



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:23 AM UTC

PDB ID : 7XLQ / pdb_00007xlq
EMDB ID : EMD-33285
Title : Structure of human R-type voltage-gated CaV2.3-alpha2/delta1-beta1 channel complex in the ligand-free (apo) state
Authors : Gao, Y.; Qiu, Y.; Wei, Y.; Dong, Y.; Zhang, X.C.; Zhao, Y.
Deposited on : 2022-04-22
Resolution : 3.10 Å(reported)
Based on initial model : 7VFS

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:

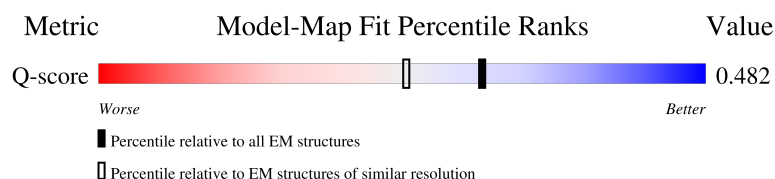
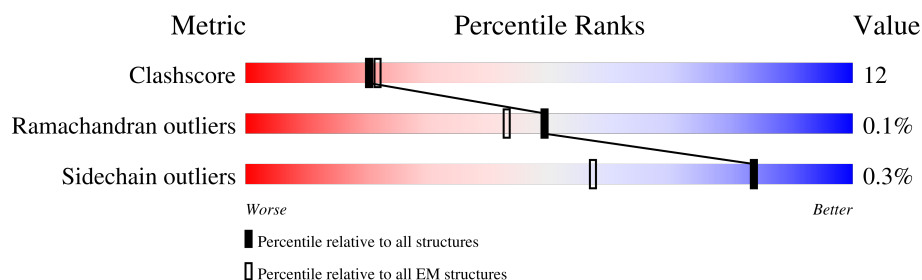
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2313	
2	D	1077	
3	B	598	
4	C	3	

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Mol	Chain	Length	Quality of chain
4	E	3	67% 33%
5	F	3	100% 67% 33%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20132 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 R-type calcium channel subunit alpha-1E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1319	Total	C	N	O	S	0	0
			10674	7007	1761	1830	76		

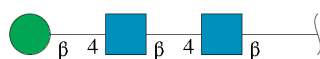
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	955	Total	C	N	O	S	0	0
			7637	4842	1281	1483	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

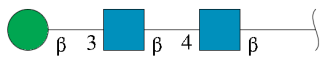
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	162	Total	C	N	O	S	0	0
			1259	805	217	232	5		

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



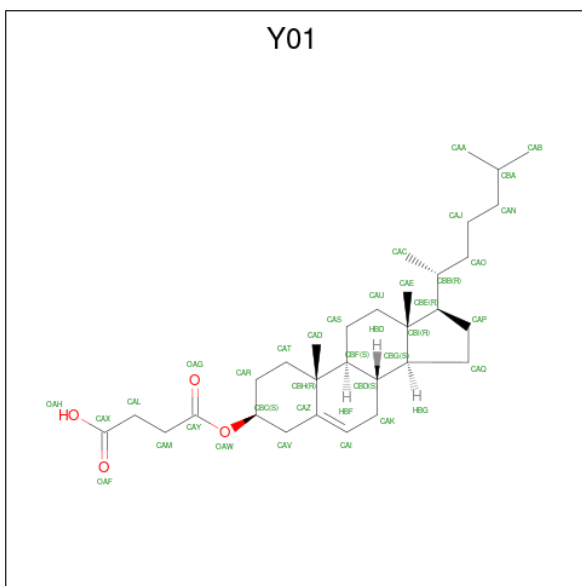
Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

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

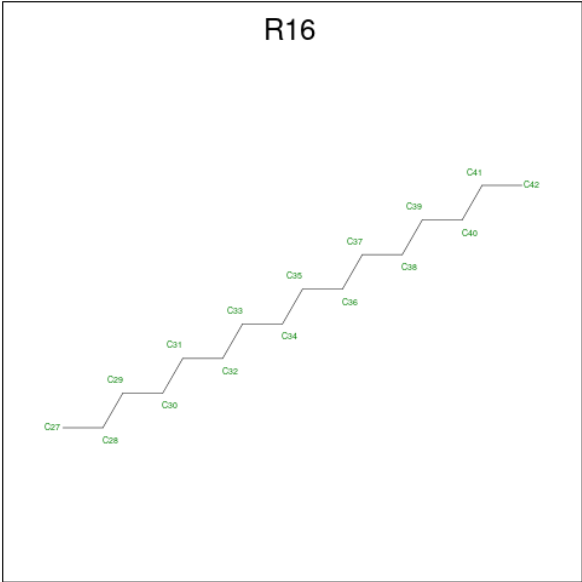


Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $\text{C}_{31}\text{H}_{50}\text{O}_4$).

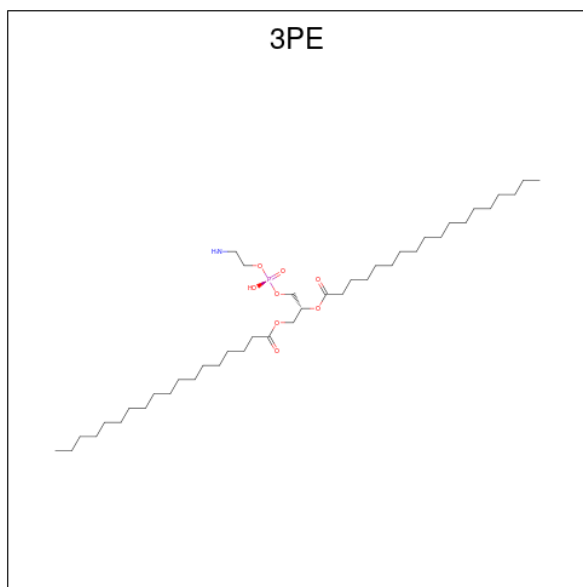
[illegible]

- Molecule 7 is HEXADECANE (CCD ID: R16) (formula: $\text{C}_{16}\text{H}_{34}$).



Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C	0
			10	10	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			13	13	
7	A	1	Total	C	0
			9	9	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			9	9	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).

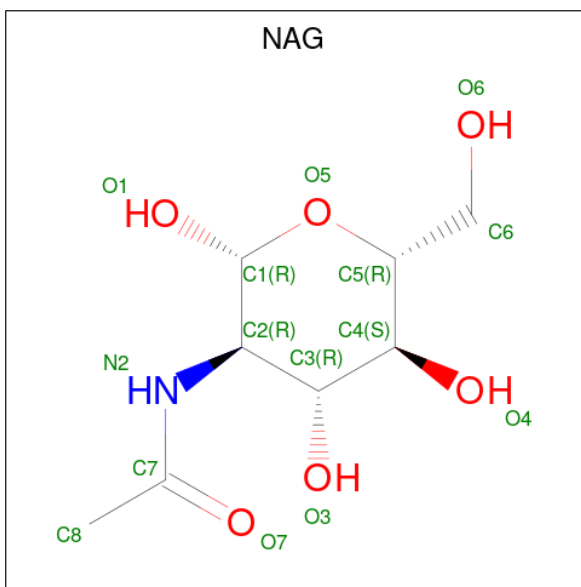


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 9 is CALCIUM ION (CCD ID: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

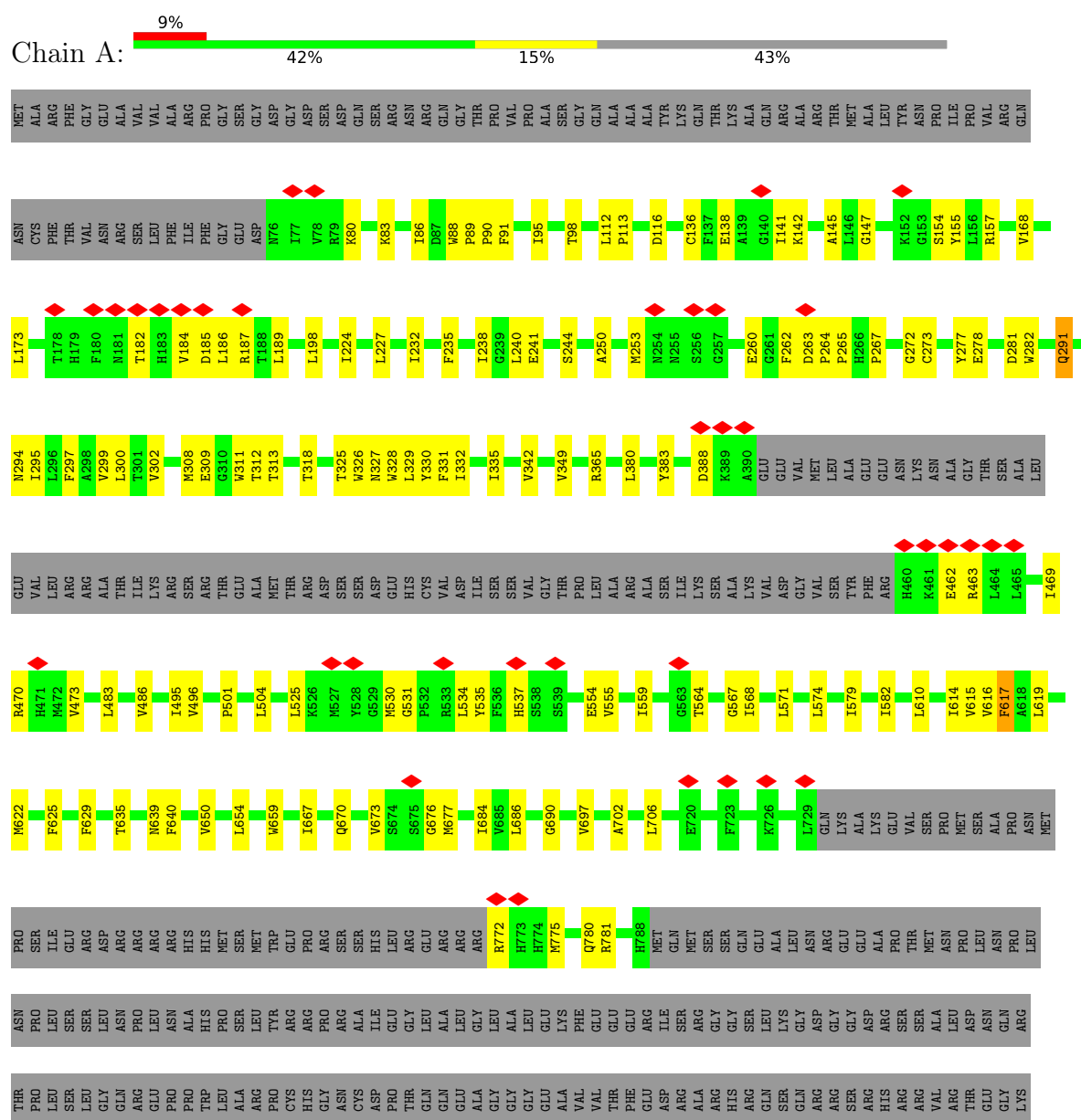


Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

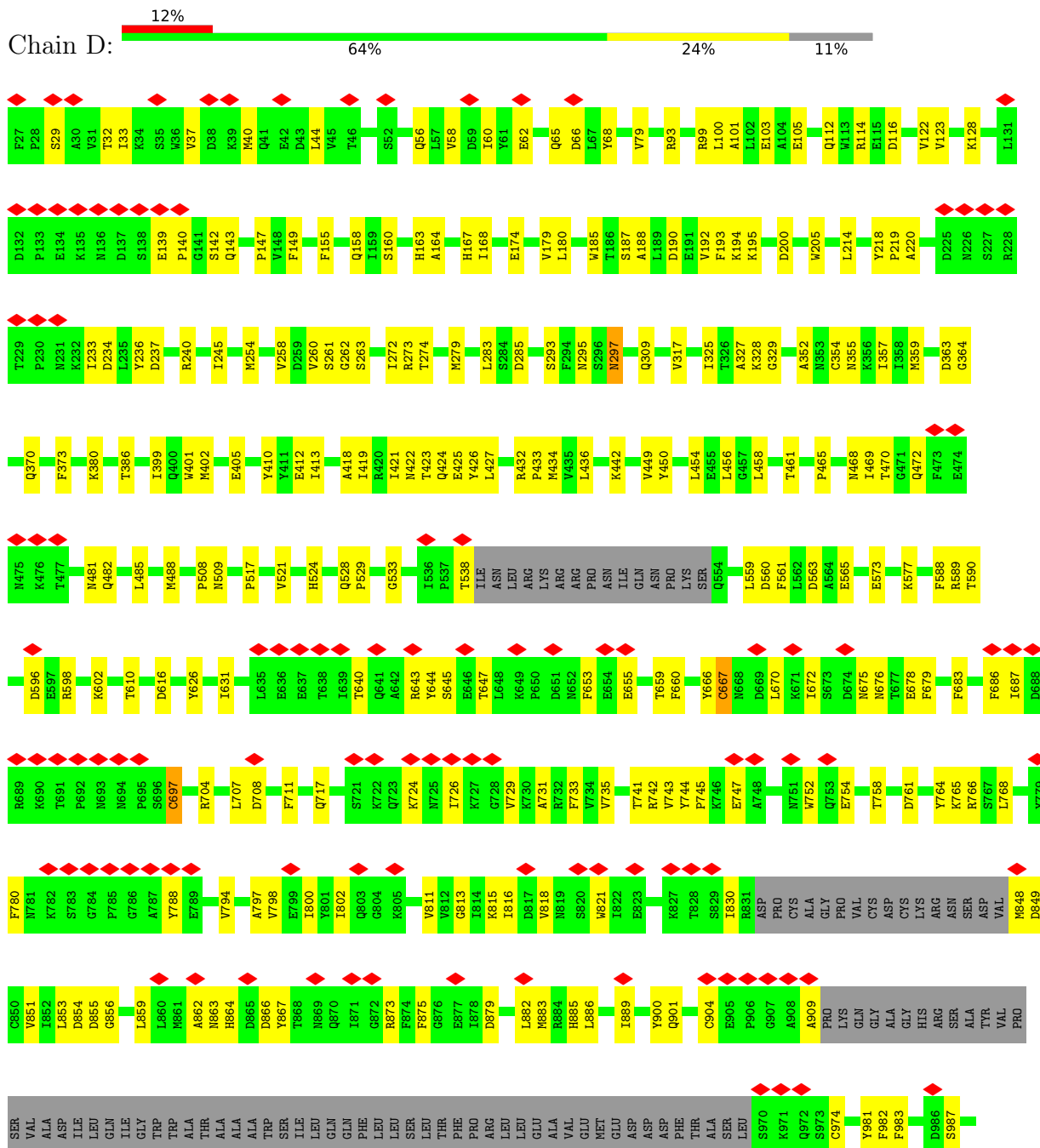
- Molecule 1: Voltage-dependent R-type calcium channel subunit alpha-1E





[illegible]

- Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1



Chain E:  67% 33%



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

Chain F:  100% 67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	257473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.112	Depositor
Minimum map value	-3.500	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, R16, CA, 3PE, BMA, 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	0.29	0/10939	0.54	4/14805 (0.0%)
2	D	0.26	0/7799	0.48	2/10578 (0.0%)
3	B	0.14	0/1280	0.40	0/1729
All	All	0.27	0/20018	0.51	6/27112 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1479	SER	N-CA-C	-8.43	101.02	114.09
2	D	697	CYS	CA-CB-SG	7.02	130.54	114.40
1	A	272	GLY	CA-C-N	5.77	128.41	120.39
1	A	272	GLY	C-N-CA	5.77	128.41	120.39
2	D	667	CYS	CA-CB-SG	5.44	126.92	114.40
1	A	1294	ILE	N-CA-C	-5.08	107.78	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10674	0	10813	277	0
2	D	7637	0	7427	182	0
3	B	1259	0	1254	32	0
4	C	39	0	34	1	0
4	E	39	0	34	3	0
5	F	39	0	34	0	0
6	A	210	0	294	49	0
7	A	89	0	180	6	0
8	A	32	0	38	1	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	D	112	0	104	2	0
All	All	20132	0	20212	492	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 (492) 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:1299:PHE:CD2	6:A:2404:Y01:HAA3	1.92	1.04
1:A:564:THR:HG21	6:A:2404:Y01:HAL2	1.39	1.02
1:A:88:TRP:CD1	1:A:90:PRO:HG2	2.05	0.92
1:A:1499:TYR:CD2	6:A:2415:Y01:HAI	2.07	0.90
2:D:524:HIS:HE1	2:D:565:GLU:OE2	1.55	0.89
1:A:295:ILE:HG21	6:A:2415:Y01:HAE3	1.56	0.85
1:A:1506:TYR:HE1	6:A:2401:Y01:CAE	1.89	0.84
2:D:655:GLU:HB3	2:D:717:GLN:HE22	1.44	0.82
1:A:295:ILE:CG2	6:A:2415:Y01:HAE3	2.11	0.81
2:D:994:LEU:HB3	2:D:1001:ARG:HB2	1.62	0.80
2:D:830:ILE:HG22	2:D:863:ASN:HB2	1.64	0.80
2:D:524:HIS:CE1	2:D:565:GLU:OE2	2.35	0.79
1:A:235:PHE:HA	1:A:238:ILE:HD12	1.65	0.79
2:D:883:MET:HA	2:D:886:LEU:HB2	1.65	0.79
2:D:240:ARG:HG3	2:D:424:GLN:HE21	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:THR:HG23	6:A:2401:Y01:HAI	1.66	0.78
1:A:564:THR:HG21	6:A:2404:Y01:CAL	2.14	0.77
1:A:1513:LEU:CD2	6:A:2401:Y01:HAB1	2.16	0.76
1:A:308:MET:SD	1:A:1661:THR:OG1	2.44	0.75
1:A:1513:LEU:HD22	6:A:2401:Y01:HAB1	1.68	0.75
2:D:528:GLN:O	2:D:901:GLN:NE2	2.21	0.73
1:A:1506:TYR:HE1	6:A:2401:Y01:HAE1	1.53	0.73
1:A:83:LYS:HG3	1:A:141:ILE:HG13	1.71	0.72
1:A:1617:LEU:HD22	1:A:1713:LEU:HD12	1.72	0.71
3:B:229:MET:HE2	3:B:316:LEU:HD12	1.72	0.71
1:A:295:ILE:CG2	6:A:2415:Y01:CAE	2.69	0.71
1:A:1460:MET:HB3	1:A:1462:GLN:HG2	1.72	0.70
1:A:1299:PHE:CE2	6:A:2404:Y01:HAA3	2.27	0.70
1:A:1793:MET:HB2	1:A:1815:THR:HG21	1.73	0.70
1:A:1556:GLU:OE1	1:A:1579:ARG:NH1	2.25	0.70
2:D:434:MET:HE2	2:D:465:PRO:HG3	1.72	0.69
1:A:1454:LYS:HZ3	1:A:1805:PHE:HB3	1.57	0.69
1:A:1373:GLY:HA3	1:A:1666:GLN:HE22	1.57	0.69
2:D:442:LYS:NZ	2:D:465:PRO:O	2.25	0.69
2:D:640:THR:HA	2:D:643:ARG:HE	1.58	0.69
1:A:318:THR:O	1:A:327:ASN:ND2	2.26	0.69
2:D:93:ARG:NH1	2:D:200:ASP:OD2	2.27	0.68
1:A:1506:TYR:HD1	6:A:2401:Y01:HBD	1.57	0.68
1:A:1658:ARG:NH1	1:A:1663:GLU:O	2.27	0.68
1:A:1814:ARG:HH12	1:A:1820:LYS:HB2	1.58	0.68
2:D:237:ASP:OD2	2:D:424:GLN:NE2	2.27	0.68
2:D:596:ASP:OD1	2:D:596:ASP:O	2.12	0.68
3:B:346:ILE:HG21	3:B:352:LEU:HD12	1.75	0.67
2:D:295:ASN:ND2	2:D:328:LYS:O	2.27	0.67
1:A:1441:LYS:H	1:A:1444:ARG:HB2	1.59	0.67
2:D:563:ASP:OD1	2:D:1051:ARG:NH2	2.27	0.67
1:A:241:GLU:OE1	1:A:1579:ARG:NH2	2.29	0.66
1:A:1460:MET:HE3	1:A:1461:PRO:HD2	1.76	0.66
1:A:1505:THR:CG2	6:A:2401:Y01:HAV2	2.25	0.66
1:A:273:CYS:HB3	1:A:277:TYR:HB2	1.77	0.65
1:A:1791:VAL:HA	1:A:1866:GLY:HA3	1.79	0.64
1:A:300:LEU:HD13	1:A:684:ILE:HD11	1.78	0.64
1:A:1407:PHE:HA	1:A:1411:PRO:HD2	1.80	0.64
1:A:1506:TYR:CE1	6:A:2401:Y01:CAE	2.78	0.64
2:D:670:LEU:HG	2:D:686:PHE:HD2	1.63	0.63
2:D:44:LEU:HD21	2:D:821:TRP:HE1	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1353:PHE:HD1	1:A:1364:THR:HG22	1.63	0.63
2:D:733:PHE:HB3	2:D:743:VAL:HG23	1.81	0.62
1:A:1506:TYR:HE1	6:A:2401:Y01:HAE3	1.63	0.62
1:A:1793:MET:HG3	1:A:1811:ALA:HB1	1.82	0.62
1:A:1621:TYR:HA	1:A:1624:ILE:HD12	1.81	0.62
1:A:263:ASP:HB3	1:A:264:PRO:HD3	1.80	0.62
2:D:481:ASN:OD1	4:E:1:NAG:O6	2.18	0.62
2:D:139:GLU:OE1	2:D:140:PRO:HD2	2.00	0.62
1:A:1513:LEU:CD2	6:A:2401:Y01:CAB	2.78	0.61
2:D:357:ILE:HG21	2:D:359:MET:HE2	1.81	0.61
1:A:483:LEU:HA	1:A:486:VAL:HG12	1.81	0.61
1:A:1763:GLU:HA	1:A:1766:GLU:HB3	1.82	0.61
1:A:297:PHE:CE2	7:A:2414:R16:H342	2.35	0.61
1:A:297:PHE:CE2	7:A:2414:R16:C34	2.83	0.61
1:A:706:LEU:HD21	1:A:1421:LEU:HG	1.83	0.61
1:A:1299:PHE:HE2	6:A:2404:Y01:HAB2	1.66	0.61
1:A:184:VAL:HG23	1:A:185:ASP:H	1.64	0.61
1:A:383:TYR:HB3	3:B:355:LEU:HD11	1.83	0.61
1:A:1796:PRO:HB3	1:A:1858:PRO:HB3	1.82	0.61
2:D:363:ASP:OD1	2:D:364:GLY:N	2.32	0.61
2:D:848:MET:N	2:D:1019:GLU:OE1	2.34	0.61
2:D:33:ILE:HD11	2:D:1004:HIS:HD2	1.65	0.60
2:D:704:ARG:NH1	2:D:708:ASP:OD2	2.33	0.60
2:D:573:GLU:O	2:D:577:LYS:HG2	2.02	0.60
1:A:1621:TYR:CE2	1:A:1706:PHE:HB2	2.37	0.60
2:D:469:ILE:HG23	2:D:472:GLN:HG3	1.83	0.60
1:A:1461:PRO:HG2	1:A:1469:TYR:HD2	1.67	0.60
1:A:1513:LEU:HD22	6:A:2401:Y01:CAB	2.31	0.60
1:A:1506:TYR:CE1	6:A:2401:Y01:HAE3	2.36	0.59
2:D:149:PHE:HB3	2:D:158:GLN:HB3	1.85	0.59
3:B:255:PHE:HA	3:B:258:HIS:CE1	2.37	0.59
1:A:564:THR:CG2	6:A:2404:Y01:HAL2	2.22	0.59
1:A:1814:ARG:NH2	1:A:1820:LYS:O	2.36	0.59
2:D:659:THR:HB	2:D:742:ARG:HG3	1.85	0.59
2:D:596:ASP:OD2	2:D:598:ARG:NH2	2.35	0.58
1:A:1505:THR:HG23	6:A:2401:Y01:HAV2	1.83	0.58
1:A:1335:ASP:OD2	1:A:1344:LYS:NZ	2.33	0.58
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.38	0.58
2:D:994:LEU:N	2:D:1001:ARG:O	2.31	0.58
2:D:1003:PHE:HA	2:D:1018:VAL:HA	1.85	0.58
1:A:496:VAL:HG21	1:A:1309:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:ALA:HB3	1:A:1507:GLU:HG3	1.85	0.58
2:D:58:VAL:HG13	2:D:800:ILE:HG22	1.86	0.58
1:A:1620:ILE:HG22	1:A:1624:ILE:HD11	1.86	0.58
2:D:100:LEU:HB3	2:D:488:MET:HE2	1.85	0.58
1:A:1506:TYR:CE1	6:A:2401:Y01:HAE1	2.38	0.57
1:A:312:THR:HG21	1:A:1658:ARG:HG3	1.86	0.57
1:A:83:LYS:HB3	1:A:145:ALA:HB2	1.85	0.57
1:A:1703:PHE:O	1:A:1707:ILE:HG12	2.05	0.57
1:A:1410:PHE:HB2	1:A:1411:PRO:HD3	1.87	0.57
2:D:885:HIS:O	2:D:889:ILE:HD12	2.05	0.57
1:A:186:LEU:HD12	1:A:187:ARG:N	2.19	0.57
1:A:309:GLU:HG3	1:A:659:TRP:CD1	2.40	0.57
1:A:564:THR:HG21	6:A:2404:Y01:CAX	2.35	0.57
2:D:660:PHE:HB3	2:D:676:ASN:HD21	1.69	0.57
1:A:186:LEU:HD13	1:A:189:LEU:H	1.70	0.56
1:A:1515:ILE:O	1:A:1519:MET:HG3	2.05	0.56
2:D:470:THR:HG21	4:E:1:NAG:H5	1.87	0.56
2:D:997:GLY:N	2:D:1026:CYS:SG	2.68	0.56
2:D:675:ASN:HB3	2:D:678:GLU:HG3	1.88	0.56
1:A:224:ILE:HD11	1:A:349:VAL:HG21	1.87	0.56
1:A:281:ASP:OD1	1:A:282:TRP:N	2.39	0.56
1:A:1471:VAL:HG21	1:A:1530:ILE:HG22	1.87	0.56
2:D:380:LYS:NZ	2:D:405:GLU:O	2.29	0.56
3:B:310:PHE:O	3:B:314:ARG:N	2.39	0.56
1:A:291:GLN:O	1:A:297:PHE:HB3	2.05	0.56
1:A:1658:ARG:HH12	1:A:1664:ALA:HB3	1.71	0.56
1:A:1299:PHE:CE2	6:A:2404:Y01:HAB2	2.42	0.55
1:A:1741:LEU:HD21	1:A:1813:ILE:HD11	1.87	0.55
2:D:982:PHE:HZ	4:C:1:NAG:H61	1.70	0.55
1:A:1167:SER:HB2	1:A:1265:PRO:HG3	1.88	0.55
1:A:1224:ILE:HD12	1:A:1224:ILE:H	1.71	0.55
1:A:1760:HIS:CE1	1:A:1762:THR:HG23	2.41	0.55
3:B:247:MET:HE3	3:B:251:ALA:HB2	1.89	0.55
3:B:332:LEU:HD23	3:B:332:LEU:O	2.07	0.55
1:A:571:LEU:HD21	6:A:2404:Y01:HAN2	1.87	0.55
2:D:509:ASN:ND2	2:D:626:TYR:OH	2.39	0.55
2:D:410:TYR:OH	2:D:412:GLU:OE1	2.22	0.55
1:A:198:LEU:HG	1:A:616:VAL:HG21	1.87	0.55
1:A:470:ARG:HA	1:A:473:VAL:HG12	1.89	0.55
1:A:297:PHE:CE2	7:A:2414:R16:H341	2.42	0.55
1:A:1412:PHE:O	1:A:1416:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1756:CYS:SG	1:A:1759:ILE:HA	2.48	0.54
2:D:99:ARG:HD2	2:D:195:LYS:NZ	2.23	0.54
2:D:413:ILE:HG21	2:D:419:ILE:HD13	1.90	0.54
1:A:1450:ALA:HB2	1:A:1809:LEU:HD22	1.89	0.54
2:D:788:TYR:HD1	2:D:818:VAL:HG11	1.72	0.54
1:A:1299:PHE:HD2	6:A:2404:Y01:HAA3	1.65	0.54
1:A:1744:PHE:HB2	1:A:1775:LEU:HD21	1.90	0.54
1:A:1804:HIS:CE1	1:A:1853:LEU:HD21	2.41	0.54
2:D:65:GLN:HG2	2:D:802:ILE:HD12	1.89	0.54
2:D:432:ARG:HB2	2:D:433:PRO:HD3	1.90	0.54
1:A:1265:PRO:HB2	1:A:1620:ILE:HD11	1.90	0.54
1:A:331:PHE:O	1:A:335:ILE:HG12	2.08	0.54
2:D:254:MET:HE1	2:D:279:MET:HG2	1.90	0.54
1:A:113:PRO:HD2	2:D:263:SER:HA	1.90	0.54
2:D:58:VAL:O	2:D:62:GLU:HG3	2.08	0.54
1:A:116:ASP:HB2	2:D:262:GLY:HA3	1.90	0.53
6:A:2410:Y01:HBA	6:A:2410:Y01:HBB	1.88	0.53
1:A:616:VAL:HA	1:A:619:LEU:HD12	1.90	0.53
1:A:1377:VAL:O	1:A:1381:SER:OG	2.26	0.53
1:A:1423:ILE:HG23	1:A:1723:MET:HE3	1.91	0.53
2:D:44:LEU:HD21	2:D:821:TRP:NE1	2.23	0.53
1:A:775:MET:HE3	1:A:780:GLN:HG2	1.90	0.53
1:A:1789:ARG:HH12	1:A:1812:LEU:HD23	1.74	0.53
1:A:1864:THR:O	1:A:1868:ILE:HG13	2.08	0.53
1:A:1795:MET:HE1	1:A:1808:THR:HG23	1.91	0.53
3:B:269:VAL:HG11	3:B:273:ILE:HD11	1.89	0.53
3:B:342:VAL:HG13	3:B:387:ILE:HB	1.90	0.53
1:A:311:TRP:HE1	1:A:1661:THR:HG21	1.73	0.52
1:A:1814:ARG:HG2	1:A:1821:ILE:HD11	1.91	0.52
2:D:155:PHE:HA	2:D:456:LEU:HD21	1.92	0.52
2:D:285:ASP:O	2:D:309:GLN:NE2	2.42	0.52
2:D:508:PRO:HG2	2:D:764:TYR:CE2	2.44	0.52
1:A:1790:LEU:HG	1:A:1793:MET:HE2	1.90	0.52
1:A:227:LEU:HD21	1:A:1597:LEU:HD21	1.90	0.52
2:D:56:GLN:O	2:D:60:ILE:HG13	2.10	0.52
2:D:103:GLU:HG2	2:D:192:VAL:HG21	1.91	0.52
1:A:473:VAL:HG21	1:A:525:LEU:HB3	1.92	0.52
1:A:1199:PHE:HA	1:A:1202:VAL:HG22	1.92	0.52
1:A:332:ILE:HD11	1:A:1654:MET:HE1	1.92	0.52
1:A:635:THR:OG1	1:A:639:ASN:OD1	2.26	0.52
1:A:1506:TYR:CD1	6:A:2401:Y01:HBD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:VAL:HG11	6:A:2404:Y01:HBE	1.91	0.52
1:A:253:MET:HG3	1:A:260:GLU:HB3	1.92	0.51
1:A:554:GLU:CD	1:A:567:GLY:HA2	2.34	0.51
1:A:1619:PHE:O	1:A:1623:ILE:HG12	2.10	0.51
2:D:373:PHE:CE2	2:D:402:MET:HG2	2.46	0.51
2:D:205:TRP:HE1	2:D:456:LEU:CD1	2.23	0.51
1:A:1505:THR:HG21	6:A:2401:Y01:OAH	2.11	0.51
1:A:1292:ILE:HG13	1:A:1421:LEU:HD11	1.92	0.51
2:D:273:ARG:NH2	2:D:325:ILE:O	2.43	0.51
1:A:1491:ASN:HD21	1:A:1582:ARG:HH11	1.58	0.51
2:D:560:ASP:OD1	2:D:561:PHE:N	2.44	0.51
3:B:263:ARG:HE	3:B:264:ILE:HD11	1.76	0.51
3:B:327:ASN:O	3:B:377:LEU:HD21	2.11	0.51
1:A:380:LEU:HD12	3:B:351:VAL:HG23	1.92	0.51
2:D:352:ALA:O	2:D:354:CYS:N	2.42	0.51
1:A:240:LEU:O	1:A:244:SER:HB2	2.10	0.50
1:A:328:TRP:HB2	1:A:332:ILE:HD13	1.94	0.50
6:A:2406:Y01:HAN2	6:A:2406:Y01:HAC3	1.91	0.50
1:A:1240:ALA:HB2	1:A:1254:ILE:HG21	1.93	0.50
1:A:238:ILE:HB	1:A:330:TYR:HE1	1.75	0.50
1:A:88:TRP:CD1	1:A:91:PHE:HB2	2.46	0.50
1:A:530:MET:HE3	1:A:534:LEU:O	2.12	0.50
1:A:617:PHE:CZ	1:A:686:LEU:HB2	2.46	0.50
1:A:1265:PRO:O	1:A:1268:THR:HG22	2.12	0.50
1:A:1353:PHE:CD1	1:A:1364:THR:HG22	2.47	0.50
1:A:95:ILE:HA	1:A:98:THR:HG22	1.94	0.50
2:D:99:ARG:HD2	2:D:195:LYS:HZ3	1.77	0.50
2:D:666:TYR:O	2:D:667:CYS:HB3	2.12	0.50
2:D:788:TYR:CD1	2:D:818:VAL:HG11	2.46	0.50
1:A:1262:VAL:O	1:A:1265:PRO:HD2	2.12	0.49
2:D:370:GLN:HG2	2:D:401:TRP:CH2	2.48	0.49
2:D:672:ILE:HG22	2:D:679:PHE:HE2	1.77	0.49
2:D:1049:GLN:HG2	2:D:1049:GLN:O	2.12	0.49
1:A:568:ILE:HG13	1:A:568:ILE:O	2.13	0.49
1:A:1849:LYS:O	1:A:1853:LEU:N	2.42	0.49
2:D:79:VAL:HG12	2:D:610:THR:HG22	1.94	0.49
1:A:294:ASN:HB2	1:A:297:PHE:HD2	1.78	0.49
2:D:724:LYS:HD2	2:D:744:TYR:OH	2.13	0.49
1:A:142:LYS:HD2	1:A:155:TYR:HE1	1.78	0.49
1:A:250:ALA:HB2	1:A:282:TRP:CD2	2.48	0.49
1:A:1153:ARG:HD3	1:A:1154:TYR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1617:LEU:HD11	1:A:1621:TYR:HE1	1.78	0.49
2:D:193:PHE:HB3	2:D:218:TYR:CG	2.48	0.49
1:A:1768:LEU:HD23	1:A:1777:LEU:HB2	1.95	0.49
2:D:1061:ASP:OD1	2:D:1061:ASP:N	2.45	0.49
3:B:268:ARG:HA	3:B:322:ASP:HB3	1.94	0.48
1:A:1454:LYS:NZ	1:A:1805:PHE:HB3	2.26	0.48
2:D:128:LYS:NZ	2:D:234:ASP:OD2	2.41	0.48
2:D:297:ASN:C	2:D:297:ASN:HD22	2.21	0.48
1:A:1543:ASN:O	1:A:1547:PHE:N	2.44	0.48
2:D:752:TRP:NE1	2:D:754:GLU:HB2	2.28	0.48
3:B:256:LEU:HD21	3:B:401:LEU:HD21	1.95	0.48
2:D:726:ILE:HB	2:D:729:VAL:HG22	1.94	0.48
1:A:1202:VAL:O	1:A:1206:ILE:HG12	2.12	0.48
1:A:1513:LEU:CD1	6:A:2401:Y01:HAB1	2.43	0.48
