



Full wwPDB EM Validation Report ⓘ

Dec 9, 2025 – 06:38 PM EST

PDB ID : 9PZS / pdb_00009pzs
EMDB ID : EMD-72078
Title : Native GluN1/GluN2A/GluN2B in complex with 5F11 and 3D2 Fabs (class 1), glycine and glutamate bound state
Authors : Kim, J.; Gouaux, E.
Deposited on : 2025-08-11
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

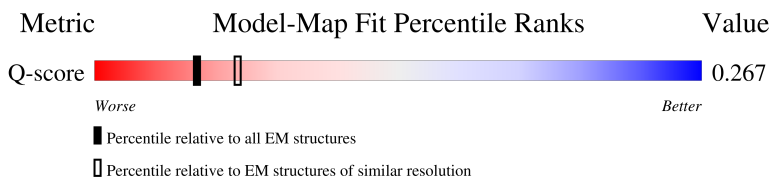
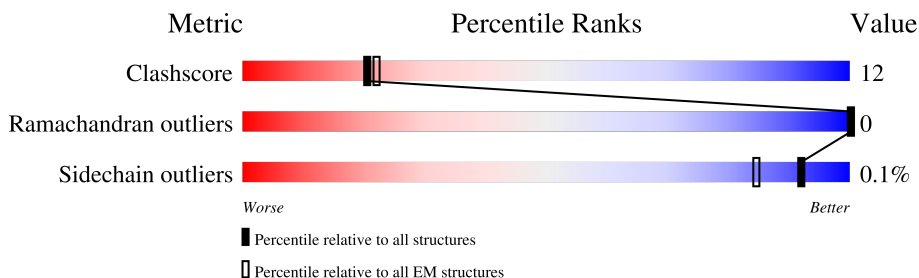
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	1482	 37% 9% 54%
2	A	938	 56% 18% 26%
2	C	938	 58% 16% 26%
3	F	277	 36% 6% 57%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	277	
4	G	244	
4	I	244	
5	B	1464	
6	J	141	
7	K	131	
8	E	2	
8	L	2	
8	N	2	
8	O	2	
8	P	2	
9	M	3	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24307 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 Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	680	Total	C	N	O	S	0	0
			4873	3129	803	915	26		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	691	Total	C	N	O	S	0	0
			5081	3221	868	966	26		
2	C	693	Total	C	N	O	S	0	0
			4925	3125	849	930	21		

- Molecule 3 is a protein called Heavy chain of GluN1-specific monoclonal Fab fragment, termed 5F11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	119	Total	C	N	O	S	0	0
			744	461	129	151	3		
3	H	119	Total	C	N	O	S	0	0
			744	461	129	151	3		

- Molecule 4 is a protein called Light chain of GluN1-specific monoclonal Fab fragment, termed 5F11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	114	Total	C	N	O	S	0	0
			755	478	126	147	4		
4	I	114	Total	C	N	O	S	0	0
			755	478	126	147	4		

- Molecule 5 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	672	Total	C	N	O	S	0	0
			4892	3136	811	920	25		

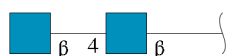
- Molecule 6 is a protein called Heavy chain of GluN2A-specific monoclonal Fab fragment, termed 3D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	110	Total	C	N	O	S	0	0
			689	435	116	136	2		

- Molecule 7 is a protein called Light chain of GluN2A-specific monoclonal Fab fragment, termed 3D2.

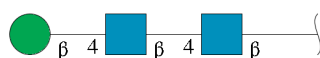
Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	101	Total	C	N	O	S	0	0
			628	391	110	125	2		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



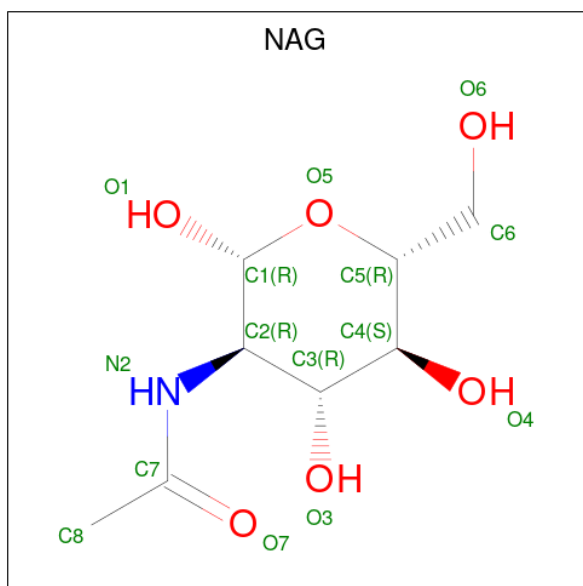
Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	2	Total	C	N	O		0	0
			28	16	2	10			
8	L	2	Total	C	N	O		0	0
			28	16	2	10			
8	N	2	Total	C	N	O		0	0
			28	16	2	10			
8	O	2	Total	C	N	O		0	0
			28	16	2	10			
8	P	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 9 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.



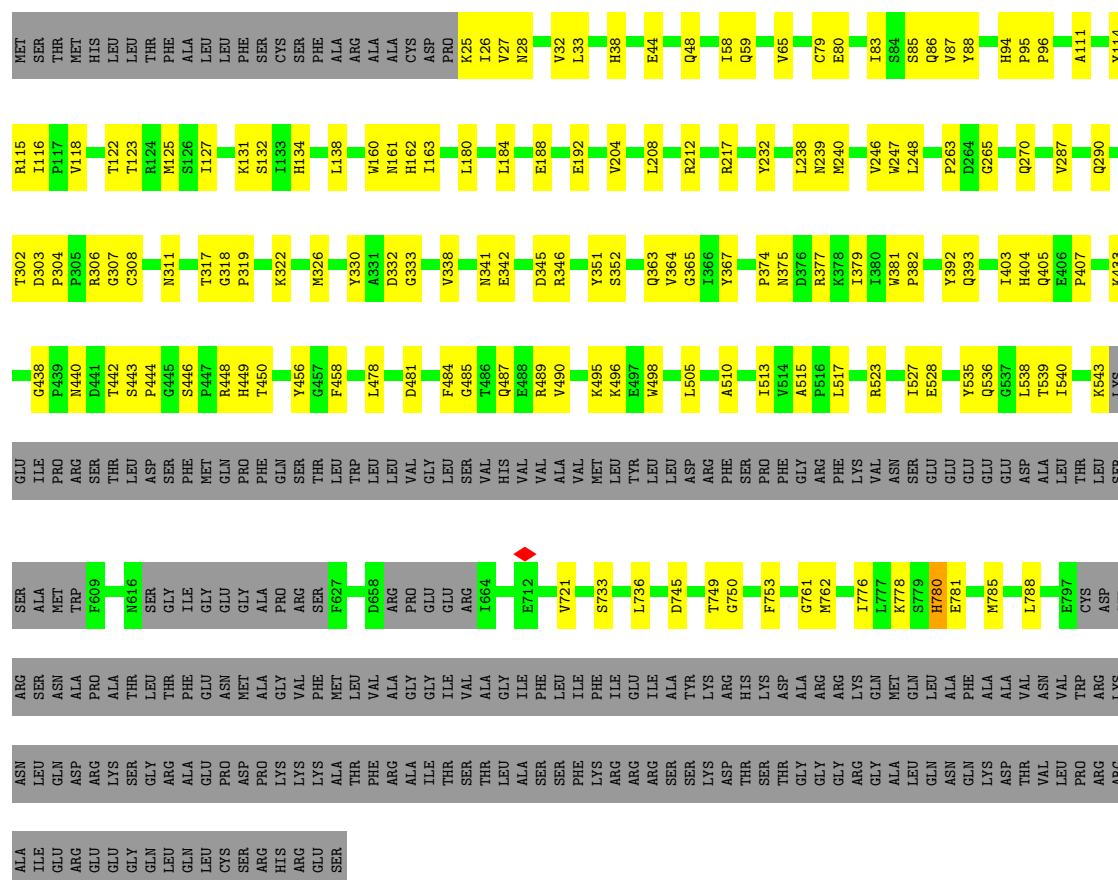
Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	3	Total	C	N	O	0	0
			39	22	2	15		

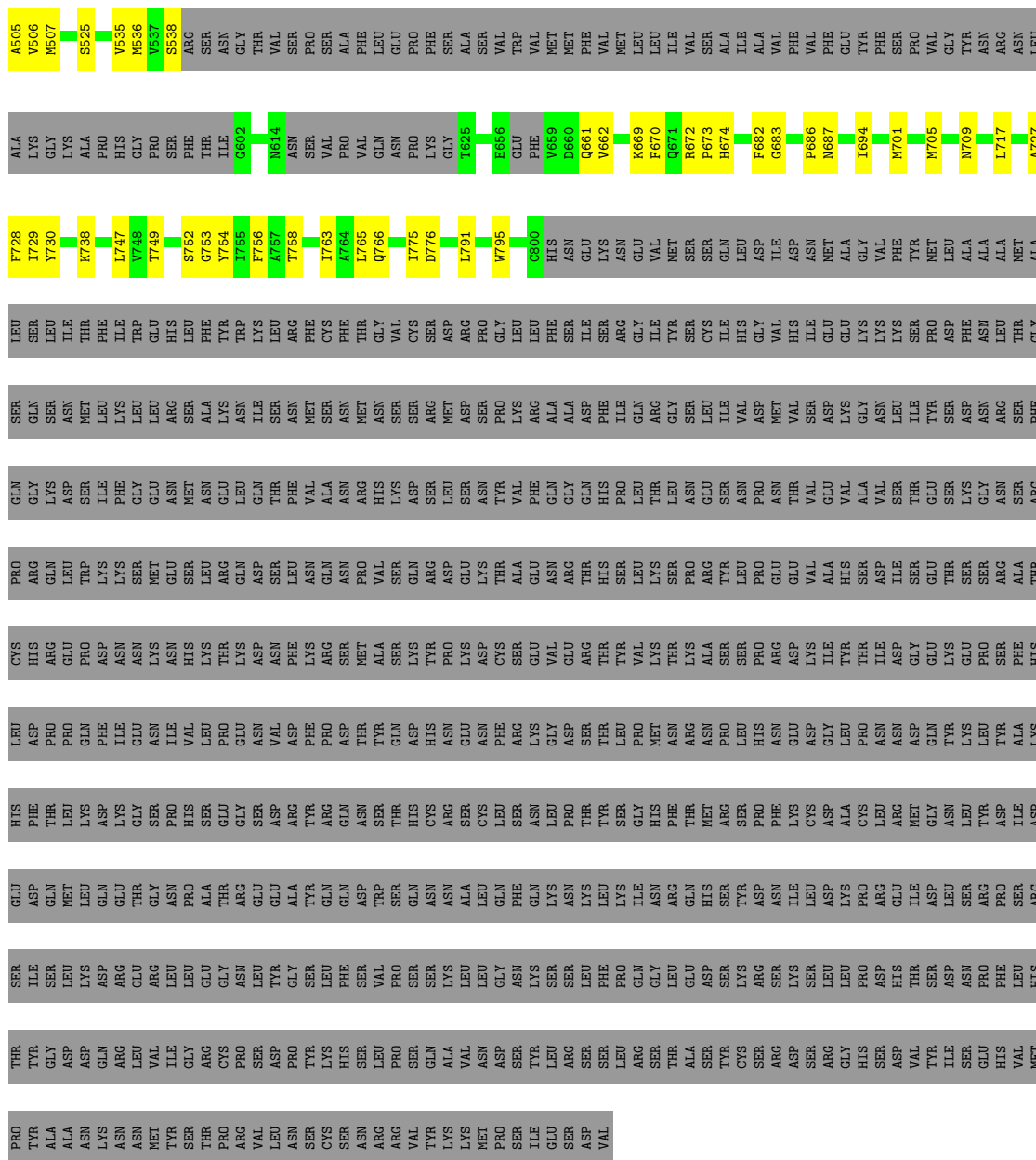
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

Chain C:  58% 16% 26%





- Molecule 6: Heavy chain of GluN2A-specific monoclonal Fab fragment, termed 3D2



- Molecule 7: Light chain of GluN2A-specific monoclonal Fab fragment, termed 3D2




- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1
MAG2

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33%  67%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	296585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (\AA)	468.38403, 468.38403, 468.38403	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.394, 1.394, 1.394	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.21	0/4969	0.37	0/6784
2	A	0.15	0/5186	0.36	0/7075
2	C	0.19	0/5028	0.38	0/6890
3	F	0.22	0/758	0.41	0/1046
3	H	0.23	0/758	0.41	0/1046
4	G	0.12	0/775	0.31	0/1070
4	I	0.12	0/775	0.31	0/1070
5	B	0.19	0/4989	0.38	0/6808
6	J	0.13	0/701	0.35	0/966
7	K	0.18	0/641	0.34	0/885
All	All	0.18	0/24580	0.37	0/33640

