	C1-O11-P-O12
9	A	2004	POV	O21-C2-C3-O31
10	A	2005	P5S	O-C-CA-N
9	A	2004	POV	O11-C1-C2-O21
10	A	2005	P5S	C3-O16-P12-O13
10	A	2005	P5S	C41-C42-C43-C44
9	A	2003	POV	O12-C11-C12-N
10	A	2005	P5S	C43-C44-C45-C46
10	A	2005	P5S	C46-C48-C49-C50
9	A	2004	POV	O11-C1-C2-C3
9	A	2003	POV	C35-C36-C37-C38
9	A	2003	POV	C11-O12-P-O11
10	A	2005	P5S	CB-OG-P12-O16
11	B	501	NAG	C1-C2-N2-C7
10	A	2005	P5S	OXT-C-CA-CB
10	A	2005	P5S	O47-C38-C39-C40
9	A	2004	POV	C1-C2-C3-O31
10	A	2005	P5S	O-C-CA-CB
9	A	2004	POV	C1-O11-P-O13

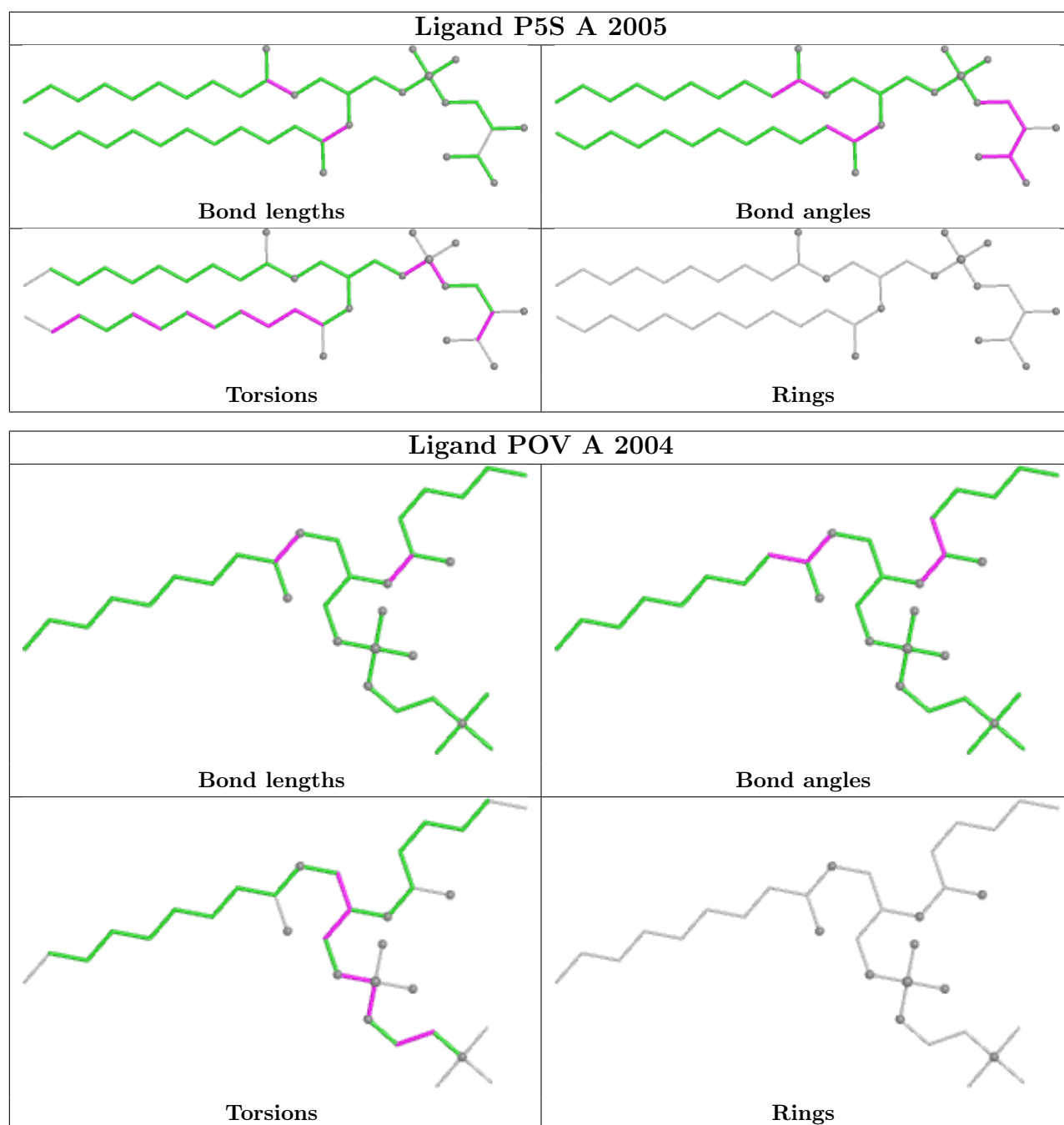
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2002	BEF	2	0
9	A	2003	POV	1	0
11	B	501	NAG	3	0
10	A	2005	P5S	5	0
9	A	2004	POV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

