



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 11:25 PM EDT

PDB ID : 7UHF
EMDB ID : EMD-26513
Title : Human L-type voltage-gated calcium channel Cav1.3 in the presence of cinarizine at 3.1 Angstrom resolution
Authors : Gao, S.; Yao, X.; Yan, N.
Deposited on : 2022-03-26
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

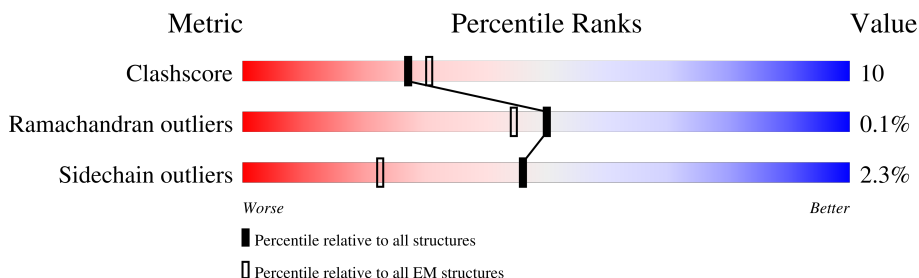
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	2161	<div> <div>28%</div> <div>44%</div> <div>12%</div> <div>43%</div> </div>
2	D	1103	<div> <div>8%</div> <div>73%</div> <div>13%</div> <div>14%</div> </div>
3	C	484	<div> <div>67%</div> <div>54%</div> <div>13%</div> <div>33%</div> </div>
4	B	3	<div> <div>67%</div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
5	E	2	<div> <div>100%</div> </div>
5	G	2	<div> <div>100%</div> </div>
5	H	2	<div> <div>50%</div> <div>100%</div> </div>
6	F	4	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20379 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 Voltage-dependent L-type calcium channel subunit alpha-1D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1230	Total	C	N	O	S	0	0
			9900	6517	1597	1715	71		

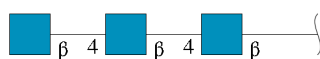
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2575	1619	467	479	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	B	3	Total	C	N	O	0	0
			42	24	3	15		

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



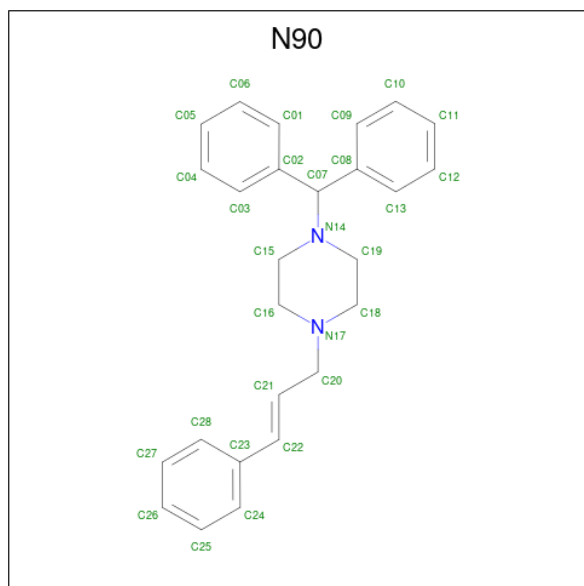
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is 1-(diphenylmethyl)-4-[(2E)-3-phenylprop-2-en-1-yl]piperazine (three-letter code: N90) (formula: C₂₆H₂₈N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N		0
			28	26	2		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).

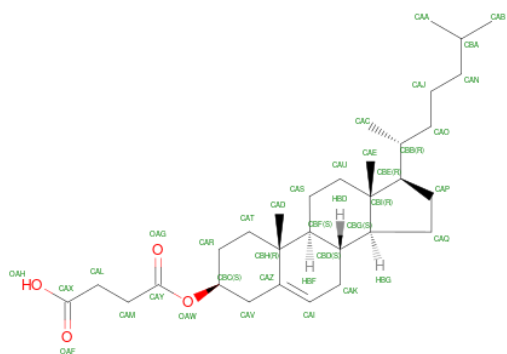


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

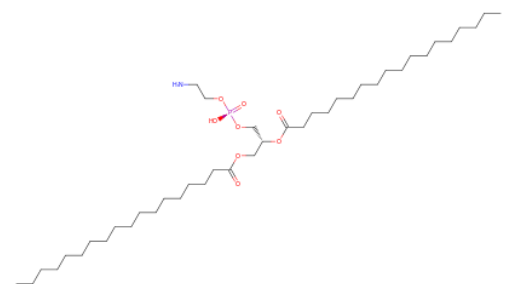
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Ca	0
			1	1	
9	D	1	Total	Ca	0
			1	1	

- Molecule 10 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



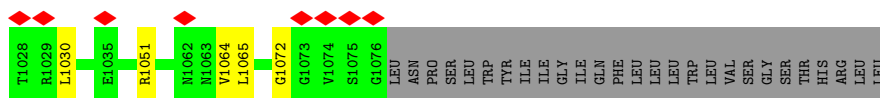
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			35	31	4	

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).

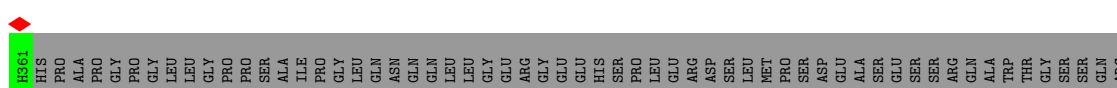
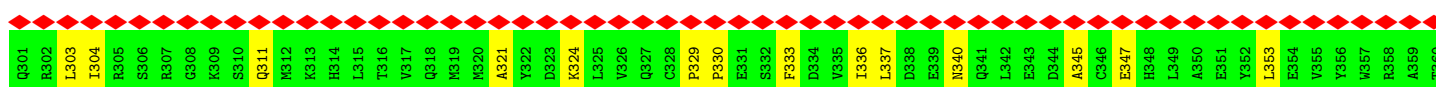
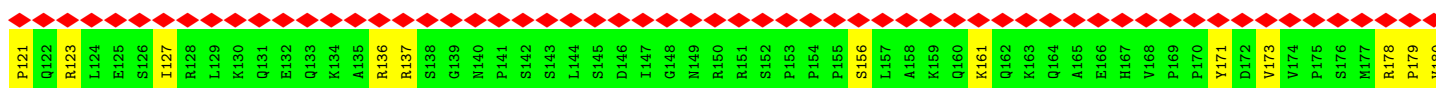
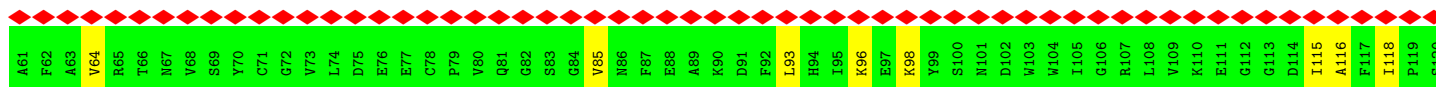
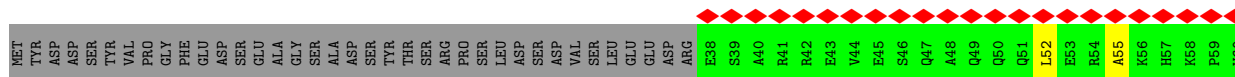


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 45	C 35	N 1	O 8	P 1	0





• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3



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



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51625	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, CA, N90, 3PE, NAG