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	D	4873	0	4462	120	0
2	A	5081	0	4722	135	0
2	C	4925	0	4437	121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	744	0	550	20	0
3	H	744	0	550	11	0
4	G	755	0	593	14	0
4	I	755	0	593	14	0
5	B	4892	0	4559	121	0
6	J	689	0	512	7	0
7	K	628	0	470	2	0
8	E	28	0	25	0	0
8	L	28	0	25	1	0
8	N	28	0	25	1	0
8	O	28	0	25	4	0
8	P	28	0	25	1	0
9	M	39	0	34	1	0
10	A	14	0	13	0	0
10	B	14	0	13	4	0
10	C	14	0	13	0	0
All	All	24307	0	21646	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (545) 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)
5:B:340:ASN:ND2	10:B:1501:NAG:C1	1.68	1.56
5:B:687:ASN:ND2	8:O:1:NAG:C1	1.71	1.49
1:D:62:LEU:CD1	1:D:64:VAL:HG13	1.65	1.25
1:D:62:LEU:CD1	1:D:64:VAL:CG1	2.16	1.23
2:C:527:ILE:HG21	2:C:762:MET:O	1.42	1.18
1:D:172:VAL:HG22	1:D:203:LEU:HB2	1.18	1.17
2:C:527:ILE:CG2	2:C:762:MET:O	1.97	1.14
1:D:62:LEU:HD13	1:D:64:VAL:HG13	1.22	1.09
1:D:760:THR:HG22	1:D:761:GLY:H	1.07	1.08
2:C:33:LEU:HD21	2:C:38:HIS:CB	1.84	1.08
2:C:95:PRO:HD3	2:C:122:THR:HG21	1.38	1.05
2:A:505:LEU:HD23	2:A:527:ILE:HD13	1.40	1.02
1:D:62:LEU:HD13	1:D:64:VAL:CG1	1.81	1.00
2:C:438:GLY:HA3	2:C:478:LEU:HD12	1.39	0.99
2:A:527:ILE:CG2	2:A:762:MET:O	2.11	0.98
5:B:231:CYS:O	5:B:261:VAL:HG22	1.61	0.97
2:C:33:LEU:HD21	2:C:38:HIS:HB2	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:527:ILE:HG23	2:A:762:MET:O	1.67	0.94
2:C:364:VAL:HG11	2:C:379:ILE:HG12	1.49	0.94
1:D:502:VAL:HG22	1:D:522:VAL:HG12	1.48	0.93
1:D:62:LEU:CD1	1:D:64:VAL:HG11	2.02	0.90
1:D:172:VAL:HG22	1:D:203:LEU:CB	2.02	0.90
5:B:231:CYS:O	5:B:261:VAL:CG2	2.19	0.90
2:C:377:ARG:NH2	3:H:123:TYR:O	2.05	0.90
1:D:182:PHE:CE1	1:D:186:ILE:HD11	2.08	0.88
1:D:172:VAL:CG2	1:D:203:LEU:HB2	2.03	0.87
2:C:505:LEU:HD23	2:C:527:ILE:CD1	2.04	0.87
2:C:33:LEU:HD21	2:C:38:HIS:HB3	1.58	0.86
5:B:68:ASN:ND2	6:J:123:ILE:HG12	1.89	0.86
1:D:760:THR:HG22	1:D:761:GLY:N	1.86	0.86
1:D:94:ILE:O	1:D:121:THR:HG21	1.74	0.85
1:D:182:PHE:CZ	1:D:186:ILE:HD11	2.12	0.85
1:D:667:SER:HA	1:D:672:GLN:HE21	1.41	0.85
2:C:505:LEU:HD23	2:C:527:ILE:HD13	1.58	0.84
1:D:502:VAL:HG22	1:D:522:VAL:CG1	2.05	0.84
2:C:95:PRO:HD3	2:C:122:THR:CG2	2.07	0.84
1:D:515:ILE:O	1:D:760:THR:HG21	1.78	0.84
2:C:505:LEU:CD2	2:C:527:ILE:HD13	2.07	0.83
1:D:62:LEU:HD12	1:D:64:VAL:HG13	1.60	0.81
1:D:182:PHE:CZ	1:D:186:ILE:CD1	2.63	0.81
5:B:68:ASN:HD22	6:J:123:ILE:HG12	1.44	0.80
1:D:62:LEU:HD12	1:D:64:VAL:HG22	1.65	0.79
1:D:172:VAL:HG21	1:D:203:LEU:HD12	1.63	0.79
2:C:527:ILE:HG23	2:C:762:MET:O	1.81	0.79
1:D:760:THR:CG2	1:D:761:GLY:H	1.91	0.79
2:A:307:GLY:HA2	2:A:311:ASN:HB2	1.65	0.79
1:D:62:LEU:HD11	1:D:64:VAL:HG11	1.64	0.78
2:A:479:VAL:HG13	2:A:481:ASP:O	1.84	0.78
1:D:62:LEU:HD11	1:D:64:VAL:CG1	2.13	0.75
2:A:255:SER:OG	3:F:75:THR:HB	1.88	0.74
2:C:364:VAL:HB	2:C:379:ILE:HD11	1.70	0.73
1:D:95:GLN:HA	1:D:121:THR:HG22	1.71	0.72
2:C:527:ILE:HG22	2:C:528:GLU:N	2.03	0.72
2:A:362:VAL:HG13	3:F:124:GLY:HA3	1.72	0.71
1:D:42:VAL:HG22	1:D:73:MET:C	2.14	0.71
2:A:217:ARG:HE	2:A:393:GLN:HE21	1.37	0.71
2:C:364:VAL:CG1	2:C:379:ILE:HG12	2.19	0.70
1:D:502:VAL:CG2	1:D:522:VAL:CG1	2.69	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:LEU:CD2	2:C:38:HIS:HB3	2.20	0.70
2:A:38:HIS:CE1	3:F:95:SER:HB3	2.27	0.70
2:C:458:PHE:HE1	2:C:788:LEU:HB3	1.56	0.70
2:A:527:ILE:HG21	2:A:762:MET:O	1.92	0.70
2:A:115:ARG:NH2	5:B:107:GLU:OE2	2.25	0.69
2:C:212:ARG:NH1	2:C:238:LEU:O	2.23	0.69
2:C:95:PRO:CD	2:C:122:THR:HG21	2.18	0.69
1:D:257:ILE:HG12	1:D:278:ILE:HB	1.75	0.69
5:B:68:ASN:ND2	6:J:123:ILE:CG1	2.55	0.68
1:D:652:ALA:HA	1:D:655:ILE:HD12	1.74	0.68
1:D:774:ARG:O	1:D:778:LEU:HG	1.93	0.68
5:B:154:GLN:NE2	5:B:279:VAL:O	2.27	0.68
2:C:26:ILE:HG22	2:C:59:GLN:HB2	1.77	0.67
2:A:341:ASN:HB3	2:A:347:LYS:HD2	1.76	0.67
5:B:536:MET:HE1	5:B:749:THR:HG22	1.76	0.67
1:D:62:LEU:CD1	1:D:64:VAL:CG2	2.73	0.66
4:G:92:GLY:HA3	4:G:97:PHE:HA	1.77	0.66
4:I:92:GLY:HA3	4:I:97:PHE:HA	1.77	0.66
5:B:763:ILE:HD11	5:B:775:ILE:HG21	1.78	0.66
2:A:115:ARG:NH2	5:B:106:GLN:OE1	2.29	0.66
5:B:340:ASN:CG	10:B:1501:NAG:C1	2.66	0.66
2:C:489:ARG:HA	2:C:496:LYS:HA	1.78	0.66
2:A:28:ASN:ND2	2:A:85:SER:O	2.30	0.65
2:C:28:ASN:ND2	2:C:85:SER:O	2.30	0.65
2:A:362:VAL:CG1	3:F:124:GLY:HA3	2.27	0.65
5:B:275:GLY:H	5:B:366:LEU:HB3	1.62	0.65
1:D:62:LEU:HD12	1:D:64:VAL:CG2	2.27	0.65
1:D:479:TYR:OH	1:D:500:GLU:OE1	2.14	0.65
1:D:172:VAL:CG2	1:D:203:LEU:HD12	2.25	0.64
2:A:506:LEU:HA	2:A:763:ARG:HH12	1.63	0.64
2:C:184:LEU:O	2:C:188:GLU:N	2.31	0.64
5:B:705:MET:SD	5:B:709:ASN:ND2	2.70	0.64
4:I:61:TRP:HB2	4:I:74:ILE:HB	1.80	0.64
2:A:399:LYS:HB3	2:A:477:HIS:HE1	1.61	0.64
1:D:299:ILE:HG22	1:D:342:VAL:HG11	1.78	0.64
5:B:416:PHE:HA	5:B:459:PHE:H	1.61	0.64
2:A:527:ILE:HG22	2:A:528:GLU:N	2.11	0.63
1:D:509:ALA:HB3	1:D:765:ALA:HB3	1.79	0.63
1:D:241:PHE:O	1:D:245:ASN:ND2	2.31	0.63
5:B:687:ASN:CG	8:O:1:NAG:C1	2.67	0.63
5:B:306:MET:HG3	5:B:313:ILE:HG13	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:MET:HB3	2:A:513:ILE:HD13	1.81	0.63
4:G:61:TRP:HB2	4:G:74:ILE:HB	1.80	0.63
4:G:61:TRP:N	4:G:74:ILE:O	2.28	0.62
5:B:340:ASN:ND2	10:B:1501:NAG:C2	2.58	0.62
1:D:231:TYR:HD1	1:D:259:PRO:HG3	1.64	0.62
2:C:83:ILE:HG21	2:C:308:CYS:H	1.65	0.62
2:C:161:ASN:N	2:C:392:TYR:OH	2.32	0.62
2:A:351:TYR:HB2	2:A:367:TYR:HB3	1.80	0.62
2:C:448:ARG:NH2	2:C:450:THR:OG1	2.32	0.62
2:C:527:ILE:CG2	2:C:528:GLU:N	2.62	0.62
5:B:78:ASP:OD1	5:B:81:SER:CB	2.48	0.62
5:B:374:LYS:O	5:B:386:ARG:NH2	2.32	0.62
2:C:527:ILE:CG2	2:C:528:GLU:H	2.13	0.62
5:B:484:LYS:NZ	5:B:686:PRO:O	2.31	0.62
2:A:27:VAL:N	2:A:59:GLN:O	2.33	0.61
5:B:78:ASP:OD1	5:B:81:SER:HB2	2.01	0.61
4:I:61:TRP:N	4:I:74:ILE:O	2.28	0.61
2:C:162:HIS:HD2	2:C:192:GLU:HB2	1.66	0.61
2:A:439:PRO:HD2	2:A:478:LEU:HD23	1.82	0.60
5:B:406:LEU:HD22	5:B:506:VAL:HG11	1.83	0.60
2:C:485:GLY:O	2:C:523:ARG:NH2	2.30	0.60
2:A:505:LEU:O	2:A:763:ARG:NH1	2.34	0.60
1:D:502:VAL:HG21	1:D:522:VAL:HG11	1.83	0.60
5:B:37:ALA:HA	5:B:70:VAL:HB	1.82	0.60
2:A:33:LEU:HD21	2:A:93:SER:OG	2.01	0.60
1:D:72:ALA:O	1:D:84:ARG:NH2	2.34	0.60
1:D:502:VAL:CG2	1:D:522:VAL:HG11	2.32	0.60
2:A:106:PRO:HB3	5:B:115:PHE:CZ	2.37	0.60
5:B:413:GLU:H	5:B:417:VAL:HB	1.66	0.60
2:C:246:VAL:HG13	2:C:381:TRP:CZ3	2.37	0.59
2:C:307:GLY:HA2	2:C:311:ASN:HB2	1.83	0.59
5:B:78:ASP:OD1	5:B:81:SER:OG	2.20	0.59
2:A:202:LYS:HA	2:A:230:THR:HG21	1.85	0.59
5:B:307:LEU:HD12	5:B:311:SER:HA	1.84	0.59
2:C:127:ILE:HG13	2:C:134:HIS:HE1	1.67	0.59
1:D:527:VAL:HG22	1:D:777:ASP:HB2	1.83	0.59
5:B:42:HIS:HA	5:B:103:ASP:HB3	1.85	0.59
2:C:405:GLN:HG3	2:C:407:PRO:HD2	1.84	0.59
2:A:158:TYR:HD1	2:A:388:LYS:HD3	1.67	0.59
2:A:217:ARG:HE	2:A:393:GLN:NE2	2.00	0.59
2:A:253:GLU:N	2:A:253:GLU:OE1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:420:CYS:HB3	2:A:433:LYS:HD2	1.85	0.58
1:D:670:LYS:HA	1:D:677:PHE:CE1	2.38	0.58
3:F:67:TRP:HZ2	3:F:70:TRP:HD1	1.51	0.58
1:D:34:SER:N	1:D:64:VAL:O	2.37	0.58
2:A:505:LEU:HD23	2:A:527:ILE:CD1	2.25	0.58
3:F:59:GLN:HB2	3:F:65:LEU:HG	1.86	0.58
3:H:67:TRP:HZ2	3:H:70:TRP:HD1	1.51	0.58
2:A:740:ALA:HA	2:A:746:LEU:HB2	1.86	0.57
2:A:264:ASP:HA	2:A:356:LEU:HD23	1.86	0.57
4:G:115:GLN:NE2	4:G:116:HIS:O	2.38	0.57
3:H:59:GLN:HB2	3:H:65:LEU:HG	1.86	0.57
4:I:115:GLN:NE2	4:I:116:HIS:O	2.38	0.57
1:D:266:THR:HG23	1:D:373:TRP:HD1	1.69	0.57
2:A:518:THR:O	2:A:523:ARG:NH1	2.37	0.57
2:C:505:LEU:HA	2:C:510:ALA:HB3	1.87	0.57
2:C:86:GLN:NE2	2:C:304:PRO:O	2.37	0.57
2:C:28:ASN:HB2	2:C:87:VAL:HA	1.87	0.57
4:G:43:CYS:O	4:G:97:PHE:N	2.34	0.57
2:A:405:GLN:HG2	2:A:516:PRO:HG3	1.86	0.57
2:C:217:ARG:NH2	2:C:393:GLN:OE1	2.36	0.57
4:I:43:CYS:O	4:I:97:PHE:N	2.34	0.57
5:B:379:GLU:OE1	5:B:382:THR:OG1	2.23	0.56
5:B:672:ARG:HD2	5:B:673:PRO:HD2	1.87	0.56
3:H:39:LYS:HA	3:H:102:GLN:HA	1.87	0.56
1:D:120:LEU:HD12	1:D:317:PRO:HG2	1.87	0.56
3:F:39:LYS:HA	3:F:102:GLN:HA	1.87	0.56
2:C:527:ILE:HG22	2:C:528:GLU:H	1.68	0.56
2:C:539:THR:OG1	2:C:540:ILE:N	2.35	0.56
2:C:338:VAL:HG22	2:C:346:ARG:NH2	2.20	0.56
1:D:515:ILE:HD12	1:D:528:PRO:HG3	1.87	0.56
2:A:153:GLU:OE1	2:A:156:ARG:NH1	2.39	0.56
2:C:322:LYS:O	2:C:326:MET:HG2	2.05	0.56
2:C:338:VAL:HG22	2:C:346:ARG:HH21	1.71	0.56
5:B:687:ASN:ND2	8:O:1:NAG:C2	2.62	0.56
2:A:527:ILE:CG2	2:A:528:GLU:N	2.68	0.56
1:D:78:PRO:HB3	1:D:111:ILE:HD13	1.88	0.55
2:C:364:VAL:HB	2:C:379:ILE:CD1	2.36	0.55
2:A:33:LEU:HB2	2:A:39:GLU:HG3	1.88	0.55
2:C:115:ARG:HB3	2:C:318:GLY:HA3	1.87	0.55
2:C:290:GLN:HB3	2:C:330:TYR:HE1	1.71	0.55
5:B:155:ALA:HA	5:B:158:MET:HE2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:VAL:HB	2:C:379:ILE:CG1	2.37	0.55
1:D:532:THR:OG1	1:D:533:GLY:N	2.40	0.55
5:B:459:PHE:HE1	5:B:791:LEU:HB3	1.72	0.55
2:A:93:SER:HB3	2:A:121:LEU:HD12	1.89	0.55
2:C:111:ALA:HB1	2:C:116:ILE:HB	1.89	0.55
2:A:33:LEU:CD2	2:A:93:SER:OG	2.55	0.55
2:A:362:VAL:HG22	3:F:124:GLY:O	2.06	0.55
1:D:667:SER:HA	1:D:672:GLN:NE2	2.18	0.55
8:N:1:NAG:H61	8:N:2:NAG:C7	2.37	0.55
1:D:62:LEU:HD11	1:D:64:VAL:CG2	2.38	0.54
5:B:157:VAL:HG21	5:B:361:LEU:HD12	1.89	0.54
5:B:244:ARG:HA	5:B:249:THR:CG2	2.37	0.54
5:B:538:SER:HA	5:B:747:LEU:HA	1.88	0.54
2:A:80:GLU:CD	5:B:80:LYS:HD2	2.32	0.54
2:A:543:LYS:HD3	2:A:721:VAL:HG13	1.88	0.54
2:C:536:GLN:HB2	2:C:733:SER:HB2	1.90	0.54
5:B:416:PHE:HD1	5:B:459:PHE:HB3	1.72	0.54
6:J:41:CYS:HB3	6:J:98:ALA:HB3	1.90	0.54
2:A:26:ILE:HG22	2:A:59:GLN:HB2	1.90	0.54
5:B:763:ILE:CD1	5:B:775:ILE:HG21	2.38	0.54
4:I:41:MET:HG2	4:I:130:THR:HG21	1.89	0.54
9:M:1:NAG:H61	9:M:2:NAG:C7	2.38	0.54
1:D:62:LEU:HD12	1:D:62:LEU:O	2.08	0.54
2:A:647:TYR:HA	2:A:650:ASN:ND2	2.23	0.54
5:B:160:LYS:NZ	5:B:164:ASP:OD2	2.39	0.54
5:B:379:GLU:HG2	5:B:380:ASN:H	1.72	0.54
5:B:487:LYS:N	5:B:494:ASN:OD1	2.39	0.54
5:B:525:SER:HB2	5:B:776:ASP:OD1	2.08	0.54
4:G:41:MET:HG2	4:G:130:THR:HG21	1.89	0.54
5:B:661:GLN:OE1	5:B:669:LYS:NZ	2.41	0.53
2:A:788:LEU:O	2:A:791:THR:OG1	2.22	0.53
3:F:58:LYS:O	3:F:66:GLU:N	2.34	0.53
8:L:1:NAG:H61	8:L:2:NAG:C7	2.38	0.53
2:C:505:LEU:HD23	2:C:527:ILE:HD11	1.85	0.53
1:D:536:VAL:HG22	1:D:730:ILE:HG23	1.91	0.53
5:B:498:GLY:O	5:B:504:ARG:NH2	2.41	0.53
2:C:212:ARG:NH2	2:C:239:ASN:O	2.41	0.53
5:B:117:SER:OG	5:B:122:ILE:O	2.19	0.53
2:A:368:ASN:N	2:A:371:HIS:O	2.35	0.53
3:H:58:LYS:O	3:H:66:GLU:N	2.34	0.53
2:A:91:LEU:HD23	2:A:121:LEU:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:180:LEU:HA	2:A:183:LEU:HD12	1.91	0.53
1:D:223:LEU:HD13	1:D:228:ILE:HG12	1.91	0.52
2:A:362:VAL:HG13	3:F:124:GLY:CA	2.38	0.52
5:B:364:ILE:HG22	5:B:374:LYS:HA	1.90	0.52
2:A:204:VAL:HG21	2:A:231:VAL:HG12	1.91	0.52
1:D:160:ILE:HD11	1:D:364:ILE:HD13	1.91	0.52
2:A:115:ARG:NH1	5:B:106:GLN:OE1	2.42	0.52
5:B:298:ILE:HD11	5:B:348:LEU:HB3	1.92	0.52
2:C:114:TYR:OH	2:C:311:ASN:O	2.24	0.52
1:D:695:ILE:HG22	1:D:703:HIS:HB2	1.91	0.52
2:A:527:ILE:CG2	2:A:528:GLU:H	2.22	0.52
5:B:279:VAL:HG22	5:B:363:VAL:HA	1.90	0.52
5:B:763:ILE:HG13	5:B:763:ILE:O	2.09	0.52
2:C:162:HIS:N	2:C:392:TYR:OH	2.43	0.52
1:D:95:GLN:HA	1:D:121:THR:CG2	2.40	0.51
5:B:172:LEU:HB3	5:B:203:VAL:HG13	1.92	0.51
2:C:438:GLY:HA3	2:C:478:LEU:CD1	2.28	0.51
8:P:1:NAG:H62	8:P:2:NAG:C7	2.40	0.51
1:D:731:TYR:HB3	1:D:736:LEU:HD11	1.92	0.51
2:A:704:ARG:O	2:A:708:LYS:NZ	2.44	0.51
5:B:149:ALA:HB2	5:B:359:PRO:HG3	1.92	0.51
2:C:377:ARG:CZ	3:H:123:TYR:O	2.59	0.51
2:C:481:ASP:N	2:C:481:ASP:OD1	2.43	0.51
5:B:459:PHE:CE1	5:B:791:LEU:HB3	2.46	0.51
1:D:662:GLN:HG3	1:D:663:VAL:HG13	1.91	0.51
2:A:153:GLU:HA	2:A:156:ARG:HD3	1.92	0.51
2:A:743:LYS:HB2	2:A:746:LEU:HG	1.92	0.51
2:C:513:ILE:HB	2:C:761:GLY:HA3	1.92	0.51
2:A:742:GLN:HA	2:A:797:GLU:HB2	1.93	0.51
2:C:490:VAL:H	2:C:495:LYS:N	2.09	0.51
1:D:129:GLY:HA2	1:D:132:MET:HE1	1.93	0.50
1:D:163:GLU:HG2	1:D:386:MET:HG3	1.93	0.50
1:D:176:PHE:CG	1:D:177:PRO:HD2	2.46	0.50
2:A:330:TYR:CD2	2:A:338:VAL:HG13	2.46	0.50
2:C:232:TYR:HB3	2:C:263:PRO:HD3	1.92	0.50
5:B:274:SER:HB2	5:B:396:PHE:HA	1.92	0.50
5:B:416:PHE:HB3	5:B:460:CYS:HB2	1.94	0.50
1:D:681:PHE:HD2	1:D:683:PHE:HD1	1.58	0.50
1:D:151:GLU:HA	1:D:185:LYS:HG2	1.94	0.50
1:D:244:ALA:O	1:D:248:GLY:N	2.44	0.50
5:B:672:ARG:HG3	5:B:674:HIS:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:1:NAG:H61	8:O:2:NAG:C7	2.41	0.50
2:C:95:PRO:HG2	2:C:96:PRO:HD3	1.92	0.50
1:D:42:VAL:HG13	1:D:74:ASN:HA	1.93	0.50
2:A:255:SER:HB3	3:F:75:THR:O	2.12	0.50
1:D:285:TRP:HE1	1:D:363:VAL:HG21	1.78	0.49
2:A:95:PRO:HD3	2:A:122:THR:HG21	1.93	0.49
2:A:133:ILE:HG23	5:B:111:GLN:OE1	2.13	0.49
2:A:49:ALA:O	2:A:53:HIS:ND1	2.39	0.49
1:D:515:ILE:HG21	2:A:531:LYS:HE2	1.94	0.49
2:A:212:ARG:NH2	2:A:238:LEU:HB3	2.26	0.49
2:A:406:GLU:N	2:A:406:GLU:OE1	2.42	0.49
1:D:164:TYR:OH	1:D:388:TYR:O	2.28	0.49
2:A:541:LEU:HD11	2:A:746:LEU:HB3	1.94	0.49
2:C:32:VAL:HG13	2:C:65:VAL:HG23	1.93	0.49
1:D:287:TYR:CE2	1:D:292:ARG:HG2	2.48	0.49
1:D:416:PHE:HD1	1:D:460:PHE:HB3	1.76	0.49
1:D:524:ASP:OD2	1:D:773:LYS:NZ	2.35	0.49
2:C:341:ASN:OD1	2:C:345:ASP:N	2.35	0.49
2:A:145:SER:HB2	2:A:179:ARG:HG2	1.95	0.49
5:B:753:GLY:HA2	5:B:756:PHE:HD2	1.78	0.49
4:I:39:VAL:HG13	4:I:104:VAL:HG21	1.94	0.49
5:B:250:GLY:H	5:B:253:PHE:HD2	1.61	0.49
1:D:270:PRO:HG2	1:D:273:PHE:CZ	2.48	0.48
2:C:163:ILE:HD11	2:C:180:LEU:HD21	1.95	0.48
1:D:233:THR:OG1	1:D:236:GLU:CD	2.56	0.48
4:G:39:VAL:HG13	4:G:104:VAL:HG21	1.94	0.48
2:A:65:VAL:HG21	2:A:78:VAL:HG22	1.95	0.48
2:A:489:ARG:HA	2:A:496:LYS:HA	1.95	0.48
5:B:244:ARG:HA	5:B:249:THR:HG23	1.94	0.48
2:A:762:MET:HB3	2:A:762:MET:HE3	1.79	0.48
5:B:535:VAL:HG22	5:B:729:ILE:HG12	1.95	0.48
2:C:287:VAL:HA	2:C:330:TYR:CE1	2.49	0.48
1:D:62:LEU:CD1	1:D:64:VAL:HG22	2.35	0.48
1:D:172:VAL:O	1:D:230:LEU:HA	2.13	0.48
1:D:534:ILE:HD12	1:D:694:ASN:HD22	1.79	0.48
2:A:685:LYS:HB2	2:A:710:ASN:HB3	1.96	0.48
5:B:752:SER:HB3	5:B:754:TYR:CZ	2.49	0.48
1:D:62:LEU:HD12	1:D:64:VAL:CG1	2.23	0.48
5:B:672:ARG:HH11	5:B:673:PRO:HG2	1.79	0.48
2:A:146:HIS:O	2:A:150:VAL:HG23	2.13	0.47
2:A:287:VAL:HG21	2:A:338:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:681:TYR:HB3	2:A:728:ALA:HB3	1.96	0.47
3:F:81:ASN:O	3:F:85:THR:N	2.47	0.47
5:B:264:ASN:HB3	5:B:267:LEU:HB3	1.96	0.47
5:B:406:LEU:HD13	5:B:507:MET:HE3	1.96	0.47
2:C:442:THR:O	2:C:446:SER:N	2.43	0.47
3:H:81:ASN:O	3:H:85:THR:N	2.47	0.47
1:D:126:ILE:O	1:D:292:ARG:NH1	2.40	0.47
2:A:88:TYR:OH	2:A:303:ASP:OD1	2.23	0.47
5:B:661:GLN:HB3	5:B:669:LYS:HZ1	1.77	0.47
1:D:62:LEU:HD11	1:D:64:VAL:HG21	1.96	0.47
1:D:671:PHE:O	1:D:674:PRO:HD3	2.13	0.47
5:B:765:LEU:HD21	5:B:775:ILE:HD12	1.96	0.47
1:D:182:PHE:CE2	1:D:186:ILE:HD12	2.50	0.47
1:D:368:ASN:OD1	1:D:368:ASN:N	2.47	0.47
2:A:668:ASN:HA	2:A:673:ARG:HH21	1.78	0.47
5:B:170:PHE:HE1	5:B:198:TRP:HB3	1.80	0.47
1:D:266:THR:HG23	1:D:373:TRP:CD1	2.48	0.47
1:D:681:PHE:CD2	1:D:683:PHE:HD1	2.32	0.47
2:A:731:TRP:HB3	2:A:736:LEU:HD11	1.96	0.47
5:B:34:LEU:HA	5:B:66:ASP:O	2.15	0.47
2:A:217:ARG:N	2:A:391:GLY:O	2.48	0.47
1:D:97:VAL:HB	1:D:123:ILE:HG23	1.97	0.47
2:A:243:SER:HA	2:A:383:GLY:HA3	1.97	0.47
5:B:251:TYR:HA	5:B:396:PHE:CE2	2.50	0.47
1:D:257:ILE:HA	1:D:278:ILE:O	2.15	0.47
2:A:790:LYS:HG2	2:A:794:ARG:HE	1.79	0.47
2:C:484:PHE:HB3	2:C:523:ARG:HH12	1.80	0.47
3:F:38:VAL:O	3:F:103:PHE:N	2.46	0.46
5:B:156:THR:OG1	5:B:186:PHE:HZ	1.97	0.46
5:B:165:TYR:CZ	5:B:390:TRP:HB2	2.50	0.46
2:A:328:SER:HB3	2:A:330:TYR:CE2	2.50	0.46
5:B:172:LEU:HD12	5:B:228:LEU:HB2	1.97	0.46
2:C:306:ARG:C	2:C:311:ASN:HD22	2.23	0.46
2:C:364:VAL:CG1	2:C:379:ILE:CG1	2.91	0.46
7:K:82:VAL:HG13	7:K:83:PRO:HD2	1.98	0.46
1:D:182:PHE:CZ	1:D:186:ILE:HD12	2.46	0.46
1:D:243:VAL:O	1:D:246:SER:OG	2.24	0.46
2:A:58:ILE:HG12	2:A:296:LEU:HD11	1.96	0.46
2:A:390:ARG:NH1	2:A:394:MET:HE3	2.30	0.46
2:A:538:LEU:C	2:A:539:THR:HG23	2.41	0.46
2:A:215:GLU:HA	2:A:393:GLN:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:240:LEU:HD12	5:B:272:PHE:CE1	2.51	0.46
5:B:462:ASP:OD2	5:B:795:TRP:NE1	2.49	0.46
5:B:505:ALA:O	5:B:766:GLN:NE2	2.47	0.46
5:B:672:ARG:NH1	5:B:673:PRO:HG2	2.31	0.46
2:C:131:LYS:NZ	2:C:342:GLU:O	2.38	0.46
2:C:290:GLN:HB3	2:C:330:TYR:CE1	2.50	0.46
1:D:536:VAL:HG22	1:D:730:ILE:HG12	1.97	0.46
3:F:121:ILE:HA	3:F:126:TYR:HA	1.98	0.46
5:B:157:VAL:O	5:B:161:ILE:HG13	2.15	0.46
2:A:527:ILE:HG22	2:A:528:GLU:H	1.79	0.46
2:C:83:ILE:HG21	2:C:308:CYS:N	2.29	0.46
2:C:539:THR:HG23	2:C:736:LEU:HD12	1.96	0.46
2:C:543:LYS:HG3	2:C:721:VAL:O	2.16	0.46
2:A:163:ILE:HA	2:A:218:VAL:HB	1.96	0.46
5:B:273:PRO:HB2	5:B:396:PHE:CD1	2.50	0.46
5:B:75:ASN:OD1	5:B:76:ARG:N	2.49	0.46
5:B:287:SER:OG	5:B:289:GLU:OE1	2.28	0.46
3:H:81:ASN:HB3	3:H:84:PHE:HD2	1.81	0.46
1:D:156:VAL:HG22	1:D:379:TRP:CE2	2.51	0.45
1:D:123:ILE:O	1:D:143:PHE:HA	2.16	0.45
1:D:314:ILE:HG23	1:D:314:ILE:O	2.16	0.45
2:A:362:VAL:CG2	3:F:124:GLY:O	2.64	0.45
5:B:411:LEU:HD23	5:B:485:HIS:CE1	2.52	0.45
5:B:683:GLY:HA2	5:B:705:MET:HG2	1.98	0.45
7:K:51:TYR:O	7:K:54:THR:OG1	2.26	0.45
2:A:330:TYR:HD2	2:A:338:VAL:HG13	1.79	0.45
2:C:438:GLY:CA	2:C:478:LEU:HD12	2.29	0.45
2:A:165:LEU:HB3	2:A:194:VAL:HA	1.97	0.45
2:A:487:GLN:HB2	2:A:498:TRP:CE2	2.52	0.45
2:C:433:LYS:HA	2:C:456:TYR:HB3	1.99	0.45
5:B:682:PHE:HB3	5:B:727:ALA:HB3	1.98	0.45
2:C:162:HIS:CD2	2:C:192:GLU:HB2	2.48	0.45
2:C:489:ARG:HA	2:C:496:LYS:CA	2.45	0.45
1:D:513:LEU:HD23	1:D:513:LEU:HA	1.75	0.45
4:G:73:LEU:O	4:G:84:VAL:HG21	2.17	0.45
2:C:458:PHE:CE1	2:C:788:LEU:HB3	2.45	0.45
4:I:43:CYS:HB3	4:I:97:PHE:HB2	1.98	0.45
1:D:101:ASP:OD1	1:D:101:ASP:N	2.49	0.45
2:A:778:LYS:O	2:A:781:GLU:HG3	2.17	0.45
4:G:43:CYS:HB3	4:G:97:PHE:HB2	1.99	0.45
2:C:88:TYR:OH	2:C:303:ASP:OD1	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:73:LEU:O	4:I:84:VAL:HG21	2.17	0.45
1:D:126:ILE:HB	1:D:292:ARG:HB3	1.98	0.45
1:D:681:PHE:HD2	1:D:683:PHE:CD1	2.35	0.45
2:A:117:PRO:HG2	2:A:321:PHE:HD2	1.82	0.45
2:A:150:VAL:HG21	2:A:351:TYR:CD2	2.51	0.45
2:A:519:ILE:HD12	2:A:532:PRO:HG3	1.98	0.45
2:A:215:GLU:O	2:A:393:GLN:HG3	2.17	0.45
4:G:89:THR:N	4:G:100:THR:O	2.48	0.45
2:A:152:PHE:CG	2:A:183:LEU:HB3	2.52	0.44
2:A:158:TYR:CD1	2:A:388:LYS:HD3	2.50	0.44
2:A:266:ILE:HG22	2:A:356:LEU:HB2	1.98	0.44
5:B:694:ILE:HG23	5:B:701:MET:HB3	1.99	0.44
2:A:367:TYR:HD1	2:A:372:VAL:HG22	1.83	0.44
2:C:27:VAL:HG23	2:C:58:ILE:HD11	2.00	0.44
2:A:163:ILE:HG22	2:A:218:VAL:HG11	2.00	0.44
3:F:121:ILE:HG12	3:F:126:TYR:HA	1.98	0.44
5:B:170:PHE:CE1	5:B:198:TRP:HB3	2.52	0.44
5:B:240:LEU:CD1	5:B:272:PHE:CD1	3.00	0.44
3:H:38:VAL:O	3:H:103:PHE:N	2.46	0.44
1:D:469:SER:OG	1:D:474:PHE:O	2.36	0.44
2:C:118:VAL:O	2:C:138:LEU:N	2.42	0.44
2:A:680:ILE:H	2:A:727:HIS:HB2	1.82	0.44
3:F:81:ASN:HB3	3:F:84:PHE:HD2	1.81	0.44
2:C:505:LEU:HD21	2:C:527:ILE:HD13	1.95	0.44
2:A:305:PRO:HB2	2:A:311:ASN:ND2	2.33	0.44
2:A:76:LEU:HD12	5:B:83:ILE:HG21	1.98	0.44
2:A:95:PRO:HG2	2:A:96:PRO:HD3	1.99	0.44
4:G:74:ILE:HG12	4:G:80:ARG:HA	2.00	0.44
5:B:154:GLN:HE22	5:B:259:SER:N	2.16	0.44
5:B:240:LEU:HD12	5:B:272:PHE:CD1	2.52	0.44
5:B:430:VAL:O	5:B:433:THR:OG1	2.32	0.44
2:C:270:GLN:HB3	2:C:352:SER:HB2	2.00	0.44
4:I:74:ILE:HG12	4:I:80:ARG:HA	2.00	0.44
2:C:33:LEU:CD2	2:C:38:HIS:CB	2.72	0.44
2:A:502:MET:SD	2:A:523:ARG:HG2	2.57	0.44
5:B:758:THR:O	2:C:535:TYR:HE2	2.00	0.44
5:B:763:ILE:CD1	5:B:765:LEU:HD11	2.48	0.44
1:D:404:ASP:O	1:D:475:THR:OG1	2.32	0.43
1:D:258:VAL:HB	1:D:262:VAL:HG21	1.99	0.43
5:B:244:ARG:HH22	5:B:397:SER:HB2	1.83	0.43
2:C:780:HIS:ND1	2:C:785:MET:HG3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LEU:HD23	1:D:748:LEU:HD22	2.00	0.43
2:A:28:ASN:HB3	2:A:87:VAL:HG12	2.00	0.43
2:A:90:ILE:HB	2:A:118:VAL:HG13	2.01	0.43
2:A:287:VAL:HG13	2:A:330:TYR:CZ	2.53	0.43
5:B:728:PHE:HE2	5:B:730:TYR:HB2	1.82	0.43
2:C:363:GLN:C	2:C:375:ASN:HD21	2.26	0.43
5:B:728:PHE:CE2	5:B:730:TYR:HB2	2.53	0.43
2:C:403:ILE:HG12	2:C:404:HIS:H	1.84	0.43
5:B:525:SER:OG	5:B:763:ILE:HG12	2.18	0.43
2:C:487:GLN:HB2	2:C:498:TRP:CZ2	2.53	0.43
1:D:37:ILE:HB	1:D:68:VAL:HG22	1.99	0.43
1:D:132:MET:HG2	1:D:261:LEU:CD2	2.48	0.43
2:A:287:VAL:CG2	2:A:338:VAL:HG11	2.48	0.43
2:A:399:LYS:HB3	2:A:477:HIS:CE1	2.49	0.43
2:A:539:THR:HG22	2:A:751:GLU:O	2.18	0.43
5:B:99:VAL:HG22	5:B:125:LEU:HD12	2.01	0.43
5:B:365:VAL:O	5:B:373:GLU:N	2.31	0.43
5:B:662:VAL:HG22	5:B:669:LYS:HD2	2.00	0.43
6:J:21:VAL:HA	6:J:45:GLY:HA3	1.99	0.43
5:B:160:LYS:NZ	5:B:383:LEU:HB3	2.34	0.43
5:B:670:PHE:HB3	5:B:701:MET:HE1	2.01	0.43
2:C:79:CYS:SG	2:C:80:GLU:N	2.92	0.43
2:C:123:THR:OG1	2:C:125:MET:HG2	2.18	0.43
2:A:106:PRO:O	2:A:110:THR:HG23	2.18	0.43
2:A:440:ASN:N	2:A:449:HIS:O	2.51	0.43
2:A:789:ASP:O	2:A:794:ARG:N	2.39	0.43
3:F:67:TRP:HZ2	3:F:70:TRP:CD1	2.35	0.43
5:B:763:ILE:HD12	5:B:765:LEU:HD11	2.00	0.43
2:C:44:GLU:OE2	2:C:48:GLN:NE2	2.48	0.43
1:D:148:PRO:HB3	1:D:360:PRO:HG2	2.01	0.43
2:A:167:VAL:HG11	2:A:173:GLY:HA2	2.01	0.43
2:A:787:ASP:O	2:A:791:THR:HG23	2.19	0.43
3:F:67:TRP:CZ2	3:F:70:TRP:HD1	2.35	0.43
2:C:365:GLY:HA2	2:C:374:PRO:HA	2.00	0.43
2:C:762:MET:HB3	2:C:762:MET:HE3	1.76	0.43
5:B:144:PHE:HE2	5:B:146:GLN:HE21	1.67	0.43
5:B:380:ASN:OD1	5:B:381:GLN:N	2.50	0.43
3:H:67:TRP:CZ2	3:H:70:TRP:HD1	2.35	0.43
2:A:353:ILE:N	2:A:365:GLY:O	2.45	0.42
2:C:440:ASN:N	2:C:449:HIS:O	2.50	0.42
2:C:443:SER:HB3	2:C:444:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:ARG:HG2	2:C:319:PRO:HD3	2.02	0.42
2:A:471:ASN:C	2:A:471:ASN:HD22	2.28	0.42
2:A:631:ILE:O	2:A:634:MET:HG2	2.19	0.42
4:G:62:TYR:HE1	4:G:115:GLN:HB3	1.84	0.42
2:C:515:ALA:O	2:C:517:LEU:N	2.52	0.42
2:A:169:ASP:O	2:A:173:GLY:N	2.52	0.42
5:B:39:LEU:O	5:B:100:PHE:HA	2.19	0.42
2:C:778:LYS:O	2:C:781:GLU:HG3	2.20	0.42
1:D:760:THR:CG2	1:D:761:GLY:N	2.59	0.42
2:C:247:TRP:O	2:C:248:LEU:HG	2.19	0.42
1:D:674:PRO:HB2	1:D:705:TYR:CZ	2.55	0.42
2:C:265:GLY:HA3	2:C:382:PRO:HG3	2.02	0.42
1:D:111:ILE:O	1:D:115:ILE:HD12	2.19	0.42
4:I:25:THR:O	4:I:44:LYS:N	2.41	0.42
2:A:293:HIS:HA	2:A:296:LEU:HD12	2.01	0.42
2:C:302:THR:OG1	2:C:317:THR:OG1	2.26	0.42
1:D:62:LEU:CD1	1:D:64:VAL:CB	2.95	0.42
2:A:414:THR:HG21	2:A:418:GLY:HA2	2.02	0.42
1:D:172:VAL:HG22	1:D:203:LEU:CG	2.49	0.42
1:D:498:ILE:O	1:D:502:VAL:HG23	2.20	0.42
1:D:177:PRO:HB3	2:C:132:SER:HB3	2.01	0.41
1:D:413:GLU:H	1:D:417:VAL:HB	1.84	0.41
2:A:743:LYS:HD2	2:A:746:LEU:HD11	2.01	0.41
4:I:62:TYR:HE1	4:I:115:GLN:HB3	1.84	0.41
2:A:212:ARG:HH22	2:A:238:LEU:HB3	1.85	0.41
1:D:534:ILE:HD13	1:D:691:THR:HG23	2.01	0.41
5:B:93:ALA:CB	6:J:123:ILE:HD13	2.50	0.41
5:B:110:ALA:HB2	5:B:131:ALA:HA	2.02	0.41
5:B:310:PHE:HB3	5:B:313:ILE:HD11	2.01	0.41
4:I:89:THR:N	4:I:100:THR:O	2.48	0.41
1:D:288:GLY:O	1:D:292:ARG:HG3	2.19	0.41
5:B:717:LEU:HD22	5:B:738:LYS:NZ	2.36	0.41
5:B:763:ILE:HG13	5:B:765:LEU:CD1	2.51	0.41
2:C:25:LYS:O	2:C:59:GLN:N	2.50	0.41
2:C:332:ASP:OD1	2:C:333:GLY:N	2.54	0.41
2:A:217:ARG:HB3	2:A:245:TYR:HA	2.03	0.41
2:A:650:ASN:OD1	2:A:651:LEU:N	2.53	0.41
5:B:251:TYR:HA	5:B:396:PHE:HE2	1.85	0.41
2:C:33:LEU:HA	2:C:94:HIS:HE1	1.85	0.41
1:D:216:ILE:HG22	1:D:243:VAL:HG11	2.03	0.41
1:D:674:PRO:HB2	1:D:705:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:732:ASP:HB3	1:D:735:VAL:HG22	2.03	0.41
2:A:150:VAL:HG21	2:A:351:TYR:HD2	1.85	0.41
4:G:63:GLN:NE2	4:G:112:TYR:OH	2.53	0.41
5:B:340:ASN:ND2	10:B:1501:NAG:C7	2.84	0.41
2:C:204:VAL:O	2:C:208:LEU:HG	2.20	0.41
2:C:351:TYR:HB2	2:C:367:TYR:HB3	2.02	0.41
6:J:53:ILE:HD13	6:J:53:ILE:HA	1.91	0.41
1:D:42:VAL:HG22	1:D:73:MET:CB	2.51	0.41
1:D:78:PRO:O	1:D:82:ILE:HG12	2.20	0.41
2:A:162:HIS:HB2	2:A:392:TYR:CE1	2.56	0.41
2:A:218:VAL:HA	2:A:246:VAL:HB	2.03	0.41
2:A:763:ARG:HA	2:A:763:ARG:HD2	1.83	0.41
2:C:776:ILE:HD13	2:C:776:ILE:HA	1.94	0.41
2:A:38:HIS:CE1	3:F:95:SER:CB	3.02	0.41
5:B:231:CYS:O	5:B:261:VAL:HG23	2.14	0.41
2:C:247:TRP:O	2:C:248:LEU:HD23	2.21	0.41
2:C:364:VAL:CB	2:C:379:ILE:CG1	2.98	0.41
2:C:489:ARG:HA	2:C:495:LYS:C	2.46	0.41
2:C:749:THR:OG1	2:C:750:GLY:N	2.52	0.41
1:D:540:ARG:N	1:D:747:LYS:O	2.41	0.40
2:C:208:LEU:HB3	2:C:240:MET:SD	2.61	0.40
2:C:543:LYS:NZ	2:C:745:ASP:OD2	2.48	0.40
2:A:541:LEU:HB2	2:A:736:LEU:HD13	2.01	0.40
4:G:25:THR:O	4:G:44:LYS:N	2.40	0.40
2:C:287:VAL:HG13	2:C:330:TYR:CZ	2.55	0.40
2:A:161:ASN:OD1	2:A:187:ARG:NH1	2.46	0.40
2:A:199:PRO:HB3	2:A:227:ASP:OD2	2.21	0.40
5:B:98:LEU:HD12	5:B:98:LEU:HA	1.90	0.40
5:B:114:ASP:OD1	5:B:144:PHE:HB3	2.21	0.40
5:B:135:MET:CG	5:B:146:GLN:HE22	2.34	0.40
2:C:160:TRP:CH2	2:C:246:VAL:HG11	2.55	0.40
2:C:538:LEU:HB2	2:C:753:PHE:CE2	2.57	0.40
5:B:416:PHE:CD1	5:B:459:PHE:HB3	2.53	0.40
2:C:364:VAL:CB	2:C:379:ILE:HG12	2.52	0.40
3:H:121:ILE:HG12	3:H:126:TYR:HA	2.03	0.40
4:I:63:GLN:NE2	4:I:112:TYR:OH	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	666/1482 (45%)	629 (94%)	37 (6%)	0	100	100
2	A	681/938 (73%)	648 (95%)	33 (5%)	0	100	100
2	C	685/938 (73%)	659 (96%)	26 (4%)	0	100	100
3	F	117/277 (42%)	116 (99%)	1 (1%)	0	100	100
3	H	117/277 (42%)	116 (99%)	1 (1%)	0	100	100
4	G	112/244 (46%)	108 (96%)	4 (4%)	0	100	100
4	I	112/244 (46%)	108 (96%)	4 (4%)	0	100	100
5	B	660/1464 (45%)	626 (95%)	34 (5%)	0	100	100
6	J	104/141 (74%)	99 (95%)	5 (5%)	0	100	100
7	K	95/131 (72%)	93 (98%)	2 (2%)	0	100	100
All	All	3349/6136 (55%)	3202 (96%)	147 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	D	463/1297 (36%)	462 (100%)	1 (0%)	92	94
2	A	505/806 (63%)	505 (100%)	0	100	100
2	C	460/806 (57%)	459 (100%)	1 (0%)	92	94
3	F	49/225 (22%)	49 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	49/225 (22%)	49 (100%)	0	100	100
4	G	60/213 (28%)	60 (100%)	0	100	100
4	I	60/213 (28%)	60 (100%)	0	100	100
5	B	485/1308 (37%)	484 (100%)	1 (0%)	92	94
6	J	44/113 (39%)	44 (100%)	0	100	100
7	K	43/106 (41%)	43 (100%)	0	100	100
All	All	2218/5312 (42%)	2215 (100%)	3 (0%)	92	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	321	CYS
5	B	147	PHE
2	C	780	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	127	HIS
1	D	153	GLN
1	D	348	ASN
1	D	662	GLN
1	D	672	GLN
1	D	694	ASN
1	D	767	GLN
1	D	775	GLN
1	D	782	GLN
2	A	38	HIS
2	A	59	GLN
2	A	73	GLN
2	A	134	HIS
2	A	280	HIS
2	A	311	ASN
2	A	393	GLN
2	A	405	GLN
2	A	453	GLN
2	A	471	ASN
2	A	477	HIS
2	A	710	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	63	GLN
5	B	68	ASN
5	B	119	GLN
5	B	146	GLN
5	B	154	GLN
5	B	702	HIS
2	C	50	ASN
2	C	73	GLN
2	C	86	GLN
2	C	134	HIS
2	C	146	HIS
2	C	147	GLN
2	C	162	HIS
2	C	311	ASN
2	C	427	ASN
2	C	477	HIS
2	C	710	ASN
4	I	63	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	$\# Z > 2$
8	NAG	E	1	8,1	14,14,15	0.28	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	E	2	8	14,14,15	0.26	0	17,19,21	0.59	0
8	NAG	L	1	8,1	14,14,15	0.26	0	17,19,21	0.71	0
8	NAG	L	2	8	14,14,15	0.27	0	17,19,21	0.62	0
9	NAG	M	1	2,9	14,14,15	0.25	0	17,19,21	0.64	0
9	NAG	M	2	9	14,14,15	0.27	0	17,19,21	0.65	0
9	BMA	M	3	9	11,11,12	0.22	0	15,15,17	0.56	0
8	NAG	N	1	2,8	14,14,15	0.28	0	17,19,21	0.63	0
8	NAG	N	2	8	14,14,15	0.27	0	17,19,21	0.66	0
8	NAG	O	1	8	14,14,15	0.24	0	17,19,21	0.67	0
8	NAG	O	2	8	14,14,15	0.28	0	17,19,21	0.61	0
8	NAG	P	1	2,8	14,14,15	0.26	0	17,19,21	0.67	0
8	NAG	P	2	8	14,14,15	0.27	0	17,19,21	0.63	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
8	NAG	E	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	E	2	8	-	0/6/23/26	0/1/1/1
8	NAG	L	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
9	NAG	M	1	2,9	-	3/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
8	NAG	N	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	NAG	O	1	8	-	3/6/23/26	0/1/1/1
8	NAG	O	2	8	-	0/6/23/26	0/1/1/1
8	NAG	P	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