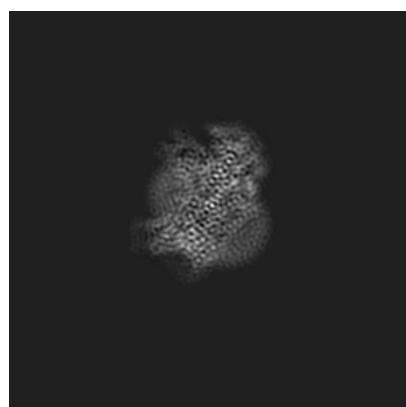
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0872. These allow visual inspection of the internal detail of the map and identification of artifacts.

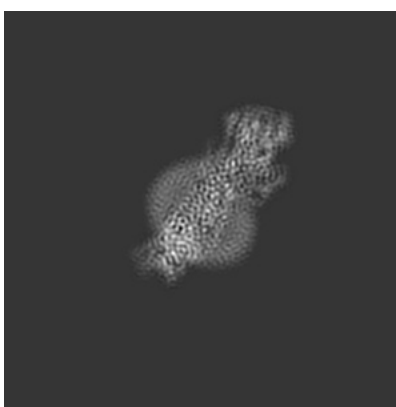
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

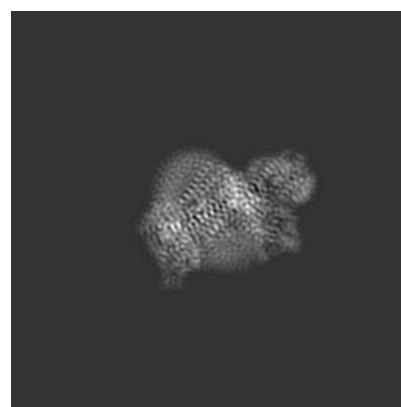
6.1.1 Primary map



X



Y

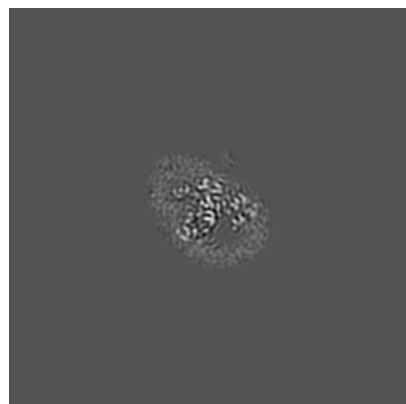


Z

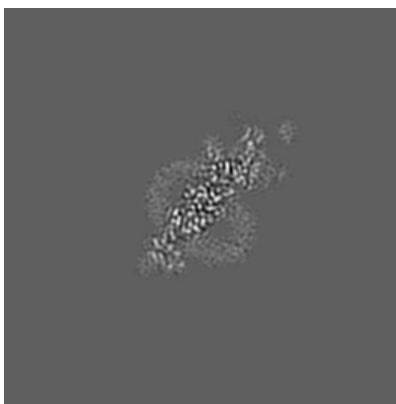
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

