



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:46 PM UTC

PDB ID : 6KZP / pdb_00006kzp
EMDB ID : EMD-0792
Title : calcium channel-ligand
Authors : Yan, N.
Deposited on : 2019-09-25
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.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

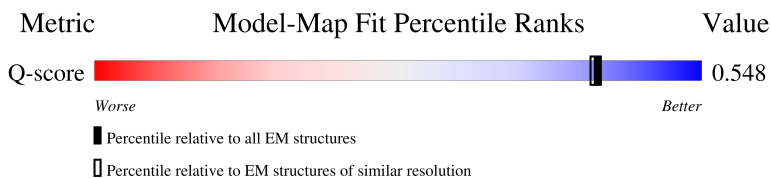
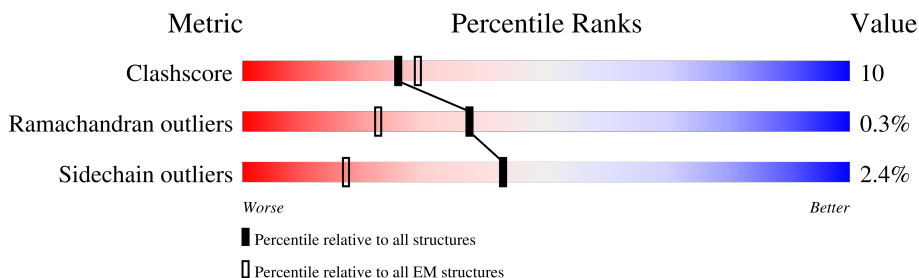
1 Overall quality at a glance

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	2146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	Y01	A	2317	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8557 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 T-type calcium channel subunit alpha-1G, Voltage-dependent T-type calcium channel subunit alpha-1G.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1014	Total	C	N	O	S	0	0
			8159	5391	1324	1379	65		

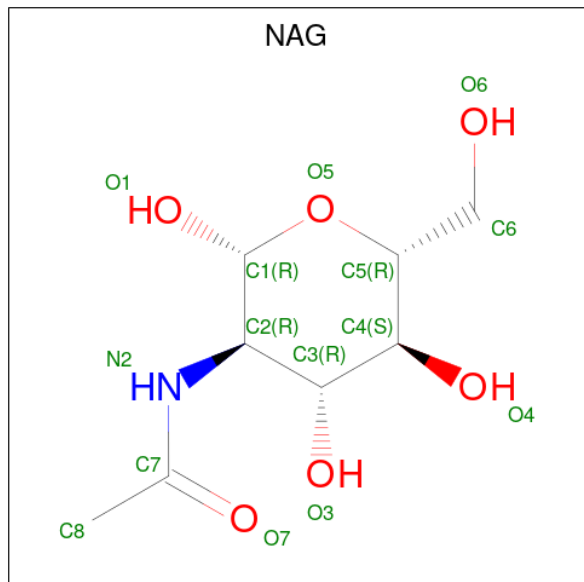
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O43497
A	-17	HIS	-	expression tag	UNP O43497
A	-16	HIS	-	expression tag	UNP O43497
A	-15	HIS	-	expression tag	UNP O43497
A	-14	HIS	-	expression tag	UNP O43497
A	-13	HIS	-	expression tag	UNP O43497
A	-12	HIS	-	expression tag	UNP O43497
A	-11	HIS	-	expression tag	UNP O43497
A	-10	HIS	-	expression tag	UNP O43497
A	-9	GLY	-	expression tag	UNP O43497
A	-8	ASP	-	expression tag	UNP O43497
A	-7	TYR	-	expression tag	UNP O43497
A	-6	LYS	-	expression tag	UNP O43497
A	-5	ASP	-	expression tag	UNP O43497
A	-4	ASP	-	expression tag	UNP O43497
A	-3	ASP	-	expression tag	UNP O43497
A	-2	ASP	-	expression tag	UNP O43497
A	-1	LYS	-	expression tag	UNP O43497
A	0	GLY	-	expression tag	UNP O43497
A	1	THR	-	expression tag	UNP O43497

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

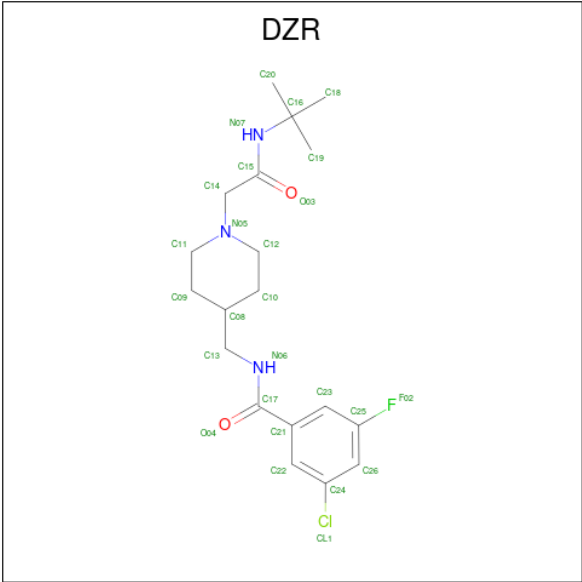
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