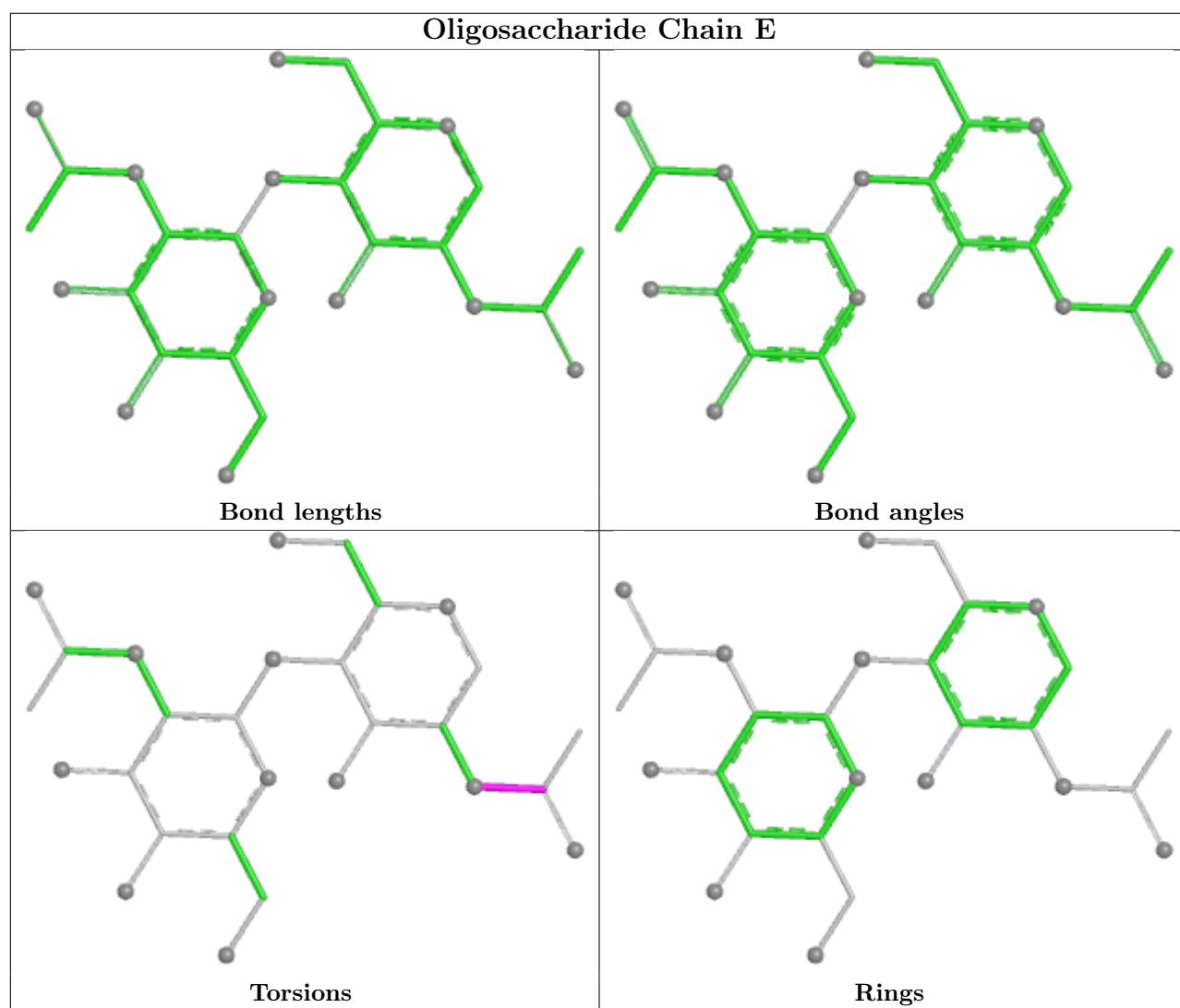
Mol	Chain	Res	Type	Atoms
8	L	1	NAG	O7-C7-N2-C2
8	O	1	NAG	C8-C7-N2-C2
8	O	1	NAG	O7-C7-N2-C2
8	P	1	NAG	C8-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2
9	M	1	NAG	C8-C7-N2-C2
9	M	1	NAG	O7-C7-N2-C2
8	E	1	NAG	C8-C7-N2-C2
8	N	1	NAG	C8-C7-N2-C2
8	N	1	NAG	O7-C7-N2-C2
8	E	1	NAG	O7-C7-N2-C2
8	L	1	NAG	C3-C2-N2-C7
8	O	1	NAG	C3-C2-N2-C7
9	M	1	NAG	C3-C2-N2-C7