2:D:58:VAL:HG22	2:D:798:VAL:HG13	1.96	0.48
2:D:991:SER:HB3	2:D:1004:HIS:ND1	2.29	0.48
1:A:278:GLU:N	1:A:278:GLU:OE2	2.47	0.48
1:A:1771:MET:HB2	1:A:1776:GLY:HA3	1.95	0.48
1:A:1358:ILE:HG21	6:A:2406:Y01:HAC1	1.95	0.48
2:D:254:MET:HE3	2:D:359:MET:HG3	1.95	0.47
2:D:418:ALA:O	2:D:422:ASN:ND2	2.46	0.47
3:B:328:HIS:HB3	3:B:331:GLN:HB2	1.96	0.47
1:A:1385:THR:O	1:A:1386:GLU:HG3	2.13	0.47
1:A:1847:SER:H	1:A:1850:MET:HE3	1.79	0.47
2:D:254:MET:SD	2:D:283:LEU:HD21	2.53	0.47
3:B:230:ARG:NH2	3:B:339:PRO:O	2.48	0.47
1:A:622:MET:HG2	1:A:640:PHE:O	2.13	0.47
2:D:168:ILE:HG12	2:D:214:LEU:CD2	2.44	0.47
1:A:495:ILE:HG22	6:A:2406:Y01:HAE2	1.95	0.47
1:A:1646:PHE:CZ	1:A:1655:LEU:HD22	2.49	0.47
2:D:386:THR:HB	2:D:399:ILE:HG23	1.95	0.47
3:B:234:LEU:HD13	3:B:342:VAL:HB	1.96	0.47
1:A:88:TRP:NE1	1:A:90:PRO:HG2	2.29	0.47
1:A:1382:VAL:O	1:A:1384:VAL:N	2.47	0.47
1:A:1625:GLY:HA2	1:A:1629:PHE:HD2	1.79	0.47
2:D:68:TYR:CD1	2:D:631:ILE:HG23	2.50	0.47
3:B:263:ARG:HE	3:B:264:ILE:CD1	2.27	0.47
1:A:1478:PRO:HB3	1:A:1481:GLU:HB2	1.97	0.47
8:A:2409:3PE:H352	8:A:2409:3PE:H241	1.96	0.47
2:D:261:SER:O	2:D:327:ALA:HB1	2.15	0.47
2:D:469:ILE:HG22	2:D:469:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:LYS:HE3	1:A:1862:ASP:HB2	1.96	0.47
2:D:33:ILE:HD11	2:D:1004:HIS:CD2	2.49	0.47
2:D:521:VAL:HG22	2:D:559:LEU:O	2.14	0.47
1:A:617:PHE:CG	1:A:686:LEU:HD13	2.50	0.47
1:A:325:THR:HG1	1:A:326:TRP:CD1	2.33	0.47
1:A:388:ASP:H	3:B:247:MET:HE2	1.79	0.47
1:A:1374:TRP:CD1	1:A:1375:PRO:HD3	2.50	0.47
2:D:245:ILE:HG12	2:D:427:LEU:CD1	2.45	0.47
1:A:1768:LEU:HB3	1:A:1777:LEU:HB3	1.97	0.46
1:A:1513:LEU:HD21	6:A:2401:Y01:CAB	2.45	0.46
2:D:174:GLU:HA	2:D:179:VAL:HG11	1.98	0.46
2:D:274:THR:HG22	2:D:419:ILE:HG21	1.98	0.46
1:A:1334:VAL:HG22	2:D:233:ILE:HD11	1.97	0.46
1:A:1486:ALA:O	1:A:1490:LEU:HG	2.16	0.46
2:D:904:CYS:HB2	2:D:974:CYS:HB3	1.43	0.46
1:A:1596:LEU:HD23	1:A:1728:TYR:HE2	1.81	0.46
2:D:508:PRO:HB2	2:D:765:LYS:HG2	1.97	0.46
1:A:1714:MET:HE2	1:A:1714:MET:HB3	1.80	0.46
2:D:485:LEU:HD22	4:E:1:NAG:H82	1.98	0.46
2:D:856:GLY:HA2	2:D:981:TYR:HB2	1.97	0.46
1:A:1363:LEU:HD22	7:A:2407:R16:H312	1.96	0.46
2:D:879:ASP:HB2	2:D:882:LEU:HD23	1.97	0.46
2:D:122:VAL:HG23	2:D:142:SER:HB3	1.98	0.46
3:B:239:LEU:HB2	3:B:242:TYR:CD2	2.51	0.46
2:D:122:VAL:HG21	2:D:180:LEU:HD22	1.98	0.46
1:A:138:GLU:HA	1:A:141:ILE:HG22	1.98	0.45
1:A:531:GLY:O	1:A:535:TYR:HB2	2.16	0.45
2:D:218:TYR:HB3	2:D:219:PRO:HD3	1.99	0.45
3:B:244:VAL:HG21	3:B:356:ILE:HG12	1.99	0.45
1:A:1835:LEU:HD23	1:A:1855:VAL:HG13	1.98	0.45
6:A:2408:Y01:HAC1	6:A:2408:Y01:HAP1	1.64	0.45
1:A:1303:PHE:CE2	6:A:2404:Y01:HAP2	2.52	0.45
1:A:1657:PHE:HB2	6:A:2408:Y01:HAQ2	1.99	0.45
2:D:644:TYR:O	2:D:647:THR:OG1	2.32	0.45
1:A:1308:VAL:O	1:A:1312:LYS:HB2	2.17	0.45
2:D:185:TRP:HA	10:D:1205:NAG:H82	1.98	0.45
1:A:1743:GLU:O	1:A:1747:VAL:HG22	2.16	0.45
2:D:357:ILE:CG2	2:D:359:MET:HE2	2.47	0.45
2:D:436:LEU:HD23	2:D:1065:LEU:HB2	1.98	0.45
2:D:735:VAL:HG12	2:D:741:THR:OG1	2.17	0.45
1:A:1173:GLU:HG2	1:A:1186:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:ARG:O	1:A:1447:ILE:HG22	2.16	0.45
2:D:37:VAL:HA	2:D:40:MET:HG2	1.98	0.45
2:D:260:VAL:HG22	2:D:293:SER:HB2	1.97	0.45
2:D:295:ASN:C	2:D:297:ASN:H	2.24	0.45
2:D:436:LEU:HD11	2:D:482:GLN:HG2	1.98	0.45
2:D:660:PHE:HB3	2:D:676:ASN:ND2	2.31	0.45
2:D:160:SER:OG	2:D:220:ALA:HB3	2.17	0.45
1:A:673:VAL:HG13	1:A:673:VAL:O	2.17	0.45
2:D:240:ARG:HG3	2:D:424:GLN:NE2	2.24	0.45
1:A:332:ILE:HD11	1:A:1654:MET:CE	2.48	0.44
2:D:640:THR:HA	2:D:643:ARG:HG2	1.99	0.44
2:D:859:LEU:HD21	2:D:867:TYR:HB3	1.99	0.44
1:A:1312:LYS:HE2	1:A:1312:LYS:HB3	1.72	0.44
1:A:1673:LEU:HD23	1:A:1699:ALA:HB3	1.99	0.44
2:D:29:SER:HB3	2:D:32:THR:HG23	2.00	0.44
2:D:588:PHE:CE2	2:D:590:THR:HG22	2.52	0.44
1:A:311:TRP:NE1	1:A:1661:THR:HG21	2.32	0.44
2:D:193:PHE:CG	2:D:218:TYR:HB2	2.52	0.44
1:A:173:LEU:HB2	1:A:189:LEU:HD21	1.99	0.44
1:A:1790:LEU:HD21	1:A:1865:VAL:HG12	1.99	0.44
6:A:2415:Y01:HAP1	6:A:2415:Y01:HAO2	1.69	0.44
1:A:496:VAL:HG21	1:A:1309:GLN:HE22	1.83	0.44
1:A:702:ALA:HB1	1:A:1417:ILE:HD13	2.00	0.44
1:A:1458:ARG:HA	1:A:1754:ALA:HB1	1.99	0.44
2:D:66:ASP:OD1	2:D:66:ASP:N	2.48	0.44
3:B:239:LEU:HB2	3:B:242:TYR:HD2	1.83	0.44
1:A:88:TRP:CD1	1:A:91:PHE:CB	3.01	0.44
1:A:154:SER:OG	1:A:157:ARG:HG2	2.17	0.44
2:D:449:VAL:HG12	2:D:458:LEU:HD22	1.99	0.44
2:D:450:TYR:HE1	2:D:461:THR:HG22	1.83	0.44
1:A:555:VAL:O	1:A:559:ILE:HG12	2.17	0.44
1:A:1243:LEU:HD23	1:A:1247:LYS:NZ	2.33	0.44
2:D:538:THR:HG23	2:D:909:ALA:HB2	1.99	0.44
2:D:862:ALA:HB3	2:D:867:TYR:HB2	1.99	0.44
3:B:341:ILE:O	3:B:386:ASP:N	2.51	0.44
3:B:342:VAL:HG22	3:B:387:ILE:HD12	1.99	0.44
2:D:745:PRO:C	2:D:747:GLU:H	2.26	0.43
1:A:1571:ASN:C	1:A:1572:MET:HE2	2.43	0.43
1:A:186:LEU:HD13	1:A:189:LEU:HB3	2.00	0.43
1:A:1201:MET:SD	1:A:1230:VAL:HG21	2.58	0.43
1:A:1795:MET:HE2	1:A:1808:THR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HB3	1:A:116:ASP:HB3	1.99	0.43
1:A:1401:ILE:HA	1:A:1404:VAL:HG12	2.01	0.43
1:A:1513:LEU:HD13	6:A:2401:Y01:HAB1	2.01	0.43
1:A:1582:ARG:HG2	1:A:1585:LYS:HE3	1.99	0.43
1:A:1836:GLN:HB3	1:A:1851:LEU:HD21	1.99	0.43
2:D:413:ILE:CG2	2:D:419:ILE:HD13	2.48	0.43
1:A:574:LEU:HD11	6:A:2404:Y01:HAB3	1.99	0.43
1:A:1201:MET:O	1:A:1205:MET:HG2	2.19	0.43
1:A:1559:LEU:HB3	1:A:1572:MET:HG3	2.00	0.43
1:A:1680:PRO:O	1:A:1681:ASP:HB3	2.19	0.43
3:B:303:GLN:O	3:B:306:ILE:HG22	2.17	0.43
1:A:88:TRP:HB2	1:A:89:PRO:HD2	1.99	0.43
1:A:147:GLY:C	1:A:154:SER:HB2	2.43	0.43
1:A:83:LYS:HA	1:A:86:ILE:HG12	2.01	0.43
1:A:265:PRO:O	1:A:267:PRO:HD3	2.18	0.43
1:A:365:ARG:HG3	1:A:365:ARG:HH11	1.84	0.43
1:A:1173:GLU:OE2	1:A:1261:ARG:NH2	2.48	0.43
1:A:1655:LEU:HD21	1:A:1668:ILE:HG21	2.01	0.43
1:A:1804:HIS:CG	1:A:1853:LEU:HD11	2.54	0.43
2:D:864:HIS:ND1	2:D:866:ASP:HB3	2.34	0.43
3:B:307:GLU:HA	3:B:310:PHE:HB2	2.01	0.43
1:A:772:ARG:O	1:A:775:MET:HG3	2.19	0.43
1:A:1616:MET:O	1:A:1620:ILE:HG12	2.18	0.43
6:A:2410:Y01:HAE2	6:A:2410:Y01:HAO1	2.00	0.43
1:A:80:LYS:O	1:A:80:LYS:HD3	2.18	0.42
1:A:383:TYR:CE2	3:B:346:ILE:HG13	2.54	0.42
1:A:654:LEU:HD22	1:A:690:GLY:HA3	2.01	0.42
1:A:670:GLN:O	1:A:676:GLY:HA3	2.19	0.42
1:A:1422:ILE:O	1:A:1426:PHE:HB2	2.19	0.42
1:A:1760:HIS:ND1	1:A:1762:THR:HG23	2.34	0.42
1:A:615:VAL:O	1:A:616:VAL:C	2.62	0.42
1:A:1629:PHE:CE1	1:A:1672:CYS:HB3	2.54	0.42
1:A:1856:PRO:HG2	1:A:1858:PRO:HD3	2.01	0.42
1:A:1475:VAL:HG11	1:A:1532:PHE:HE2	1.84	0.42
1:A:1765:TYR:O	1:A:1769:THR:HG23	2.20	0.42
2:D:423:THR:O	2:D:426:TYR:CD2	2.72	0.42
2:D:780:PHE:CE1	2:D:873:ARG:HD2	2.54	0.42
2:D:983:PHE:CD2	2:D:1007:LYS:HE3	2.54	0.42
1:A:383:TYR:CE1	3:B:392:ASN:HA	2.54	0.42
1:A:1680:PRO:C	1:A:1682:THR:H	2.26	0.42
1:A:1785:VAL:O	1:A:1788:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:VAL:HG21	2:D:1043:PRO:HG2	2.01	0.42
2:D:653:PHE:CZ	2:D:659:THR:HG22	2.55	0.42
2:D:766:ARG:HH22	2:D:855:ASP:HB2	1.84	0.42
1:A:262:PHE:HE1	1:A:277:TYR:CZ	2.38	0.42
1:A:1537:TYR:CE1	1:A:1543:ASN:HB3	2.54	0.42
1:A:1658:ARG:NH1	1:A:1668:ILE:HD11	2.34	0.42
1:A:650:VAL:HG13	1:A:686:LEU:HD11	2.02	0.42
2:D:517:PRO:CG	2:D:616:ASP:HB2	2.50	0.42
2:D:645:SER:HB2	2:D:687:ILE:HG21	2.01	0.42
2:D:764:TYR:O	2:D:768:LEU:HD23	2.19	0.42
1:A:1736:LEU:HD11	1:A:1775:LEU:HD13	2.02	0.42
2:D:62:GLU:O	2:D:65:GLN:HG3	2.20	0.42
2:D:167:HIS:CE1	2:D:236:TYR:HD1	2.38	0.42
2:D:258:VAL:HG13	2:D:272:ILE:HG21	2.02	0.42
2:D:670:LEU:HG	2:D:686:PHE:CD2	2.47	0.42
2:D:879:ASP:OD1	2:D:879:ASP:N	2.52	0.42
1:A:1383:ASP:OD1	1:A:1393:ARG:HA	2.20	0.42
1:A:1548:ILE:HA	1:A:1551:ILE:HG22	2.02	0.42
2:D:164:ALA:HA	2:D:218:TYR:O	2.19	0.42
2:D:528:GLN:H	2:D:901:GLN:HE22	1.68	0.42
3:B:328:HIS:CG	3:B:329:PRO:HD2	2.54	0.42
1:A:232:ILE:HG23	1:A:302:VAL:HG13	2.01	0.42
1:A:469:ILE:O	1:A:473:VAL:HG12	2.19	0.42
2:D:421:ILE:O	2:D:425:GLU:HG2	2.19	0.42
2:D:675:ASN:CB	2:D:678:GLU:HG3	2.49	0.42
1:A:297:PHE:HE2	7:A:2414:R16:H342	1.85	0.41
1:A:1159:ILE:HG13	1:A:1200:GLU:HG3	2.02	0.41
1:A:1314:LYS:HB3	1:A:1384:VAL:CG2	2.50	0.41
1:A:1383:ASP:O	1:A:1391:PRO:HB3	2.20	0.41
1:A:1618:PHE:CD2	6:A:2408:Y01:HAP2	2.55	0.41
1:A:1620:ILE:O	1:A:1624:ILE:HG13	2.20	0.41
2:D:667:CYS:HB2	2:D:697:CYS:HB3	1.68	0.41
2:D:683:PHE:CZ	2:D:687:ILE:HD11	2.55	0.41
2:D:707:LEU:HD21	2:D:711:PHE:CE2	2.55	0.41
1:A:1360:TRP:O	1:A:1364:THR:HG23	2.19	0.41
1:A:1526:VAL:HA	1:A:1529:VAL:HG22	2.01	0.41
2:D:187:SER:O	2:D:190:ASP:HB2	2.19	0.41
1:A:326:TRP:HE3	1:A:329:LEU:HD12	1.85	0.41
1:A:625:PHE:HB3	1:A:629:PHE:CE1	2.55	0.41
1:A:667:ILE:HD13	1:A:677:MET:HG3	2.03	0.41
1:A:781:ARG:HA	1:A:781:ARG:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:TRP:CZ2	7:A:2407:R16:H282	2.55	0.41
2:D:468:ASN:OD1	2:D:470:THR:HG23	2.20	0.41
2:D:589:ARG:HD3	2:D:602:LYS:HE3	2.02	0.41
1:A:1308:VAL:C	1:A:1310:LEU:H	2.29	0.41
1:A:1460:MET:HG2	1:A:1754:ALA:HB3	2.02	0.41
6:A:2408:Y01:HAN1	6:A:2408:Y01:HAC3	2.02	0.41
2:D:101:ALA:O	2:D:105:GLU:HG3	2.20	0.41
2:D:260:VAL:HG11	2:D:325:ILE:HG12	2.02	0.41
2:D:454:LEU:O	2:D:456:LEU:HD12	2.21	0.41
2:D:533:GLY:N	2:D:900:TYR:O	2.45	0.41
2:D:758:THR:HA	2:D:761:ASP:OD2	2.21	0.41
1:A:534:LEU:HA	1:A:537:HIS:CD2	2.55	0.41
1:A:1455:PRO:C	1:A:1456:LEU:HD12	2.46	0.41
1:A:1463:ASN:HB3	1:A:1465:HIS:HB2	2.03	0.41
2:D:245:ILE:HG12	2:D:427:LEU:HD13	2.02	0.41
2:D:987:SER:O	2:D:1007:LYS:HD3	2.21	0.41
3:B:245:THR:O	3:B:249:GLN:HG2	2.21	0.41
1:A:1431:ASP:HB2	1:A:1436:GLU:HG3	2.01	0.41
2:D:194:LYS:HG2	2:D:218:TYR:OH	2.20	0.41
1:A:1456:LEU:HD21	1:A:1748:TRP:HB3	2.01	0.41
2:D:731:ALA:HB3	2:D:815:LYS:HB2	2.03	0.41
1:A:136:CYS:HA	1:A:168:VAL:HG21	2.02	0.41
1:A:1629:PHE:CD1	1:A:1672:CYS:HB3	2.56	0.41
6:A:2415:Y01:HAO1	6:A:2415:Y01:HBA	1.43	0.41
2:D:112:GLN:O	2:D:112:GLN:HG2	2.21	0.41
2:D:240:ARG:NH2	2:D:423:THR:OG1	2.54	0.41
2:D:355:ASN:O	2:D:357:ILE:HG13	2.21	0.41
2:D:851:VAL:HG23	2:D:1016:ILE:HB	2.03	0.41
2:D:854:ASP:OD1	2:D:854:ASP:N	2.51	0.41
1:A:157:ARG:HA	1:A:157:ARG:HD2	1.91	0.41
1:A:299:VAL:HA	1:A:302:VAL:HG12	2.03	0.41
1:A:311:TRP:HE1	1:A:1661:THR:CG2	2.34	0.41
2:D:123:VAL:HA	2:D:143:GLN:O	2.21	0.41
2:D:205:TRP:HE3	2:D:219:PRO:HD2	1.85	0.41
2:D:258:VAL:HG12	2:D:260:VAL:HG13	2.03	0.41
1:A:235:PHE:HD1	1:A:330:TYR:CE1	2.39	0.41
1:A:1304:ALA:O	1:A:1308:VAL:HG23	2.21	0.41
1:A:1523:LEU:O	1:A:1527:LEU:HB2	2.21	0.41
1:A:1723:MET:HA	1:A:1726:PHE:HB2	2.03	0.41
2:D:254:MET:HE1	2:D:279:MET:CG	2.50	0.41
2:D:1043:PRO:HA	2:D:1046:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:HE2	3:B:346:ILE:HG13	1.87	0.40
1:A:501:PRO:HD2	1:A:504:LEU:HD12	2.03	0.40
1:A:614:ILE:HG12	1:A:654:LEU:HD11	2.03	0.40
1:A:1275:LEU:HD21	1:A:1616:MET:HE1	2.03	0.40
2:D:116:ASP:OD1	2:D:116:ASP:N	2.54	0.40
2:D:188:ALA:O	2:D:192:VAL:HG23	2.22	0.40
2:D:254:MET:CE	2:D:359:MET:HG3	2.51	0.40
2:D:261:SER:HB2	2:D:329:GLY:O	2.21	0.40
2:D:733:PHE:CZ	2:D:813:GLY:HA3	2.56	0.40
1:A:1658:ARG:HH11	1:A:1668:ILE:HD11	1.86	0.40
2:D:794:VAL:HG21	2:D:816:ILE:HD12	2.01	0.40
2:D:853:LEU:HD11	2:D:875:PHE:CD2	2.56	0.40
1:A:579:ILE:O	1:A:582:ILE:HG12	2.21	0.40
2:D:114:ARG:HH22	10:D:1205:NAG:H62	1.86	0.40
2:D:797:ALA:HA	2:D:811:VAL:HG22	2.04	0.40
1:A:89:PRO:N	1:A:90:PRO:HD2	2.36	0.40
1:A:462:GLU:O	1:A:463:ARG:HD2	2.22	0.40
1:A:610:LEU:HD11	1:A:697:VAL:HG11	2.02	0.40
1:A:1361:ALA:O	1:A:1365:LEU:HB2	2.22	0.40
1:A:1389:ARG:NH1	1:A:1389:ARG:HG2	2.37	0.40
2:D:849:ASP:HA	2:D:863:ASN:OD1	2.21	0.40
1:A:1814:ARG:NH1	1:A:1819:ILE:O	2.54	0.40
6:A:2404:Y01:HAN1	6:A:2404:Y01:HAC3	2.04	0.40
6:A:2415:Y01:HAC2	6:A:2415:Y01:HAJ2	1.74	0.40
2:D:626:TYR:CE1	2:D:768:LEU:HD12	2.56	0.40
3:B:252:LEU:HD12	3:B:252:LEU:HA	1.89	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	1309/2313 (57%)	1191 (91%)	117 (9%)	1 (0%)	48	78
2	D	947/1077 (88%)	878 (93%)	68 (7%)	1 (0%)	48	78
3	B	158/598 (26%)	150 (95%)	8 (5%)	0	100	100
All	All	2414/3988 (60%)	2219 (92%)	193 (8%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1682	THR
2	D	529	PRO