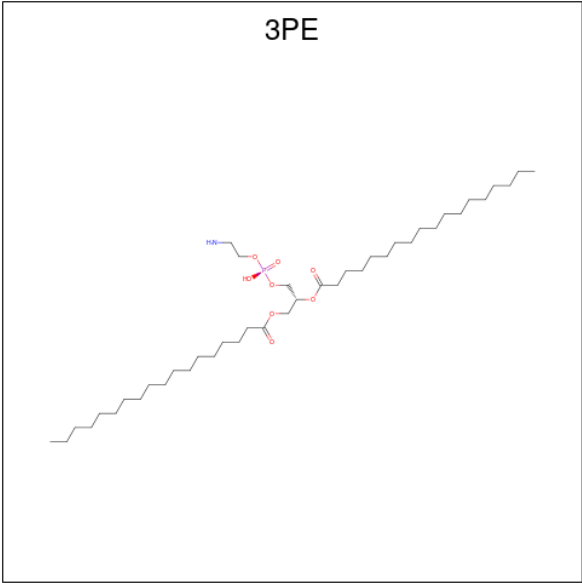
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is {N}-[[1-[2-({tert}-butylamino)-2-oxidanylidene-ethyl]piperidin-4-yl]methyl]-3-chloranyl-5-fluoranyl-benzamide (CCD ID: DZR) (formula: $C_{19}H_{27}ClFN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
4	A	1	26	19	1	1	3	2	0

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	31	21	1	8	1	0
5	A	1	31	21	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total C 14 14					0
5	A	1	Total C N O P 33 23 1 8 1					0
5	A	1	Total C 13 13					0
5	A	1	Total C N O P 36 26 1 8 1					0
5	A	1	Total C 16 16					0
5	A	1	Total C N O P 35 25 1 8 1					0

- # Y01

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138449	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	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: CA, Y01, 3PE, DZR, 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	0.36	0/8337	0.68	4/11298 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	742	SER	CA-C-N	5.34	131.74	121.54
1	A	742	SER	C-N-CA	5.34	131.74	121.54
1	A	768	PRO	CA-C-N	5.16	131.39	121.54
1	A	768	PRO	C-N-CA	5.16	131.39	121.54