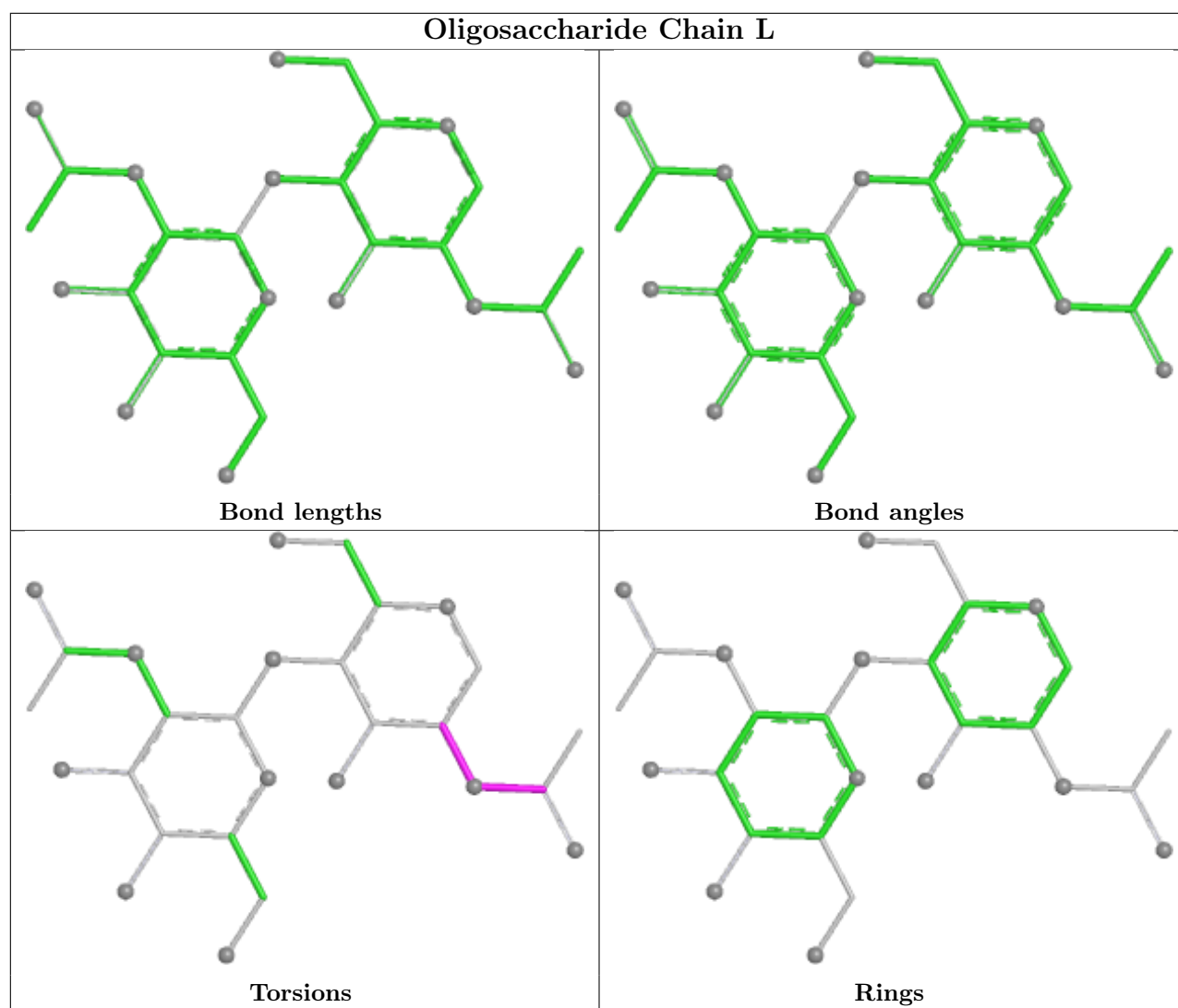
There are no ring outliers.