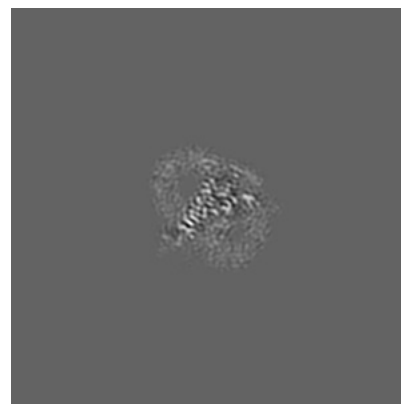
6.2.1 Primary map



X Index: 142



Y Index: 142

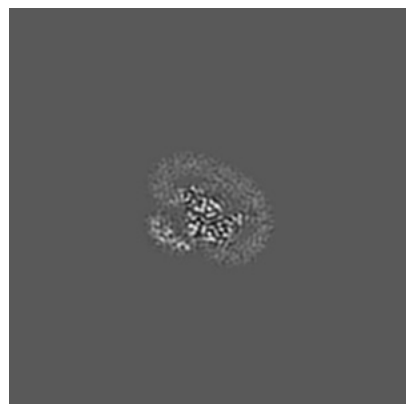


Z Index: 142

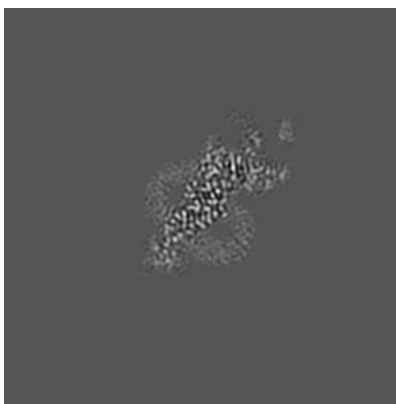
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

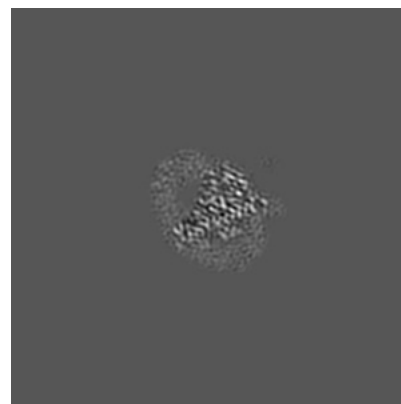
6.3.1 Primary map



X Index: 132



Y Index: 144

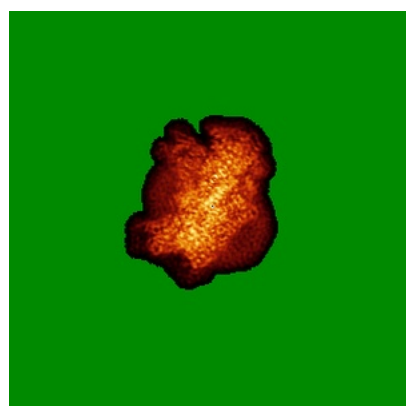


Z Index: 148

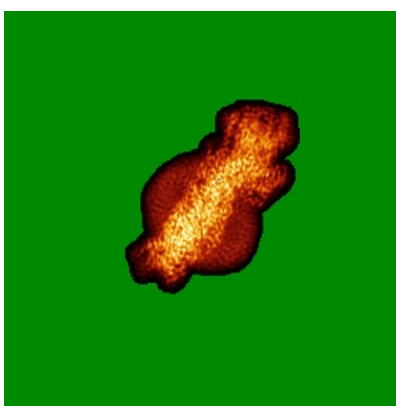
The images above show the largest variance slices of the map in three orthogonal directions.