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	8159	0	8358	161	0
2	A	2	0	0	0	0
3	A	56	0	52	0	0
4	A	26	0	0	1	0
5	A	209	0	282	15	0
6	A	105	0	147	34	0
All	All	8557	0	8839	179	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 (179) 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)
6:A:2316:Y01:HAN1	6:A:2316:Y01:HAP1	1.23	1.11
1:A:1326:LEU:HD21	1:A:1366:LEU:HD11	1.38	1.01
1:A:1400:PHE:CE2	6:A:2317:Y01:HAB1	1.97	0.99
6:A:2316:Y01:HAN1	6:A:2316:Y01:CAP	1.95	0.97
1:A:125:PHE:HE2	1:A:163:GLY:HA3	1.27	0.96
1:A:1326:LEU:HD21	1:A:1366:LEU:CD1	2.00	0.91
1:A:1624:ASN:HD21	1:A:1695:ARG:HH22	0.96	0.89
1:A:101:PHE:HE1	1:A:180:ARG:NH2	1.73	0.87
1:A:780:ILE:HG12	1:A:822:ILE:HD11	1.58	0.86
1:A:1400:PHE:HE2	6:A:2317:Y01:HAB1	1.40	0.86
5:A:2313:3PE:H31	5:A:2313:3PE:H222	1.58	0.86
6:A:2316:Y01:HAP1	6:A:2316:Y01:CAN	2.06	0.86
1:A:835:THR:HG21	5:A:2315:3PE:H352	1.58	0.85
1:A:757:THR:HA	1:A:760:MET:HE2	1.56	0.85
1:A:1624:ASN:ND2	1:A:1695:ARG:HH22	1.75	0.83
1:A:128:PHE:CE2	1:A:189:ARG:NH1	2.48	0.82
5:A:2313:3PE:H31	5:A:2313:3PE:C22	2.09	0.80
1:A:1270:ILE:HG12	1:A:1364:ARG:HH11	1.45	0.80
1:A:1354:LEU:HD22	1:A:1354:LEU:O	1.83	0.79
1:A:1448:ASN:ND2	6:A:2316:Y01:HAD1	1.99	0.78
1:A:1359:LEU:HD13	1:A:1740:GLU:HG2	1.65	0.78
1:A:1717:LEU:O	1:A:1717:LEU:HD13	1.83	0.77
1:A:762:ILE:HG22	6:A:2316:Y01:CAK	2.13	0.77
1:A:288:LEU:HB3	1:A:315:ASN:HB2	1.67	0.77
1:A:762:ILE:HG22	6:A:2316:Y01:HAK1	1.67	0.76
1:A:1270:ILE:CG1	1:A:1364:ARG:HH11	1.97	0.76
1:A:1670:GLU:HG2	1:A:1685:ILE:HG23	1.68	0.76
1:A:1400:PHE:CD2	6:A:2317:Y01:HAB1	2.19	0.76
1:A:1688:MET:HA	1:A:1688:MET:HE3	1.68	0.76
1:A:1688:MET:HE3	1:A:1688:MET:CA	2.17	0.74
1:A:839:MET:HG3	5:A:2315:3PE:H3A1	1.68	0.74
1:A:1403:PHE:CZ	5:A:2315:3PE:H281	2.24	0.72
1:A:1450:GLY:O	6:A:2317:Y01:HAD2	1.90	0.71
1:A:1355:ARG:NE	1:A:1358:ARG:HH11	1.89	0.71
1:A:813:VAL:O	1:A:817:ILE:HG12	1.90	0.71
1:A:1717:LEU:HD13	1:A:1717:LEU:C	2.16	0.70
1:A:835:THR:CG2	5:A:2315:3PE:H352	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2317:Y01:CAO	6:A:2317:Y01:HAA2	2.21	0.70
1:A:767:GLN:HB2	1:A:768:PRO:HD2	1.73	0.70
1:A:1364:ARG:N	1:A:1365:PRO:HD2	2.05	0.70
6:A:2317:Y01:HAA2	6:A:2317:Y01:HAO2	1.73	0.69
1:A:1366:LEU:C	1:A:1366:LEU:HD12	2.18	0.68
6:A:2317:Y01:HAO2	6:A:2317:Y01:CAA	2.23	0.68
1:A:771:LEU:O	1:A:775:LEU:HG	1.93	0.68
1:A:1709:LEU:O	1:A:1712:THR:HG23	1.93	0.67
1:A:101:PHE:CE1	1:A:180:ARG:NH2	2.62	0.67
1:A:1688:MET:HA	1:A:1688:MET:CE	2.25	0.66
1:A:1624:ASN:HD21	1:A:1695:ARG:NH2	1.81	0.66
1:A:1693:ILE:O	1:A:1696:VAL:HG12	1.96	0.66
1:A:125:PHE:CE2	1:A:163:GLY:HA3	2.20	0.66
1:A:1400:PHE:CD2	6:A:2317:Y01:CAB	2.79	0.65
1:A:763:GLU:HG2	1:A:1412:LYS:HD3	1.79	0.65
1:A:1450:GLY:CA	6:A:2317:Y01:CAD	2.75	0.64
4:A:2307:DZR:C12	5:A:2313:3PE:O14	2.46	0.64
1:A:960:VAL:HG22	1:A:1506:LEU:HD11	1.78	0.63
1:A:1355:ARG:CZ	1:A:1358:ARG:HH11	2.13	0.62