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	0.25	0/10127	0.46	0/13716
2	D	0.26	0/7728	0.47	0/10477
3	C	0.23	0/2624	0.47	0/3544
All	All	0.25	0/20479	0.47	0/27737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9900	0	10071	242	0
2	D	7570	0	7370	99	0
3	C	2575	0	2619	38	0
4	B	42	0	37	2	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
6	F	56	0	49	2	0
7	A	28	0	0	3	0
8	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	28	0	26	0	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	35	0	49	8	0
11	A	45	0	64	4	0
All	All	20379	0	20373	391	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (391) 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:1155:PHE:HB3	1:A:1464:MET:CG	1.65	1.26
1:A:1155:PHE:CB	1:A:1464:MET:HG3	1.72	1.17
1:A:1015:ILE:CD1	1:A:1019:MET:HG2	1.74	1.17
1:A:1018:ILE:HG21	1:A:1146:ILE:CG2	1.78	1.13
1:A:1015:ILE:HD13	1:A:1019:MET:HG2	1.21	1.12
1:A:1018:ILE:HG21	1:A:1146:ILE:HG22	1.29	1.09
1:A:550:TRP:O	1:A:554:ILE:HG22	1.52	1.08
2:D:516:ASP:OD1	2:D:517:PRO:HD2	1.56	1.04
1:A:1086:ASN:HD22	10:A:2204:Y01:HAT1	1.25	1.00
1:A:1015:ILE:CD1	1:A:1019:MET:CG	2.38	1.00
1:A:1015:ILE:HD13	1:A:1019:MET:CG	1.93	0.98
1:A:269:VAL:N	1:A:270:PRO:HD2	1.83	0.94
1:A:1008:VAL:HG22	1:A:1457:ASN:HD21	1.35	0.90
1:A:550:TRP:O	1:A:554:ILE:CG2	2.20	0.90
2:D:516:ASP:OD1	2:D:517:PRO:CD	2.23	0.85
1:A:1156:GLN:HB3	1:A:1464:MET:CE	2.07	0.84
1:A:1155:PHE:HE2	1:A:1465:ASP:HA	1.43	0.84
1:A:1391:THR:HG22	1:A:1393:PRO:HD2	1.58	0.83
1:A:1360:LEU:HD22	1:A:1454:LEU:HD12	1.59	0.82
1:A:1015:ILE:HD12	1:A:1019:MET:HG2	1.63	0.81
1:A:269:VAL:H	1:A:270:PRO:HD2	1.43	0.80
1:A:1015:ILE:HD12	1:A:1019:MET:CG	2.09	0.80
1:A:563:LEU:HD21	1:A:599:ILE:HD13	1.63	0.80
1:A:1018:ILE:HG21	1:A:1146:ILE:HG21	1.63	0.80
1:A:334:ARG:HH21	1:A:334:ARG:HG3	1.47	0.79
1:A:1155:PHE:HD2	1:A:1464:MET:O	1.64	0.79
1:A:386:PHE:O	1:A:390:VAL:HG23	1.82	0.77
1:A:1008:VAL:HG22	1:A:1457:ASN:ND2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ILE:HD13	1:A:727:ILE:O	1.86	0.76
1:A:751:ALA:O	1:A:755:LEU:HB3	1.86	0.75
1:A:269:VAL:N	1:A:270:PRO:CD	2.48	0.75
1:A:361:ILE:O	1:A:394:SER:HB3	1.88	0.74
2:D:37:VAL:HG11	2:D:1006:GLU:HG2	1.69	0.74
1:A:334:ARG:HG3	1:A:334:ARG:NH2	1.99	0.74
8:A:2202:NAG:O7	8:A:2202:NAG:O3	2.05	0.72
1:A:1267:ASP:HB3	1:A:1270:ASN:HB2	1.70	0.71
1:A:1155:PHE:CD2	1:A:1464:MET:O	2.43	0.71
1:A:348:ASP:HB2	1:A:1227:TYR:HB2	1.72	0.71
1:A:1142:PHE:O	1:A:1146:ILE:HG23	1.91	0.70
1:A:1086:ASN:ND2	10:A:2204:Y01:HAT1	2.04	0.70
1:A:178:LEU:O	1:A:178:LEU:HG	1.92	0.69
1:A:271:LEU:C	1:A:271:LEU:HD23	2.13	0.69
1:A:543:GLU:HG3	1:A:555:GLN:HE22	1.58	0.68
1:A:747:PHE:HB3	1:A:1144:MET:HG2	1.75	0.68
1:A:1086:ASN:HD22	10:A:2204:Y01:CAT	2.02	0.68
1:A:1015:ILE:CD1	1:A:1019:MET:HG3	2.21	0.68
2:D:860:LEU:HD12	2:D:1013:LEU:HD21	1.74	0.68
2:D:732:ARG:HG2	2:D:814:ILE:HG22	1.76	0.68
2:D:676:ASN:HD22	2:D:756:PRO:HB3	1.58	0.68
1:A:1185:LEU:HD23	1:A:1486:LYS:HE2	1.77	0.67
1:A:425:LEU:HD22	1:A:757:ASP:OD2	1.95	0.66
1:A:402:LEU:HD21	1:A:1147:PHE:CZ	2.30	0.66
1:A:516:CYS:SG	1:A:517:ARG:NH1	2.69	0.66
1:A:755:LEU:C	1:A:755:LEU:HD23	2.16	0.66
2:D:496:ASP:OD1	2:D:499:ARG:NH2	2.28	0.65
2:D:993:VAL:HG22	2:D:1002:ILE:HG22	1.79	0.65
1:A:761:LEU:C	1:A:761:LEU:HD23	2.17	0.65
1:A:1147:PHE:O	1:A:1151:VAL:HG13	1.96	0.65
3:C:274:ILE:HD12	3:C:280:LEU:HD22	1.79	0.65
3:C:293:LYS:HD2	3:C:336:ILE:HD11	1.79	0.64
1:A:278:VAL:HG22	1:A:397:VAL:HG11	1.80	0.64
1:A:910:ARG:NH1	1:A:1424:GLU:OE2	2.31	0.64
1:A:269:VAL:H	1:A:270:PRO:CD	2.11	0.63
1:A:1049:LYS:HE3	1:A:1054:GLU:HB3	1.80	0.63
2:D:357:ILE:HG22	2:D:383:ARG:HB2	1.80	0.63
1:A:1155:PHE:HB3	1:A:1464:MET:HG3	0.78	0.63
2:D:591:LEU:HA	2:D:602:LYS:HA	1.80	0.63
2:D:79:VAL:HG12	2:D:610:THR:HG22	1.79	0.63
2:D:727:LYS:NZ	2:D:820:SER:OG	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:GLN:HA	1:A:1464:MET:HE1	1.80	0.63
1:A:1008:VAL:HG13	1:A:1453:PHE:CZ	2.33	0.62
2:D:204:LEU:HD12	2:D:456:LEU:HD21	1.81	0.62
1:A:1008:VAL:O	1:A:1012:ILE:HG22	2.00	0.62
1:A:543:GLU:OE1	1:A:1035:GLN:NE2	2.33	0.62
1:A:1460:VAL:HG12	1:A:1460:VAL:O	2.00	0.62
3:C:173:VAL:H	3:C:226:ARG:HH12	1.47	0.62
2:D:970:SER:OG	2:D:971:LYS:N	2.32	0.61
1:A:1013:ARG:HD2	1:A:1013:ARG:O	2.01	0.61
1:A:425:LEU:CD2	1:A:757:ASP:OD2	2.49	0.61
1:A:910:ARG:HB3	1:A:913:SER:HB3	1.83	0.61
1:A:1156:GLN:HB3	1:A:1464:MET:HE3	1.83	0.61
3:C:207:ARG:NH2	3:C:347:GLU:OE2	2.31	0.61
3:C:321:ALA:HA	3:C:324:LYS:HE2	1.83	0.61
1:A:1013:ARG:HH11	1:A:1013:ARG:CG	2.14	0.61
1:A:551:LEU:O	1:A:555:GLN:HB3	2.00	0.61
1:A:1152:ILE:O	1:A:1152:ILE:HG22	2.00	0.60
1:A:643:LEU:O	1:A:647:MET:HG2	2.01	0.60
1:A:1401:ARG:HH11	1:A:1411:ILE:HD11	1.66	0.60
1:A:367:THR:HG21	1:A:1401:ARG:HG3	1.84	0.60
1:A:1156:GLN:CB	1:A:1464:MET:CE	2.80	0.60
1:A:1155:PHE:HD2	1:A:1464:MET:C	2.04	0.60
1:A:406:SER:HB2	1:A:748:LEU:HD13	1.83	0.60
2:D:289:VAL:HG12	2:D:310:ALA:HB2	1.82	0.60
1:A:1477:LEU:HD22	1:A:1558:LEU:HD13	1.83	0.60
1:A:1155:PHE:CE2	1:A:1465:ASP:HA	2.32	0.60
3:C:266:LEU:HD21	3:C:353:LEU:HD23	1.84	0.60
1:A:271:LEU:HD23	1:A:271:LEU:O	2.02	0.60
1:A:661:ILE:HD11	1:A:702:LEU:HD11	1.83	0.60
2:D:848:MET:HA	2:D:1019:GLU:HA	1.84	0.59
1:A:653:LEU:HG	1:A:746:VAL:HG22	1.83	0.59
3:C:229:LEU:HB3	3:C:232:PRO:HG3	1.85	0.59
1:A:301:CYS:HA	1:A:333:CYS:HB3	1.83	0.59
1:A:1015:ILE:HG12	1:A:1150:PHE:HE2	1.66	0.59
1:A:953:ASN:OD1	1:A:954:TYR:N	2.36	0.59
3:C:52:LEU:HD13	3:C:115:ILE:HD12	1.85	0.59
1:A:1326:LEU:HG	1:A:1330:LEU:HD13	1.84	0.59
2:D:109:ALA:HA	2:D:470:THR:HG22	1.83	0.59
1:A:1472:ARG:HG2	1:A:1474:TRP:CE2	2.38	0.59
3:C:180:VAL:HB	3:C:268:VAL:HG12	1.86	0.58
2:D:516:ASP:CG	2:D:517:PRO:HD2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:NAG:H3	6:F:4:NAG:H83	1.85	0.58
1:A:359:GLN:OE1	1:A:712:TYR:OH	2.20	0.58
2:D:105:GLU:OE2	2:D:442:LYS:NZ	2.34	0.58
1:A:1013:ARG:HH11	1:A:1013:ARG:HG3	1.68	0.57
1:A:1018:ILE:CG2	1:A:1146:ILE:HG21	2.32	0.57
3:C:178:ARG:NH1	3:C:285:LEU:O	2.37	0.57
1:A:761:LEU:HD23	1:A:761:LEU:O	2.03	0.57
1:A:1025:LEU:HD13	1:A:1138:ILE:HD12	1.87	0.57
3:C:136:ARG:O	3:C:137:ARG:NH1	2.37	0.57
1:A:1537:PRO:HG2	1:A:1548:ALA:HB1	1.86	0.57
1:A:361:ILE:O	1:A:394:SER:CB	2.53	0.57
1:A:1151:VAL:HG22	1:A:1152:ILE:HG12	1.85	0.57
2:D:149:PHE:CE1	2:D:222:PRO:HD3	2.40	0.57
2:D:864:HIS:O	2:D:866:ASP:N	2.38	0.57
1:A:268:MET:O	1:A:268:MET:HG3	2.03	0.56
1:A:1012:ILE:O	1:A:1012:ILE:HG13	2.06	0.56
2:D:734:VAL:HG22	2:D:812:VAL:HG12	1.87	0.56
1:A:266:LYS:O	1:A:266:LYS:HG3	2.04	0.56
1:A:334:ARG:HH21	1:A:334:ARG:CG	2.15	0.56
3:C:64:VAL:HG23	3:C:93:LEU:HD21	1.88	0.56
2:D:730:LYS:HG3	2:D:817:ASP:HB3	1.87	0.56
3:C:181:VAL:HG22	3:C:269:LEU:HB2	1.87	0.56
1:A:615:ILE:O	1:A:619:ARG:HG3	2.05	0.55
4:B:2:NAG:H83	4:B:2:NAG:H3	1.87	0.55
2:D:66:ASP:O	2:D:634:LYS:NZ	2.39	0.55
3:C:260:LEU:HG	3:C:267:VAL:HG21	1.87	0.55
1:A:406:SER:OG	1:A:1152:ILE:HG21	2.06	0.55
1:A:434:ASP:O	3:C:340:ASN:ND2	2.39	0.55
1:A:1156:GLN:CA	1:A:1464:MET:CE	2.85	0.55
2:D:254:MET:HB3	2:D:289:VAL:HG23	1.88	0.54
1:A:1155:PHE:CD2	1:A:1464:MET:C	2.80	0.54
3:C:291:PHE:HB2	3:C:333:PHE:CD2	2.43	0.54
3:C:223:LEU:HA	3:C:225:LYS:HE2	1.89	0.54
1:A:1151:VAL:HA	1:A:1460:VAL:HG22	1.89	0.54
7:A:2201:N90:C01	7:A:2201:N90:C15	2.85	0.54
1:A:1156:GLN:CA	1:A:1464:MET:HE1	2.38	0.54
2:D:676:ASN:HD22	2:D:756:PRO:CB	2.21	0.54
1:A:1393:PRO:HB2	11:A:2205:3PE:H31	1.90	0.54
1:A:768:GLU:HA	1:A:768:GLU:OE2	2.07	0.53
2:D:508:PRO:HG2	2:D:764:TYR:CE2	2.43	0.53
2:D:844:ASN:ND2	2:D:865:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:3:NAG:H83	6:F:3:NAG:H3	1.89	0.53
1:A:1018:ILE:CG2	1:A:1146:ILE:CG2	2.69	0.53
1:A:1495:GLU:HG2	1:A:1497:LYS:HG3	1.91	0.53
2:D:704:ARG:NH1	2:D:708:ASP:OD2	2.42	0.53
1:A:396:PHE:O	1:A:399:ASN:HB3	2.09	0.53
1:A:237:LYS:H	1:A:237:LYS:HD2	1.74	0.53
2:D:673:SER:HB2	2:D:679:PHE:HB2	1.91	0.53
1:A:1103:TRP:CD1	1:A:1104:PRO:HD3	2.44	0.53
3:C:85:VAL:HG11	3:C:118:ILE:HG13	1.90	0.53
2:D:240:ARG:NH1	2:D:420:ARG:O	2.41	0.53
2:D:508:PRO:HG2	2:D:764:TYR:HE2	1.74	0.53
2:D:560:ASP:OD1	2:D:561:PHE:N	2.42	0.53
7:A:2201:N90:C15	7:A:2201:N90:C09	2.85	0.52
2:D:295:ASN:ND2	2:D:328:LYS:O	2.32	0.52
2:D:240:ARG:NH2	2:D:278:GLU:O	2.43	0.52
7:A:2201:N90:C22	7:A:2201:N90:C18	2.86	0.52
2:D:589:ARG:HE	2:D:602:LYS:NZ	2.08	0.52
2:D:716:VAL:HA	2:D:720:TRP:HB2	1.92	0.52
1:A:1009:PHE:HA	1:A:1012:ILE:CG2	2.40	0.52
10:A:2204:Y01:HAU2	10:A:2204:Y01:HAC1	1.92	0.52
3:C:212:ILE:HG13	3:C:266:LEU:HB3	1.91	0.52
1:A:274:ILE:O	1:A:278:VAL:HG23	2.10	0.52
1:A:1367:ILE:O	1:A:1371:MET:HG2	2.10	0.52
3:C:179:PRO:HG2	3:C:287:PRO:HB3	1.91	0.52
1:A:179:LYS:HE3	1:A:192:TYR:O	2.10	0.51
1:A:1168:LEU:HB2	1:A:1172:GLN:HB2	1.92	0.51
1:A:1375:VAL:HA	1:A:1421:CYS:HB3	1.92	0.51
1:A:192:TYR:CD2	1:A:193:VAL:HG23	2.46	0.51
2:D:1064:VAL:HG13	2:D:1065:LEU:HD12	1.92	0.51
1:A:1156:GLN:CB	1:A:1464:MET:HE1	2.41	0.51
1:A:1358:ALA:HA	11:A:2205:3PE:H3E2	1.92	0.51
2:D:147:PRO:HG2	2:D:149:PHE:CE2	2.46	0.51
2:D:410:TYR:HB3	2:D:1072:GLY:HA3	1.92	0.51
1:A:145:ILE:HG13	1:A:161:LEU:HD11	1.92	0.51
1:A:1160:GLU:HB2	1:A:1467:PHE:CE2	2.45	0.51
1:A:364:GLU:HG3	1:A:707:TRP:CD1	2.46	0.51
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.93	0.51
1:A:1207:PHE:O	1:A:1211:MET:HG2	2.11	0.50
1:A:1151:VAL:HG21	1:A:1459:PHE:HB3	1.93	0.50
2:D:373:PHE:HE2	2:D:402:MET:HG2	1.75	0.50