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

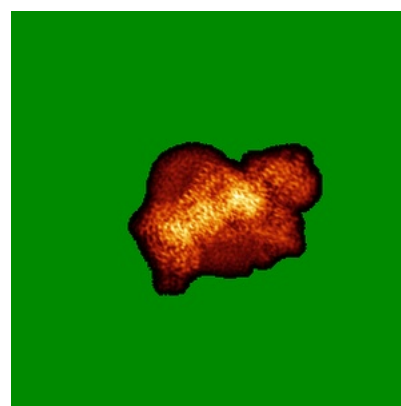
6.4.1 Primary map



X



Y

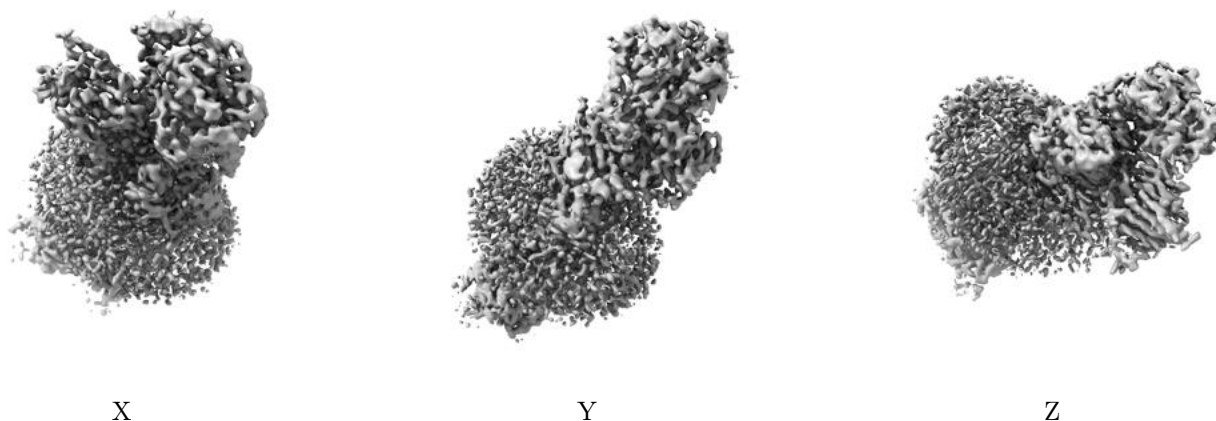


Z

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

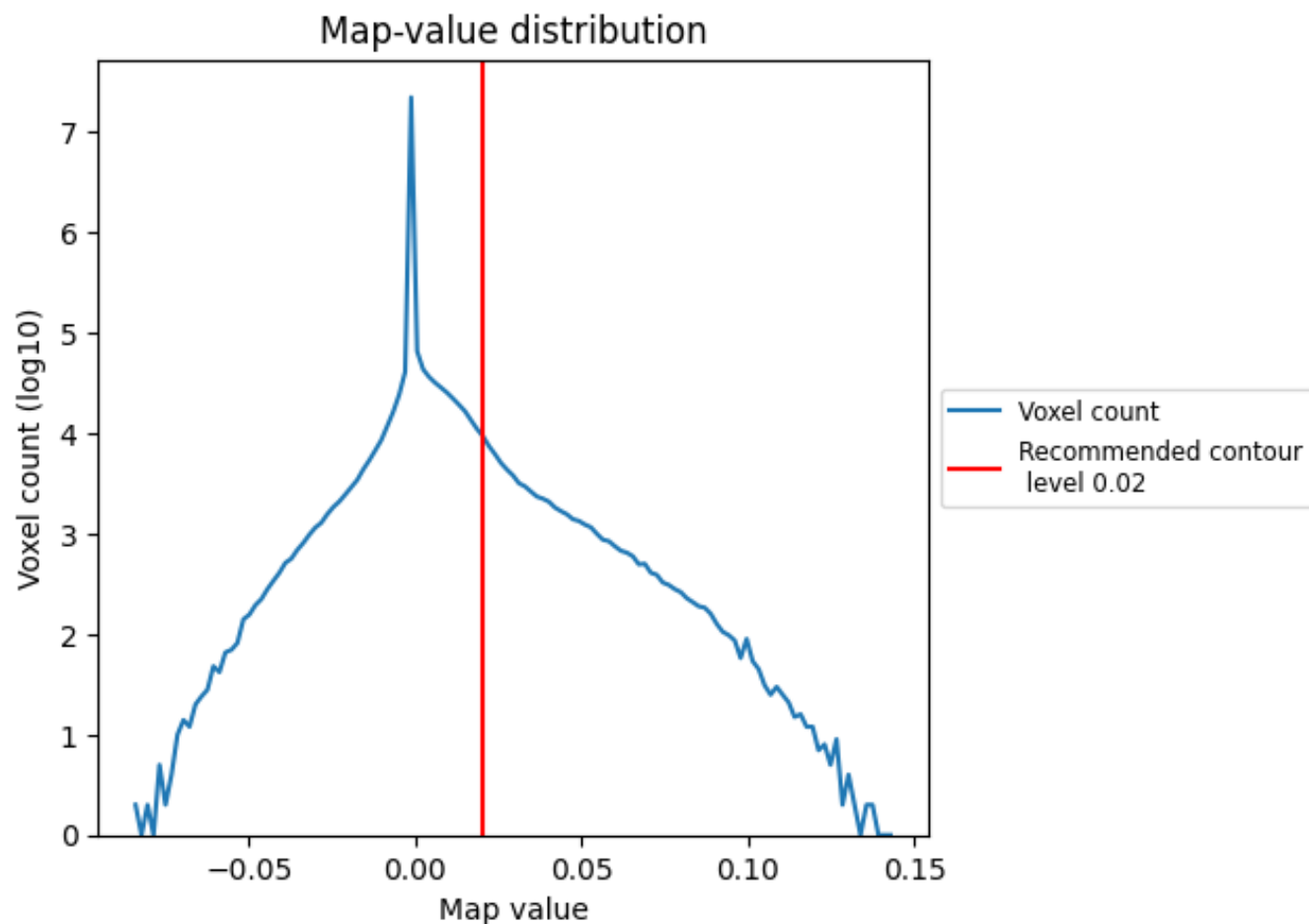
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