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	1160/2023 (57%)	1154 (100%)	6 (0%)	81	85
2	D	846/950 (89%)	845 (100%)	1 (0%)	88	90
3	B	131/510 (26%)	131 (100%)	0	100	100
All	All	2137/3483 (61%)	2130 (100%)	7 (0%)	84	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	A	313	THR
1	A	342	VAL
1	A	617	PHE
1	A	1284	THR
1	A	1483	THR
2	D	297	ASN

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

Mol	Chain	Res	Type
1	A	248	HIS
1	A	286	ASN
1	A	291	GLN
1	A	374	GLN
1	A	541	ASN
1	A	632	ASN
1	A	1666	GLN
1	A	1804	HIS
2	D	111	HIS
2	D	120	ASN
2	D	136	ASN
2	D	163	HIS
2	D	167	HIS
2	D	391	GLN
2	D	422	ASN
2	D	424	GLN
2	D	482	GLN
2	D	509	ASN
2	D	524	HIS
2	D	676	ASN
2	D	684	ASN
2	D	770	ASN
2	D	1004	HIS
3	B	392	ASN
3	B	400	HIS

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](#)

9 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	C	1	4,2	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	C	2	4	14,14,15	0.15	0	17,19,21	0.46	0
4	BMA	C	3	4	11,11,12	0.57	0	15,15,17	0.94	1 (6%)
4	NAG	E	1	4,2	14,14,15	0.39	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	BMA	E	3	4	11,11,12	0.57	0	15,15,17	0.68	0
5	NAG	F	1	5,2	14,14,15	0.86	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.46	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.70	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	C	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	O5-C1	2.96	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	4.38	118.06	112.19
4	C	3	BMA	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

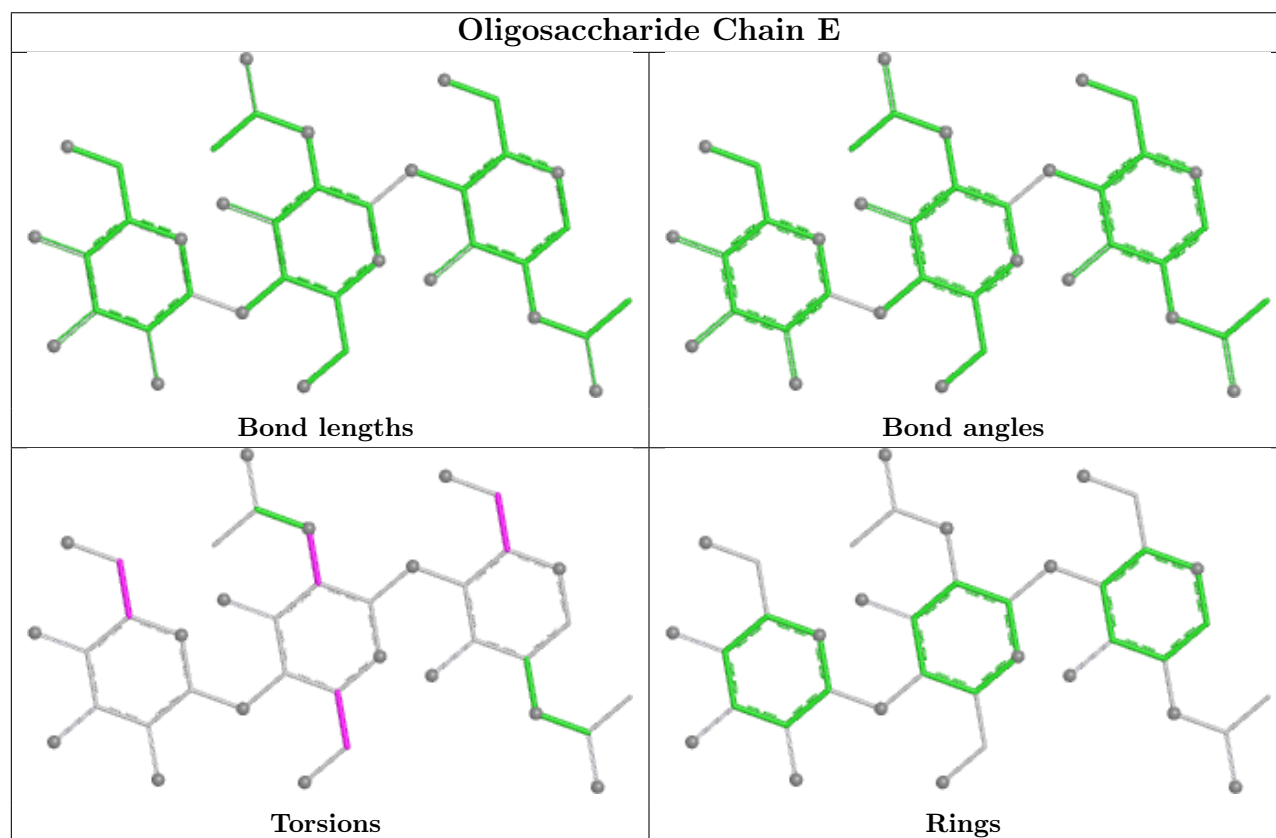
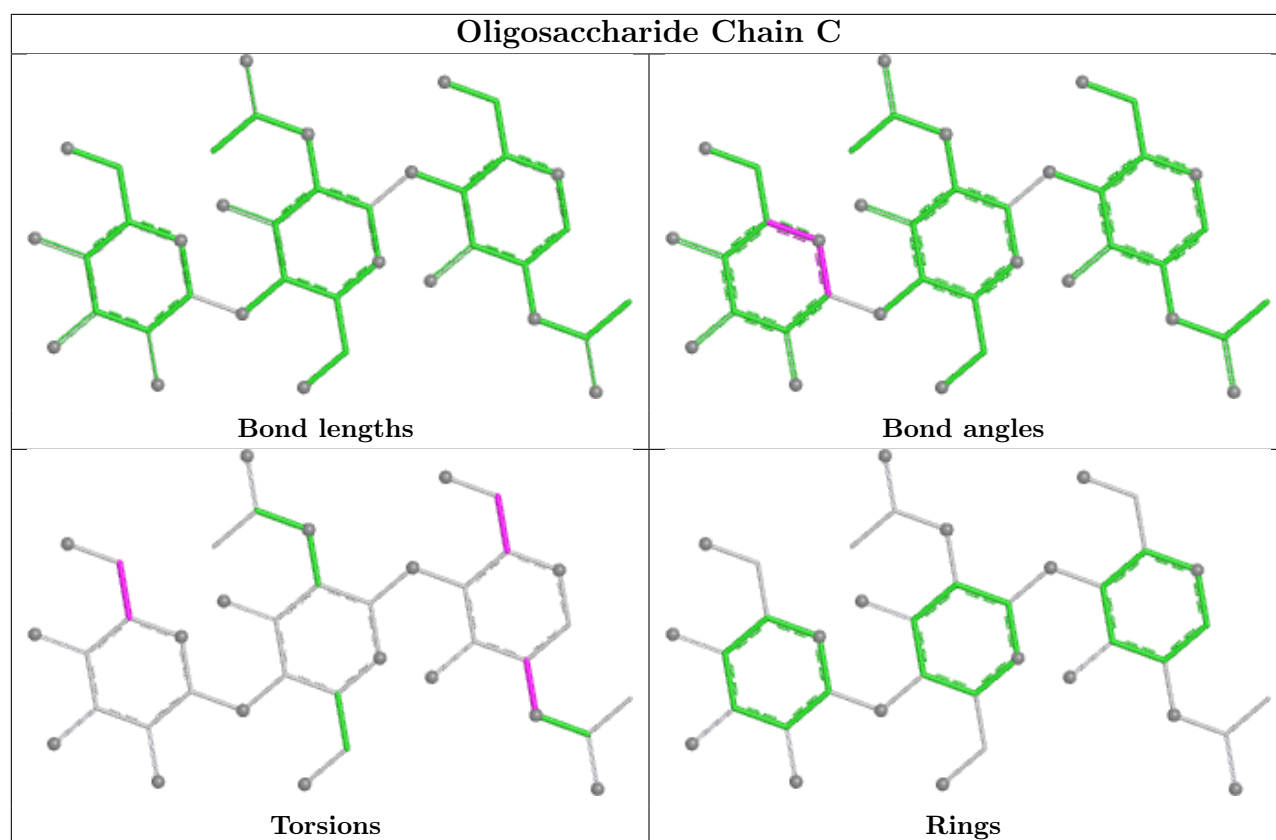
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	C	1	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
5	F	2	NAG	C4-C5-C6-O6