2:D:76:ARG:NH2	2:D:584:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:594:SER:OG	2:D:596:ASP:O	2.27	0.50
1:A:960:MET:HA	1:A:963:VAL:HG12	1.94	0.50
1:A:1481:HIS:HB3	1:A:1516:LEU:HD22	1.94	0.50
1:A:554:ILE:O	1:A:554:ILE:HG13	2.11	0.49
2:D:661:ILE:H	2:D:676:ASN:HD21	1.59	0.49
1:A:1144:MET:O	1:A:1144:MET:HG3	2.11	0.49
1:A:1147:PHE:CD1	1:A:1147:PHE:C	2.85	0.49
2:D:651:ASP:OD1	2:D:652:ASN:N	2.45	0.49
3:C:221:LEU:H	3:C:273:THR:HG21	1.77	0.49
3:C:304:ILE:HG23	3:C:311:GLN:HB2	1.94	0.49
1:A:416:ALA:HA	1:A:419:ARG:HG2	1.95	0.49
1:A:421:ASP:OD1	1:A:422:PHE:N	2.46	0.49
1:A:1382:GLN:HG3	1:A:1410:GLU:HB3	1.94	0.49
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.47	0.49
1:A:1376:ALA:H	1:A:1421:CYS:HA	1.78	0.49
1:A:896:ILE:HG23	1:A:897:MET:HE3	1.94	0.49
1:A:1252:MET:HE2	1:A:1277:VAL:HG11	1.94	0.49
2:D:560:ASP:OD2	2:D:1051:ARG:NH1	2.46	0.49
2:D:49:LYS:NZ	2:D:55:ASN:OD1	2.46	0.48
2:D:637:GLU:OE1	2:D:640:THR:N	2.43	0.48
2:D:843:ARG:NH2	2:D:865:ASP:OD1	2.37	0.48
1:A:760:SER:HA	1:A:763:THR:HB	1.96	0.48
3:C:121:PRO:HG3	3:C:171:TYR:HD2	1.78	0.48
1:A:1156:GLN:N	1:A:1464:MET:HE3	2.29	0.48
3:C:180:VAL:HA	3:C:288:ILE:HB	1.94	0.48
1:A:1156:GLN:HB3	1:A:1464:MET:HE1	1.92	0.48
2:D:676:ASN:ND2	2:D:756:PRO:HB3	2.26	0.48
2:D:515:ILE:HG22	2:D:618:SER:HB3	1.95	0.48
1:A:307:ASP:OD1	1:A:334:ARG:NH1	2.45	0.48
1:A:1584:THR:HA	1:A:1587:LYS:HD3	1.95	0.48
4:B:1:NAG:H61	4:B:2:NAG:H82	1.96	0.48
1:A:1155:PHE:CG	1:A:1464:MET:HG3	2.46	0.47
1:A:755:LEU:HD23	1:A:755:LEU:O	2.14	0.47
1:A:197:TRP:NE1	1:A:258:GLN:OE1	2.44	0.47
1:A:995:ILE:HA	1:A:1001:LEU:HD23	1.96	0.47
1:A:1155:PHE:CD2	1:A:1464:MET:HB3	2.49	0.47
2:D:468:ASN:HB3	2:D:481:ASN:HA	1.95	0.47
1:A:394:SER:O	1:A:398:LEU:CB	2.63	0.47
1:A:1153:VAL:HG13	1:A:1153:VAL:O	2.13	0.47
1:A:1422:ASP:N	1:A:1422:ASP:OD1	2.45	0.47
1:A:1427:TYR:HE1	1:A:1432:GLU:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:534:VAL:HA	2:D:975:ILE:HD11	1.97	0.47
1:A:1155:PHE:HE2	1:A:1465:ASP:CA	2.19	0.47
2:D:75:ALA:O	2:D:79:VAL:HG23	2.15	0.47
1:A:1034:VAL:O	1:A:1038:LYS:HB2	2.15	0.47
1:A:207:VAL:HG11	1:A:242:PHE:CG	2.50	0.46
1:A:639:LEU:HD12	1:A:643:LEU:HD13	1.96	0.46
1:A:214:LEU:HD23	1:A:236:VAL:HG23	1.97	0.46
1:A:1013:ARG:CG	1:A:1013:ARG:NH1	2.73	0.46
2:D:859:LEU:HD21	2:D:862:ALA:HB2	1.97	0.46
3:C:173:VAL:O	3:C:284:SER:OG	2.33	0.46
10:A:2204:Y01:HAS2	10:A:2204:Y01:HAE1	1.55	0.46
2:D:526:ASN:ND2	2:D:564:ALA:O	2.47	0.46
3:C:123:ARG:O	3:C:123:ARG:NH1	2.48	0.46
1:A:406:SER:HA	1:A:409:PHE:HD2	1.81	0.46
1:A:1512:ILE:HB	1:A:1517:GLY:HA3	1.97	0.46
1:A:257:LEU:HD11	1:A:655:LEU:HD22	1.98	0.46
1:A:1392:PHE:HB3	1:A:1393:PRO:HD3	1.97	0.46
2:D:73:ASN:HD21	2:D:506:LEU:HD23	1.81	0.46
1:A:551:LEU:HA	1:A:554:ILE:HG23	1.97	0.46
2:D:886:LEU:HD22	2:D:891:VAL:HG11	1.98	0.46
1:A:1009:PHE:HA	1:A:1012:ILE:HG22	1.97	0.45
1:A:1079:ASN:ND2	1:A:1083:ASN:HD22	2.13	0.45
2:D:877:GLU:HA	2:D:1030:LEU:HD22	1.98	0.45
1:A:526:TYR:O	1:A:530:ILE:HG12	2.16	0.45
1:A:1456:ILE:HD12	1:A:1456:ILE:HA	1.80	0.45
1:A:699:PHE:O	1:A:703:THR:HG23	2.16	0.45
1:A:1172:GLN:HG3	1:A:1559:LYS:HE3	1.99	0.45
2:D:106:LYS:HE2	2:D:106:LYS:HB3	1.70	0.45
2:D:312:VAL:HG21	2:D:532:ILE:HD11	1.98	0.45
2:D:802:ILE:HG22	2:D:803:GLN:HG2	1.99	0.45
1:A:176:THR:HA	1:A:179:LYS:HB3	1.98	0.45
2:D:373:PHE:CE2	2:D:402:MET:HG2	2.51	0.45
2:D:654:GLU:HG3	2:D:746:LYS:HD2	1.97	0.45
2:D:744:TYR:HB3	2:D:745:PRO:HD3	1.98	0.45
1:A:268:MET:HB3	1:A:741:TYR:OH	2.17	0.45
1:A:661:ILE:CD1	1:A:702:LEU:HD11	2.47	0.45
1:A:937:LYS:NZ	1:A:956:ASN:OD1	2.50	0.45
2:D:123:VAL:HG12	2:D:145:ILE:HD11	1.98	0.45
1:A:181:ILE:HD11	1:A:192:TYR:HB3	1.99	0.45
1:A:413:ARG:O	1:A:417:LYS:N	2.49	0.45
1:A:442:ILE:HG12	3:C:303:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:767:SER:OG	2:D:795:SER:OG	2.25	0.45
1:A:274:ILE:HD13	1:A:1339:LEU:HD21	1.98	0.45
2:D:116:ASP:OD1	2:D:116:ASP:N	2.50	0.45
1:A:301:CYS:CA	1:A:333:CYS:HB3	2.47	0.45
1:A:1155:PHE:O	1:A:1159:GLY:HA3	2.16	0.45
2:D:149:PHE:CZ	2:D:222:PRO:HD3	2.52	0.44
2:D:1021:LYS:HB3	2:D:1021:LYS:HE2	1.83	0.44
2:D:459:VAL:HG12	2:D:493:SER:HA	1.99	0.44
3:C:55:ALA:O	3:C:96:LYS:NZ	2.41	0.44
3:C:329:PRO:HA	3:C:330:PRO:HD3	1.93	0.44
1:A:402:LEU:CD2	1:A:1147:PHE:CZ	3.00	0.44
1:A:1151:VAL:O	1:A:1464:MET:HG2	2.17	0.44
1:A:1156:GLN:CA	1:A:1464:MET:HE3	2.47	0.44
1:A:1453:PHE:CD1	1:A:1453:PHE:O	2.70	0.44
1:A:600:THR:O	1:A:604:LEU:HD23	2.18	0.44
1:A:1462:VAL:O	1:A:1462:VAL:HG13	2.17	0.44
2:D:886:LEU:O	2:D:891:VAL:HG12	2.18	0.44
3:C:292:VAL:HG12	3:C:337:LEU:HD23	1.98	0.44
1:A:392:PHE:CD1	1:A:392:PHE:O	2.70	0.44
1:A:761:LEU:C	1:A:761:LEU:CD2	2.85	0.44
2:D:363:ASP:OD1	2:D:364:GLY:N	2.43	0.44
1:A:139:ASN:OD1	1:A:246:ARG:HD2	2.18	0.44
1:A:1018:ILE:HA	1:A:1021:VAL:HG12	1.98	0.44
2:D:708:ASP:OD1	2:D:736:THR:OG1	2.29	0.44
2:D:817:ASP:OD1	2:D:820:SER:HB3	2.18	0.44
3:C:98:LYS:HE3	3:C:98:LYS:HB2	1.88	0.44
3:C:156:SER:HB2	3:C:161:LYS:HE2	1.98	0.44
1:A:199:LEU:O	1:A:203:VAL:HG23	2.18	0.43
1:A:960:MET:SD	1:A:960:MET:N	2.91	0.43
1:A:1008:VAL:HG13	1:A:1453:PHE:HZ	1.83	0.43
1:A:1393:PRO:HB3	11:A:2205:3PE:H322	2.00	0.43
2:D:147:PRO:HB3	2:D:163:HIS:NE2	2.34	0.43
2:D:786:GLY:HA2	2:D:790:SER:HB3	2.00	0.43
1:A:148:PRO:HG3	1:A:669:MET:HG2	1.99	0.43
1:A:149:PHE:HB3	1:A:153:ASP:HB3	1.99	0.43
1:A:424:LYS:O	1:A:428:LYS:HG2	2.18	0.43
1:A:736:PHE:O	1:A:740:ASN:HB2	2.18	0.43
2:D:241:ARG:HA	2:D:241:ARG:HD2	1.84	0.43
1:A:1187:ARG:HD3	1:A:1187:ARG:HA	1.75	0.43
1:A:1502:HIS:HA	1:A:1505:VAL:HG23	1.99	0.43
2:D:513:PHE:O	2:D:513:PHE:CG	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HD11	1:A:192:TYR:CB	2.49	0.43
1:A:1036:LEU:HD13	1:A:1128:ILE:HD11	2.00	0.43
2:D:157:ARG:NH1	2:D:222:PRO:O	2.51	0.43
2:D:319:LYS:HE3	2:D:319:LYS:HB2	1.81	0.43
1:A:140:CYS:SG	1:A:247:PRO:HB3	2.59	0.43
1:A:1156:GLN:HA	1:A:1464:MET:CE	2.45	0.43
11:A:2205:3PE:H242	11:A:2205:3PE:H271	1.75	0.43
3:C:123:ARG:HH22	3:C:127:ILE:HD13	1.84	0.43
1:A:1469:TYR:HD1	1:A:1472:ARG:HD2	1.84	0.43
1:A:1046:ASP:HB3	1:A:1059:PHE:CE2	2.54	0.43
1:A:1155:PHE:CD2	1:A:1464:MET:HG3	2.54	0.43
2:D:261:SER:O	2:D:264:VAL:HG22	2.19	0.43
2:D:713:ASN:HB2	2:D:742:ARG:HH12	1.83	0.43
1:A:192:TYR:HD2	1:A:193:VAL:HG23	1.83	0.43
1:A:299:LYS:O	1:A:317:CYS:N	2.37	0.43
1:A:626:ILE:O	1:A:629:VAL:HG22	2.19	0.43
1:A:136:ILE:HD13	1:A:249:ARG:HB2	2.01	0.42
1:A:173:THR:OG1	1:A:205:VAL:HG13	2.19	0.42
1:A:610:MET:H	1:A:610:MET:HG2	1.64	0.42
1:A:937:LYS:HB3	1:A:937:LYS:HE2	1.86	0.42
1:A:1374:LYS:O	1:A:1421:CYS:HB2	2.18	0.42
1:A:1420:LEU:HD13	1:A:1433:TYR:CE2	2.54	0.42
1:A:1427:TYR:CE1	1:A:1432:GLU:HG2	2.53	0.42
3:C:178:ARG:HB3	3:C:288:ILE:HG13	2.00	0.42
1:A:535:LEU:O	1:A:539:THR:HG23	2.20	0.42
1:A:1376:ALA:HB2	1:A:1422:ASP:N	2.35	0.42
2:D:720:TRP:CH2	2:D:734:VAL:HG23	2.54	0.42
2:D:704:ARG:NH2	2:D:737:ASP:HB3	2.35	0.42
1:A:1197:LYS:O	1:A:1201:VAL:HG23	2.19	0.42
1:A:1213:VAL:HA	1:A:1216:MET:HG2	2.00	0.42
2:D:76:ARG:O	2:D:80:GLU:HG3	2.19	0.42
1:A:1009:PHE:O	1:A:1012:ILE:HG23	2.19	0.42
1:A:1079:ASN:HD21	1:A:1083:ASN:HD22	1.68	0.42
10:A:2204:Y01:HAC3	10:A:2204:Y01:HAJ1	1.78	0.42
1:A:1401:ARG:NH1	1:A:1411:ILE:HD11	2.33	0.42
1:A:280:PHE:CE2	1:A:284:ILE:HD11	2.55	0.42
1:A:297:MET:SD	1:A:373:MET:HE2	2.60	0.42
1:A:664:PHE:HD2	1:A:735:LEU:HD13	1.83	0.42
1:A:1079:ASN:OD1	1:A:1080:SER:N	2.53	0.42
3:C:180:VAL:HG22	3:C:288:ILE:HD12	2.02	0.42
2:D:264:VAL:O	2:D:269:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:LEU:HD12	2:D:680:LEU:HD11	2.01	0.41
1:A:1015:ILE:HD12	1:A:1015:ILE:O	2.20	0.41
1:A:1459:PHE:HA	1:A:1463:ILE:CG2	2.50	0.41
1:A:1015:ILE:HD12	1:A:1019:MET:HG3	1.94	0.41
1:A:570:MET:HE1	1:A:582:TYR:CZ	2.55	0.41
1:A:747:PHE:HA	1:A:750:ILE:HG22	2.01	0.41
2:D:637:GLU:HB3	2:D:640:THR:HG22	2.02	0.41
2:D:676:ASN:HA	2:D:679:PHE:HB3	2.03	0.41
3:C:337:LEU:HD11	3:C:345:ALA:HA	2.03	0.41
10:A:2204:Y01:HAD3	10:A:2204:Y01:HBD	1.71	0.41
2:D:755:ASN:OD1	2:D:756:PRO:HD2	2.21	0.41
1:A:905:ALA:O	1:A:915:ARG:NH1	2.54	0.41
1:A:1377:MET:SD	1:A:1385:ARG:HA	2.60	0.41
1:A:395:PHE:HD1	1:A:395:PHE:HA	1.73	0.41
1:A:1211:MET:O	1:A:1215:ILE:HG12	2.20	0.41
1:A:591:ASP:O	1:A:595:VAL:HG23	2.21	0.41
1:A:1025:LEU:HD12	1:A:1142:PHE:CE2	2.56	0.41
1:A:1025:LEU:HD23	1:A:1025:LEU:HA	1.85	0.41
1:A:603:ILE:HG13	1:A:604:LEU:HD22	2.03	0.41
1:A:1547:ASN:HA	1:A:1550:LEU:HG	2.03	0.41
10:A:2204:Y01:HAQ2	10:A:2204:Y01:HAK1	1.68	0.41
2:D:113:TRP:HH2	2:D:178:ILE:HD13	1.85	0.41
2:D:296:SER:HA	2:D:332:ASP:HB2	2.03	0.41
2:D:402:MET:O	2:D:406:ASN:ND2	2.43	0.41
2:D:589:ARG:HE	2:D:602:LYS:HZ3	1.69	0.41
1:A:420:GLY:HA2	1:A:423:GLN:HE22	1.86	0.40
1:A:1341:TRP:CE3	1:A:1344:ILE:HD11	2.55	0.40
1:A:1488:ILE:HG22	1:A:1508:LEU:HD12	2.03	0.40
2:D:727:LYS:HE3	2:D:727:LYS:HB3	1.89	0.40
2:D:788:TYR:OH	2:D:869:ASN:HA	2.21	0.40
1:A:1015:ILE:HG21	1:A:1146:ILE:HB	2.03	0.40
1:A:1153:VAL:HA	1:A:1156:GLN:HG2	2.02	0.40
3:C:85:VAL:HB	3:C:116:ALA:HB1	2.03	0.40
3:C:191:GLU:O	3:C:195:MET:HG2	2.20	0.40
1:A:160:ASN:O	1:A:164:VAL:HG23	2.21	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	A	1214/2161 (56%)	1140 (94%)	71 (6%)	3 (0%)	44	74
2	D	936/1103 (85%)	885 (95%)	51 (5%)	0	100	100
3	C	322/484 (66%)	308 (96%)	14 (4%)	0	100	100
All	All	2472/3748 (66%)	2333 (94%)	136 (6%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	1153	VAL
1	A	1462	VAL