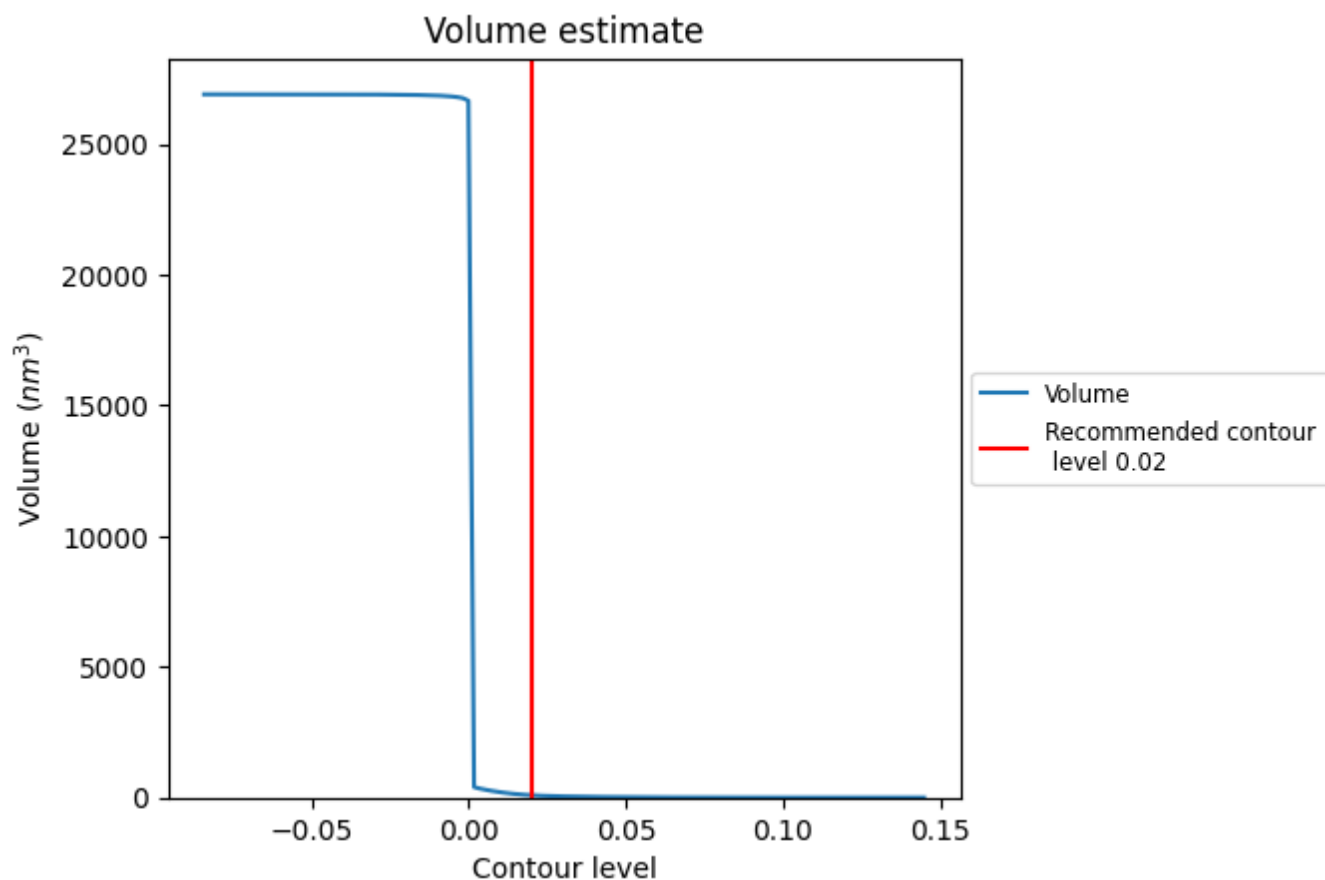
This section contains the results of statistical analysis of the map.

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.