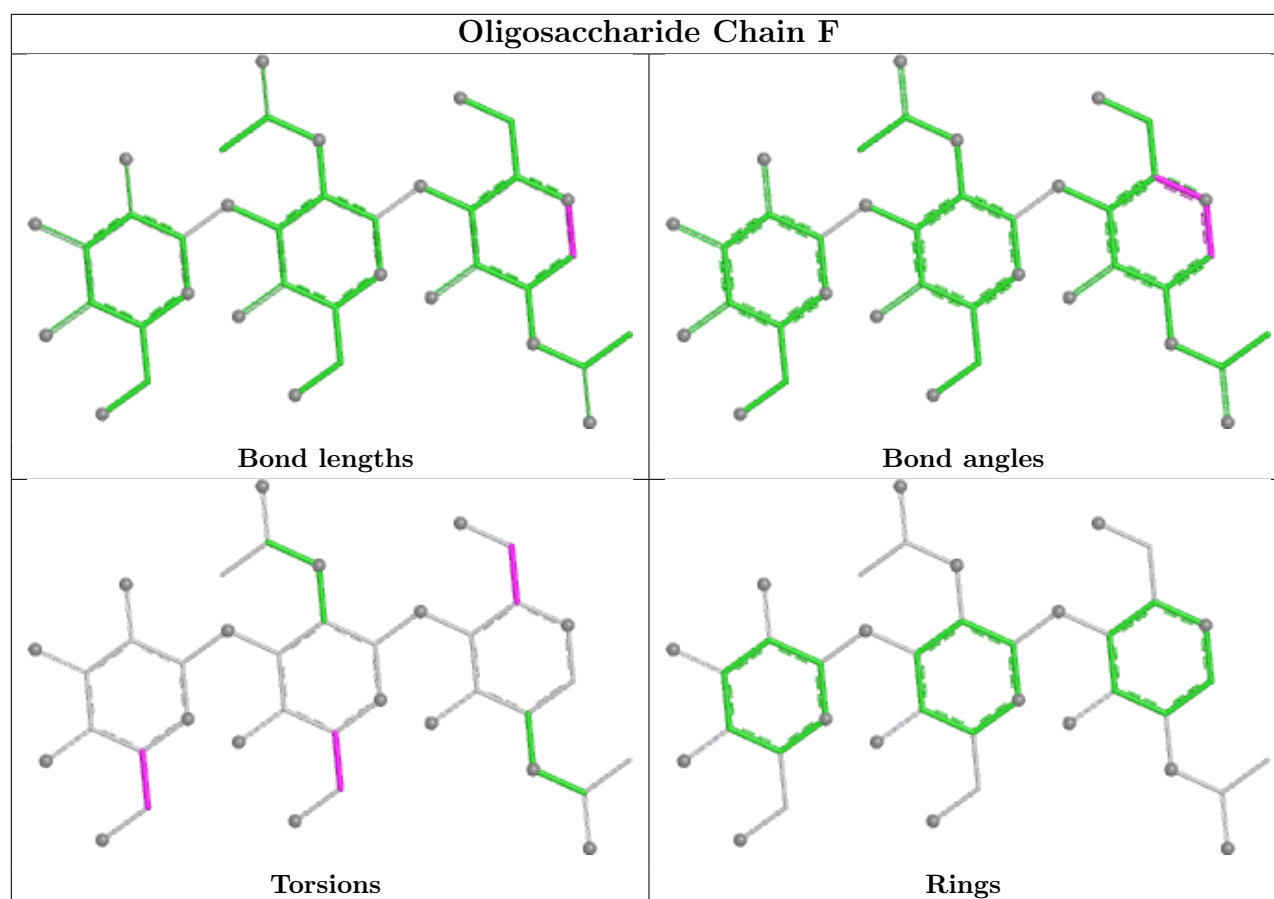
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	1	0
4	E	1	NAG	3	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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	Y01	A	2415	-	38,38,38	0.46	0	57,57,57	0.45	0
10	NAG	D	1204	2	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
8	3PE	A	2409	-	31,31,50	0.36	0	34,36,55	0.42	0
7	R16	A	2407	-	12,12,15	0.14	0	11,11,14	0.09	0
6	Y01	A	2406	-	38,38,38	0.44	0	57,57,57	0.61	0
10	NAG	D	1207	2	14,14,15	0.37	0	17,19,21	0.63	1 (5%)
6	Y01	A	2401	-	38,38,38	0.47	0	57,57,57	0.54	0
10	NAG	D	1209	2	14,14,15	0.18	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	D	1201	2	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
7	R16	A	2412	-	15,15,15	0.11	0	14,14,14	0.08	0
7	R16	A	2414	-	8,8,15	0.28	0	7,7,14	0.15	0
10	NAG	D	1202	2	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	D	1205	2	14,14,15	0.24	0	17,19,21	0.48	0
10	NAG	D	1203	2	14,14,15	0.28	0	17,19,21	0.51	0
7	R16	A	2402	-	9,9,15	0.12	0	8,8,14	0.08	0
6	Y01	A	2408	-	38,38,38	0.50	0	57,57,57	0.80	1 (1%)
7	R16	A	2411	-	8,8,15	0.12	0	7,7,14	0.09	0
6	Y01	A	2410	-	38,38,38	0.44	0	57,57,57	0.87	3 (5%)
6	Y01	A	2404	-	38,38,38	0.46	0	57,57,57	0.69	0
10	NAG	D	1208	2	14,14,15	0.26	0	17,19,21	0.43	0
7	R16	A	2405	-	15,15,15	0.14	0	14,14,14	0.11	0
7	R16	A	2403	-	15,15,15	0.11	0	14,14,14	0.18	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
6	Y01	A	2415	-	-	17/19/77/77	0/4/4/4
10	NAG	D	1204	2	-	1/6/23/26	0/1/1/1
8	3PE	A	2409	-	-	9/35/35/54	-
7	R16	A	2407	-	-	0/10/10/13	-
6	Y01	A	2406	-	-	10/19/77/77	0/4/4/4
10	NAG	D	1207	2	-	2/6/23/26	0/1/1/1
6	Y01	A	2401	-	-	13/19/77/77	0/4/4/4
10	NAG	D	1209	2	-	4/6/23/26	0/1/1/1
10	NAG	D	1201	2	-	2/6/23/26	0/1/1/1
7	R16	A	2412	-	-	1/13/13/13	-
7	R16	A	2414	-	-	2/6/6/13	-
10	NAG	D	1202	2	-	2/6/23/26	0/1/1/1
10	NAG	D	1205	2	-	0/6/23/26	0/1/1/1
10	NAG	D	1203	2	-	2/6/23/26	0/1/1/1
7	R16	A	2402	-	-	0/7/7/13	-
6	Y01	A	2408	-	-	9/19/77/77	0/4/4/4
7	R16	A	2411	-	-	0/6/6/13	-
6	Y01	A	2410	-	-	10/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	A	2404	-	-	13/19/77/77	0/4/4/4
10	NAG	D	1208	2	-	0/6/23/26	0/1/1/1
7	R16	A	2405	-	-	1/13/13/13	-
7	R16	A	2403	-	-	3/13/13/13	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2408	Y01	CBI-CBE-CBB	3.05	124.21	119.50
6	A	2410	Y01	CBG-CBI-CBE	-2.98	96.68	100.10
10	D	1201	NAG	C1-O5-C5	2.75	115.88	112.19
10	D	1207	NAG	C1-O5-C5	2.16	115.09	112.19
6	A	2410	Y01	CBI-CBE-CBB	2.11	122.75	119.50
6	A	2410	Y01	CAP-CBE-CBB	2.07	115.32	112.18
10	D	1204	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2401	Y01	OAG-CAY-OAW-CBC
6	A	2401	Y01	CAM-CAY-OAW-CBC
6	A	2401	Y01	CAX-CAL-CAM-CAY
6	A	2408	Y01	CAO-CBB-CBE-CBI
6	A	2415	Y01	CAM-CAY-OAW-CBC
6	A	2415	Y01	CAX-CAL-CAM-CAY
8	A	2409	3PE	C1-O11-P-O14
8	A	2409	3PE	C2-C1-O11-P
6	A	2404	Y01	CAV-CBC-OAW-CAY
6	A	2410	Y01	CAR-CBC-OAW-CAY
6	A	2415	Y01	CAO-CAJ-CAN-CBA
6	A	2404	Y01	CAC-CBB-CBE-CAP
6	A	2404	Y01	CAC-CBB-CBE-CBI
6	A	2404	Y01	OAG-CAY-OAW-CBC
6	A	2415	Y01	OAG-CAY-OAW-CBC
6	A	2404	Y01	CAM-CAY-OAW-CBC
6	A	2404	Y01	CAJ-CAO-CBB-CAC
10	D	1202	NAG	O5-C5-C6-O6
10	D	1207	NAG	O5-C5-C6-O6
6	A	2404	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
6	A	2404	Y01	CAO-CBB-CBE-CBI
10	D	1203	NAG	O5-C5-C6-O6
10	D	1201	NAG	O5-C5-C6-O6
6	A	2410	Y01	CAM-CAY-OAW-CBC
10	D	1202	NAG	C4-C5-C6-O6
10	D	1207	NAG	C4-C5-C6-O6
6	A	2404	Y01	CAJ-CAO-CBB-CBE
6	A	2415	Y01	CAJ-CAO-CBB-CBE
10	D	1201	NAG	C4-C5-C6-O6
10	D	1203	NAG	C4-C5-C6-O6
6	A	2415	Y01	CAJ-CAO-CBB-CAC
6	A	2408	Y01	CAC-CBB-CBE-CAP
6	A	2410	Y01	OAG-CAY-OAW-CBC
6	A	2410	Y01	CAO-CBB-CBE-CBI
6	A	2415	Y01	CAN-CAJ-CAO-CBB
6	A	2406	Y01	CAO-CBB-CBE-CBI
6	A	2415	Y01	CAO-CBB-CBE-CBI
6	A	2406	Y01	CAM-CAY-OAW-CBC
6	A	2410	Y01	CAC-CBB-CBE-CBI
6	A	2401	Y01	CAO-CAJ-CAN-CBA
6	A	2410	Y01	CAC-CBB-CBE-CAP
6	A	2408	Y01	CAO-CBB-CBE-CAP
6	A	2406	Y01	OAG-CAY-OAW-CBC
6	A	2406	Y01	CAC-CBB-CBE-CBI
6	A	2406	Y01	CAC-CBB-CBE-CAP
6	A	2401	Y01	CAN-CAJ-CAO-CBB
7	A	2403	R16	C33-C34-C35-C36
6	A	2415	Y01	CAJ-CAN-CBA-CAB
6	A	2415	Y01	CAC-CBB-CBE-CBI
6	A	2415	Y01	CAC-CBB-CBE-CAP
6	A	2408	Y01	CAC-CBB-CBE-CBI
10	D	1209	NAG	C4-C5-C6-O6
6	A	2401	Y01	CAJ-CAN-CBA-CAB
6	A	2415	Y01	CAJ-CAN-CBA-CAA
7	A	2414	R16	C28-C29-C30-C31
10	D	1209	NAG	O5-C5-C6-O6
6	A	2415	Y01	CAO-CBB-CBE-CAP
8	A	2409	3PE	O31-C31-C32-C33
6	A	2404	Y01	CAN-CAJ-CAO-CBB
6	A	2401	Y01	CAJ-CAN-CBA-CAA
8	A	2409	3PE	O21-C2-C3-O31
10	D	1209	NAG	C1-C2-N2-C7

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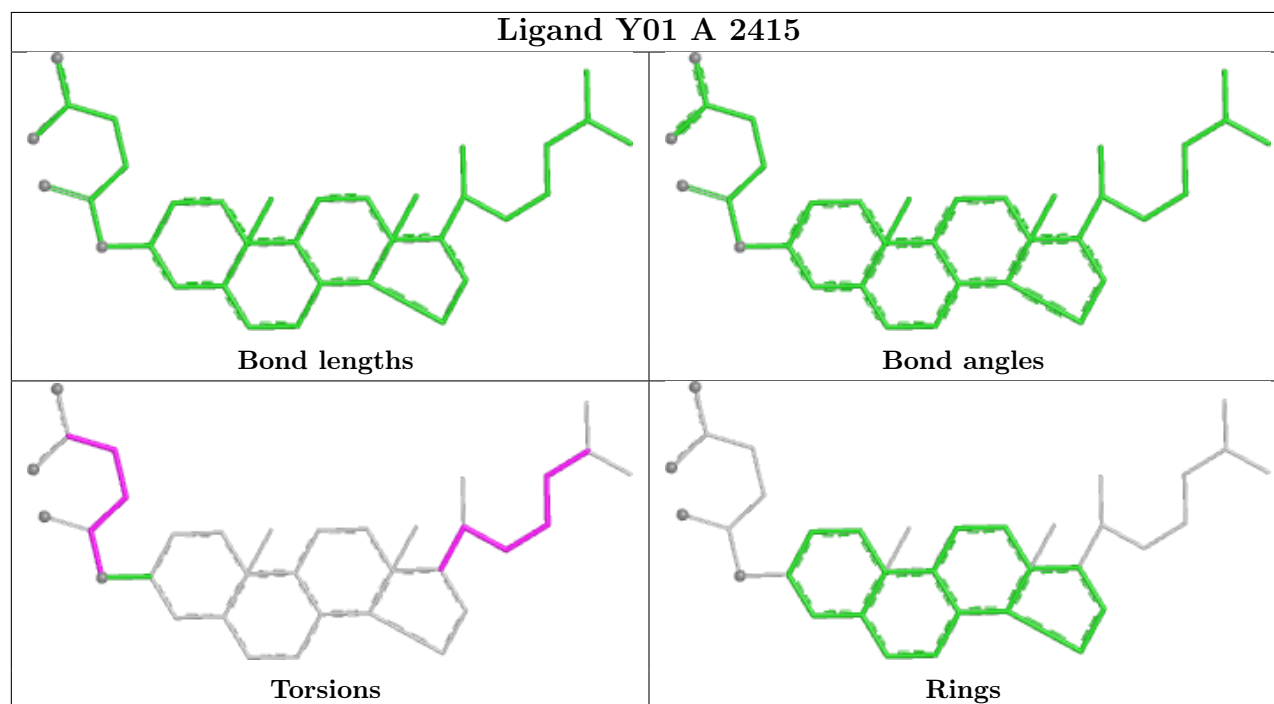
Mol	Chain	Res	Type	Atoms
6	A	2406	Y01	CAO-CBB-CBE-CAP
8	A	2409	3PE	O21-C21-C22-C23
6	A	2406	Y01	CAN-CAJ-CAO-CBB
10	D	1204	NAG	C3-C2-N2-C7
6	A	2410	Y01	CAO-CAJ-CAN-CBA
6	A	2401	Y01	CAO-CBB-CBE-CAP
6	A	2408	Y01	CAL-CAM-CAY-OAW
6	A	2408	Y01	CAJ-CAO-CBB-CBE
7	A	2403	R16	C32-C33-C34-C35
6	A	2401	Y01	CAO-CBB-CBE-CBI
6	A	2401	Y01	CAC-CBB-CBE-CBI
6	A	2404	Y01	CAX-CAL-CAM-CAY
6	A	2401	Y01	CAM-CAL-CAX-OAH
8	A	2409	3PE	O32-C31-C32-C33
8	A	2409	3PE	C22-C23-C24-C25
6	A	2408	Y01	CAM-CAL-CAX-OAF
7	A	2414	R16	C30-C31-C32-C33
6	A	2408	Y01	CAM-CAL-CAX-OAH
6	A	2408	Y01	CAV-CBC-OAW-CAY
7	A	2405	R16	C36-C37-C38-C39
6	A	2401	Y01	CAM-CAL-CAX-OAF
6	A	2415	Y01	CAM-CAL-CAX-OAH
6	A	2406	Y01	CAM-CAL-CAX-OAH
10	D	1209	NAG	C3-C2-N2-C7
6	A	2410	Y01	CAM-CAL-CAX-OAH
6	A	2401	Y01	CAC-CBB-CBE-CAP
6	A	2406	Y01	CAM-CAL-CAX-OAF
6	A	2410	Y01	CAM-CAL-CAX-OAF
6	A	2410	Y01	CAV-CBC-OAW-CAY
6	A	2415	Y01	CAM-CAL-CAX-OAF
6	A	2415	Y01	CAL-CAM-CAY-OAW
6	A	2404	Y01	CAM-CAL-CAX-OAF
7	A	2403	R16	C39-C40-C41-C42
6	A	2404	Y01	CAM-CAL-CAX-OAH
8	A	2409	3PE	C1-C2-O21-C21
8	A	2409	3PE	O22-C21-C22-C23
6	A	2415	Y01	CAL-CAM-CAY-OAG
7	A	2412	R16	C30-C31-C32-C33
6	A	2406	Y01	CAL-CAM-CAY-OAW

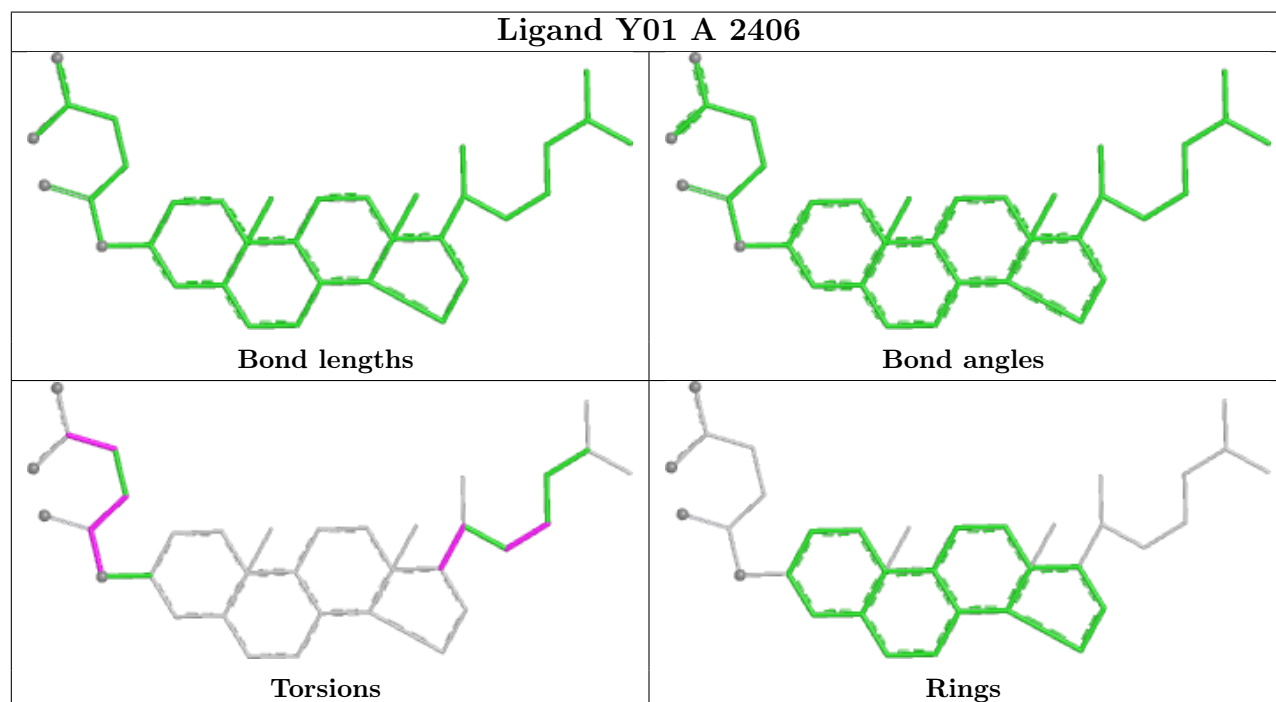
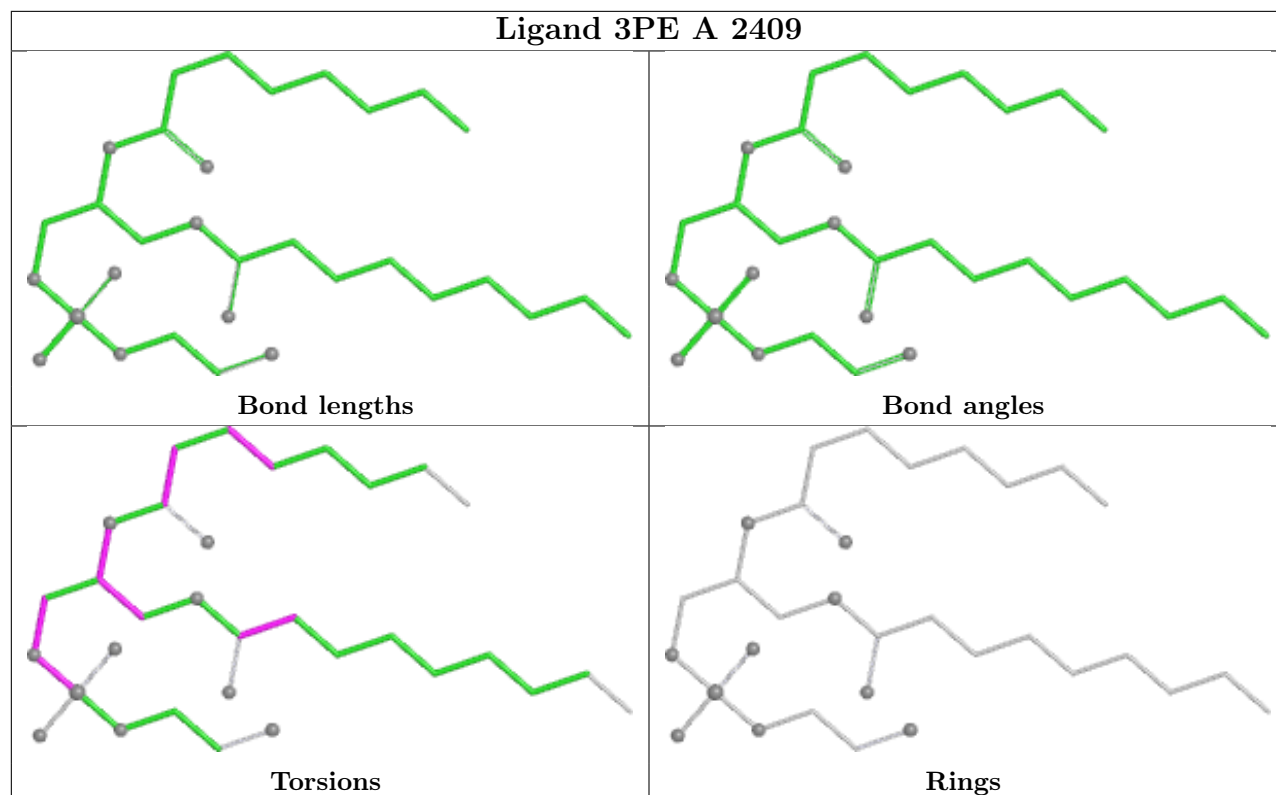
There are no ring outliers.