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	A	1086/1902 (57%)	1039 (96%)	47 (4%)	25	55
2	D	837/971 (86%)	834 (100%)	3 (0%)	89	94
3	C	287/426 (67%)	287 (100%)	0	100	100
All	All	2210/3299 (67%)	2160 (98%)	50 (2%)	46	70

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	170	ILE
1	A	173	THR
1	A	174	VAL
1	A	178	LEU
1	A	266	LYS
1	A	269	VAL
1	A	271	LEU
1	A	334	ARG
1	A	363	MET
1	A	394	SER
1	A	395	PHE
1	A	554	ILE
1	A	555	GLN
1	A	559	ASN
1	A	562	LEU
1	A	724	SER
1	A	726	MET
1	A	727	ILE
1	A	729	CYS
1	A	763	THR
1	A	765	GLN
1	A	766	LYS
1	A	768	GLU
1	A	876	ARG
1	A	1012	ILE
1	A	1013	ARG
1	A	1018	ILE
1	A	1114	ASN
1	A	1146	ILE
1	A	1147	PHE
1	A	1150	PHE
1	A	1151	VAL
1	A	1154	THR
1	A	1160	GLU
1	A	1162	GLU
1	A	1328	LYS
1	A	1455	ILE
1	A	1456	ILE
1	A	1458	LEU
1	A	1463	ILE
1	A	1464	MET
1	A	1466	ASN

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Mol	Chain	Res	Type
1	A	1467	PHE
1	A	1468	ASP
1	A	1499	ARG
1	A	1510	ARG
2	D	476	LYS
2	D	515	ILE
2	D	678	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	555	GLN
1	A	1017	ASN
1	A	1457	ASN
2	D	676	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
4	NAG	B	1	4,2	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	B	2	4	14,14,15	0.43	0	17,19,21	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	3	4	14,14,15	0.34	0	17,19,21	0.39	0
5	NAG	E	1	5,2	14,14,15	0.40	0	17,19,21	0.57	0
5	NAG	E	2	5	14,14,15	0.47	0	17,19,21	0.78	0
6	NAG	F	1	6,2	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	F	2	6	14,14,15	0.30	0	17,19,21	0.45	0
6	NAG	F	3	6	14,14,15	0.94	1 (7%)	17,19,21	1.72	2 (11%)
6	NAG	F	4	6	14,14,15	0.56	0	17,19,21	1.33	2 (11%)
5	NAG	G	1	5,2	14,14,15	0.53	0	17,19,21	0.61	0
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.55	0
5	NAG	H	1	5,2	14,14,15	0.43	0	17,19,21	0.52	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	6/6/23/26	0/1/1/1
4	NAG	B	3	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	6/6/23/26	0/1/1/1
6	NAG	F	4	6	-	4/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.03	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	NAG	C1-O5-C5	4.65	118.42	112.19
6	F	3	NAG	C2-N2-C7	4.59	129.05	122.90
6	F	4	NAG	C2-N2-C7	4.56	129.01	122.90
4	B	2	NAG	C2-N2-C7	4.51	128.95	122.90
6	F	4	NAG	C1-C2-N2	2.08	113.72	110.43
4	B	2	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	3	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	3	NAG	C8-C7-N2-C2
4	B	3	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
6	F	3	NAG	C8-C7-N2-C2
6	F	3	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
6	F	2	NAG	C4-C5-C6-O6
4	B	3	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
4	B	3	NAG	O5-C5-C6-O6

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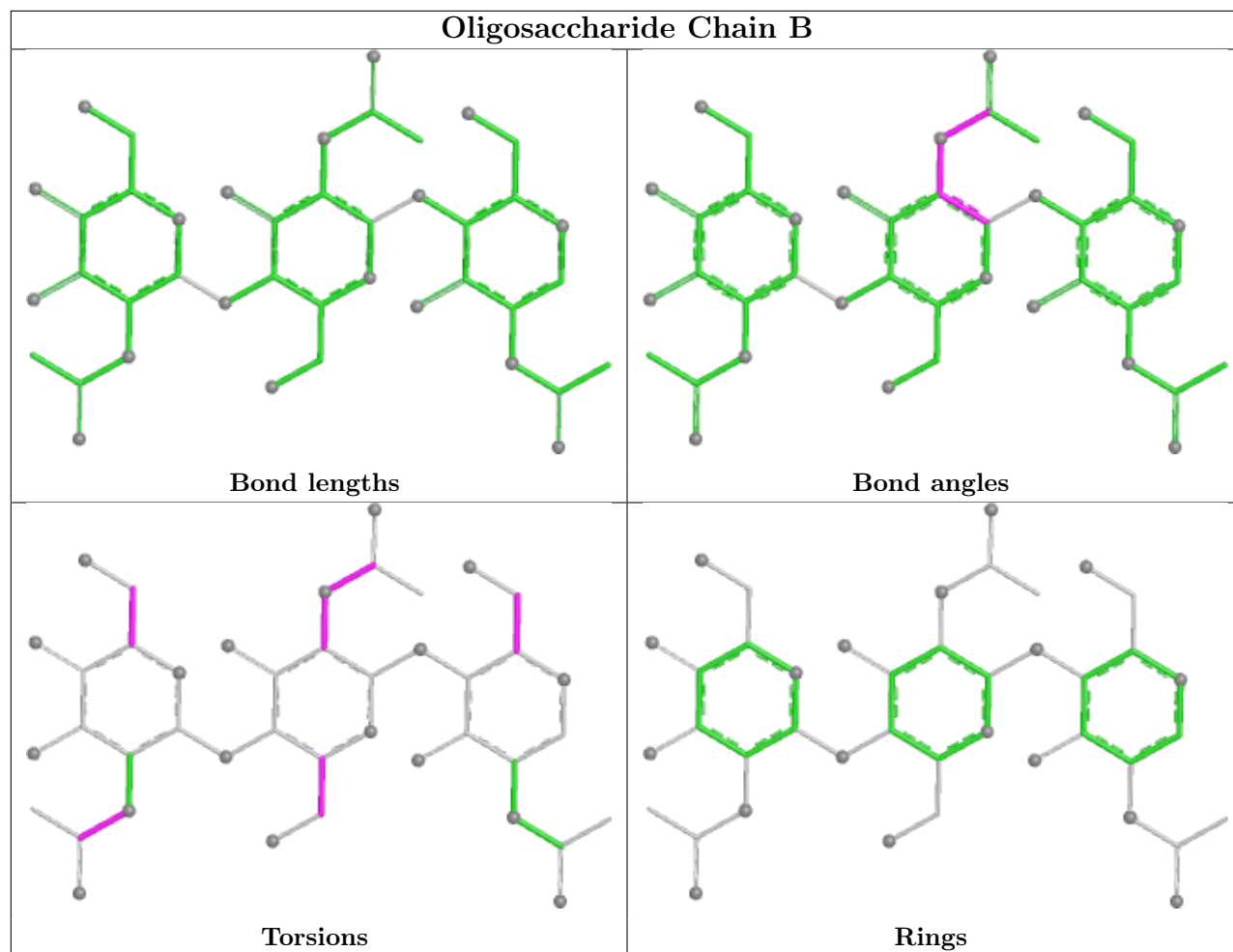
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C1-C2-N2-C7
5	E	1	NAG	C3-C2-N2-C7
4	B	2	NAG	C1-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7
6	F	3	NAG	C1-C2-N2-C7
6	F	4	NAG	C1-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
6	F	3	NAG	C3-C2-N2-C7
6	F	4	NAG	C3-C2-N2-C7

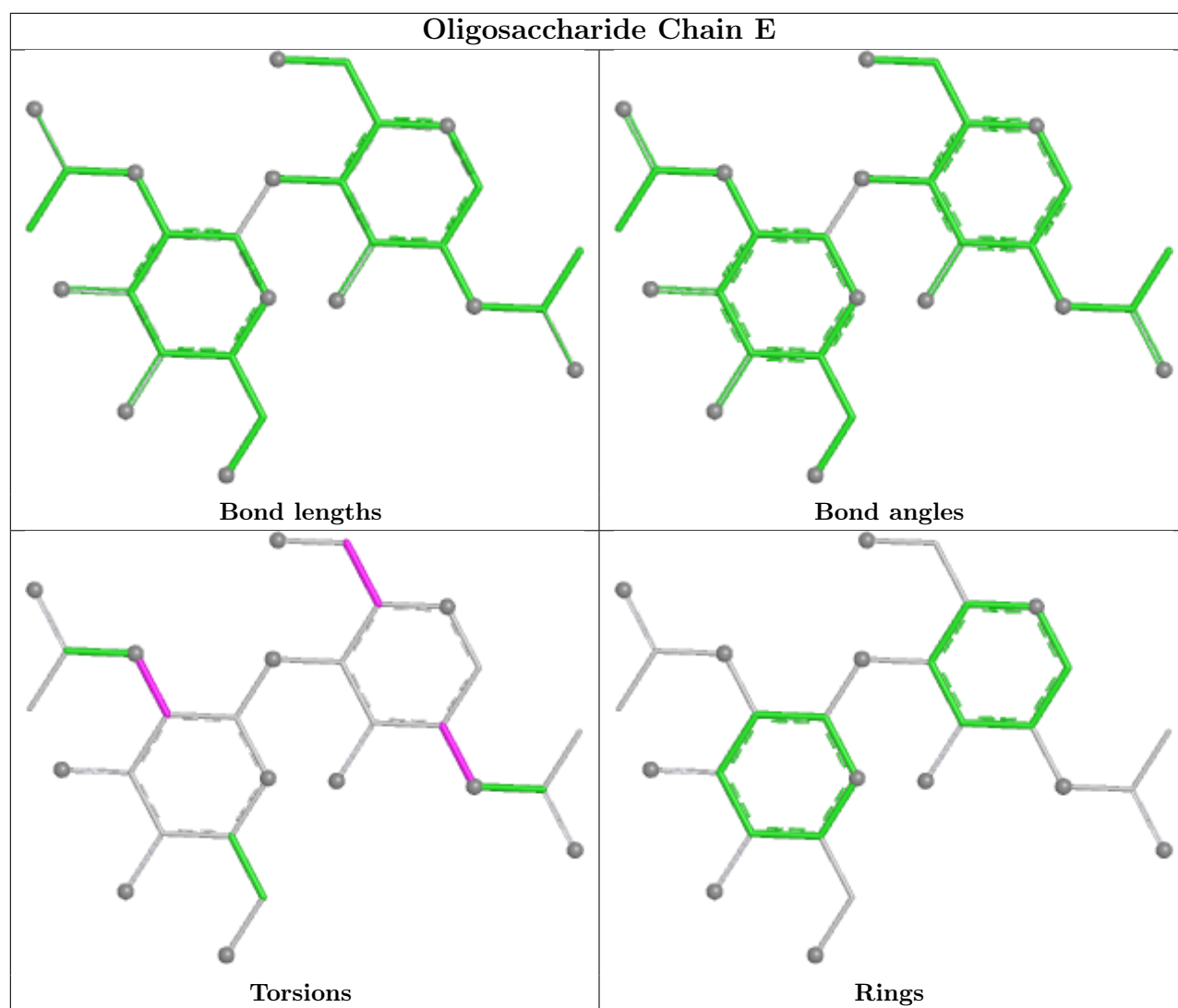
There are no ring outliers.