1:A:112:GLN:O	1:A:116:ILE:HG22	1.99	0.60
1:A:754:LEU:O	1:A:758:LEU:HD22	2.00	0.60
1:A:809:ILE:HD12	1:A:809:ILE:C	2.26	0.60
1:A:921:THR:HG21	1:A:1465:TRP:HE1	1.66	0.60
1:A:823:VAL:HG23	1:A:823:VAL:O	2.02	0.59
1:A:839:MET:CG	5:A:2315:3PE:H3A1	2.32	0.59
1:A:1459:LEU:HD23	1:A:1465:TRP:HB2	1.85	0.59
1:A:921:THR:HG21	1:A:1465:TRP:NE1	2.18	0.59
1:A:347:ILE:HG23	1:A:378:LEU:HD21	1.85	0.58
1:A:204:LEU:HD12	1:A:958:LEU:HD22	1.84	0.58
1:A:766:GLU:HA	1:A:766:GLU:OE1	2.03	0.58
1:A:1400:PHE:HD2	6:A:2317:Y01:CAB	2.16	0.58
1:A:125:PHE:HE2	1:A:163:GLY:CA	2.09	0.57
1:A:128:PHE:CD2	1:A:189:ARG:NH1	2.71	0.57
1:A:93:LEU:HD11	1:A:120:PHE:CD2	2.39	0.57
6:A:2316:Y01:HAR1	6:A:2316:Y01:OAG	2.07	0.55
1:A:93:LEU:HD11	1:A:120:PHE:CE2	2.42	0.54
1:A:127:PHE:CD1	1:A:127:PHE:C	2.85	0.54
1:A:1688:MET:CA	1:A:1688:MET:CE	2.86	0.54
1:A:1716:ALA:HB2	1:A:1829:LYS:HB2	1.89	0.54
1:A:1448:ASN:HD22	6:A:2316:Y01:HAD1	1.71	0.54
1:A:1716:ALA:HB2	1:A:1829:LYS:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:LEU:CD2	1:A:1821:ASN:ND2	2.71	0.53
1:A:123:PHE:C	1:A:123:PHE:CD1	2.87	0.53
1:A:768:PRO:HB2	1:A:770:GLU:OE1	2.08	0.53
1:A:832:VAL:HG23	5:A:2315:3PE:H321	1.90	0.53
6:A:2317:Y01:CAO	6:A:2317:Y01:CAA	2.86	0.53
6:A:2317:Y01:HAR1	6:A:2317:Y01:OAG	2.08	0.53
1:A:1450:GLY:HA3	6:A:2317:Y01:HAD1	1.90	0.52
1:A:233:TRP:HA	1:A:236:LEU:HD12	1.91	0.52
1:A:1709:LEU:O	1:A:1712:THR:CG2	2.58	0.52
1:A:767:GLN:CB	1:A:768:PRO:HD2	2.37	0.52
1:A:1450:GLY:CA	6:A:2317:Y01:HAD1	2.41	0.52
1:A:1403:PHE:CE1	5:A:2315:3PE:H281	2.45	0.51
1:A:1753:CYS:SG	1:A:1790:ARG:NH2	2.84	0.51
1:A:805:ASN:HD22	1:A:806:PRO:HD2	1.76	0.51
1:A:93:LEU:HD12	1:A:124:ILE:HD11	1.93	0.51
1:A:1366:LEU:HD12	1:A:1366:LEU:O	2.10	0.51
1:A:313:CYS:SG	1:A:314:VAL:N	2.85	0.50
1:A:1354:LEU:HD22	1:A:1354:LEU:C	2.33	0.50
1:A:766:GLU:O	1:A:766:GLU:HG3	2.12	0.50
1:A:1717:LEU:C	1:A:1717:LEU:CD1	2.85	0.50
1:A:1260:LEU:HD12	1:A:1371:ARG:HB3	1.93	0.50
1:A:1270:ILE:CG1	1:A:1364:ARG:NH1	2.73	0.49
1:A:1355:ARG:CZ	1:A:1358:ARG:NH1	2.76	0.49
1:A:1364:ARG:N	1:A:1365:PRO:CD	2.74	0.49
1:A:371:ASN:ND2	6:A:2318:Y01:HAR2	2.28	0.49
1:A:1717:LEU:N	1:A:1718:PRO:HD2	2.28	0.49
1:A:1719:GLN:HA	1:A:1719:GLN:OE1	2.13	0.49
1:A:921:THR:CG2	1:A:1465:TRP:HE1	2.25	0.49
1:A:1378:VAL:HG21	1:A:1722:ASN:HB3	1.94	0.48
1:A:1403:PHE:HZ	5:A:2315:3PE:H281	1.76	0.48
1:A:1591:ASP:HB2	1:A:1702:MET:HE1	1.94	0.48
1:A:1681:ASN:HD22	1:A:1682:PRO:HD2	1.78	0.48
1:A:1333:ILE:HD13	1:A:1360:LEU:HB3	1.95	0.48
1:A:1375:LEU:O	1:A:1379:VAL:HG23	2.14	0.48
1:A:820:TRP:CD1	1:A:820:TRP:C	2.91	0.47
1:A:1450:GLY:C	6:A:2317:Y01:HAD2	2.39	0.47
1:A:100:MET:HB2	1:A:113:ARG:HH12	1.79	0.47
1:A:1382:LEU:HD22	1:A:1821:ASN:ND2	2.28	0.47
1:A:1505:VAL:HG11	5:A:2313:3PE:H32	1.97	0.47
1:A:1359:LEU:HD13	1:A:1740:GLU:CG	2.41	0.47
1:A:288:LEU:C	1:A:288:LEU:HD13	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:GLY:C	6:A:2317:Y01:CAD	2.88	0.47