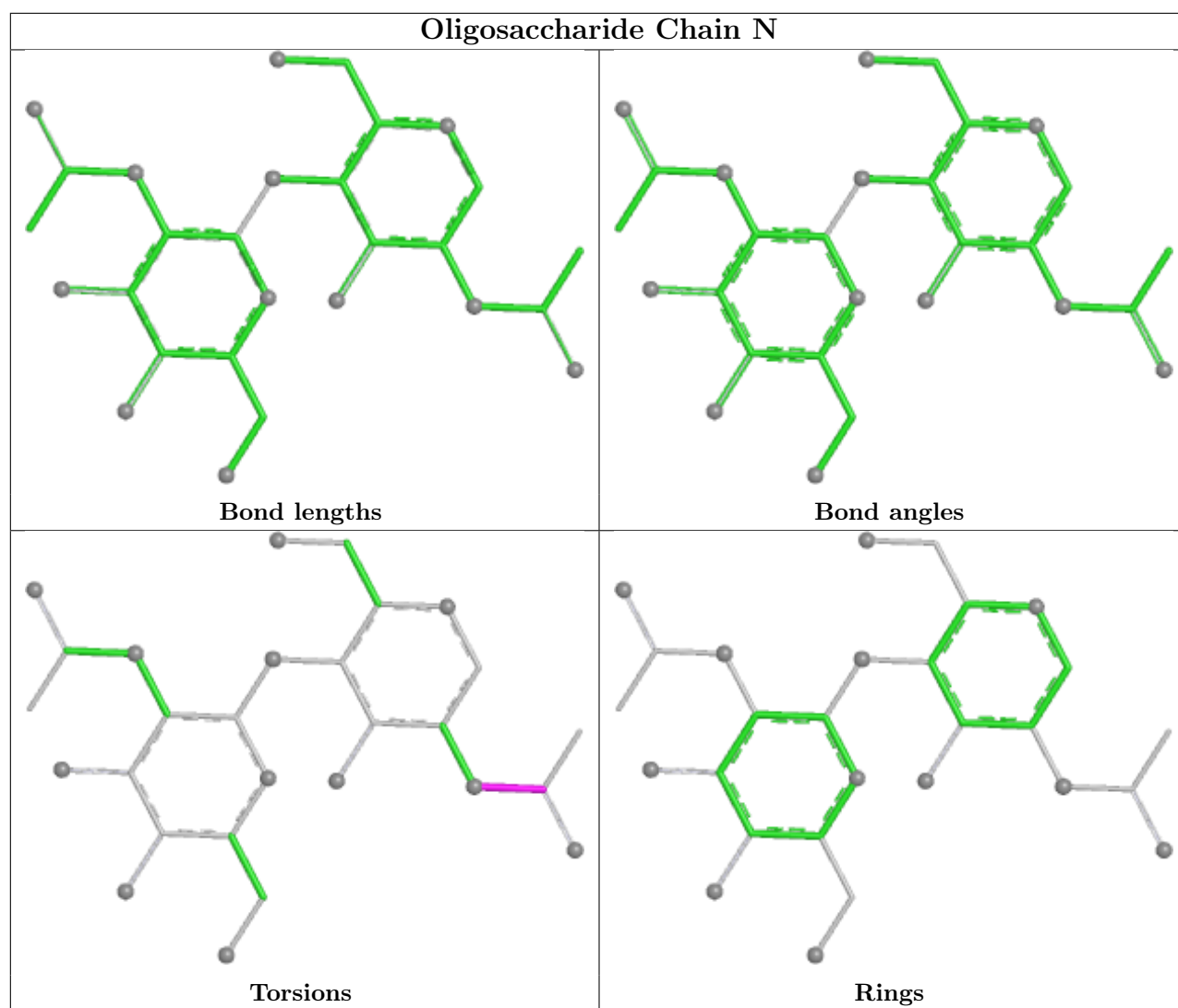
10 monomers are involved in 8 short contacts:

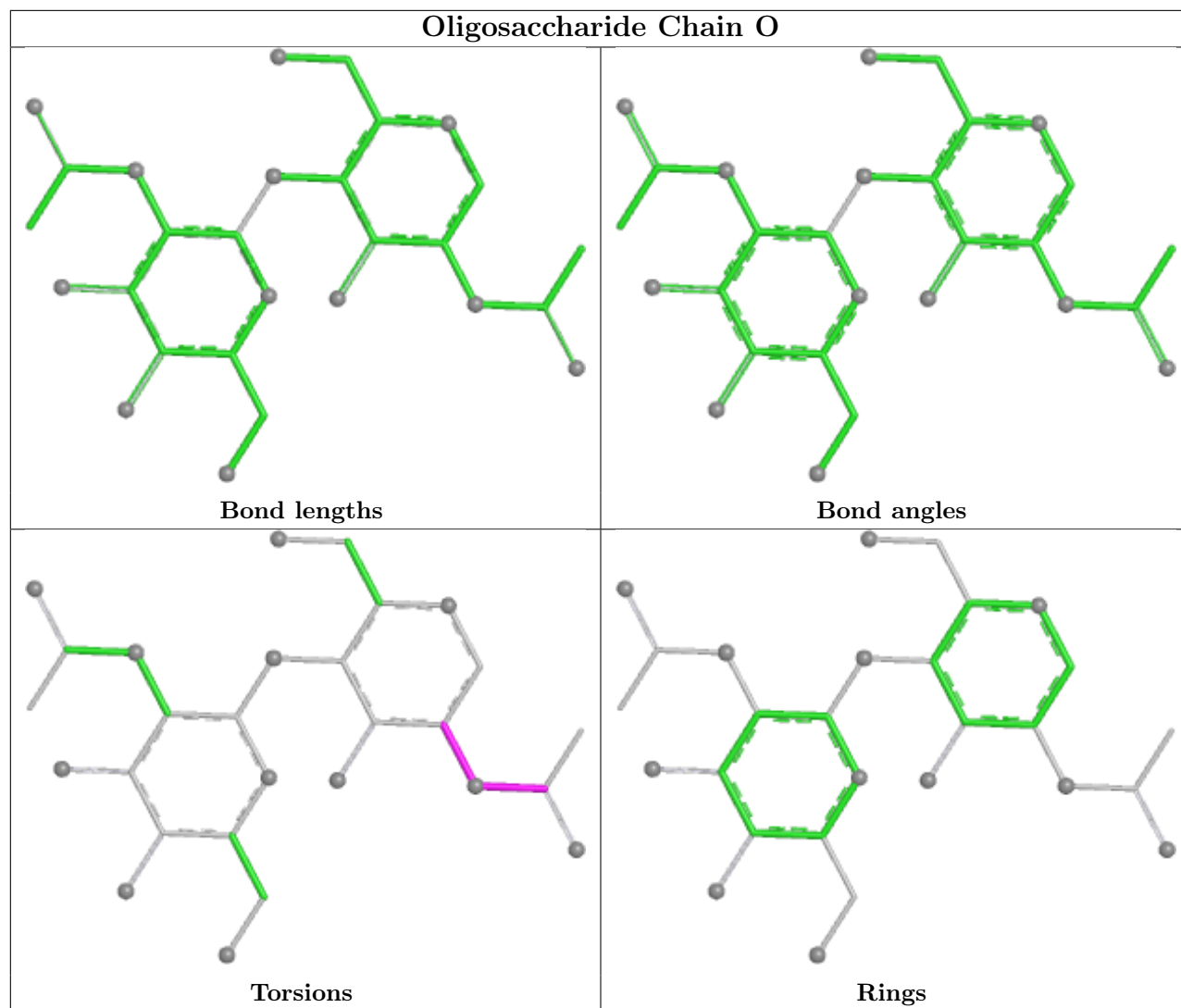
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1	NAG	1	0
8	L	1	NAG	1	0
8	P	1	NAG	1	0
8	L	2	NAG	1	0
8	O	2	NAG	1	0
8	N	2	NAG	1	0
8	O	1	NAG	4	0
8	N	1	NAG	1	0
9	M	2	NAG	1	0
8	P	2	NAG	1	0

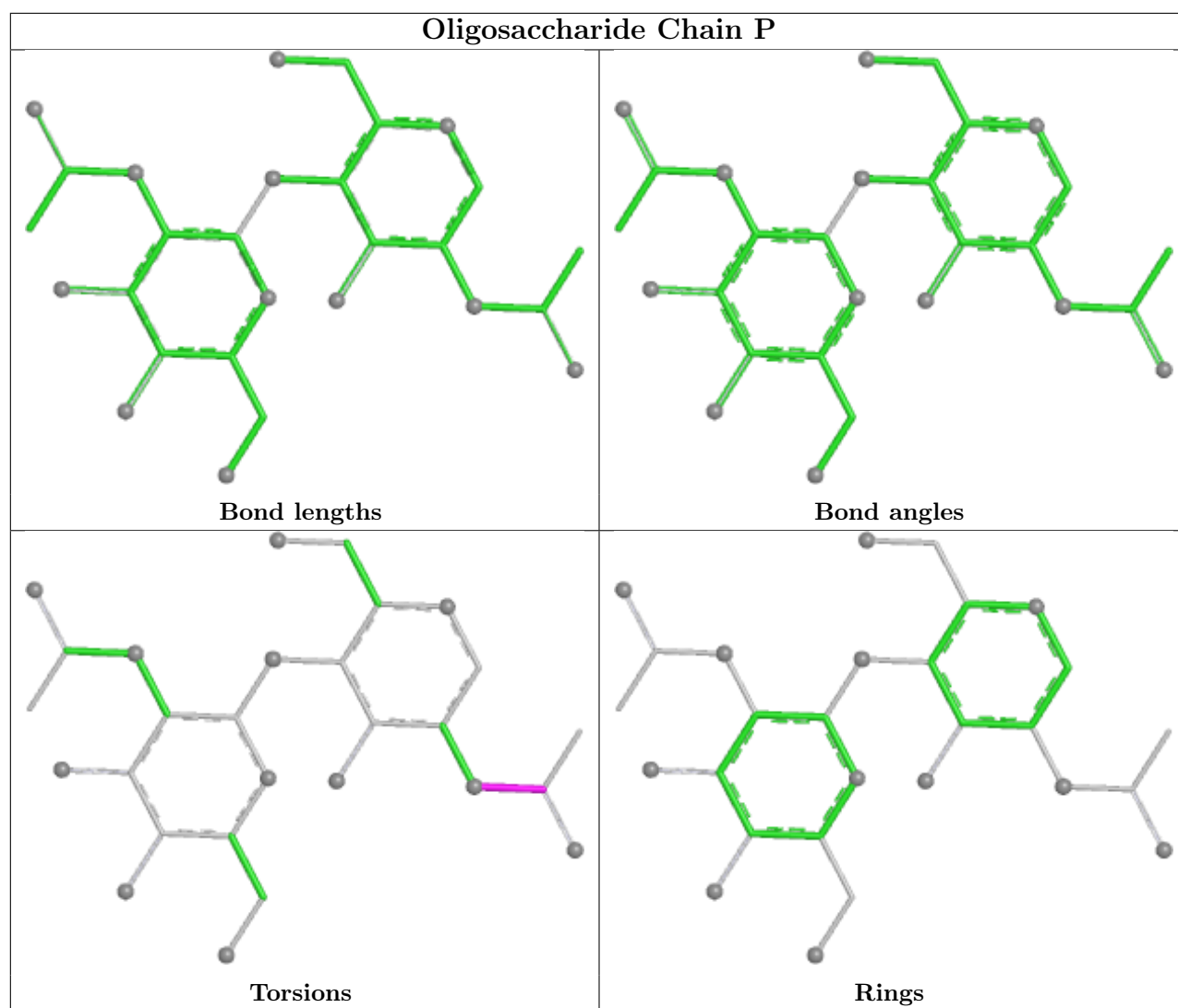
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

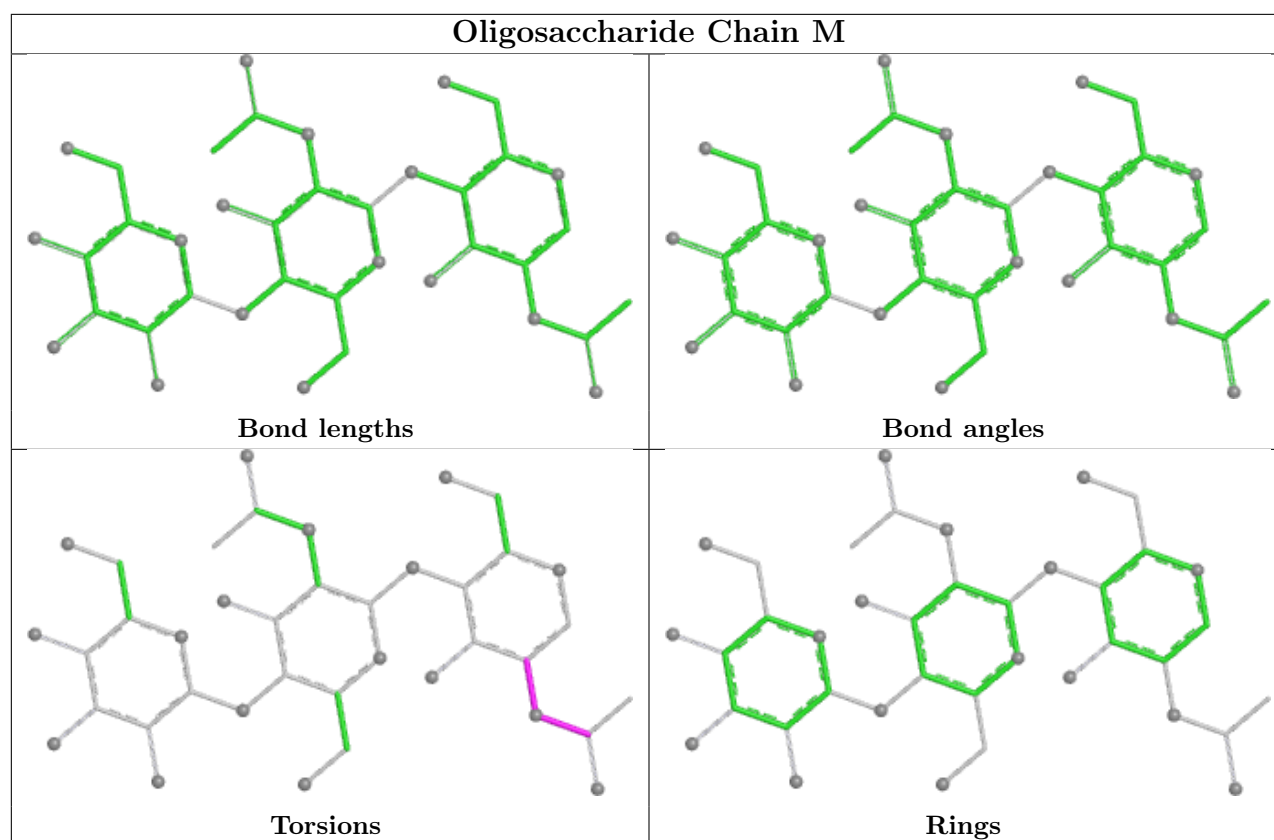












5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	B	1501	-	14,14,15	0.28	0	17,19,21	0.66	0
10	NAG	A	1001	2	14,14,15	0.26	0	17,19,21	0.70	0
10	NAG	C	1001	2	14,14,15	0.25	0	17,19,21	0.69	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
10	NAG	B	1501	-	-	2/6/23/26	0/1/1/1
10	NAG	A	1001	2	-	3/6/23/26	0/1/1/1
10	NAG	C	1001	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1001	NAG	C3-C2-N2-C7
10	A	1001	NAG	C8-C7-N2-C2
10	A	1001	NAG	O7-C7-N2-C2
10	C	1001	NAG	C3-C2-N2-C7
10	C	1001	NAG	O7-C7-N2-C2
10	C	1001	NAG	C8-C7-N2-C2
10	B	1501	NAG	O7-C7-N2-C2
10	B	1501	NAG	C8-C7-N2-C2