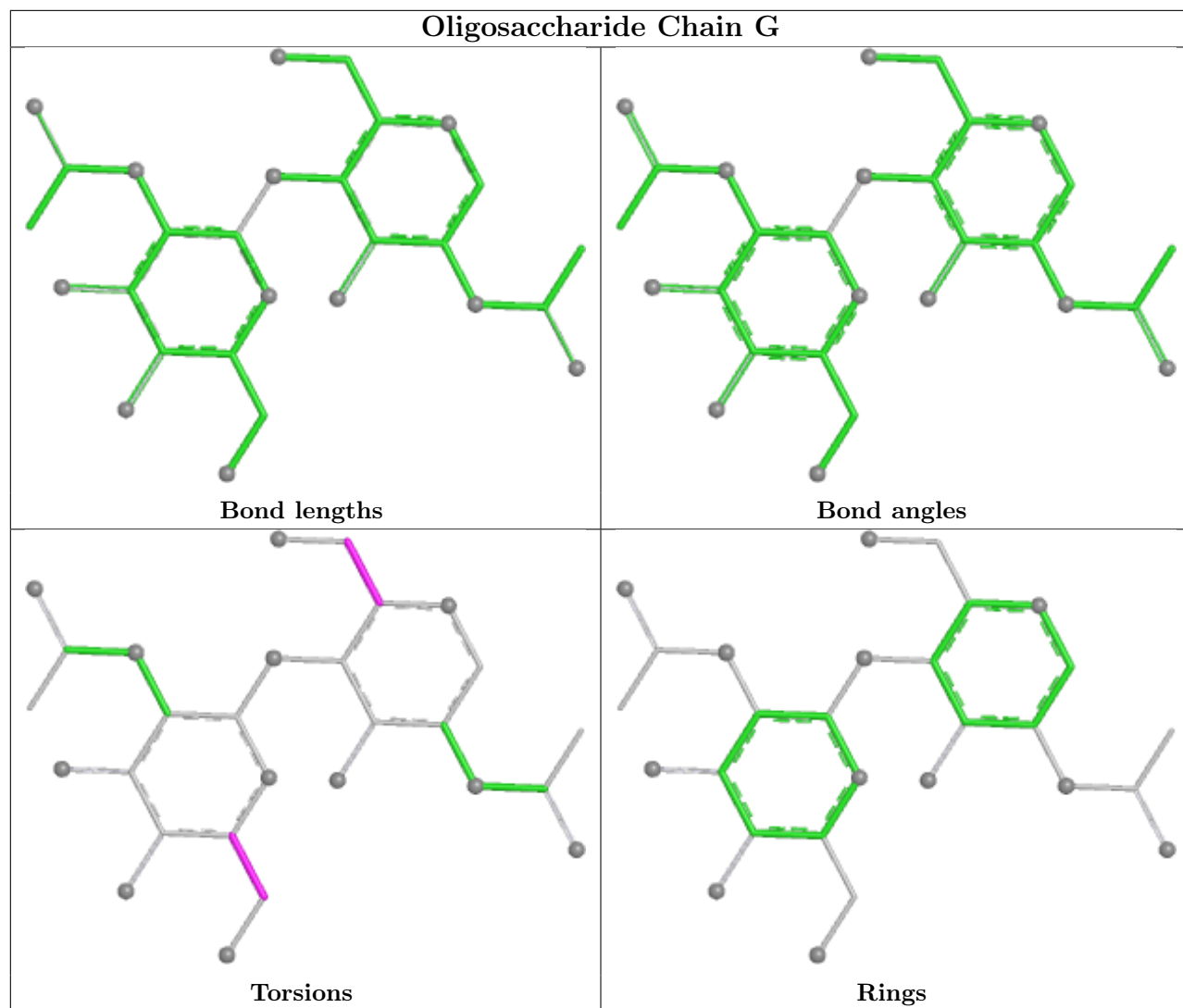
4 monomers are involved in 4 short contacts:

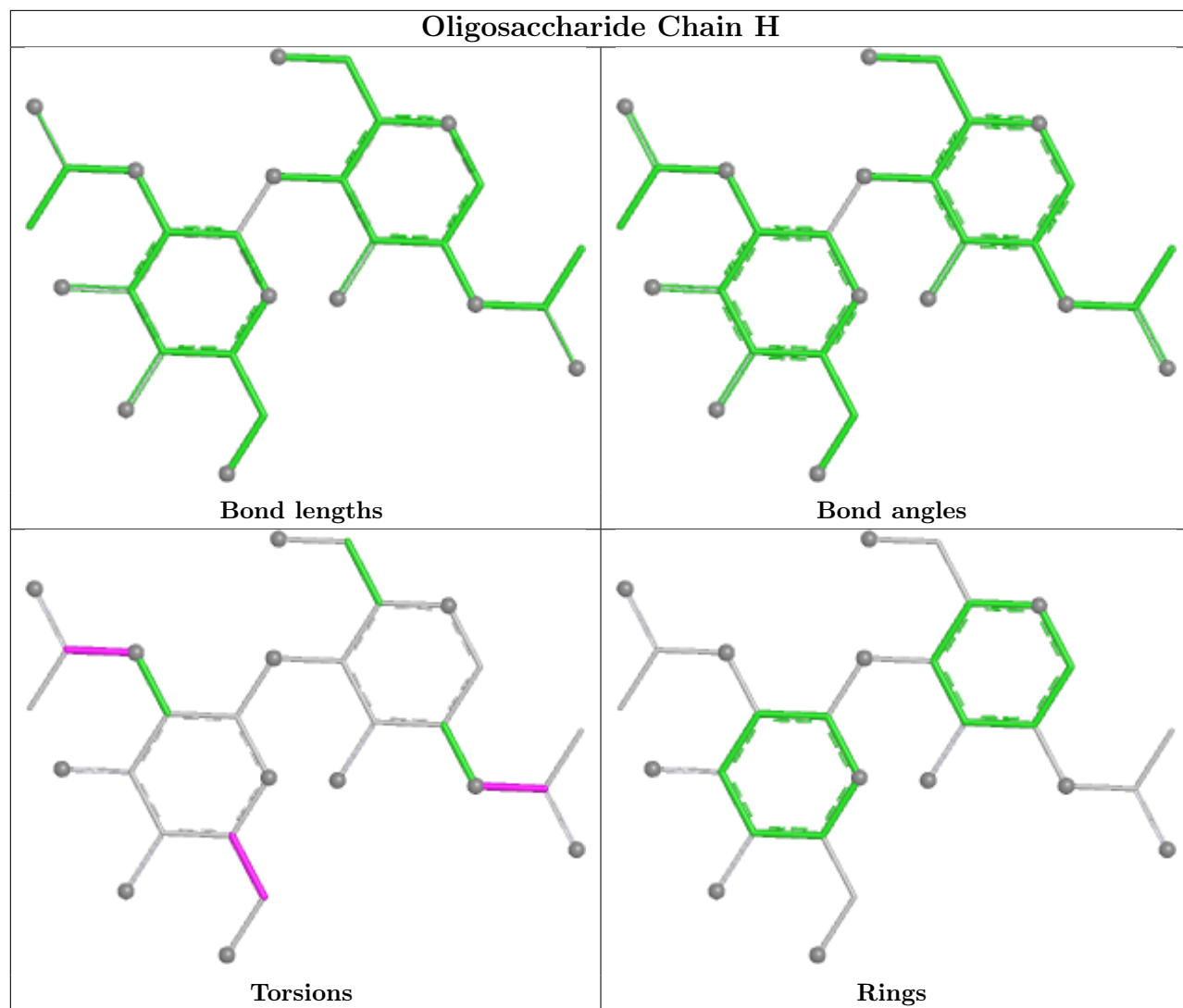
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3	NAG	1	0
4	B	2	NAG	2	0
4	B	1	NAG	1	0
6	F	4	NAG	1	0

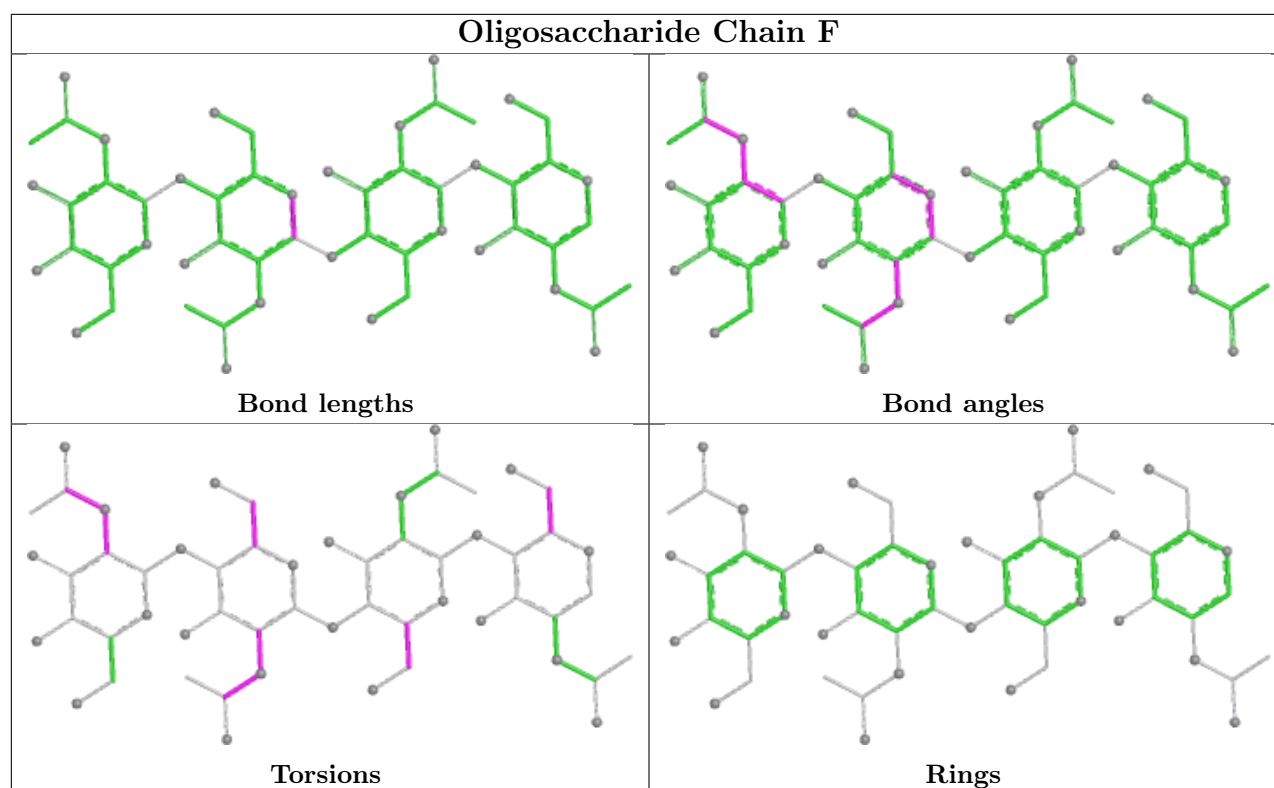
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are 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
7	N90	A	2201	-	31,31,31	3.53	13 (41%)	40,40,40	1.36	6 (15%)
11	3PE	A	2205	-	44,44,50	0.53	0	47,49,55	0.68	2 (4%)
8	NAG	D	1201	2	14,14,15	0.31	0	17,19,21	0.54	0
8	NAG	D	1202	-	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	A	2202	-	14,14,15	0.27	0	17,19,21	0.52	0
10	Y01	A	2204	-	38,38,38	2.42	11 (28%)	57,57,57	4.54	32 (56%)

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
7	N90	A	2201	-	-	5/18/28/28	0/4/4/4
11	3PE	A	2205	-	-	22/48/48/54	-
8	NAG	D	1201	2	-	2/6/23/26	0/1/1/1
8	NAG	D	1202	-	-	2/6/23/26	0/1/1/1
8	NAG	A	2202	-	-	4/6/23/26	0/1/1/1
10	Y01	A	2204	-	-	12/19/77/77	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2201	N90	C07-N14	-11.50	1.29	1.48
7	A	2201	N90	C20-N17	-8.54	1.34	1.47
10	A	2204	Y01	CAK-CBD	6.96	1.64	1.53
10	A	2204	Y01	CBD-CBG	-6.39	1.41	1.53
7	A	2201	N90	C15-N14	-6.03	1.36	1.47
7	A	2201	N90	C02-C07	5.11	1.60	1.52
7	A	2201	N90	C19-N14	-4.96	1.38	1.47
10	A	2204	Y01	CAI-CAZ	4.71	1.42	1.33
7	A	2201	N90	C18-N17	-3.94	1.36	1.46
10	A	2204	Y01	CAU-CBI	-3.88	1.47	1.54
10	A	2204	Y01	CAK-CAI	-3.86	1.42	1.50
7	A	2201	N90	C23-C22	3.51	1.57	1.47
7	A	2201	N90	C16-N17	-3.40	1.37	1.46
10	A	2204	Y01	CAL-CAX	3.38	1.58	1.50
10	A	2204	Y01	CAV-CBC	3.28	1.59	1.52
7	A	2201	N90	C27-C28	-2.90	1.34	1.38
10	A	2204	Y01	CAV-CAZ	-2.80	1.46	1.51
10	A	2204	Y01	CBB-CBE	-2.79	1.49	1.54
7	A	2201	N90	C08-C07	2.67	1.56	1.52
7	A	2201	N90	C09-C08	-2.62	1.35	1.39
7	A	2201	N90	C06-C05	2.60	1.43	1.38
7	A	2201	N90	C27-C26	2.18	1.43	1.38
10	A	2204	Y01	CAE-CBI	2.17	1.57	1.54
10	A	2204	Y01	CBH-CBF	-2.13	1.52	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2204	Y01	CAD-CBH-CAT	12.50	128.45	109.43
10	A	2204	Y01	CAK-CBD-CBG	-10.29	96.36	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2204	Y01	CAD-CBH-CAZ	-9.65	93.63	108.38
10	A	2204	Y01	CAQ-CBG-CBD	-8.59	105.39	119.10
10	A	2204	Y01	CBD-CAK-CAI	-8.55	100.92	112.76
10	A	2204	Y01	CBI-CBE-CBB	-8.32	106.65	119.50
10	A	2204	Y01	CAV-CAZ-CBH	-7.82	106.40	116.42
10	A	2204	Y01	CBH-CBF-CBD	-7.60	101.60	112.71
10	A	2204	Y01	CAV-CAZ-CAI	7.19	130.32	120.57
10	A	2204	Y01	CAT-CBH-CBF	-7.15	99.27	108.74
10	A	2204	Y01	CBG-CBI-CBE	-6.46	92.69	100.10
10	A	2204	Y01	CBI-CBG-CBD	-6.24	105.55	114.41
10	A	2204	Y01	CAP-CAQ-CBG	-5.67	94.04	105.14
10	A	2204	Y01	CAE-CBI-CBE	5.31	121.32	111.68
10	A	2204	Y01	CAE-CBI-CAU	-5.25	102.86	110.61
10	A	2204	Y01	OAW-CAY-CAM	4.96	122.21	111.48
10	A	2204	Y01	CAS-CAU-CBI	-4.19	105.67	112.74
10	A	2204	Y01	CAC-CBB-CAO	4.17	116.80	110.34
10	A	2204	Y01	OAW-CBC-CAV	3.95	116.18	108.04
7	A	2201	N90	C08-C07-N14	3.88	117.16	111.50
7	A	2201	N90	C20-N17-C18	3.86	114.51	110.49
10	A	2204	Y01	OAW-CAY-OAG	-3.64	115.19	123.70
10	A	2204	Y01	CBF-CBD-CBG	-3.52	104.48	109.09
10	A	2204	Y01	CBF-CBH-CAZ	3.39	114.62	109.65
10	A	2204	Y01	CAR-CAT-CBH	-3.37	105.61	112.78
10	A	2204	Y01	CAO-CBB-CBE	-3.37	103.35	110.33
7	A	2201	N90	C20-C21-C22	-3.31	119.46	124.72
10	A	2204	Y01	CAS-CBF-CBD	3.20	116.25	111.78
10	A	2204	Y01	CAQ-CBG-CBI	3.02	107.39	103.84
11	A	2205	3PE	C2-O21-C21	3.00	124.99	117.80
10	A	2204	Y01	CAU-CAS-CBF	-2.98	108.07	113.14
7	A	2201	N90	C23-C22-C21	-2.87	119.95	126.99
10	A	2204	Y01	CAC-CBB-CBE	-2.61	108.97	112.88
11	A	2205	3PE	O12-P-O14	2.45	123.86	112.44
10	A	2204	Y01	CAP-CBE-CBI	2.20	106.43	103.84
7	A	2201	N90	C18-C19-N14	2.12	114.34	110.61
7	A	2201	N90	C19-N14-C07	-2.11	107.41	111.64
10	A	2204	Y01	CBC-CAV-CAZ	2.06	114.49	111.45
10	A	2204	Y01	CAT-CBH-CAZ	2.03	112.25	108.74
10	A	2204	Y01	CAU-CBI-CBG	2.03	110.28	107.25