1:A:1774:ARG:HH21	1:A:1780:ASN:HB3	1.80	0.46
1:A:1368:VAL:O	1:A:1368:VAL:HG22	2.16	0.46
1:A:206:ASP:OD2	1:A:404:ARG:NH1	2.48	0.46
1:A:1389:ILE:HG22	1:A:1392:ILE:HD12	1.98	0.46
1:A:1366:LEU:CD1	1:A:1366:LEU:C	2.89	0.46
1:A:1697:LEU:C	1:A:1699:LEU:H	2.24	0.45
5:A:2313:3PE:C22	5:A:2313:3PE:C3	2.88	0.45
1:A:1450:GLY:HA2	6:A:2317:Y01:CAD	2.46	0.45
1:A:231:GLN:NE2	1:A:1608:GLU:OE1	2.50	0.45
1:A:1664:ILE:HA	1:A:1667:ILE:HG22	1.99	0.45
1:A:1350:ILE:HD12	1:A:1350:ILE:O	2.15	0.45
1:A:1697:LEU:C	1:A:1699:LEU:N	2.73	0.45
1:A:1720:VAL:HG22	1:A:1822:VAL:HG13	1.97	0.45
1:A:1382:LEU:HD21	1:A:1821:ASN:ND2	2.32	0.45
1:A:1696:VAL:O	1:A:1696:VAL:HG22	2.16	0.45
1:A:839:MET:HG3	5:A:2315:3PE:C3A	2.44	0.44
1:A:1597:VAL:HG11	1:A:1630:ILE:HD11	1.99	0.44
1:A:1355:ARG:O	1:A:1359:LEU:HD23	2.17	0.44
1:A:1400:PHE:HD2	6:A:2317:Y01:HAB3	1.81	0.44
1:A:1697:LEU:O	1:A:1699:LEU:N	2.51	0.44
1:A:224:ILE:HA	1:A:1693:ILE:HD11	2.00	0.44
1:A:769:GLU:CD	1:A:769:GLU:C	2.85	0.44
1:A:921:THR:HG23	1:A:921:THR:O	2.18	0.44
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.78	0.43
1:A:227:ILE:HG21	1:A:1605:MET:HE2	1.99	0.43
1:A:1379:VAL:O	1:A:1383:MET:HG2	2.19	0.43
1:A:345:ILE:HD11	5:A:2310:3PE:H2C2	2.00	0.43
1:A:1513:VAL:HG13	1:A:1828:MET:HE3	2.00	0.43
1:A:821:GLU:HB3	1:A:833:LEU:HD13	1.99	0.43
1:A:1817:PHE:O	1:A:1821:ASN:ND2	2.51	0.43
6:A:2317:Y01:HAC3	6:A:2317:Y01:HAJ1	1.75	0.43
1:A:1722:ASN:HD22	1:A:1722:ASN:HA	1.71	0.42
6:A:2318:Y01:HAE2	6:A:2318:Y01:HBB	1.79	0.42
1:A:101:PHE:CE1	1:A:180:ARG:CZ	3.02	0.42
6:A:2317:Y01:HAS2	6:A:2317:Y01:HAE1	1.85	0.42
1:A:1454:MET:HE2	6:A:2317:Y01:HAU2	2.02	0.42
1:A:1717:LEU:HB3	1:A:1718:PRO:HD3	2.02	0.42
1:A:1408:VAL:O	1:A:1412:LYS:HB2	2.20	0.42
1:A:1464:GLY:HA3	1:A:1782:ASN:HD21	1.83	0.42
1:A:848:LEU:HA	1:A:849:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:LEU:HD23	1:A:1459:LEU:HD12	2.01	0.42
1:A:1631:PHE:HB3	1:A:1660:VAL:HG22	2.02	0.41
1:A:121:ASP:OD2	1:A:186:ARG:NH1	2.51	0.41
6:A:2317:Y01:HAB3	6:A:2317:Y01:HAJ2	1.84	0.41
1:A:371:ASN:HD22	1:A:371:ASN:HA	1.61	0.41
1:A:1270:ILE:HG12	1:A:1364:ARG:NH1	2.24	0.41
1:A:1350:ILE:HD13	1:A:1350:ILE:HA	1.75	0.41
1:A:756:ASN:C	1:A:756:ASN:ND2	2.78	0.41
1:A:125:PHE:CD1	1:A:125:PHE:C	2.99	0.41
1:A:1278:ASP:HB2	1:A:1281:SER:HB2	2.03	0.41
1:A:239:ASN:HA	1:A:325:ALA:HA	2.02	0.40
1:A:340:ILE:HD12	1:A:340:ILE:HA	1.93	0.40
1:A:948:MET:HE2	1:A:948:MET:HB3	1.90	0.40
1:A:1376:LYS:O	1:A:1380:GLU:HG3	2.21	0.40
1:A:767:GLN:HB2	1:A:768:PRO:CD	2.49	0.40
1:A:1450:GLY:HA2	6:A:2317:Y01:HAD3	2.02	0.40
1:A:1711:ASP:O	1:A:1715:GLN:HG3	2.20	0.40
6:A:2318:Y01:HAP1	6:A:2318:Y01:HAO2	1.82	0.40
1:A:1506:LEU:HD12	1:A:1506:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	992/2146 (46%)	956 (96%)	33 (3%)	3 (0%)	36 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	909	LEU
1	A	764	TYR