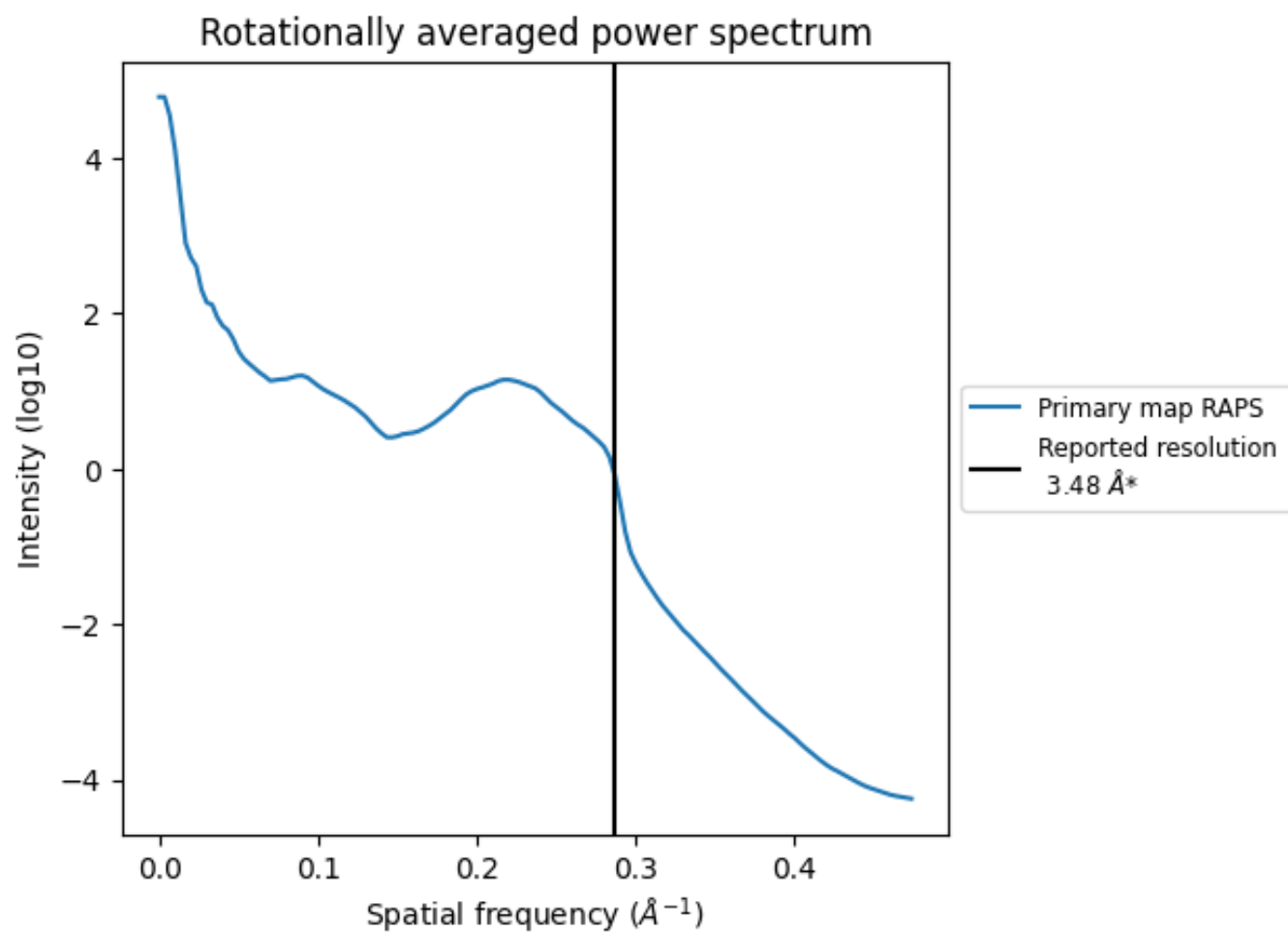
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm^3 ; this corresponds to an approximate mass of 79 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 0.287 Å⁻¹