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2201	N90	C21-C20-N17-C16
7	A	2201	N90	C21-C20-N17-C18
8	A	2202	NAG	C3-C2-N2-C7
11	A	2205	3PE	C1-O11-P-O12
11	A	2205	3PE	C1-O11-P-O13
11	A	2205	3PE	C11-O13-P-O14
11	A	2205	3PE	O13-C11-C12-N
8	D	1202	NAG	O5-C5-C6-O6
7	A	2201	N90	C21-C22-C23-C24
8	D	1202	NAG	C4-C5-C6-O6
10	A	2204	Y01	CAJ-CAO-CBB-CAC
8	A	2202	NAG	C8-C7-N2-C2
7	A	2201	N90	C21-C22-C23-C28
11	A	2205	3PE	C32-C31-O31-C3
11	A	2205	3PE	O32-C31-O31-C3
8	A	2202	NAG	O7-C7-N2-C2
7	A	2201	N90	N17-C20-C21-C22
10	A	2204	Y01	CAN-CAJ-CAO-CBB
11	A	2205	3PE	C39-C3A-C3B-C3C
11	A	2205	3PE	C22-C23-C24-C25
11	A	2205	3PE	C33-C34-C35-C36
11	A	2205	3PE	C25-C26-C27-C28
8	A	2202	NAG	O5-C5-C6-O6
11	A	2205	3PE	C24-C25-C26-C27
11	A	2205	3PE	O11-C1-C2-C3
11	A	2205	3PE	C32-C33-C34-C35
10	A	2204	Y01	CAJ-CAN-CBA-CAA
10	A	2204	Y01	CAV-CBC-OAW-CAY
10	A	2204	Y01	CAJ-CAN-CBA-CAB
11	A	2205	3PE	C34-C35-C36-C37
10	A	2204	Y01	CAJ-CAO-CBB-CBE
11	A	2205	3PE	C2A-C2B-C2C-C2D
10	A	2204	Y01	CAX-CAL-CAM-CAY
11	A	2205	3PE	O11-C1-C2-O21
10	A	2204	Y01	CAR-CBC-OAW-CAY
8	D	1201	NAG	C3-C2-N2-C7
11	A	2205	3PE	C11-O13-P-O11
11	A	2205	3PE	C11-O13-P-O12
11	A	2205	3PE	C3-C2-O21-C21
10	A	2204	Y01	CAO-CBB-CBE-CBI
8	D	1201	NAG	C1-C2-N2-C7
10	A	2204	Y01	CAC-CBB-CBE-CBI
11	A	2205	3PE	C38-C39-C3A-C3B

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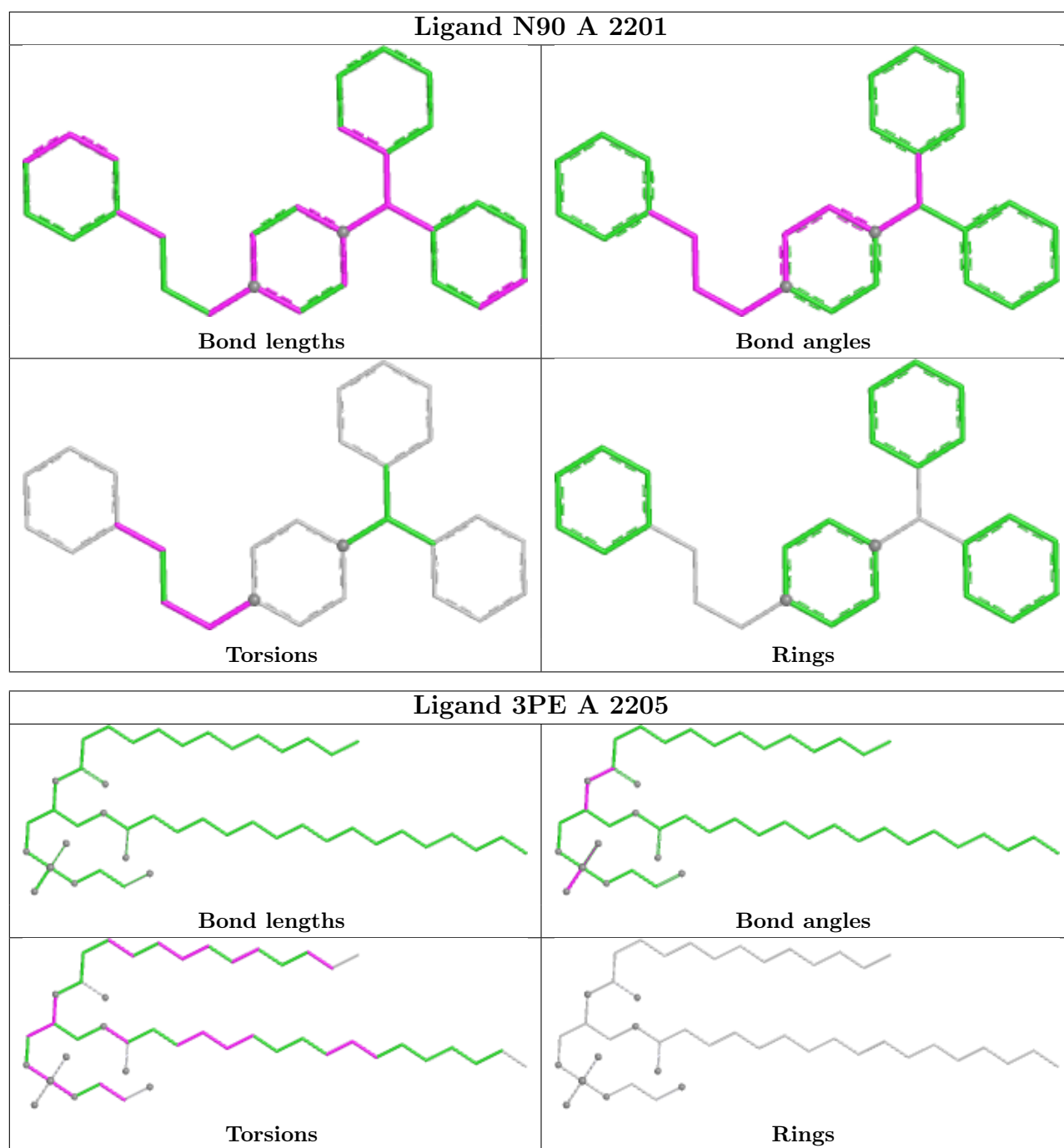
Mol	Chain	Res	Type	Atoms
11	A	2205	3PE	C27-C28-C29-C2A
10	A	2204	Y01	CAL-CAM-CAY-OAW
11	A	2205	3PE	C1-C2-O21-C21
10	A	2204	Y01	OAG-CAY-OAW-CBC

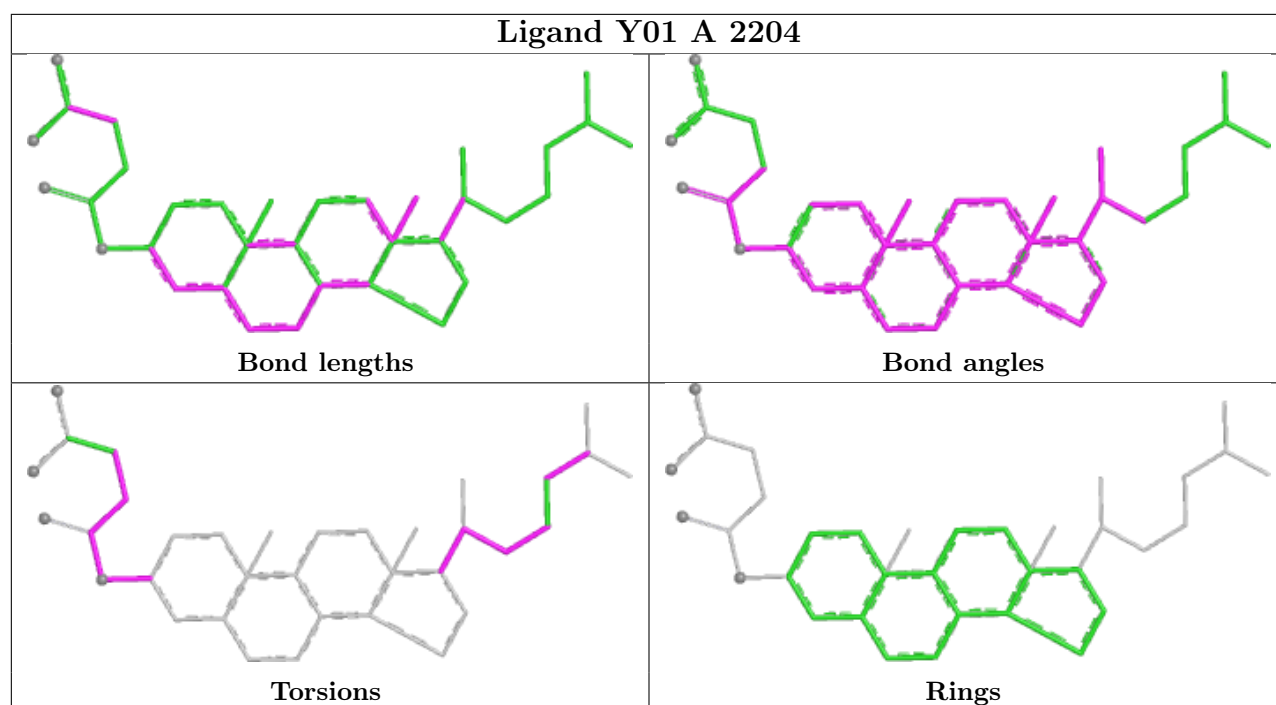
There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2201	N90	3	0
11	A	2205	3PE	4	0
8	A	2202	NAG	1	0
10	A	2204	Y01	8	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.

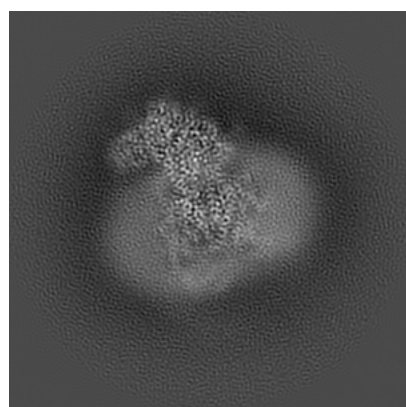
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26513. These allow visual inspection of the internal detail of the map and identification of artifacts.