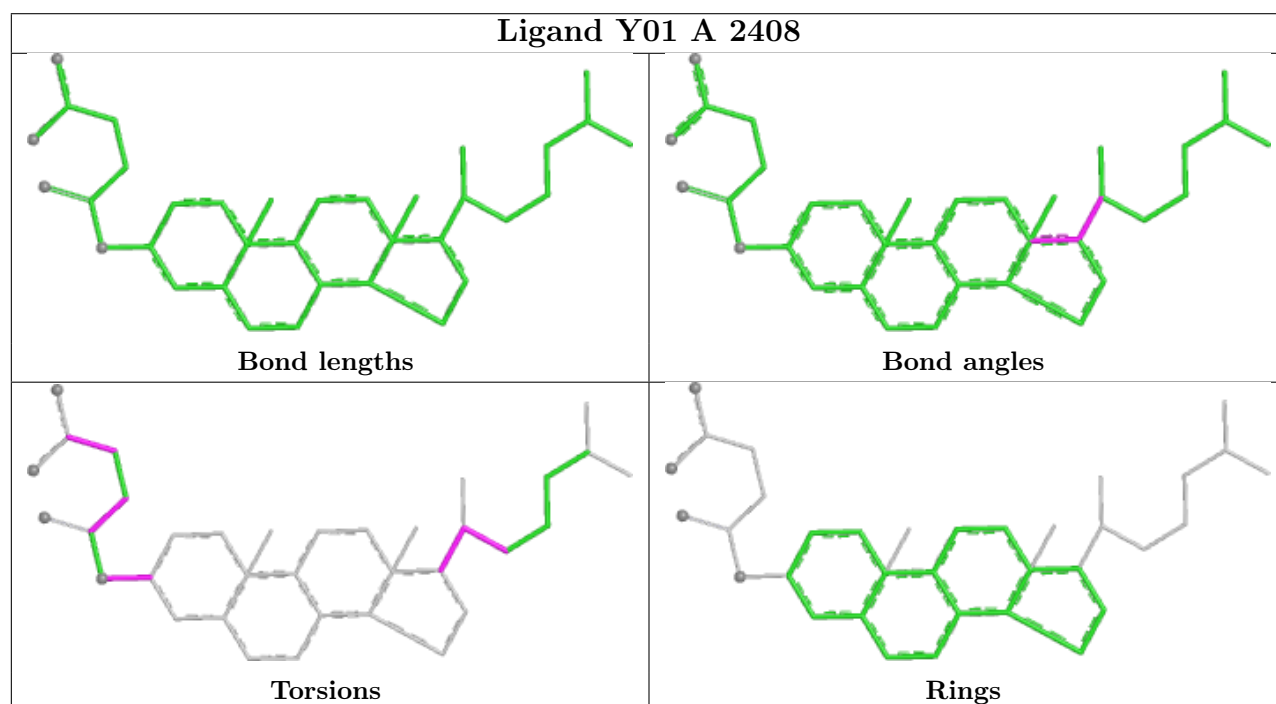
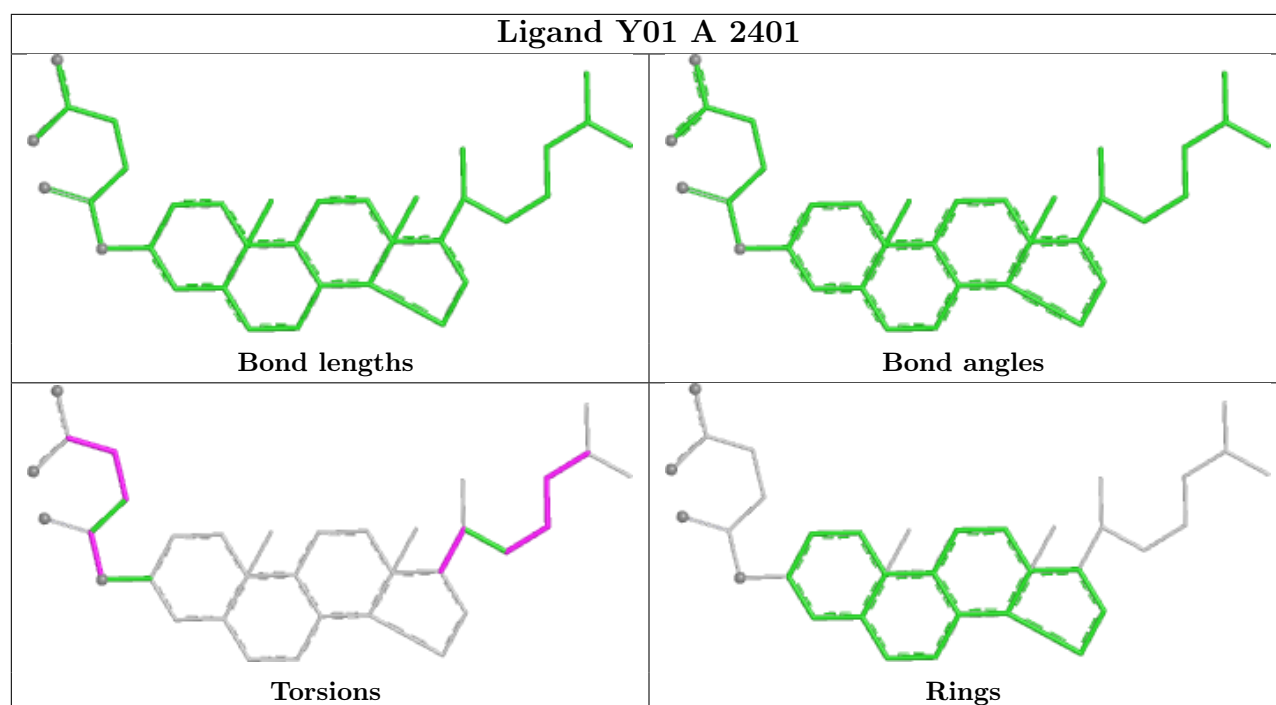
10 monomers are involved in 58 short contacts:

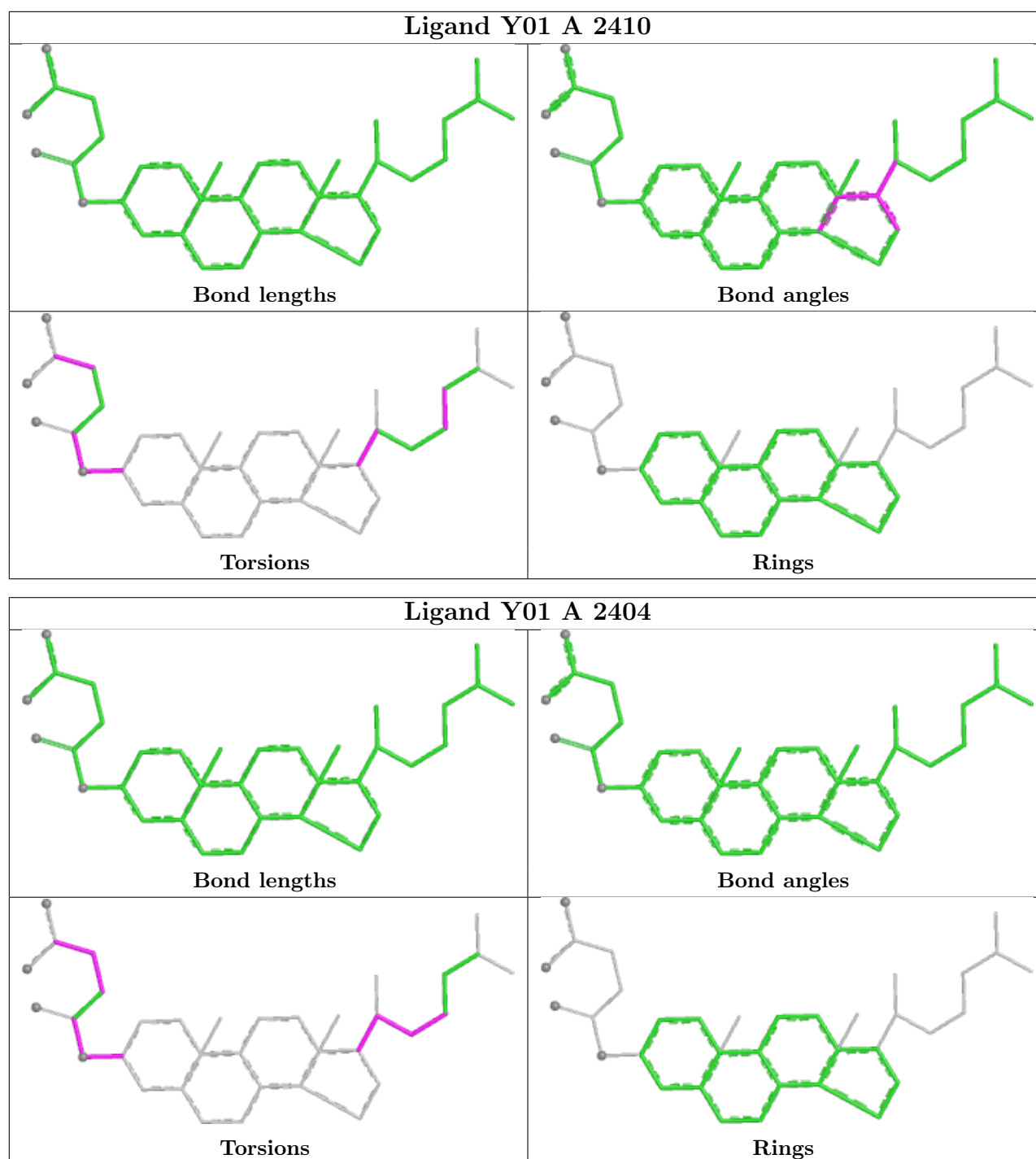
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2415	Y01	7	0
8	A	2409	3PE	1	0
7	A	2407	R16	2	0
6	A	2406	Y01	3	0
6	A	2401	Y01	19	0
7	A	2414	R16	4	0
10	D	1205	NAG	2	0
6	A	2408	Y01	4	0
6	A	2410	Y01	2	0
6	A	2404	Y01	14	0

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.

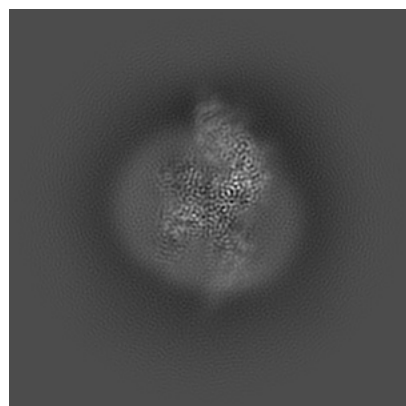
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33285. These allow visual inspection of the internal detail of the map and identification of artifacts.

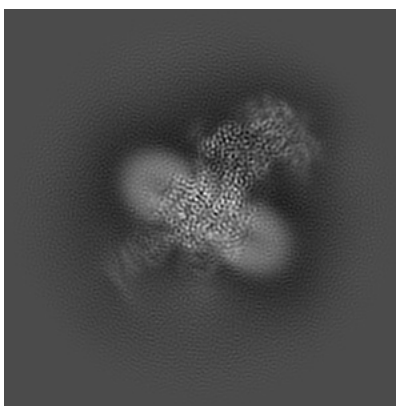
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

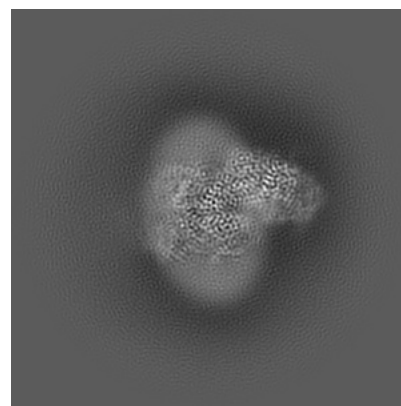
6.1.1 Primary map



X

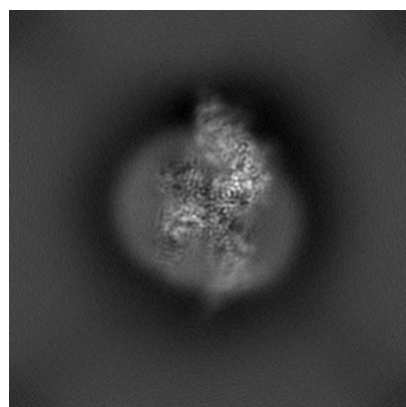


Y

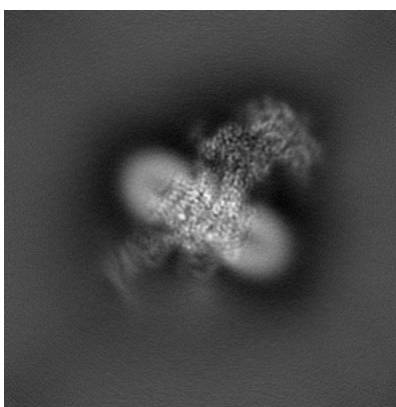


Z

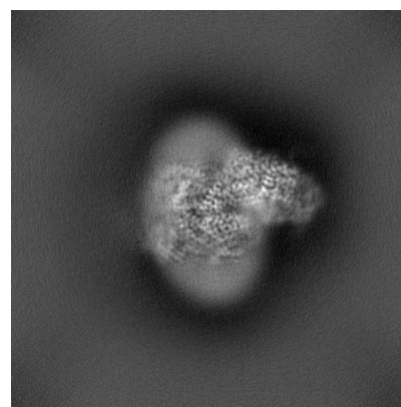
6.1.2 Raw map



X



Y

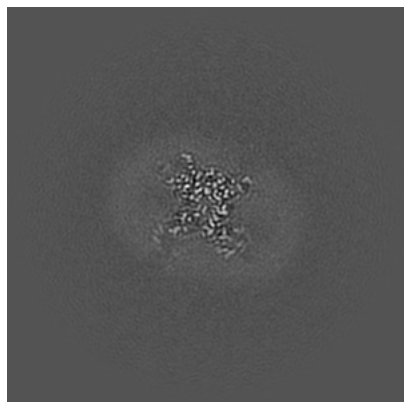


Z

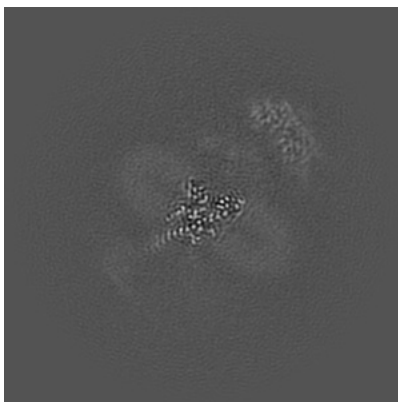
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