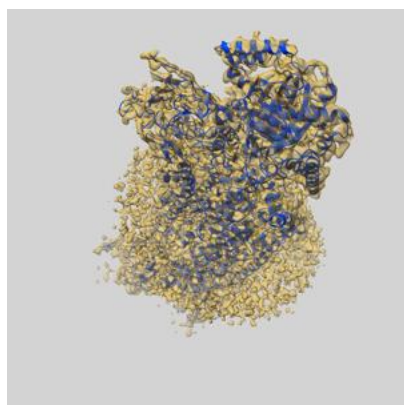
8 Fourier-Shell correlation

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

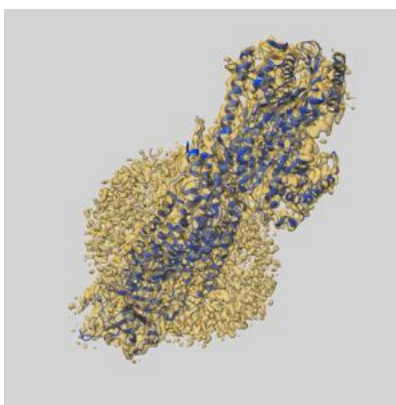
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0872 and PDB model 6LCP. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

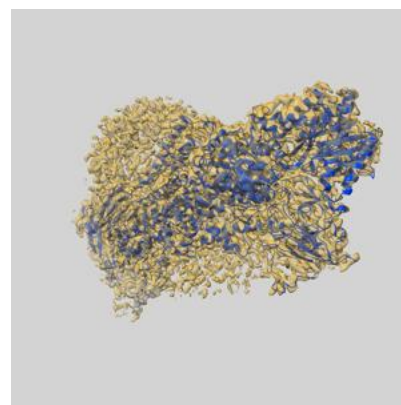
9.1 Map-model overlay [i](#)



X



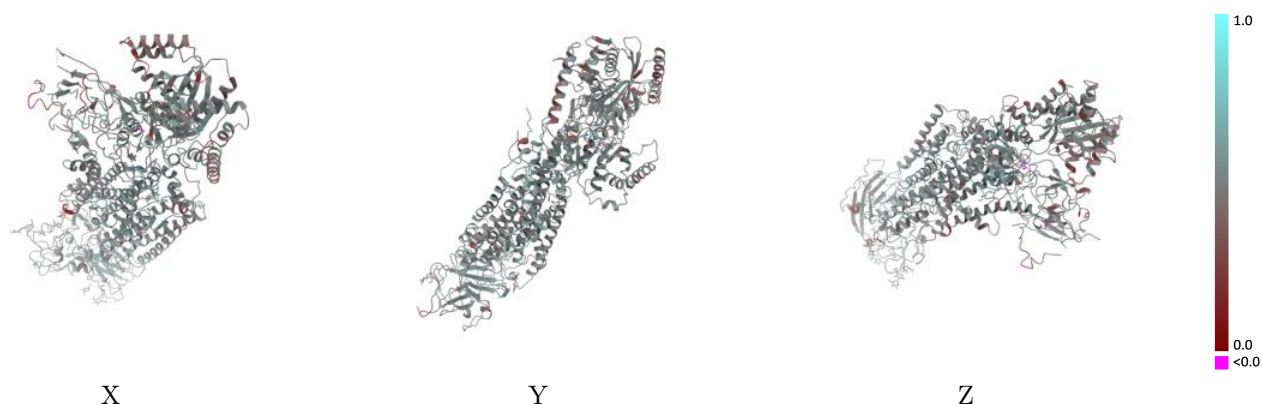
Y



Z

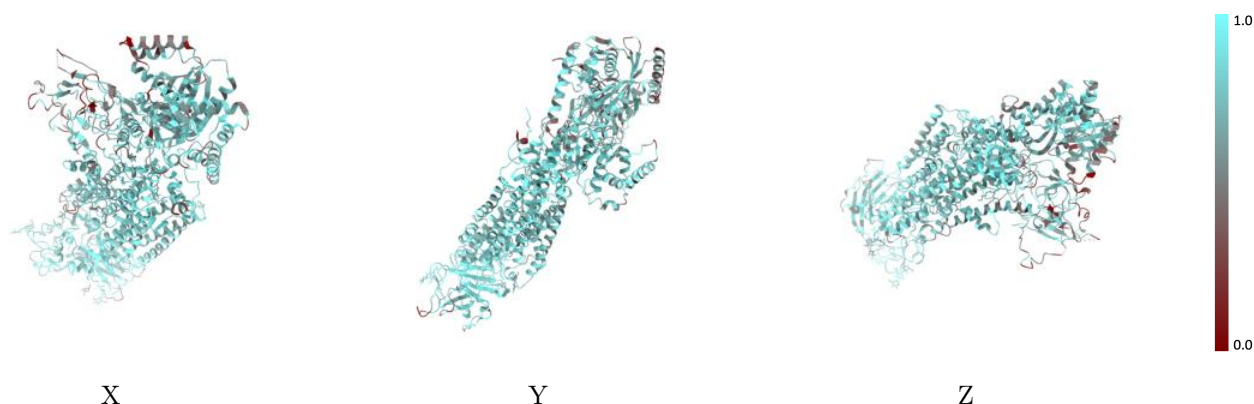
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