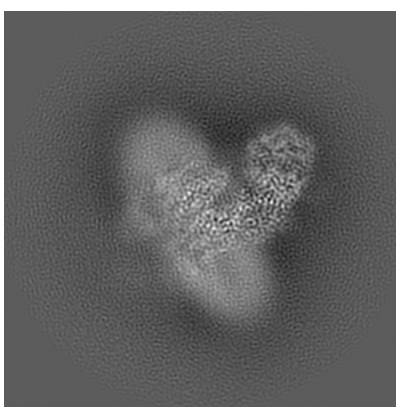
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

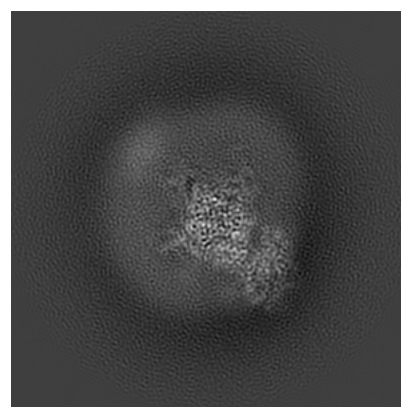
6.1.1 Primary map



X



Y

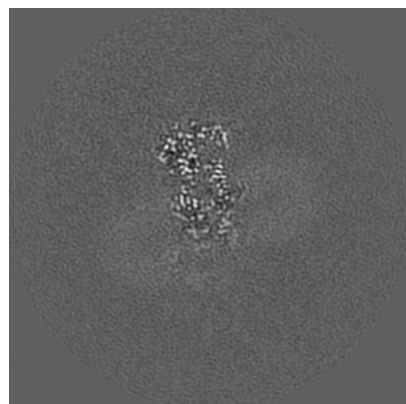


Z

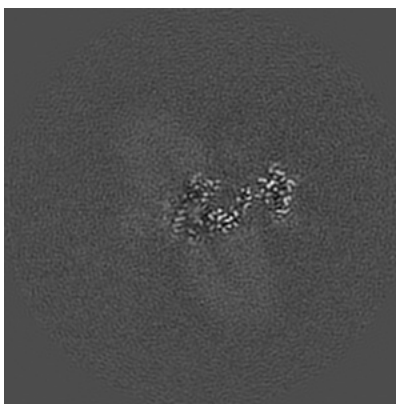
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

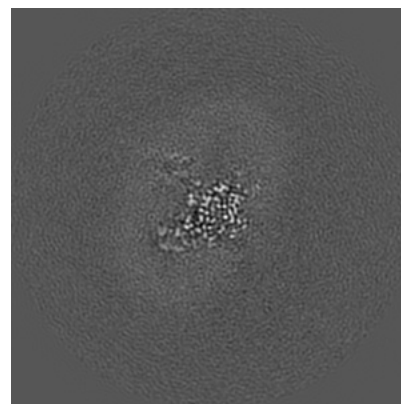
6.2.1 Primary map



X Index: 140



Y Index: 140

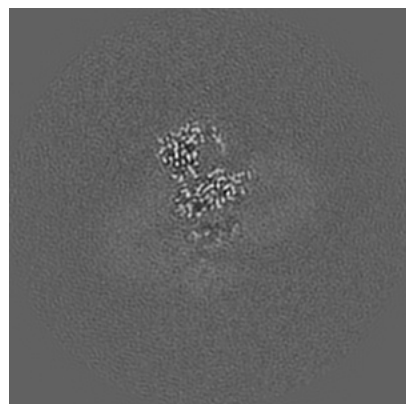


Z Index: 140

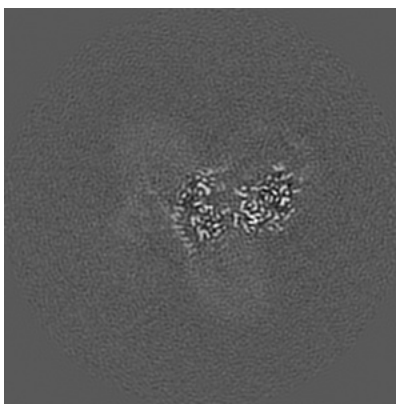
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

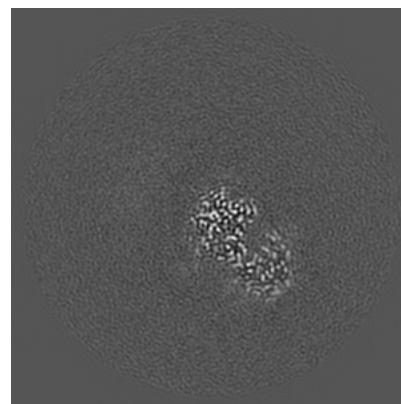
6.3.1 Primary map



X Index: 135



Y Index: 130

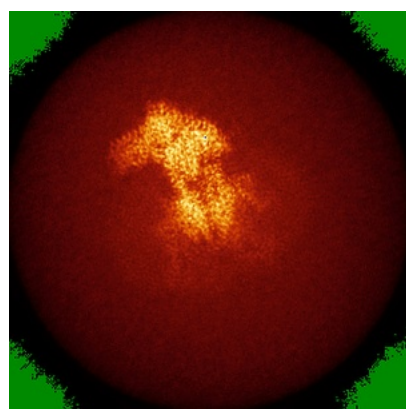


Z Index: 190

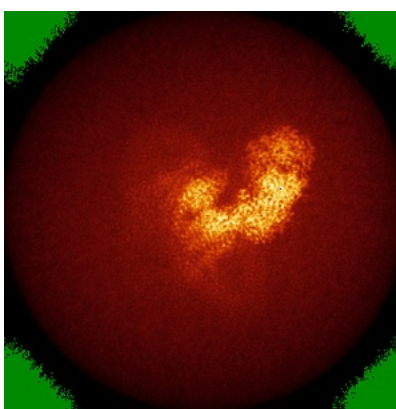
The images above show the largest variance slices of the map in three orthogonal directions.

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

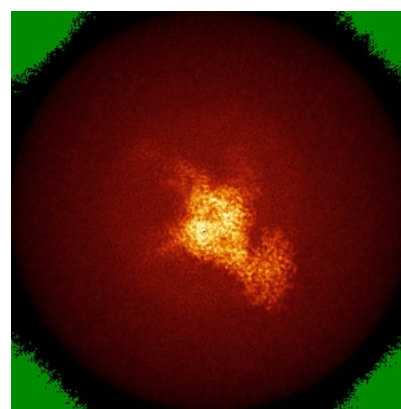
6.4.1 Primary map



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

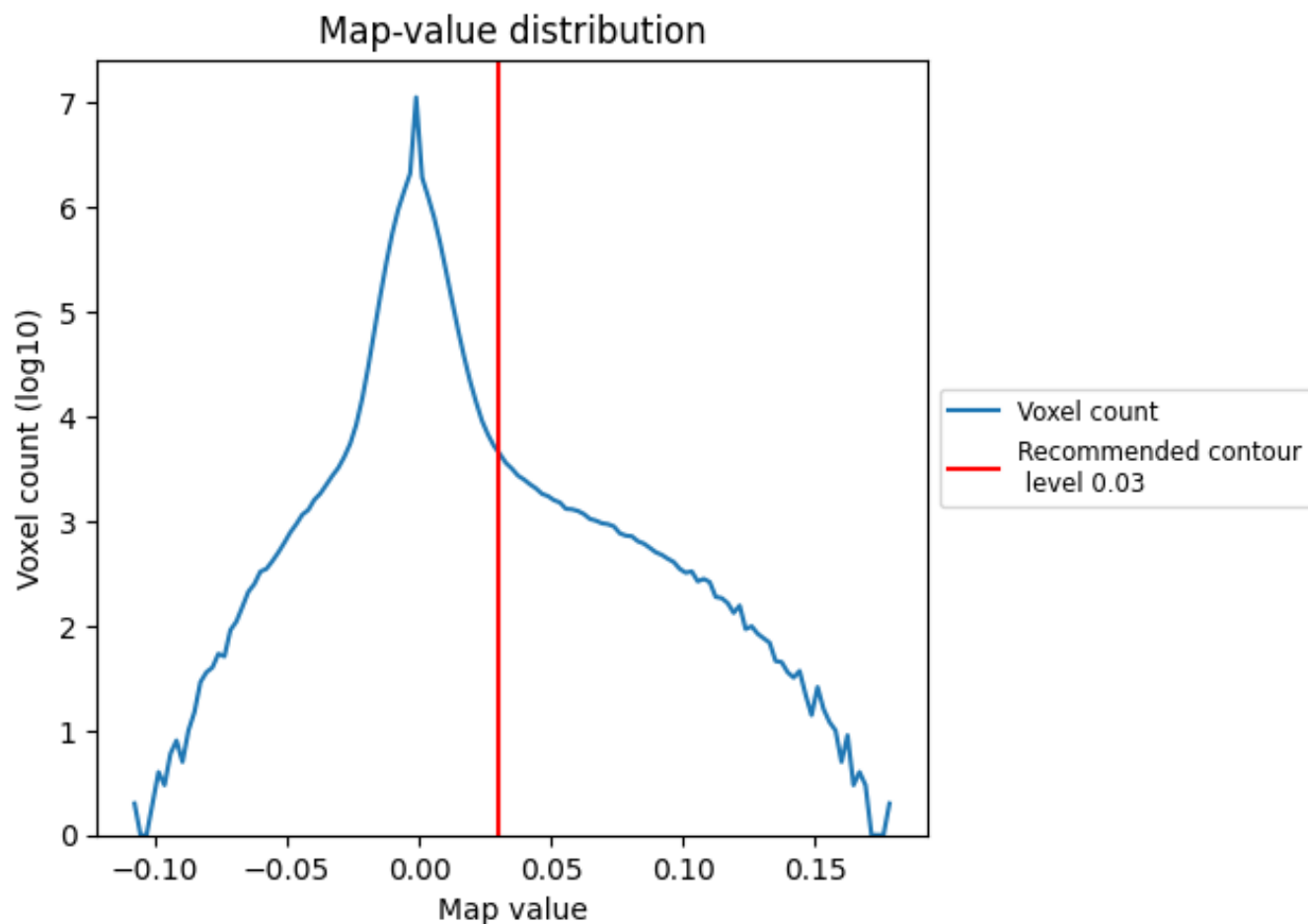
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

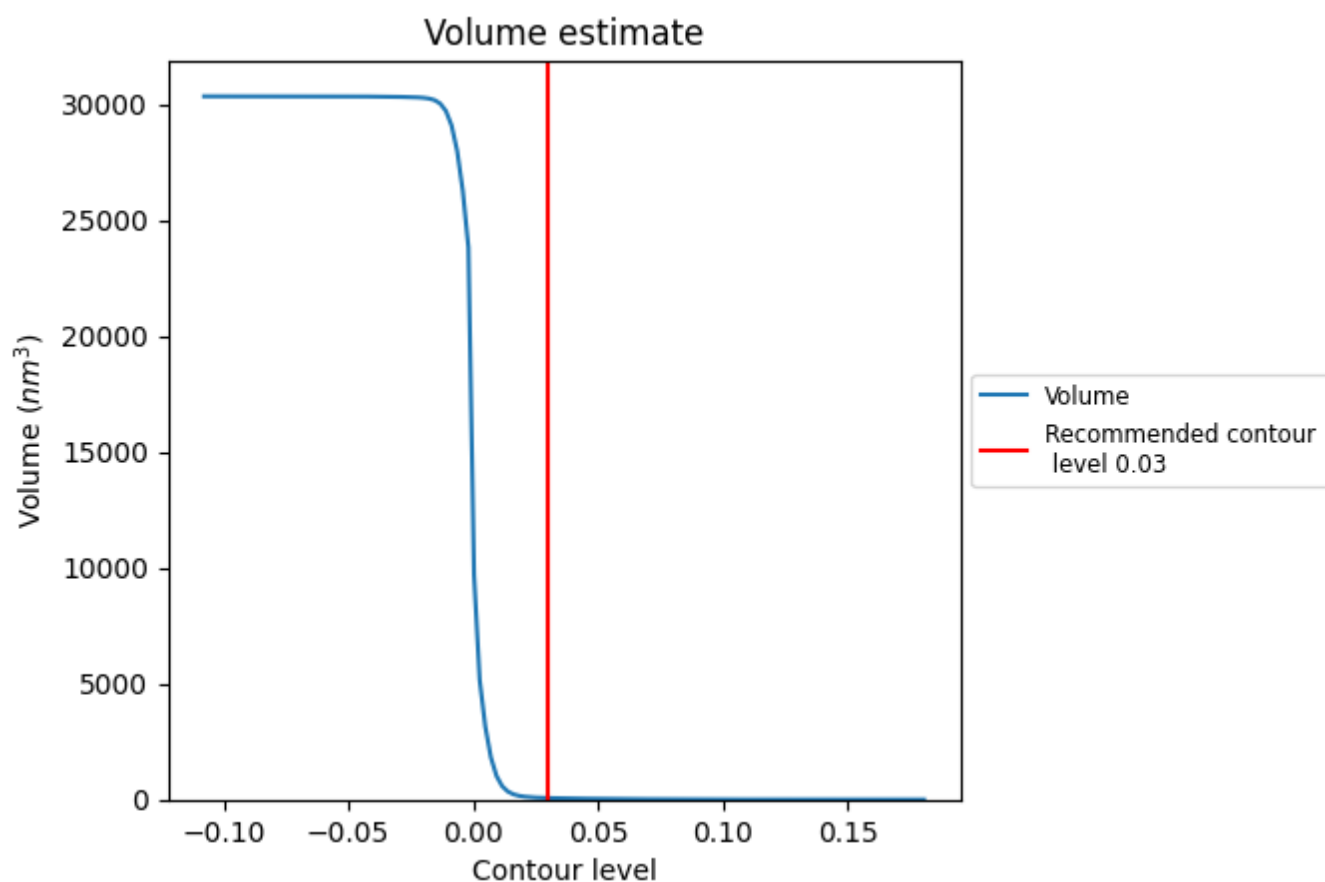
This section contains the results of statistical analysis of the map.