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Mol	Chain	Res	Type
1	A	1698	LYS

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	902/1852 (49%)	880 (98%)	22 (2%)	43	69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	116	ILE
1	A	243	LEU
1	A	314	VAL
1	A	758	LEU
1	A	769	GLU
1	A	809	ILE
1	A	811	ASP
1	A	848	LEU
1	A	921	THR
1	A	1350	ILE
1	A	1354	LEU
1	A	1355	ARG
1	A	1361	ARG
1	A	1366	LEU
1	A	1381	THR
1	A	1476	VAL
1	A	1630	ILE
1	A	1687	ILE
1	A	1697	LEU
1	A	1712	THR
1	A	1789	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	260	GLN
1	A	805	ASN
1	A	918	GLN
1	A	957	ASN
1	A	1280	HIS
1	A	1442	HIS
1	A	1486	HIS
1	A	1518	HIS
1	A	1624	ASN
1	A	1649	GLN
1	A	1675	ASN
1	A	1681	ASN
1	A	1722	ASN
1	A	1751	HIS
1	A	1780	ASN
1	A	1821	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
5	3PE	A	2310	-	13,13,50	0.20	0	12,12,55	1.02	0
3	NAG	A	2306	1	14,14,15	0.71	1 (7%)	17,19,21	2.45	4 (23%)
5	3PE	A	2314	-	15,15,50	0.25	0	14,14,55	0.87	0
5	3PE	A	2308	-	30,30,50	1.18	5 (16%)	33,35,55	1.36	4 (12%)
5	3PE	A	2315	-	34,34,50	1.18	3 (8%)	37,39,55	1.48	6 (16%)
3	NAG	A	2305	1	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
3	NAG	A	2303	1	14,14,15	1.55	2 (14%)	17,19,21	1.33	1 (5%)
5	3PE	A	2311	-	32,32,50	1.15	4 (12%)	35,37,55	1.28	3 (8%)
6	Y01	A	2318	-	38,38,38	4.22	12 (31%)	57,57,57	2.16	16 (28%)
6	Y01	A	2317	-	38,38,38	4.21	12 (31%)	57,57,57	2.50	20 (35%)
4	DZR	A	2307	-	27,27,27	2.75	7 (25%)	38,38,38	1.68	11 (28%)
3	NAG	A	2304	1	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
5	3PE	A	2312	-	12,12,50	0.28	0	11,11,55	0.90	0
5	3PE	A	2309	-	30,30,50	1.20	4 (13%)	33,35,55	1.28	3 (9%)
6	Y01	A	2316	-	38,38,38	4.19	12 (31%)	57,57,57	2.24	15 (26%)
5	3PE	A	2313	-	35,35,50	1.09	4 (11%)	38,40,55	1.29	4 (10%)