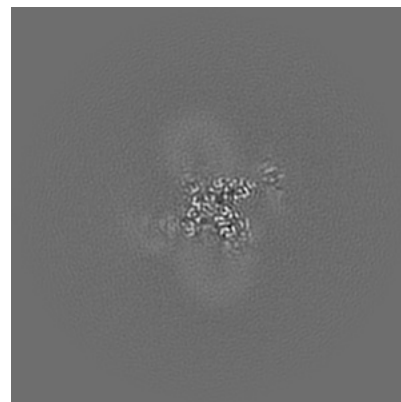
6.2.1 Primary map



X Index: 160

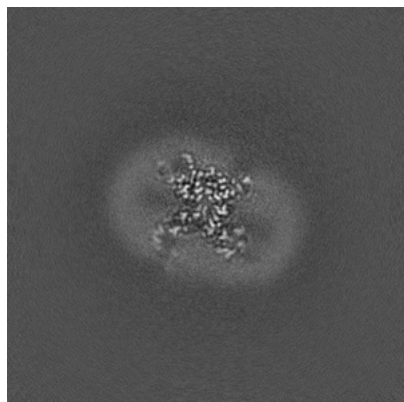


Y Index: 160

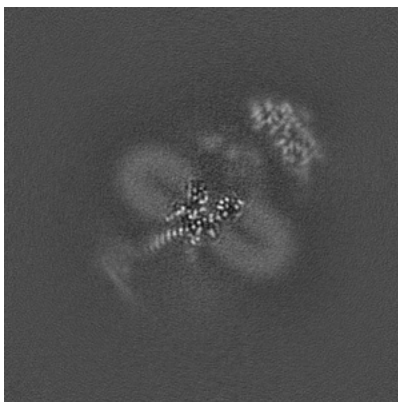


Z Index: 160

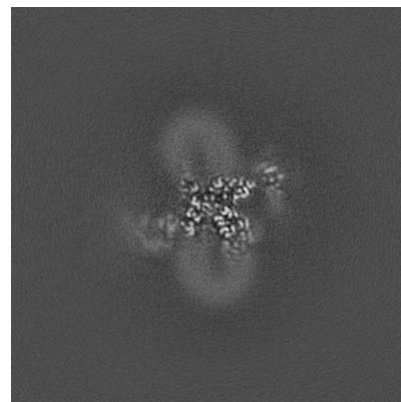
6.2.2 Raw map



X Index: 160



Y Index: 160

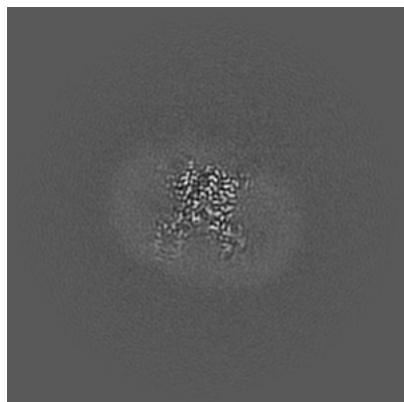


Z Index: 160

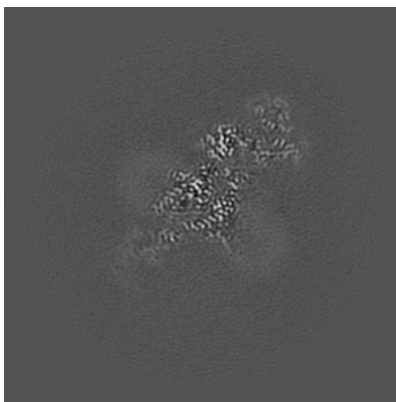
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

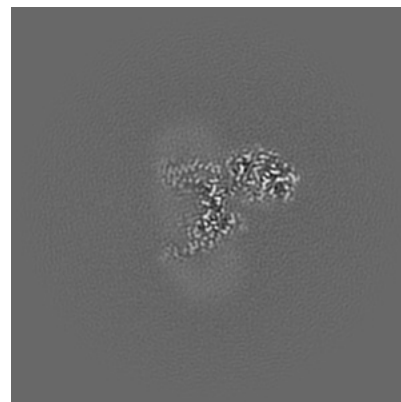
6.3.1 Primary map



X Index: 163

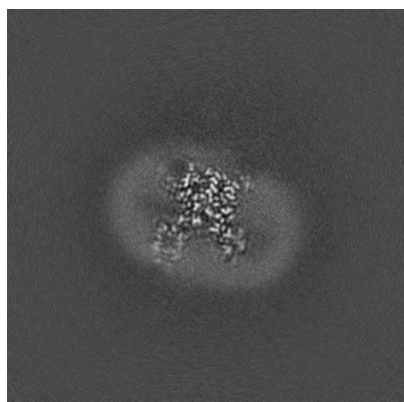


Y Index: 175

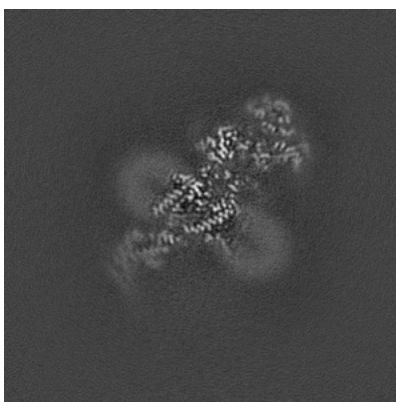


Z Index: 180

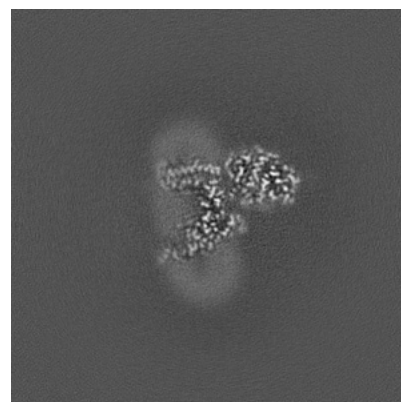
6.3.2 Raw map



X Index: 163



Y Index: 175

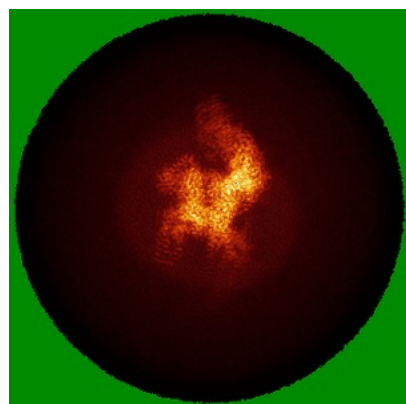


Z Index: 180

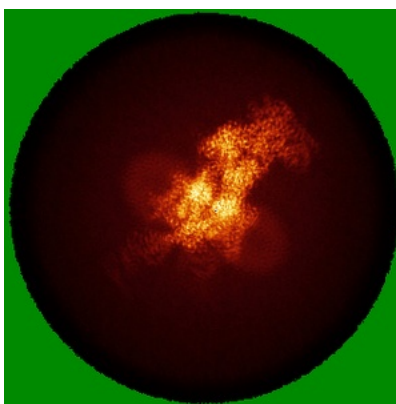
The images above show the largest variance slices of the map in three orthogonal directions.

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

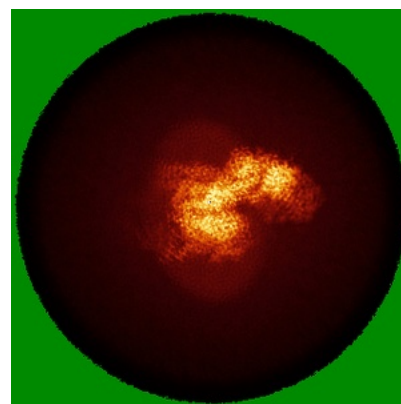
6.4.1 Primary map



X

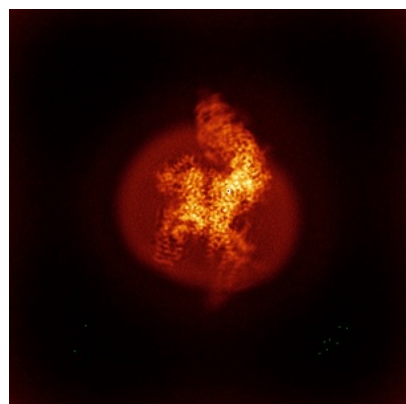


Y

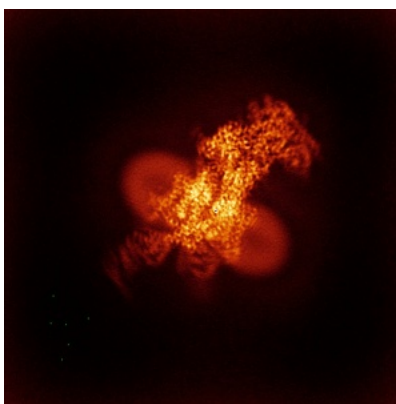


Z

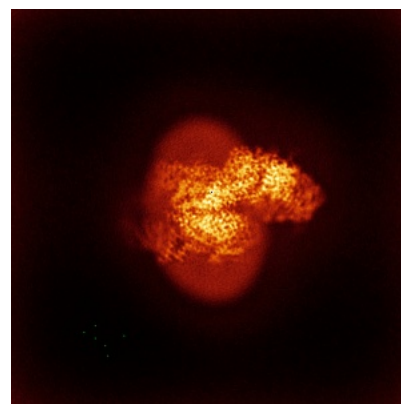
6.4.2 Raw map



X



Y

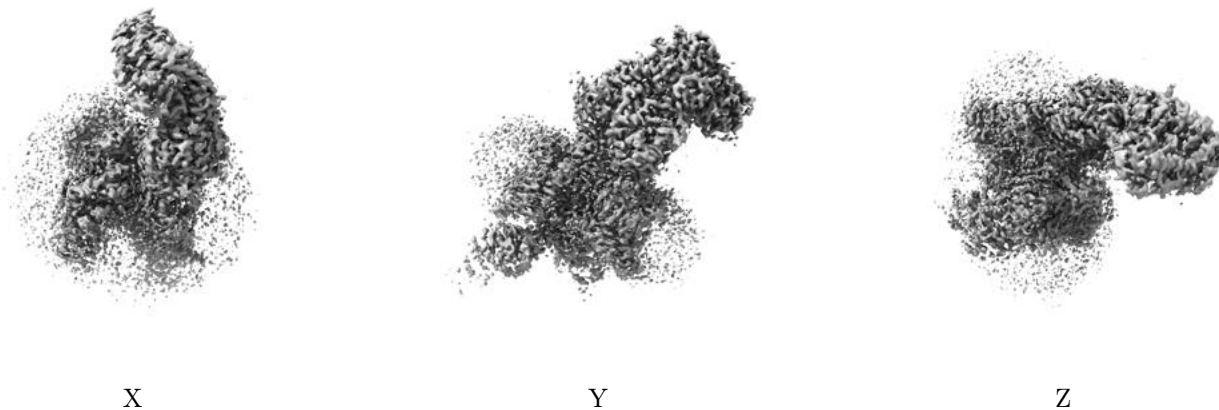


Z

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.

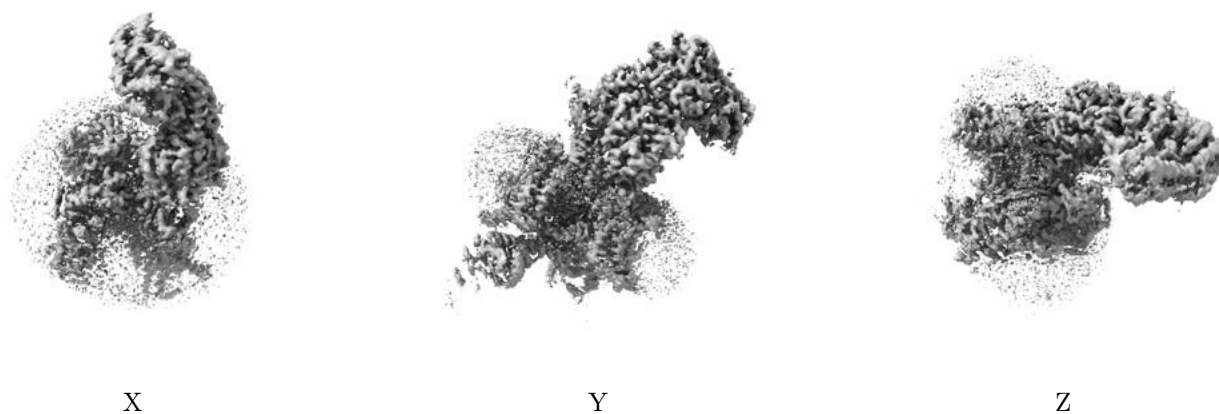
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

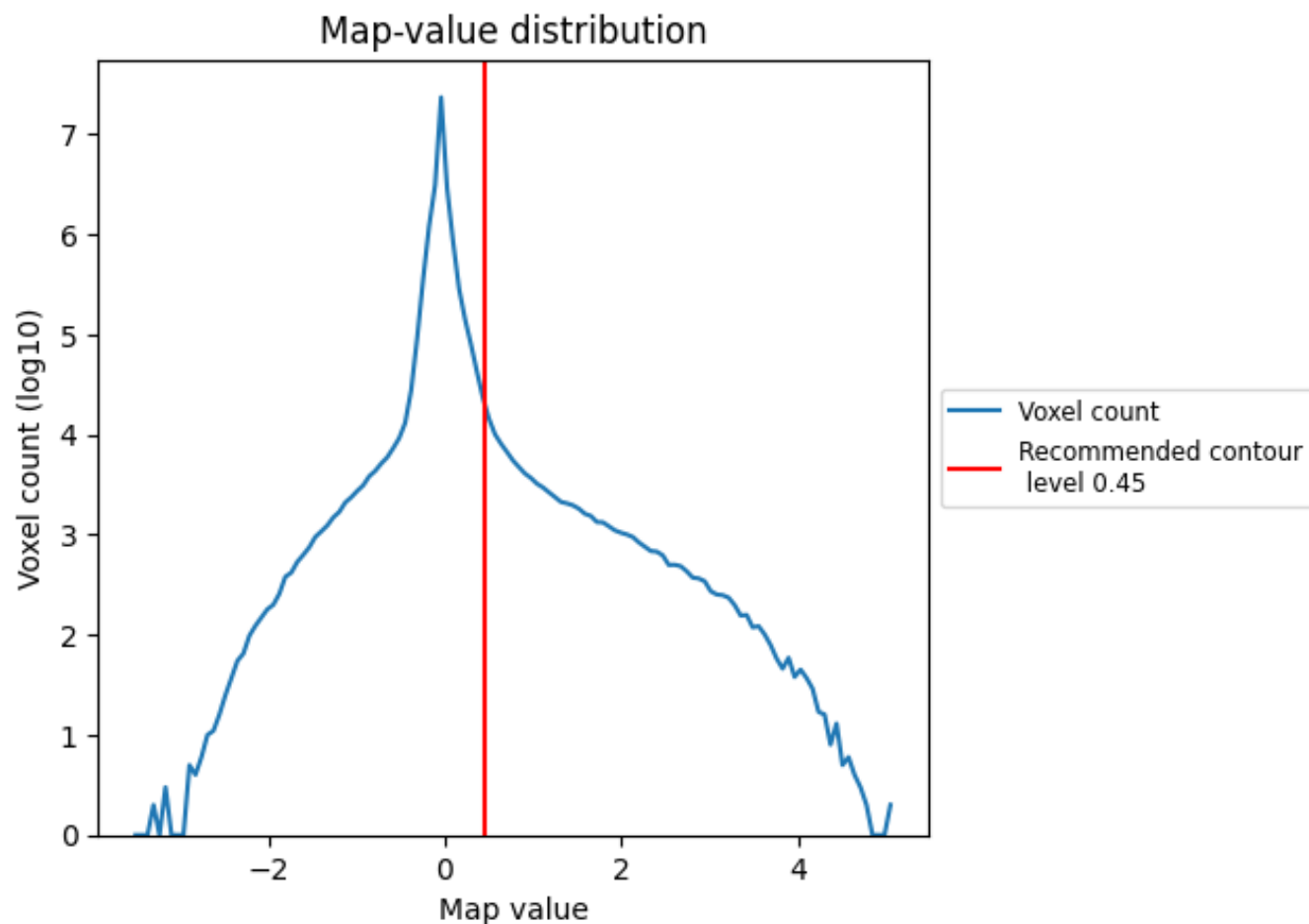
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

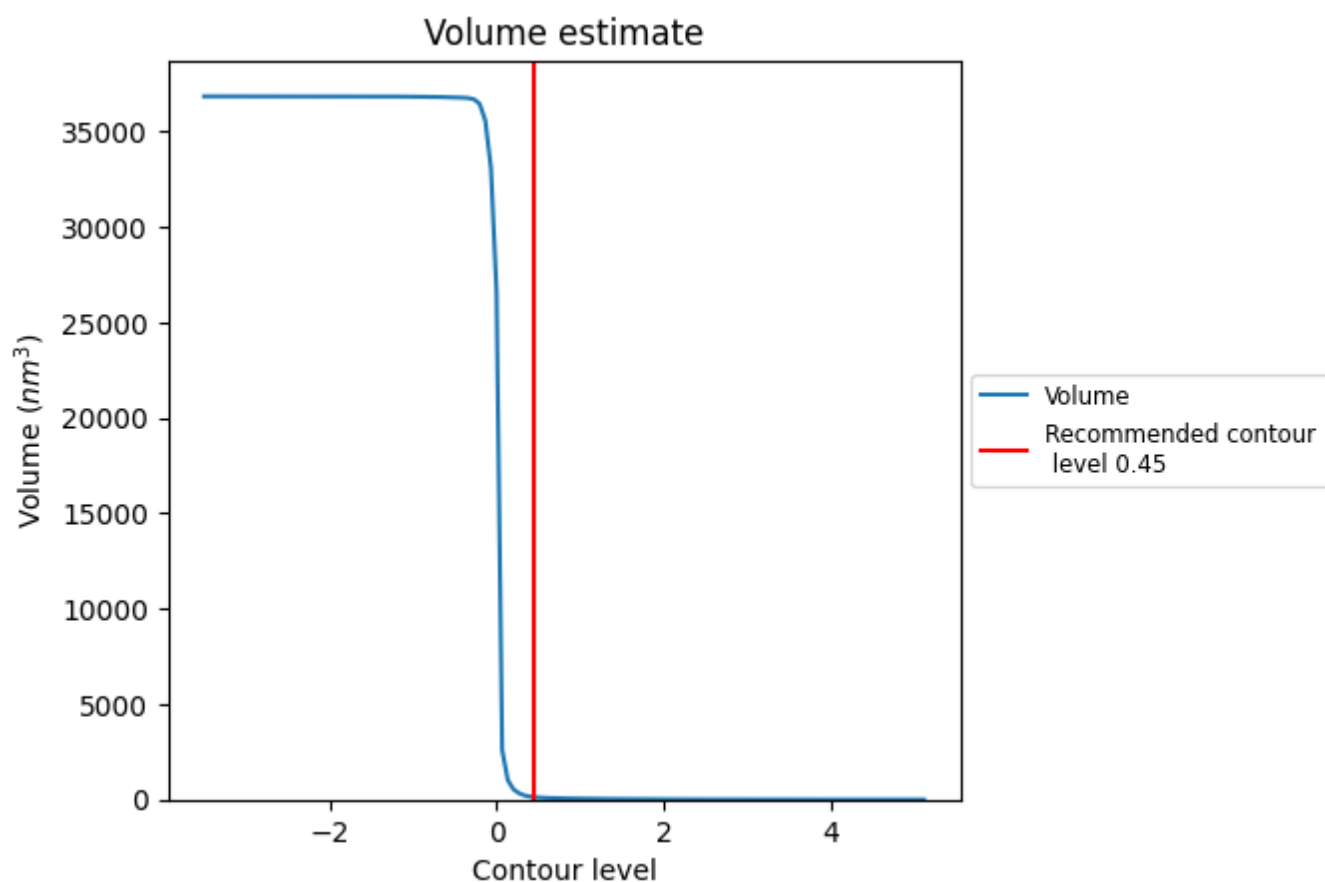
This section contains the results of statistical analysis of the map.