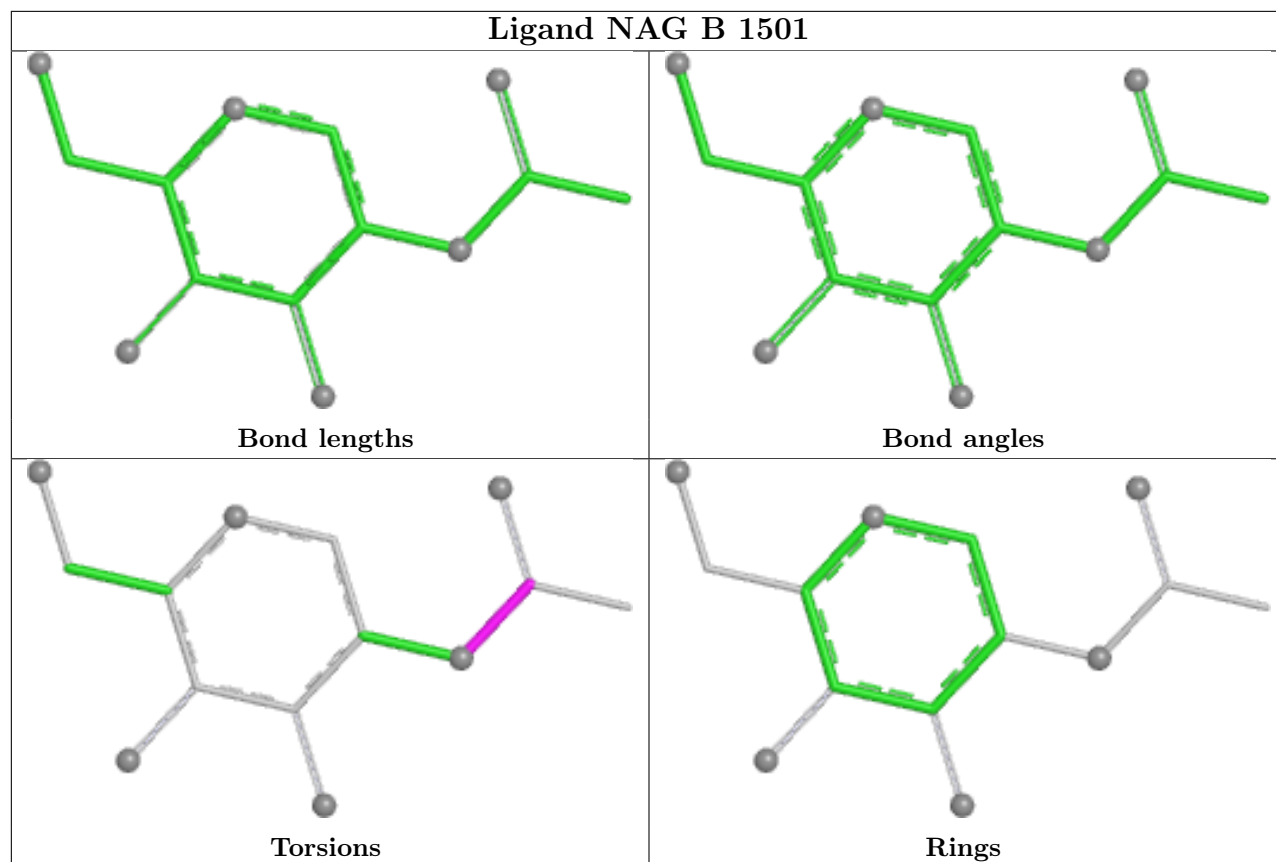
There are no ring outliers.

1 monomer is involved in 4 short contacts:

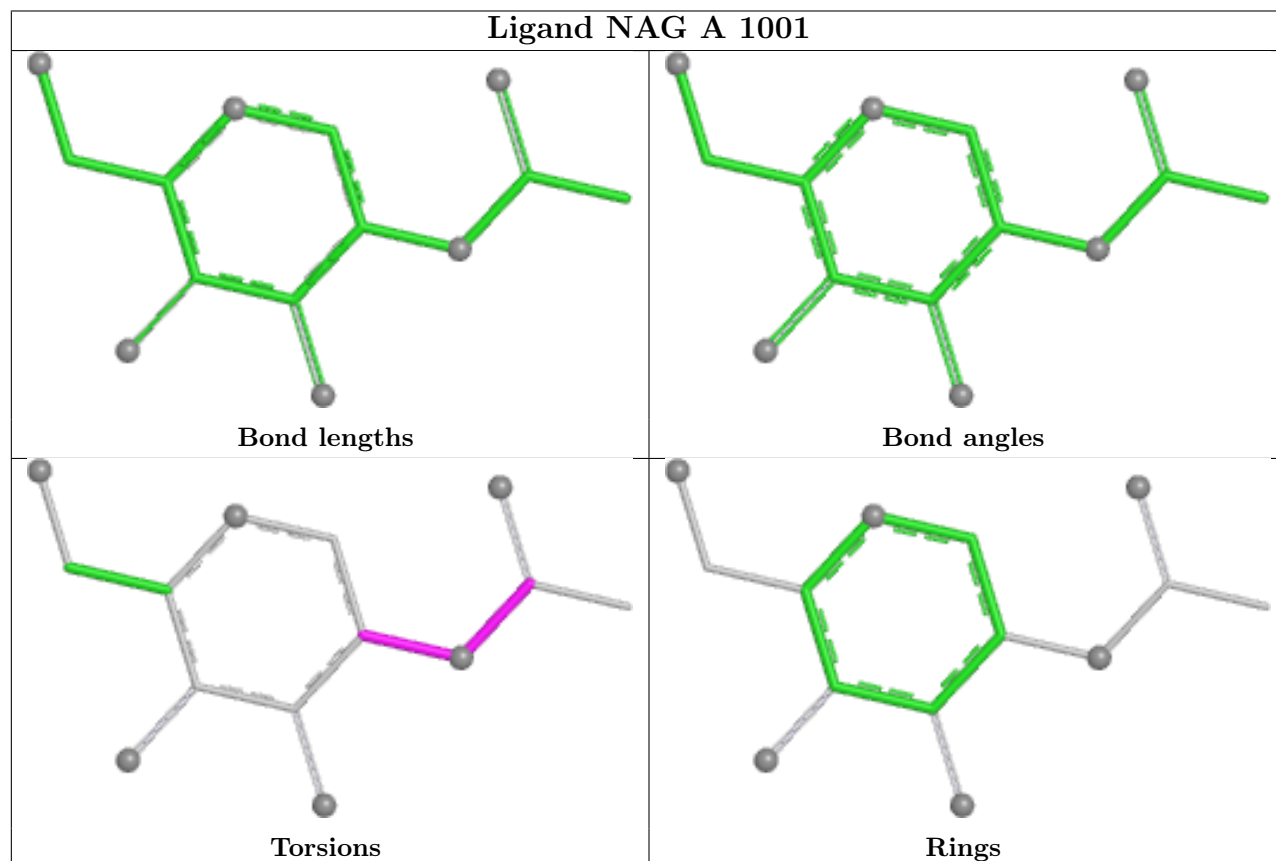
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1501	NAG	4	0

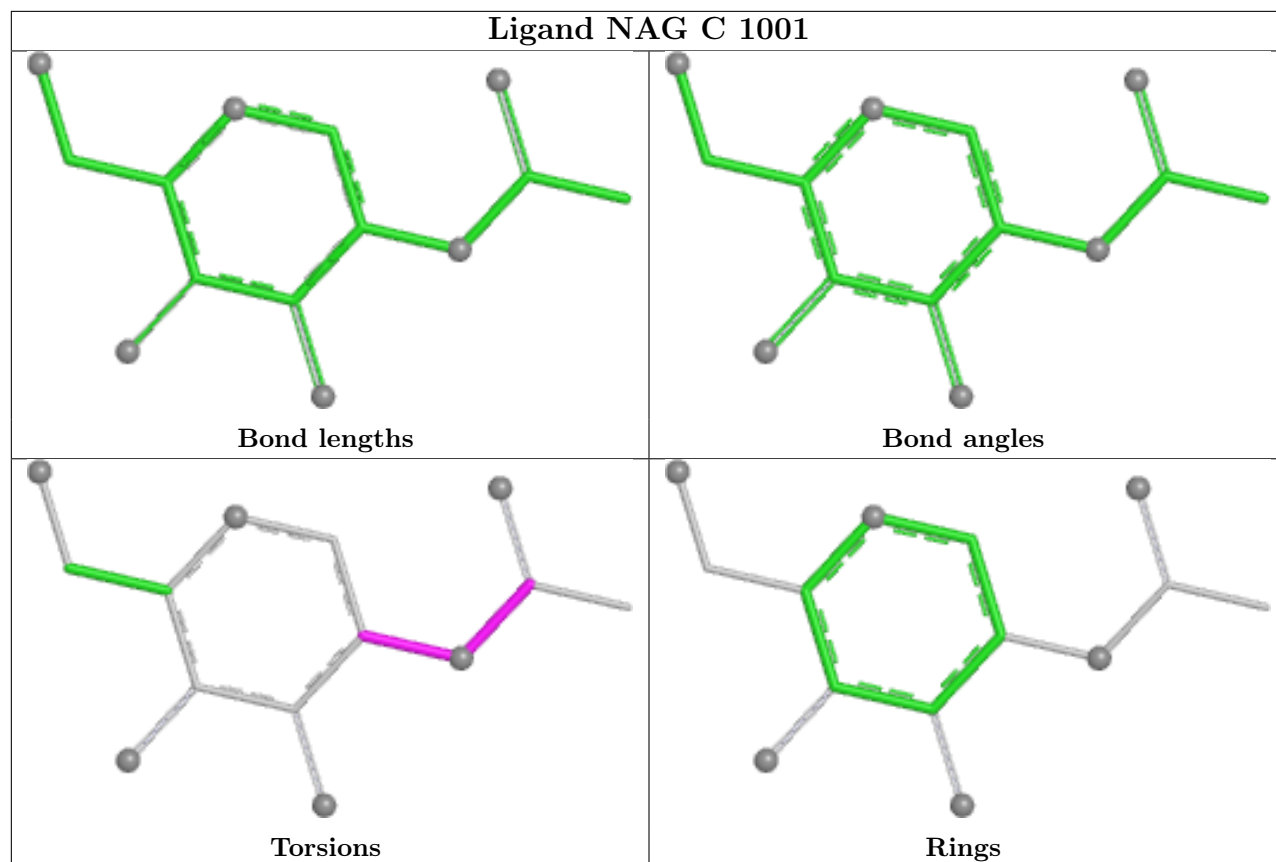
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAG B 1501



Ligand NAG A 1001





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.

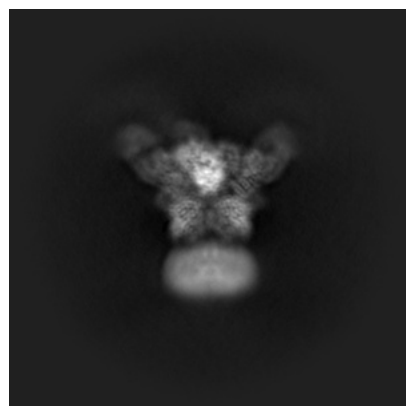
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72078. These allow visual inspection of the internal detail of the map and identification of artifacts.

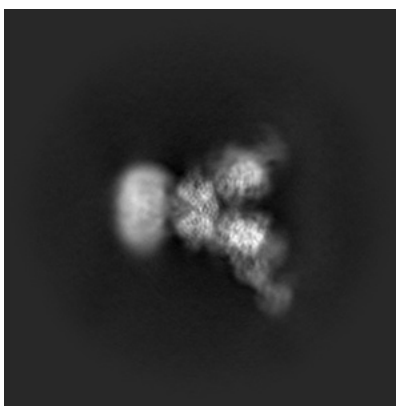
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

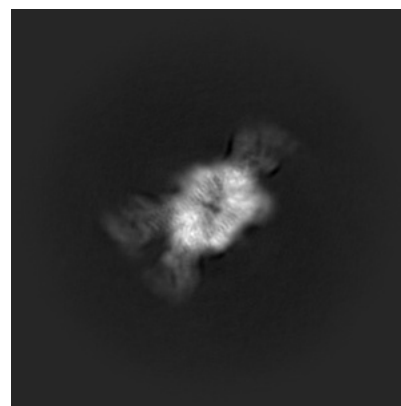
6.1.1 Primary map



X

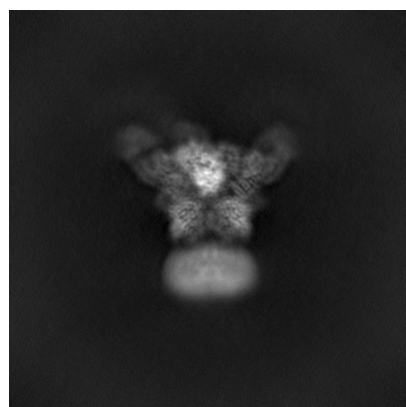


Y

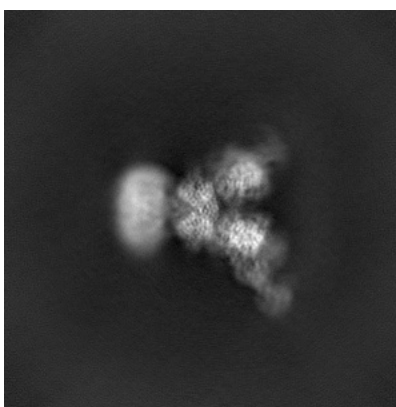


Z

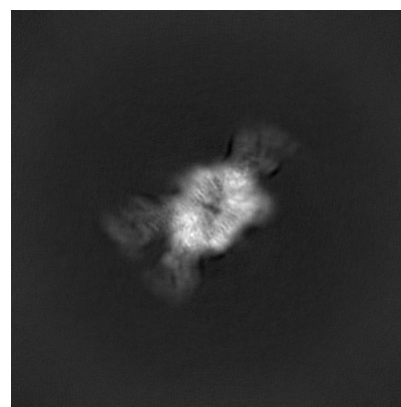
6.1.2 Raw map



X



Y

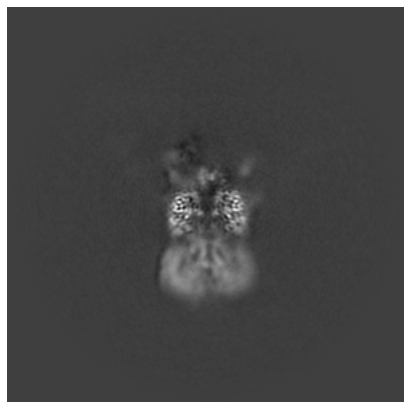


Z

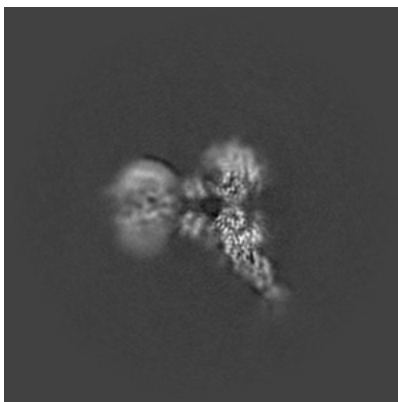
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

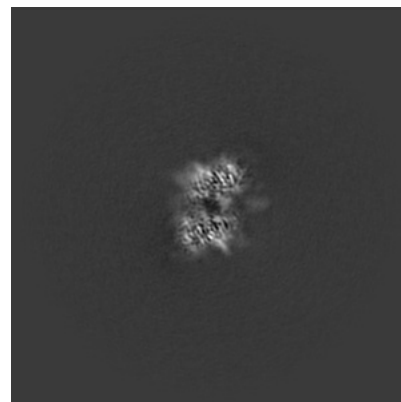
6.2.1 Primary map



X Index: 168

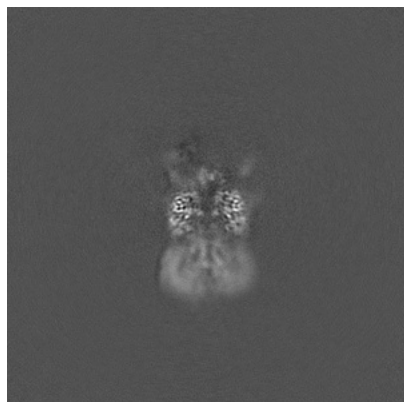


Y Index: 168

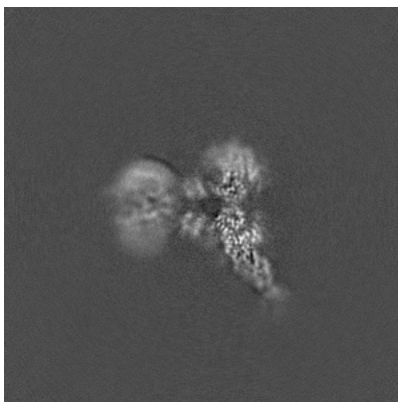


Z Index: 168

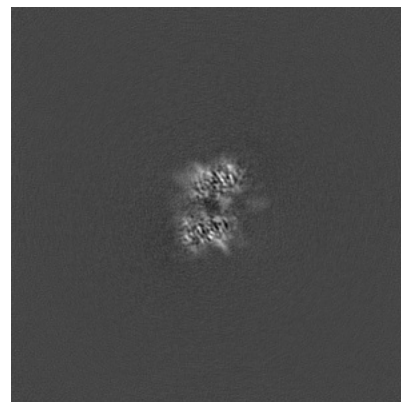
6.2.2 Raw map



X Index: 168



Y Index: 168

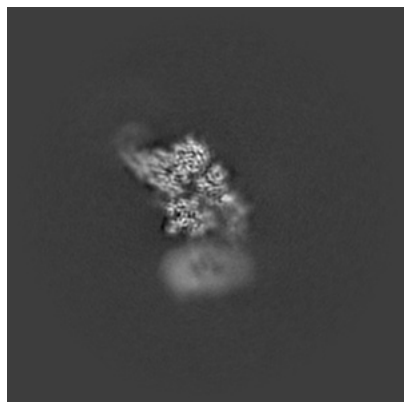


Z Index: 168

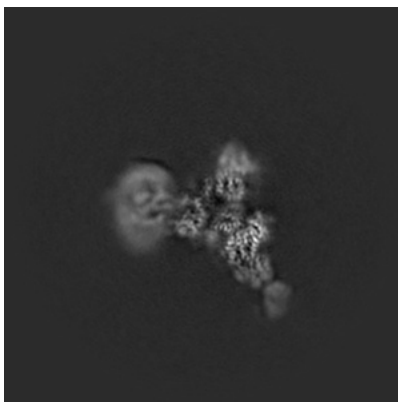
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