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
5	3PE	A	2310	-	-	4/11/11/54	-
3	NAG	A	2306	1	-	6/6/23/26	0/1/1/1
5	3PE	A	2314	-	-	6/13/13/54	-
5	3PE	A	2308	-	-	16/34/34/54	-
5	3PE	A	2315	-	-	11/38/38/54	-
3	NAG	A	2305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2303	1	-	0/6/23/26	0/1/1/1
5	3PE	A	2311	-	-	16/36/36/54	-
6	Y01	A	2318	-	-	13/19/77/77	0/4/4/4
6	Y01	A	2317	-	-	11/19/77/77	0/4/4/4
4	DZR	A	2307	-	-	2/18/28/28	0/2/2/2
3	NAG	A	2304	1	-	2/6/23/26	0/1/1/1
5	3PE	A	2312	-	-	2/10/10/54	-
5	3PE	A	2309	-	-	18/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	A	2316	-	-	15/19/77/77	0/4/4/4
5	3PE	A	2313	-	-	23/39/39/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2317	Y01	CAI-CAZ	17.61	1.69	1.33
6	A	2318	Y01	CAI-CAZ	17.56	1.69	1.33
6	A	2316	Y01	CAI-CAZ	17.30	1.68	1.33
6	A	2318	Y01	CBH-CBF	7.44	1.67	1.56
6	A	2316	Y01	CBH-CBF	7.34	1.67	1.56
6	A	2317	Y01	CAU-CBI	-7.09	1.41	1.54
6	A	2317	Y01	CBH-CBF	7.05	1.67	1.56
4	A	2307	DZR	C14-N05	-7.04	1.31	1.47
6	A	2317	Y01	CAQ-CAP	7.03	1.73	1.54
6	A	2318	Y01	CAQ-CAP	6.98	1.73	1.54
6	A	2316	Y01	CAU-CBI	-6.98	1.42	1.54
6	A	2318	Y01	CAU-CBI	-6.93	1.42	1.54
6	A	2316	Y01	CAQ-CAP	6.76	1.72	1.54
4	A	2307	DZR	C15-N07	6.67	1.45	1.34
6	A	2318	Y01	CAK-CBD	6.64	1.63	1.53
6	A	2317	Y01	CBB-CBE	-6.47	1.43	1.54
6	A	2318	Y01	CAU-CAS	6.42	1.66	1.53
6	A	2316	Y01	CAU-CAS	6.40	1.66	1.53
6	A	2317	Y01	CAU-CAS	6.28	1.65	1.53
6	A	2316	Y01	CAK-CBD	6.26	1.63	1.53
6	A	2317	Y01	CAK-CBD	6.07	1.62	1.53
6	A	2316	Y01	CBB-CBE	-6.04	1.44	1.54
6	A	2316	Y01	CBI-CBE	6.02	1.66	1.55
4	A	2307	DZR	C11-N05	-5.71	1.31	1.46
6	A	2318	Y01	CBI-CBE	5.66	1.65	1.55
6	A	2317	Y01	CBI-CBE	5.48	1.65	1.55
4	A	2307	DZR	C12-N05	-5.45	1.32	1.46
4	A	2307	DZR	C17-N06	5.27	1.45	1.33
6	A	2318	Y01	CAQ-CBG	5.20	1.65	1.54
6	A	2318	Y01	CBB-CBE	-5.13	1.45	1.54
6	A	2317	Y01	CAQ-CBG	5.09	1.64	1.54
6	A	2316	Y01	CAQ-CBG	4.91	1.64	1.54
3	A	2303	NAG	O5-C1	4.63	1.51	1.43
5	A	2315	3PE	O31-C31	3.37	1.43	1.33
3	A	2303	NAG	C1-C2	3.19	1.56	1.52
6	A	2318	Y01	OAW-CAY	3.06	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2317	Y01	OAW-CAY	2.99	1.42	1.34
5	A	2309	3PE	O21-C2	-2.94	1.39	1.46
6	A	2318	Y01	CAO-CBB	2.89	1.61	1.54
6	A	2316	Y01	OAW-CAY	2.82	1.42	1.34
5	A	2311	3PE	O21-C2	-2.74	1.40	1.46
6	A	2317	Y01	CBH-CAZ	-2.61	1.47	1.52
5	A	2308	3PE	O21-C21	2.59	1.41	1.34
6	A	2316	Y01	CBH-CAZ	-2.54	1.48	1.52
5	A	2313	3PE	O21-C2	-2.52	1.40	1.46
5	A	2315	3PE	C3-C2	2.47	1.58	1.50
5	A	2311	3PE	O31-C31	2.46	1.40	1.33
5	A	2309	3PE	O31-C31	2.42	1.40	1.33
6	A	2316	Y01	CAO-CBB	2.39	1.60	1.54
6	A	2318	Y01	CBH-CAZ	-2.39	1.48	1.52
5	A	2313	3PE	O31-C31	2.32	1.40	1.33
5	A	2308	3PE	O31-C3	-2.31	1.40	1.45
5	A	2308	3PE	O31-C31	2.21	1.39	1.33
5	A	2309	3PE	O31-C3	-2.20	1.40	1.45
5	A	2311	3PE	O31-C3	-2.18	1.40	1.45
5	A	2309	3PE	O21-C21	2.17	1.40	1.34
5	A	2311	3PE	O21-C21	2.13	1.40	1.34
4	A	2307	DZR	O04-C17	-2.13	1.18	1.23
5	A	2315	3PE	C32-C31	2.13	1.56	1.50
4	A	2307	DZR	O03-C15	-2.12	1.19	1.23
5	A	2313	3PE	O21-C21	2.12	1.40	1.34
5	A	2313	3PE	P-O12	-2.07	1.45	1.55
3	A	2306	NAG	C1-C2	2.04	1.55	1.52
5	A	2308	3PE	O21-C2	-2.03	1.41	1.46
6	A	2317	Y01	CAO-CBB	2.03	1.59	1.54
5	A	2308	3PE	P-O12	-2.01	1.46	1.55