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.

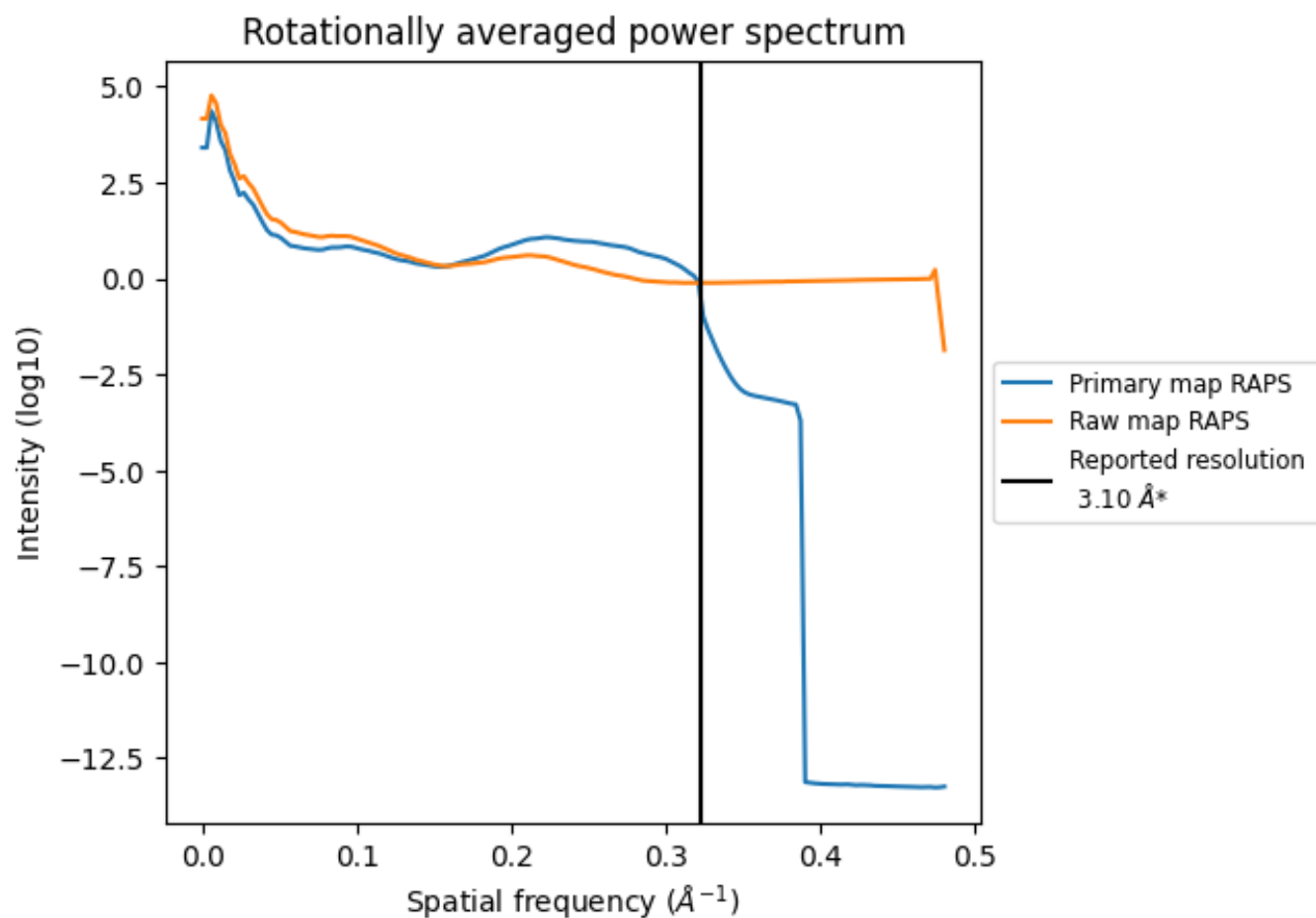
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 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 ⓘ

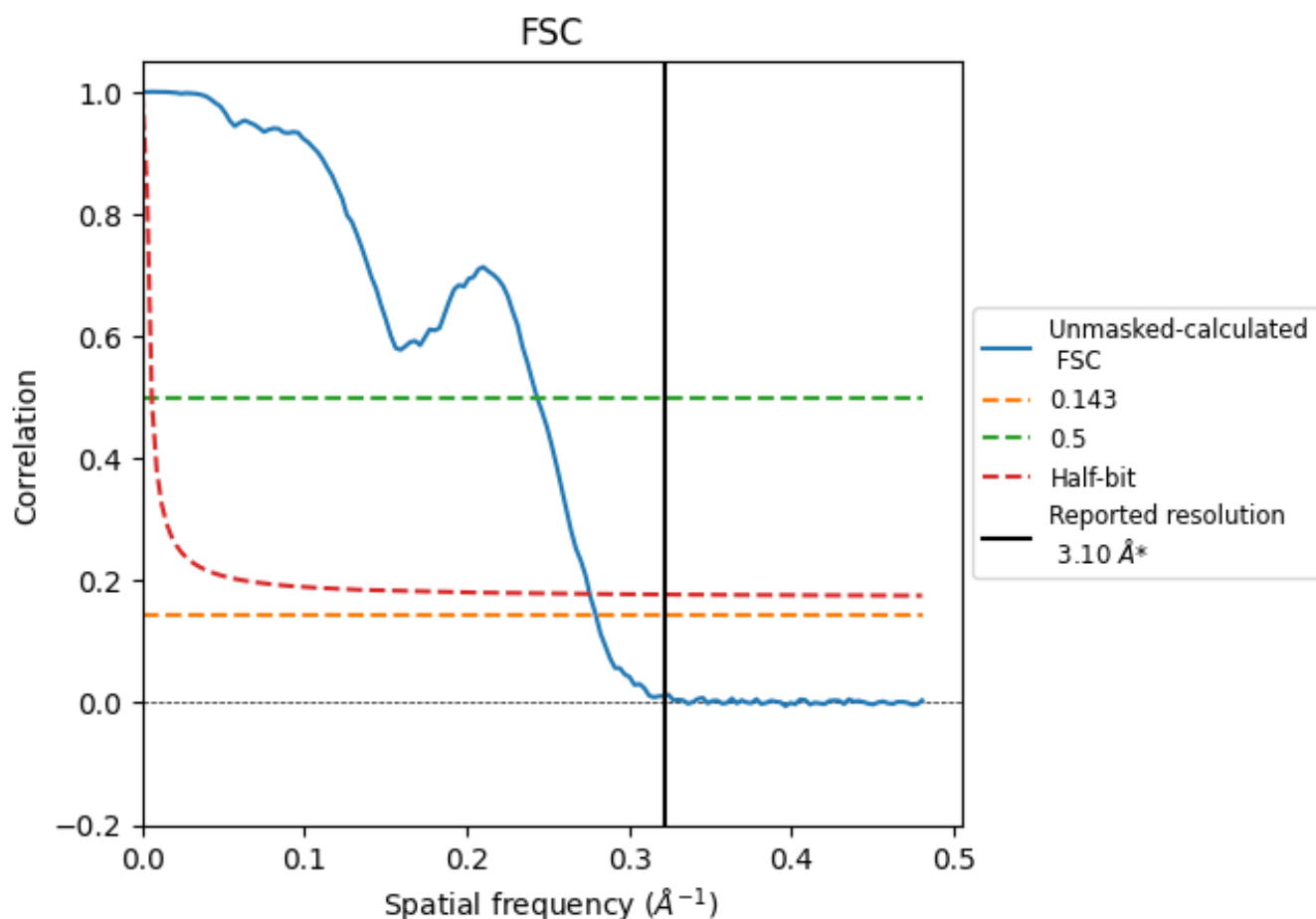


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

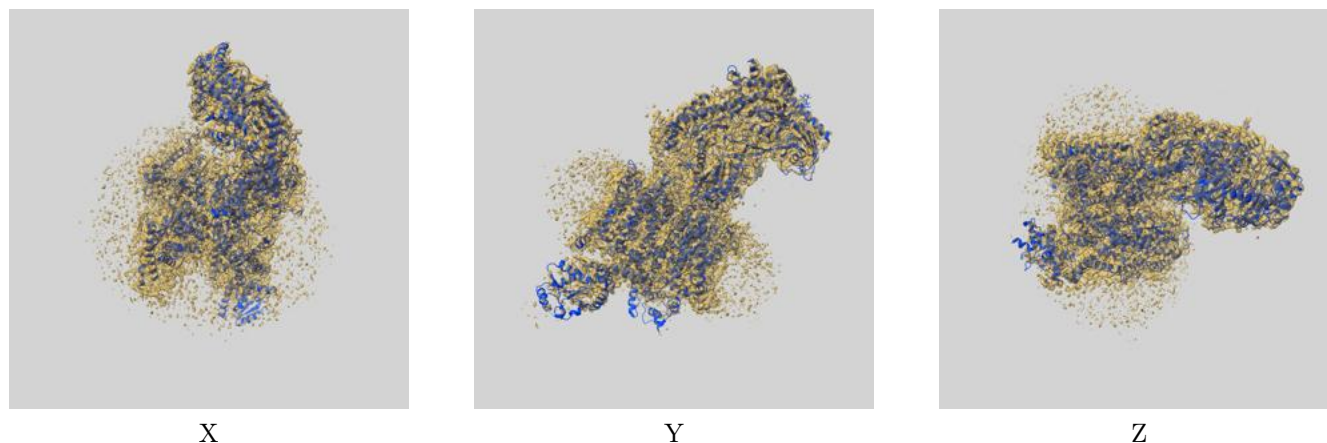
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.11	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

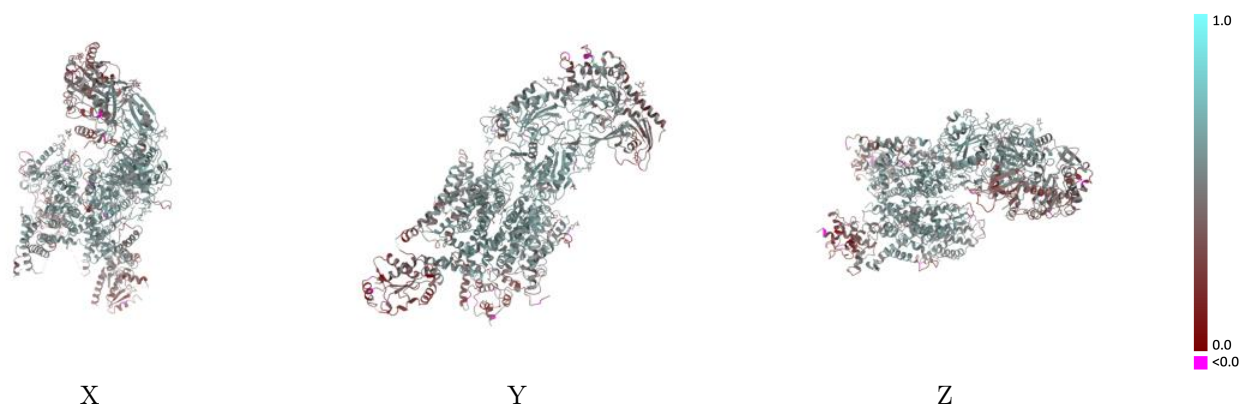
This section contains information regarding the fit between EMDB map EMD-33285 and PDB model 7XLQ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



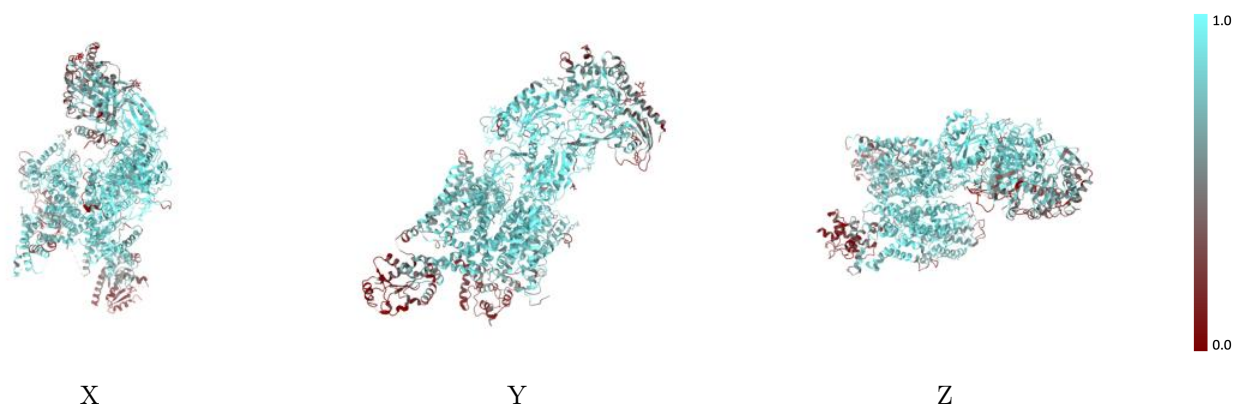
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



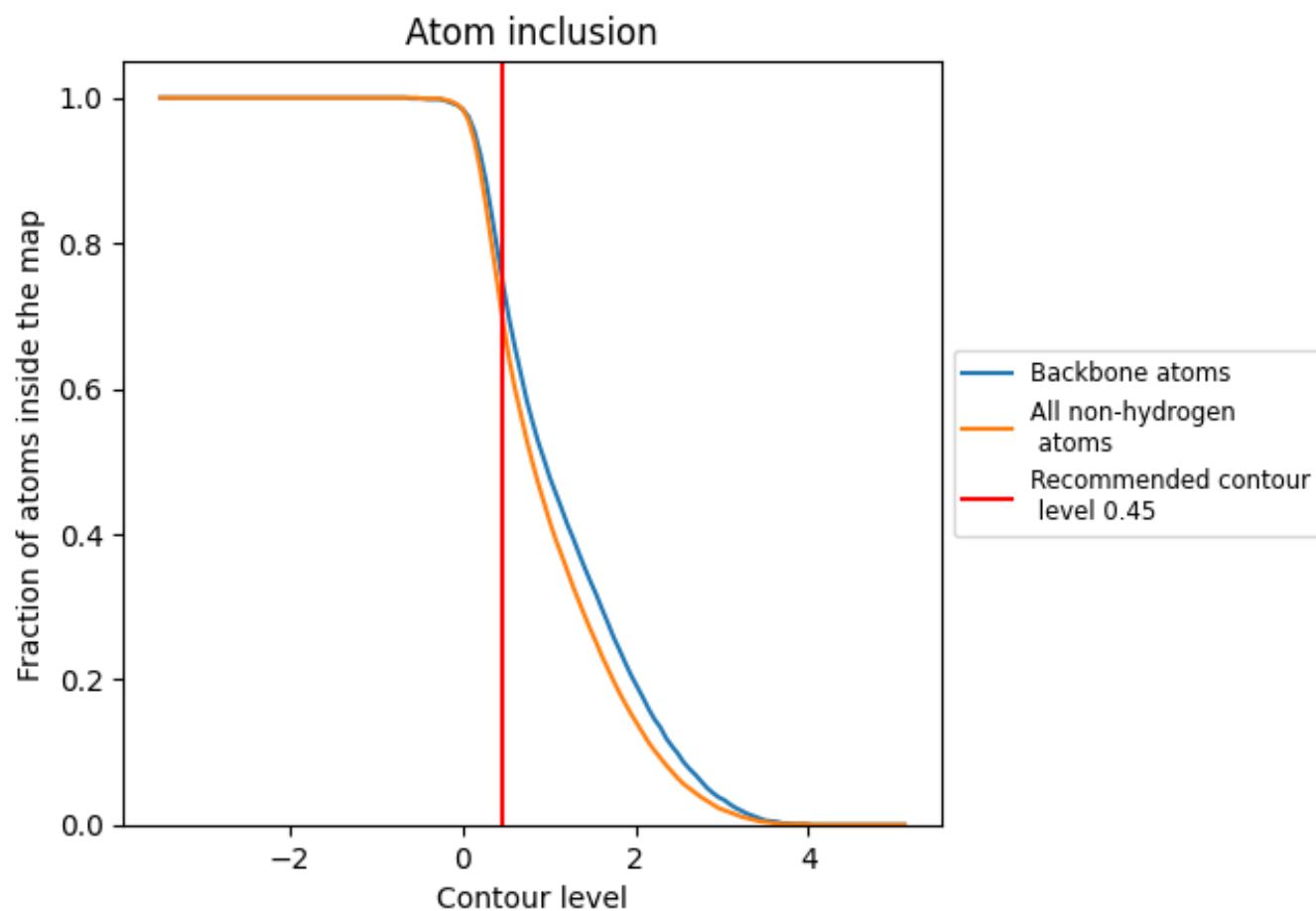
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.4820
A	0.7330	0.4950
B	0.2870	0.3080
C	0.5130	0.3910
D	0.7340	0.4940
E	0.9490	0.5530
F	0.1030	0.3340

1.0

0.0

<0.0