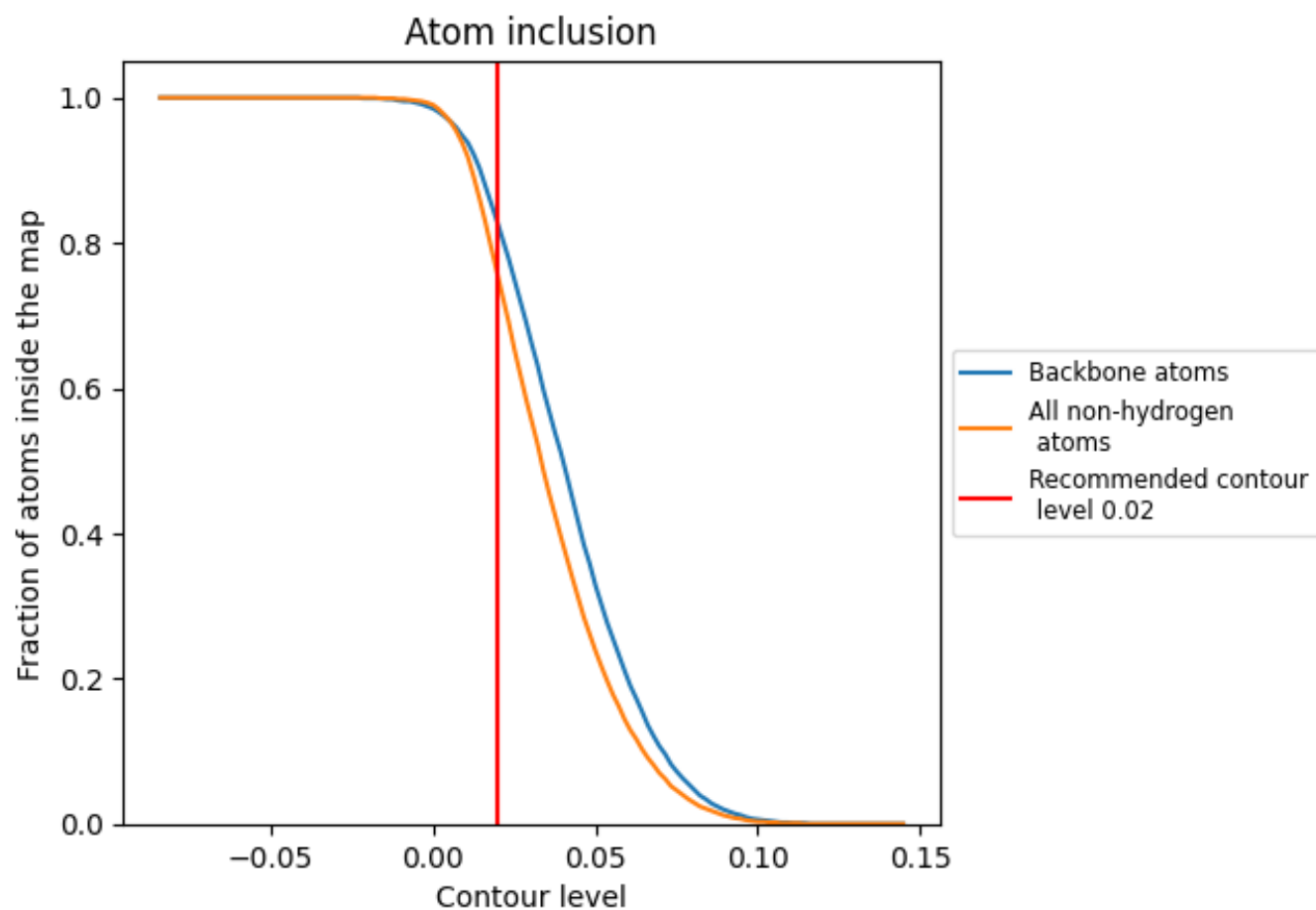
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.4960
A	0.7320	0.4930
B	0.8170	0.5080
C	0.5910	0.2730
D	0.7690	0.4900
E	0.8000	0.4990
F	0.7860	0.4860

1.0

0.0

<0.0