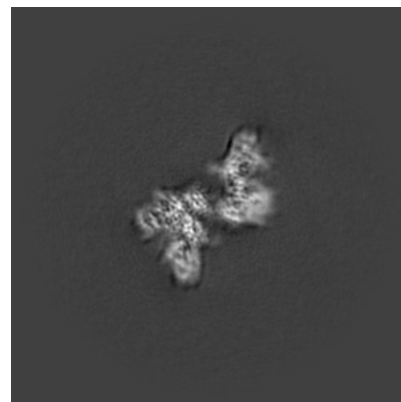
6.3.1 Primary map



X Index: 149

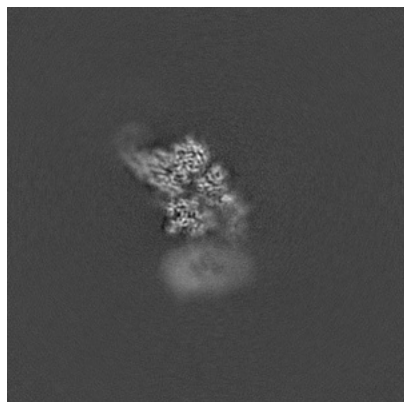


Y Index: 162



Z Index: 199

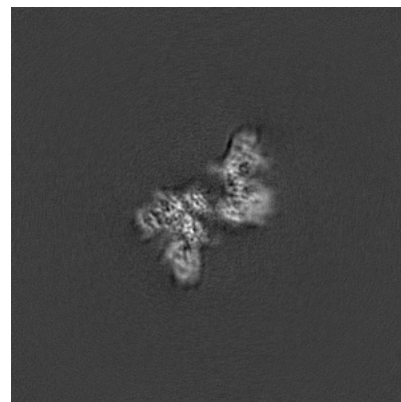
6.3.2 Raw map



X Index: 149



Y Index: 162



Z Index: 199

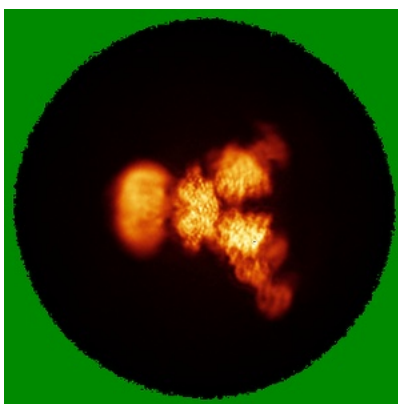
The images above show the largest variance slices of the map in three orthogonal directions.

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

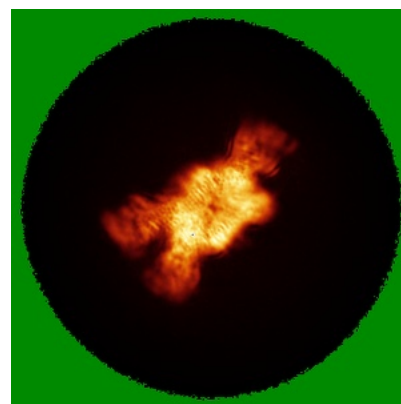
6.4.1 Primary map



X

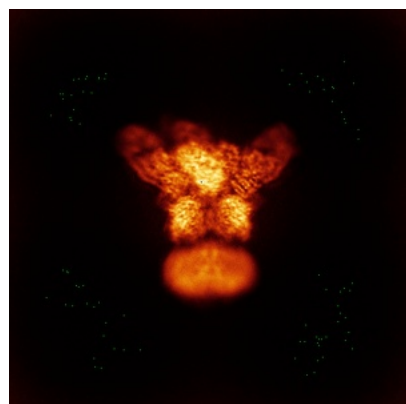


Y

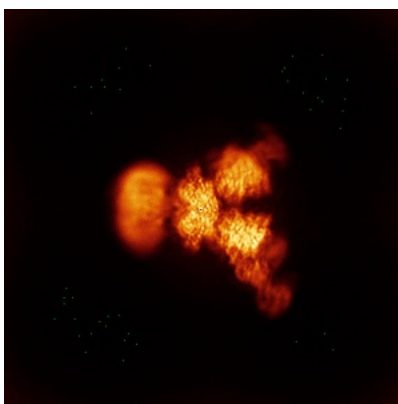


Z

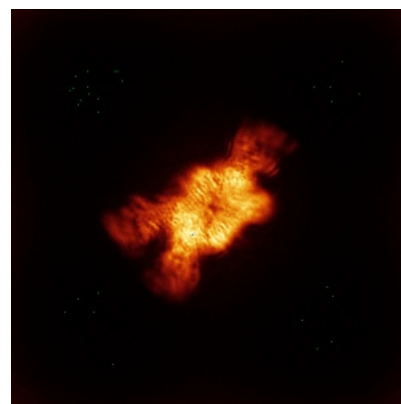
6.4.2 Raw map



X



Y

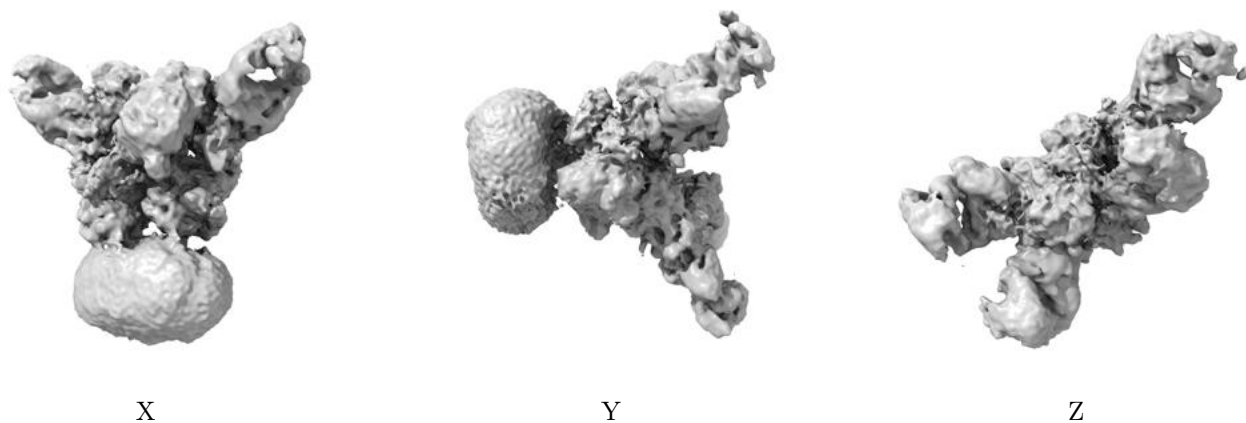


Z

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.

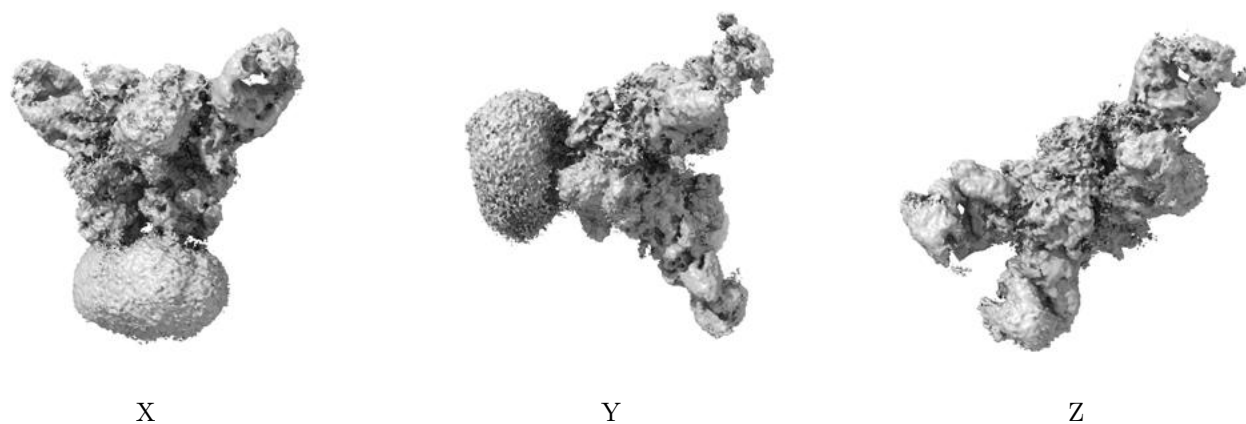
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

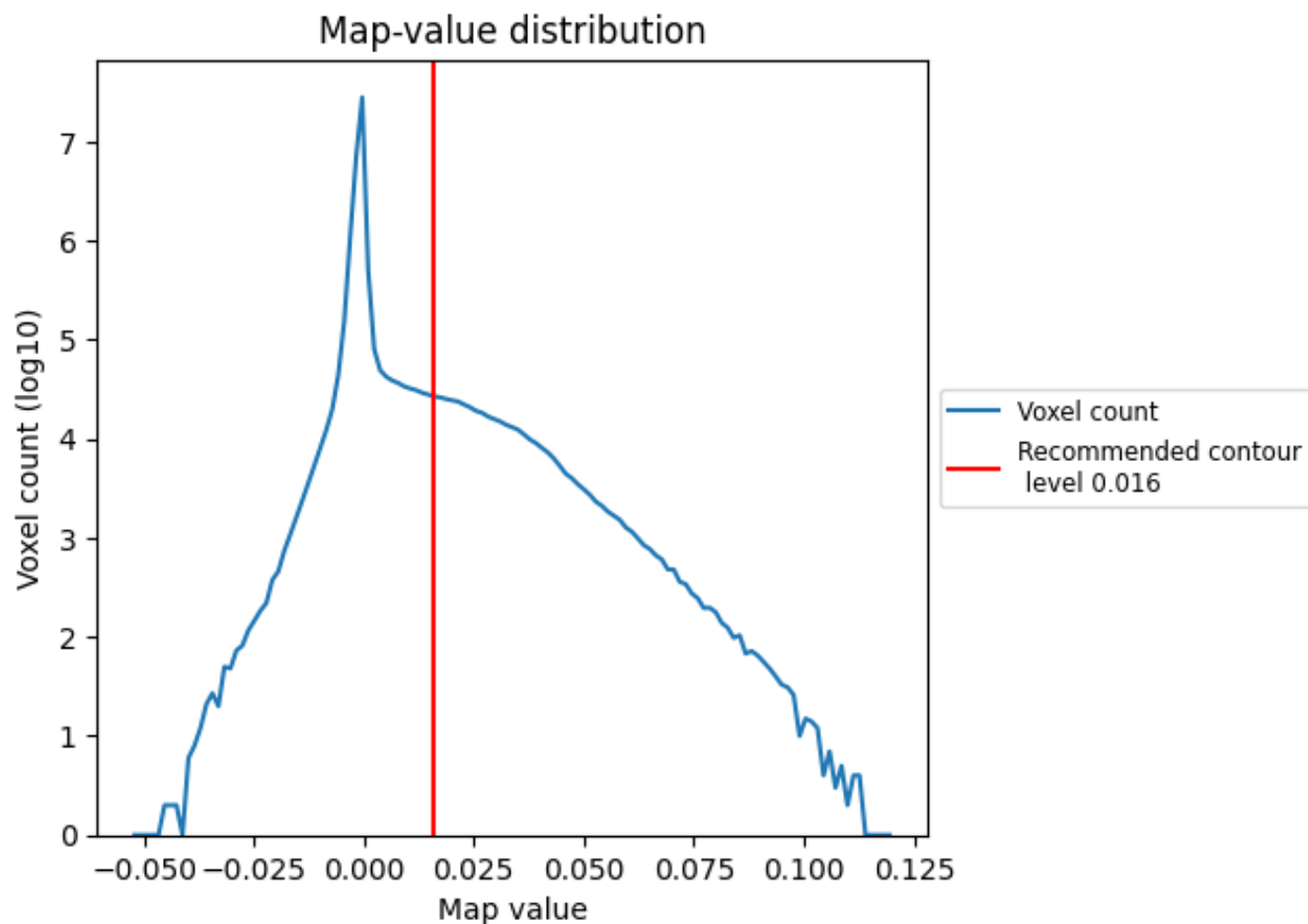
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

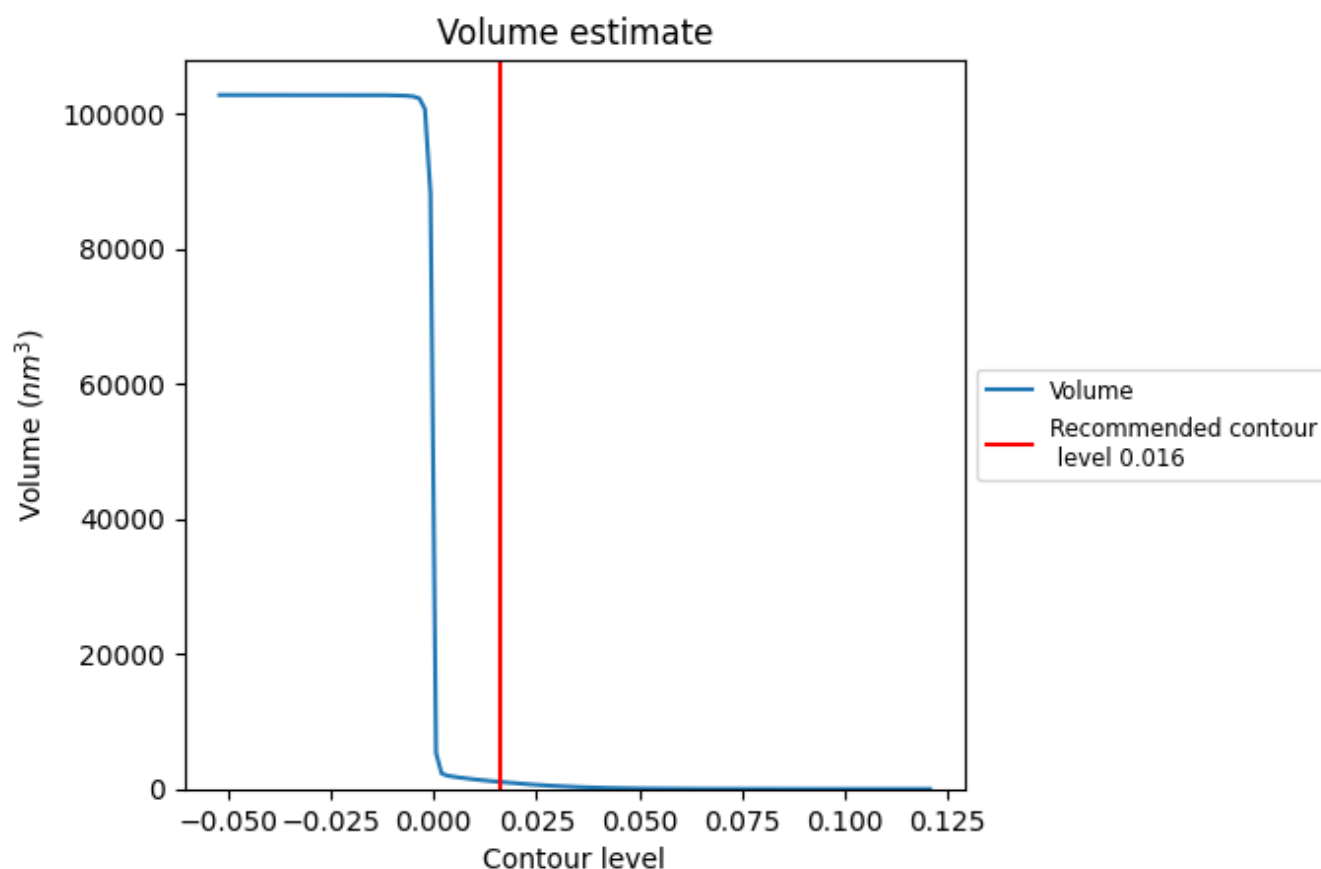
This section contains the results of statistical analysis of the map.

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.