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.

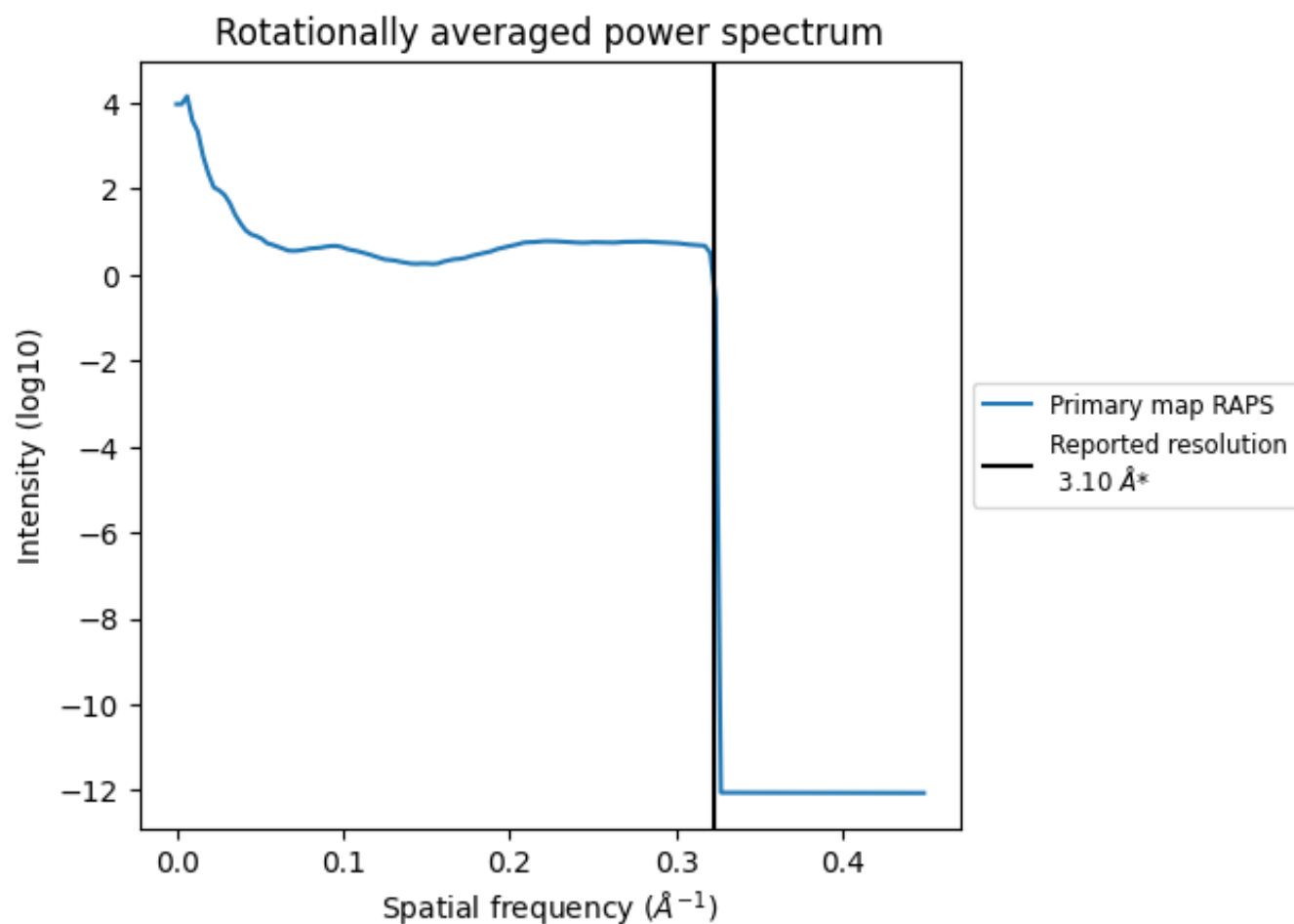
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 0.323 Å⁻¹

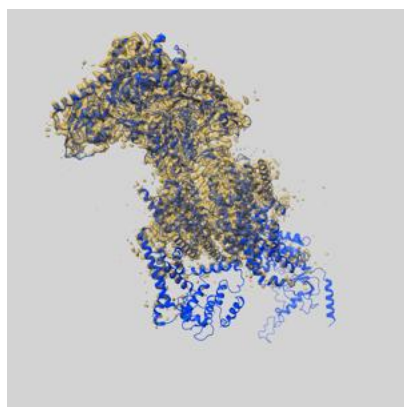
8 Fourier-Shell correlation

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

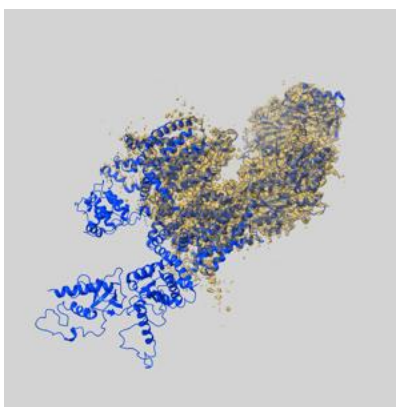
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26513 and PDB model 7UHF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

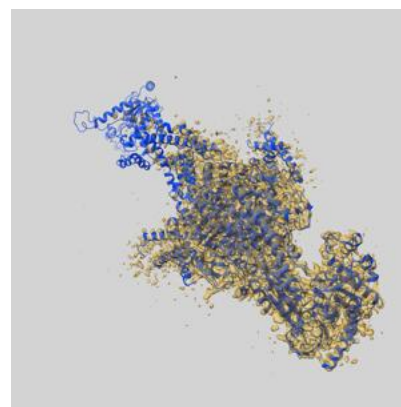
9.1 Map-model overlay [i](#)



X



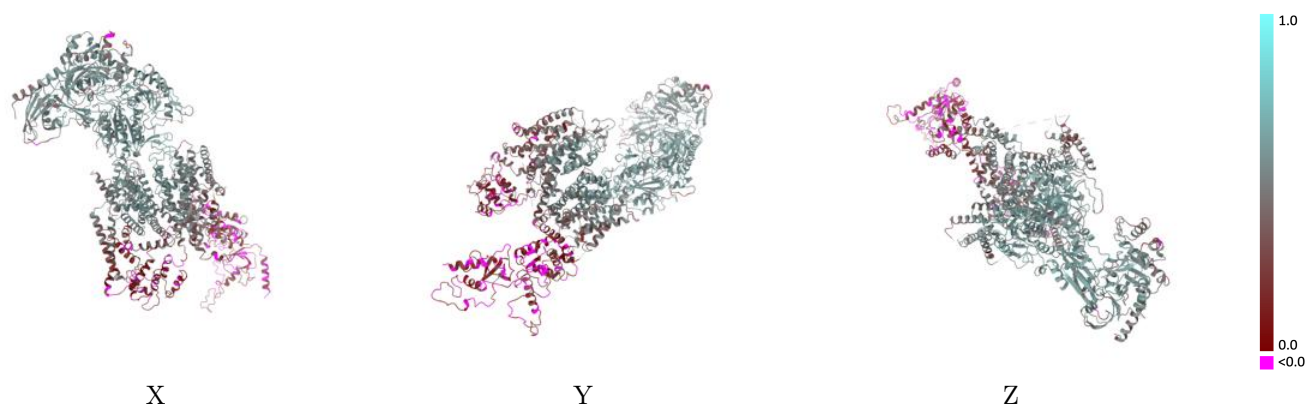
Y



Z

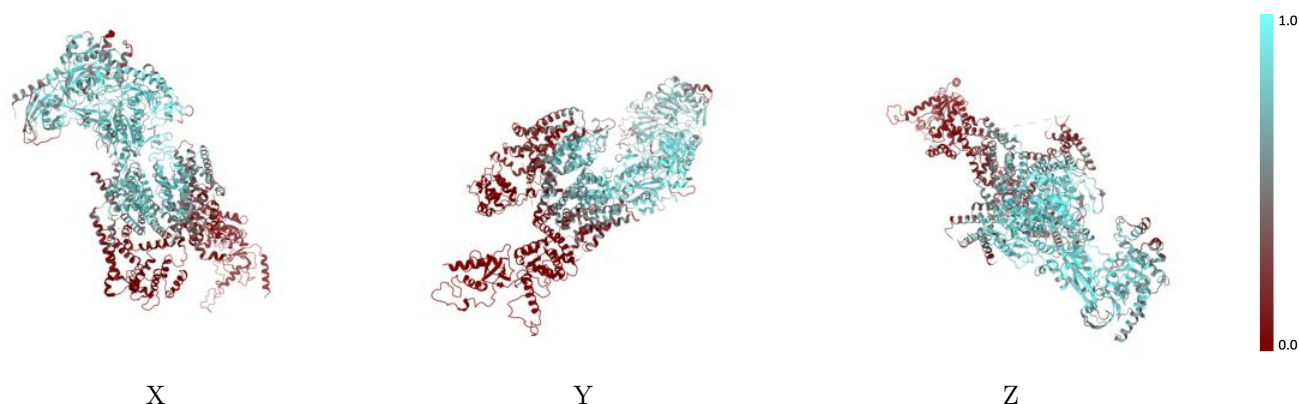
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



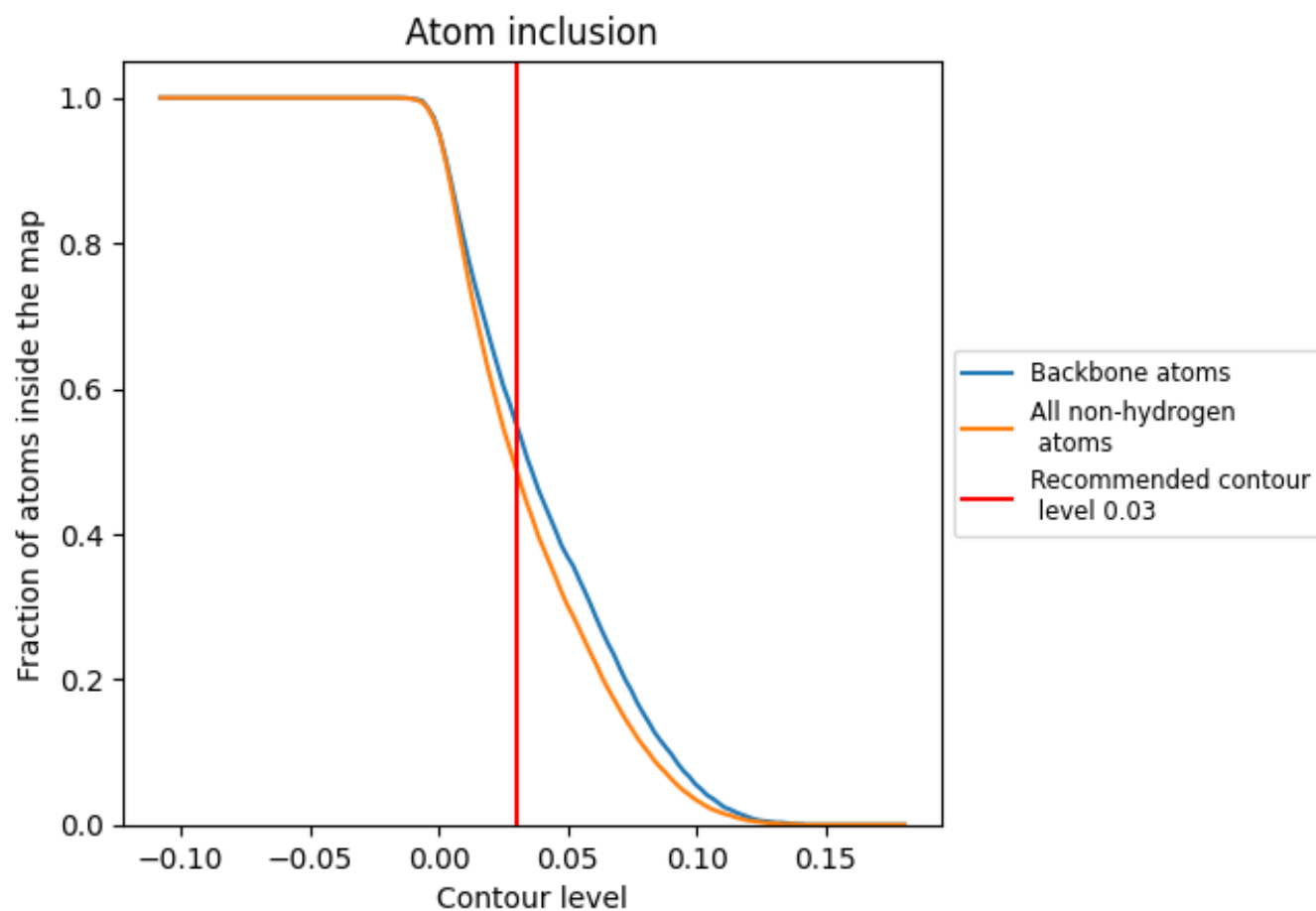
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 49% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4900	<div></div> 0.4250
A	<div></div> 0.4320	<div></div> 0.4200
B	<div></div> 0.3090	<div></div> 0.3180
C	<div></div> 0.0000	<div></div> 0.0910
D	<div></div> 0.7370	<div></div> 0.5460
E	<div></div> 0.1070	<div></div> 0.2590
F	<div></div> 0.4460	<div></div> 0.4180
G	<div></div> 0.1790	<div></div> 0.2810
H	<div></div> 0.3930	<div></div> 0.4310

1.0

0.0

<0.0