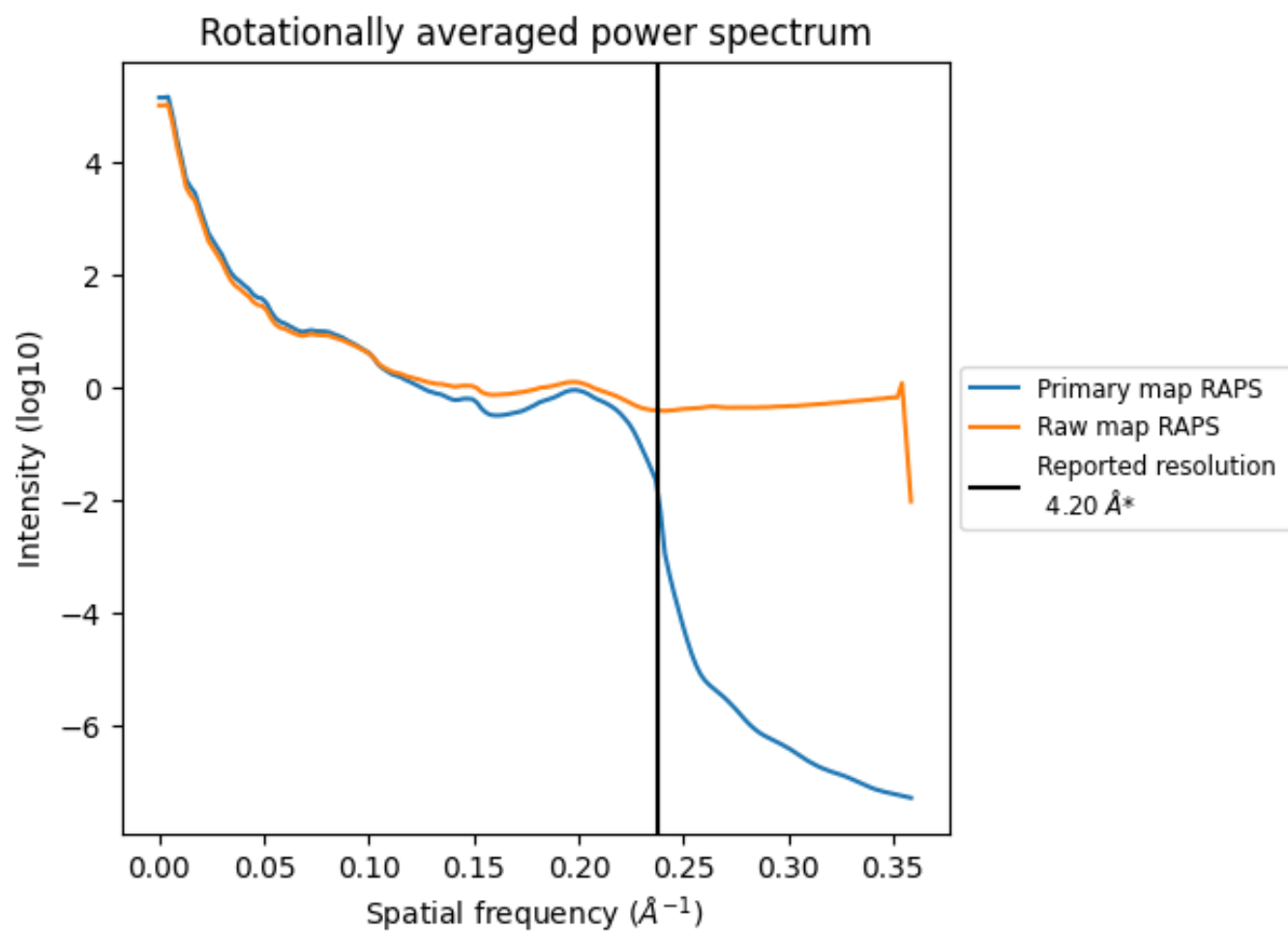
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1051 nm^3 ; this corresponds to an approximate mass of 949 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 ⓘ

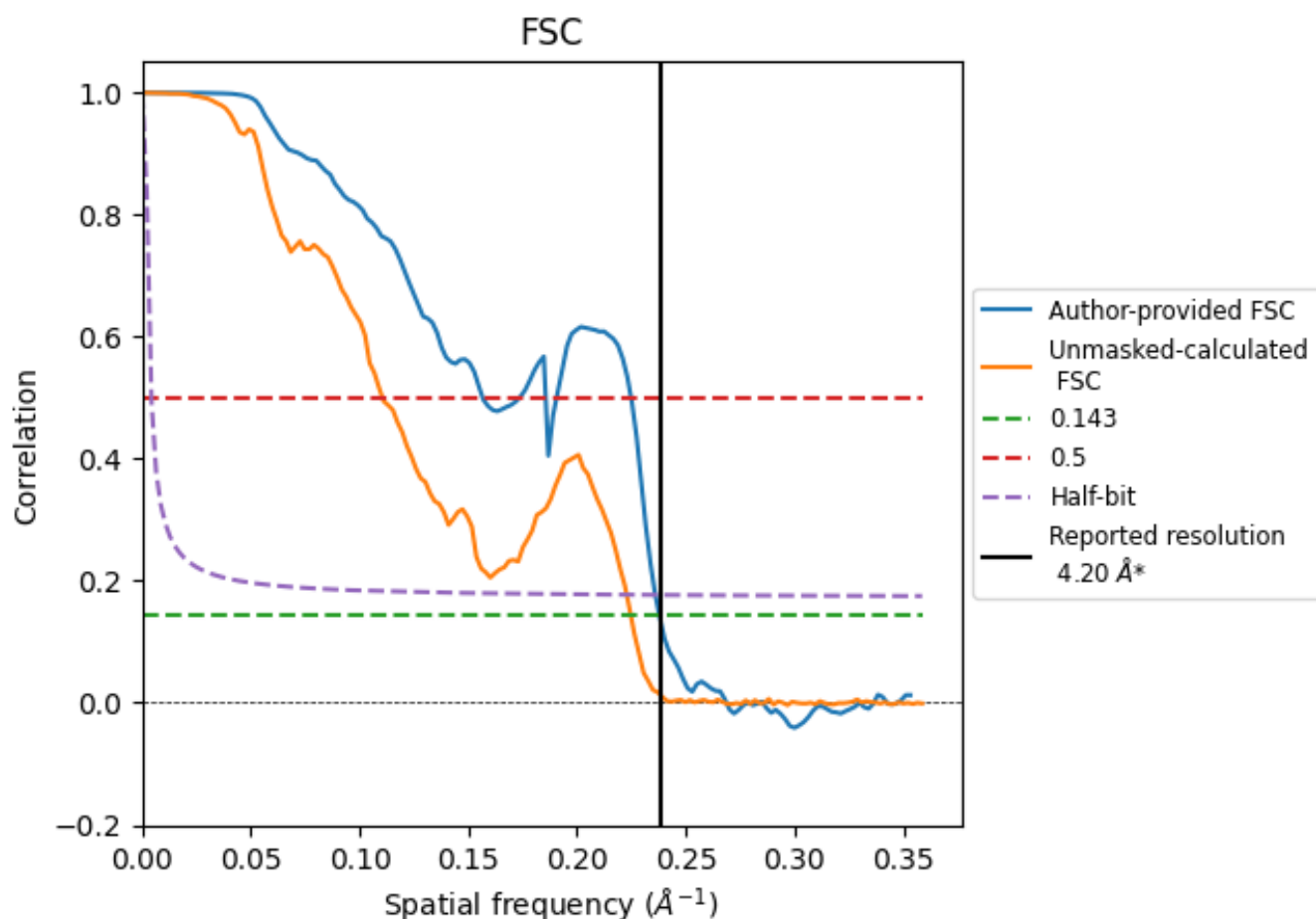


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

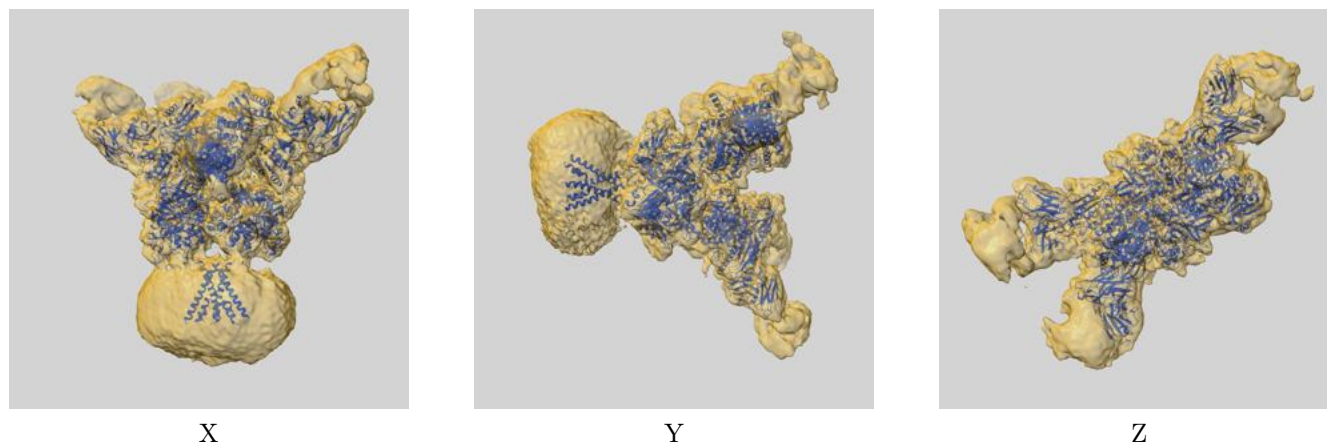
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	6.39	4.24
Unmasked-calculated*	4.45	9.05	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

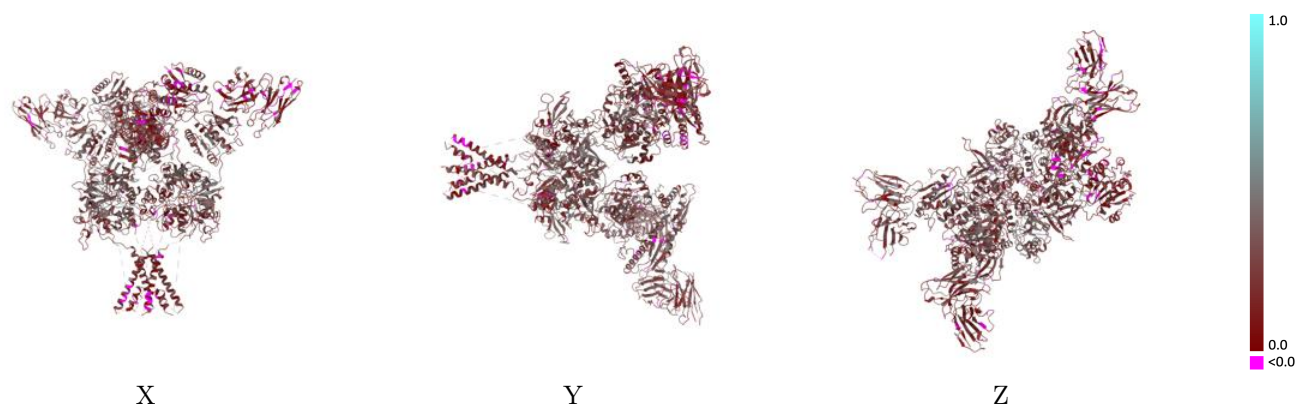
This section contains information regarding the fit between EMDB map EMD-72078 and PDB model 9PZS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



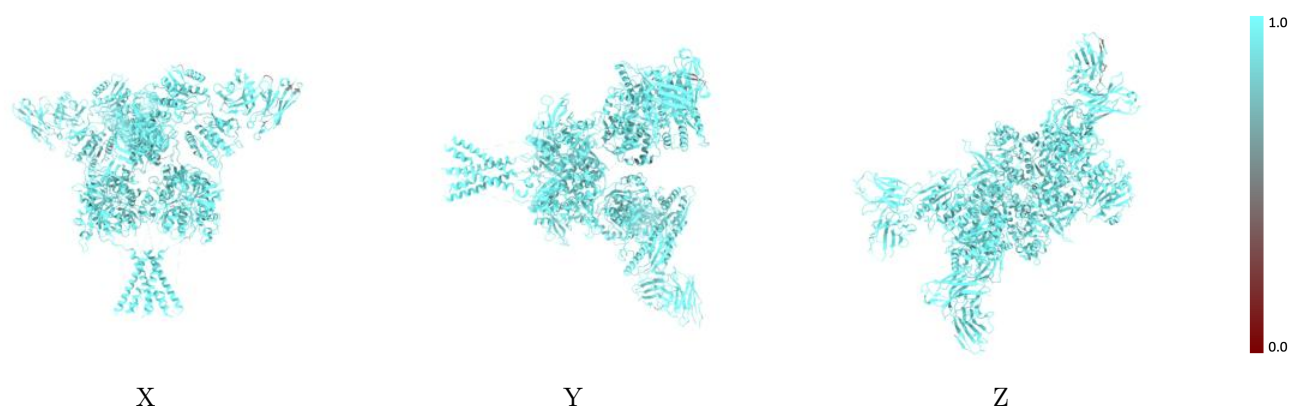
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



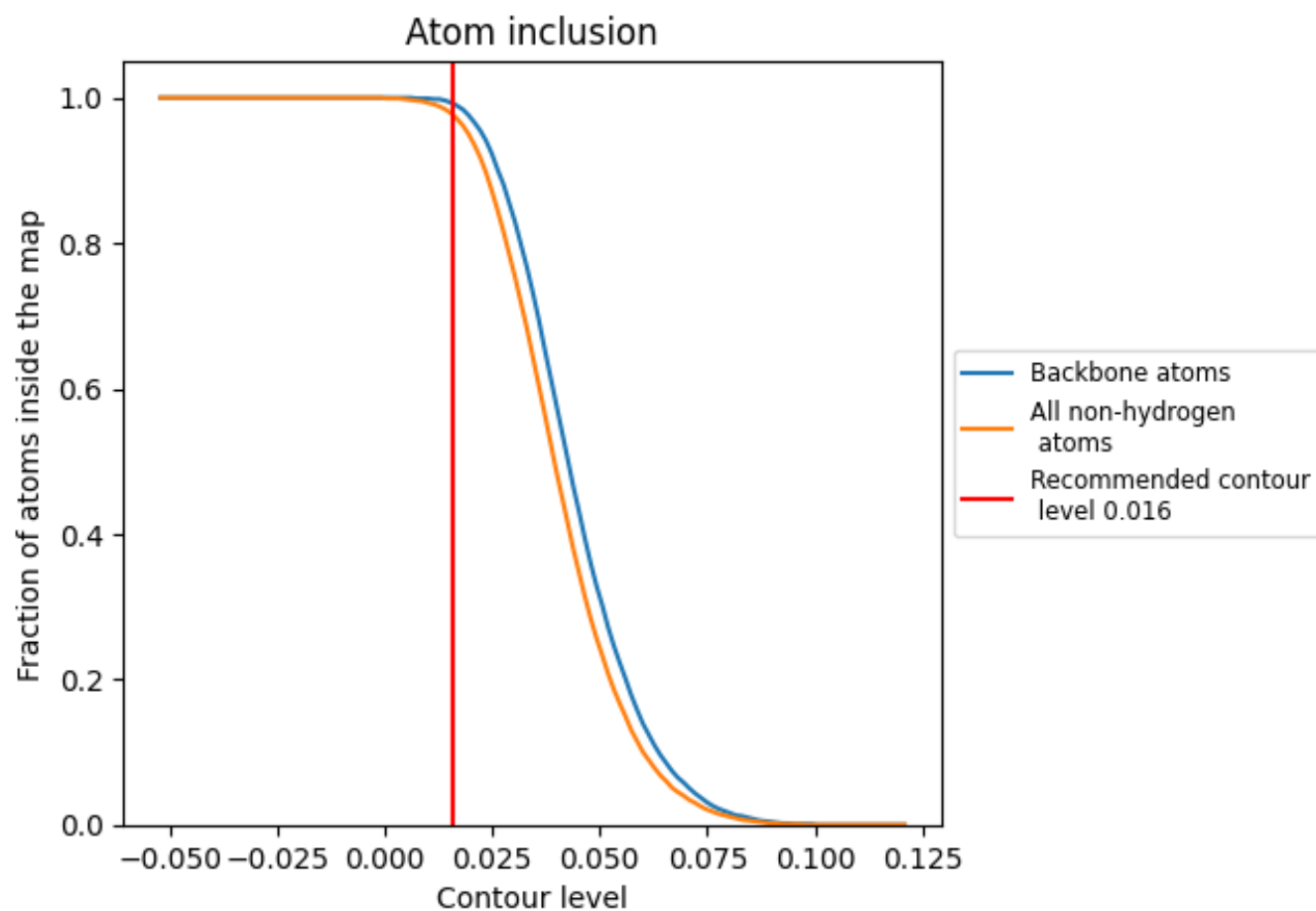
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.2670
A	 0.9740	 0.2890
B	 0.9760	 0.2860
C	 0.9750	 0.2660
D	 0.9830	 0.2730
E	 1.0000	 0.2420
F	 0.9930	 0.2490
G	 0.9730	 0.1820
H	 0.9760	 0.1760
I	 0.9450	 0.1680
J	 0.9680	 0.2670
K	 0.9710	 0.2620
L	 0.9640	 0.2820
M	 1.0000	 0.2840
N	 1.0000	 0.2130
O	 1.0000	 0.2480
P	 1.0000	 0.3120