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2306	NAG	C2-N2-C7	8.38	134.13	122.90
6	A	2317	Y01	CBI-CBE-CBB	-6.80	108.99	119.50
6	A	2317	Y01	CBG-CBI-CBE	6.35	107.38	100.10
6	A	2316	Y01	CAK-CAI-CAZ	-5.93	115.01	125.02
6	A	2317	Y01	CAV-CAZ-CBH	-5.85	108.94	116.42
5	A	2315	3PE	O21-C21-C22	5.83	124.09	111.48
6	A	2318	Y01	CAK-CAI-CAZ	-5.55	115.65	125.02
6	A	2316	Y01	CBI-CBE-CBB	-5.42	111.13	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2316	Y01	CBG-CBI-CBE	5.33	106.21	100.10
3	A	2303	NAG	C1-O5-C5	5.09	119.01	112.19
6	A	2317	Y01	CAK-CAI-CAZ	-4.89	116.76	125.02
6	A	2318	Y01	CBH-CAZ-CAI	-4.87	115.81	122.93
6	A	2318	Y01	CAD-CBH-CBF	-4.72	106.36	111.66
6	A	2316	Y01	CAE-CBI-CAU	-4.50	103.97	110.61
5	A	2308	3PE	O21-C21-C22	4.40	120.99	111.48
6	A	2318	Y01	OAW-CAY-CAM	4.26	120.69	111.48
6	A	2318	Y01	CAU-CBI-CBE	4.23	122.83	116.60
6	A	2317	Y01	CBH-CAZ-CAI	-4.20	116.79	122.93
6	A	2317	Y01	CBI-CBG-CBD	-4.18	108.48	114.41
5	A	2309	3PE	O21-C21-C22	4.16	120.48	111.48
5	A	2313	3PE	O21-C21-C22	4.10	120.36	111.48
6	A	2317	Y01	CAE-CBI-CAU	-4.09	104.58	110.61
5	A	2311	3PE	O21-C21-C22	4.08	120.30	111.48
6	A	2317	Y01	CAU-CBI-CBE	4.07	122.60	116.60
6	A	2316	Y01	CBH-CAZ-CAI	-4.05	117.01	122.93
3	A	2306	NAG	C1-C2-N2	3.88	116.55	110.43
6	A	2317	Y01	CAE-CBI-CBG	-3.88	104.64	111.68
6	A	2316	Y01	OAW-CAY-CAM	3.78	119.66	111.48
6	A	2317	Y01	CAE-CBI-CBE	-3.74	104.89	111.68
4	A	2307	DZR	C12-N05-C11	3.74	116.89	108.84
6	A	2317	Y01	OAW-CAY-CAM	3.73	119.55	111.48
6	A	2318	Y01	CAE-CBI-CBG	-3.68	105.01	111.68
6	A	2318	Y01	CAE-CBI-CBE	-3.63	105.08	111.68
4	A	2307	DZR	C16-N07-C15	-3.63	121.49	126.14
6	A	2316	Y01	CAU-CBI-CBE	3.62	121.93	116.60
6	A	2318	Y01	CBI-CBE-CBB	-3.59	113.96	119.50
6	A	2318	Y01	CAU-CBI-CBG	3.59	112.61	107.25
6	A	2316	Y01	CAD-CBH-CBF	-3.57	107.65	111.66
6	A	2318	Y01	CBG-CBI-CBE	3.56	104.18	100.10
6	A	2318	Y01	CAK-CBD-CBF	3.54	113.81	109.72
6	A	2316	Y01	CAP-CBE-CBI	3.49	107.95	103.84
6	A	2316	Y01	CAE-CBI-CBG	-3.48	105.37	111.68
6	A	2317	Y01	CAS-CBF-CBH	-3.39	108.91	113.08
6	A	2318	Y01	CAE-CBI-CAU	-3.37	105.64	110.61
4	A	2307	DZR	C10-C12-N05	3.25	116.34	111.08
4	A	2307	DZR	O03-C15-N07	-3.11	118.15	123.09
6	A	2316	Y01	CAU-CBI-CBG	3.06	111.83	107.25
6	A	2317	Y01	CAD-CBH-CBF	-2.99	108.30	111.66
6	A	2316	Y01	CAE-CBI-CBE	-2.99	106.26	111.68
6	A	2317	Y01	CBF-CBH-CAZ	2.91	113.91	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2305	NAG	C1-O5-C5	2.91	116.08	112.19
5	A	2311	3PE	O31-C31-C32	2.89	119.92	111.15
4	A	2307	DZR	C09-C11-N05	2.86	115.71	111.08
6	A	2317	Y01	CAK-CBD-CBF	2.86	113.02	109.72
5	A	2315	3PE	O31-C31-O32	-2.85	116.51	123.63
5	A	2315	3PE	O21-C21-O22	-2.74	117.30	123.70
5	A	2308	3PE	O12-P-O14	-2.70	99.86	112.44
3	A	2306	NAG	C1-O5-C5	2.70	115.81	112.19
6	A	2316	Y01	CAC-CBB-CBE	-2.69	108.84	112.88
5	A	2308	3PE	O31-C31-C32	2.69	120.03	111.83
5	A	2313	3PE	O31-C31-C32	2.68	120.00	111.83
5	A	2309	3PE	O31-C31-C32	2.66	119.95	111.83
6	A	2316	Y01	CAV-CAZ-CBH	-2.66	113.02	116.42
4	A	2307	DZR	C26-C25-C23	-2.60	120.34	123.50
6	A	2317	Y01	CAU-CBI-CBG	2.60	111.13	107.25
6	A	2316	Y01	CAK-CBD-CBF	2.52	112.64	109.72
5	A	2315	3PE	O12-P-O14	-2.51	100.79	112.44
4	A	2307	DZR	C14-C15-N07	2.50	119.44	114.94
6	A	2317	Y01	CAQ-CBG-CBD	2.49	123.08	119.10
6	A	2317	Y01	CAQ-CBG-CBI	2.47	106.75	103.84
5	A	2311	3PE	O12-P-O14	-2.45	101.04	112.44
5	A	2313	3PE	O12-P-O14	-2.45	101.05	112.44
5	A	2315	3PE	O31-C31-C32	2.39	119.11	111.83
6	A	2318	Y01	CAC-CBB-CBE	-2.34	109.37	112.88
6	A	2318	Y01	CAQ-CBG-CBD	2.28	122.74	119.10
3	A	2304	NAG	C1-O5-C5	2.27	115.22	112.19
5	A	2309	3PE	O12-P-O14	-2.25	101.99	112.44
6	A	2318	Y01	CAO-CBB-CBE	2.23	114.95	110.33
5	A	2308	3PE	C2-O21-C21	2.20	123.07	117.80
4	A	2307	DZR	C14-N05-C11	2.19	114.55	111.14
5	A	2315	3PE	C3-C2-C1	2.19	116.89	111.78
6	A	2317	Y01	CAC-CBB-CBE	-2.18	109.61	112.88
3	A	2306	NAG	C8-C7-N2	2.16	119.70	116.12
5	A	2313	3PE	O31-C3-C2	2.14	114.57	108.40
6	A	2318	Y01	CAT-CAR-CBC	2.08	113.72	110.33
4	A	2307	DZR	C14-N05-C12	2.04	114.32	111.14
4	A	2307	DZR	C13-N06-C17	-2.03	118.81	122.54
6	A	2317	Y01	CAJ-CAO-CBB	-2.01	109.46	115.08
4	A	2307	DZR	C24-C26-C25	2.00	119.90	117.64

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2308	3PE	C1-O11-P-O12
5	A	2309	3PE	C1-O11-P-O12
5	A	2309	3PE	C1-O11-P-O13
5	A	2309	3PE	C1-O11-P-O14
5	A	2309	3PE	C11-O13-P-O11
5	A	2309	3PE	C11-O13-P-O12
5	A	2309	3PE	C11-O13-P-O14
5	A	2309	3PE	O13-C11-C12-N
5	A	2309	3PE	O22-C21-O21-C2
5	A	2311	3PE	C1-O11-P-O12
5	A	2311	3PE	C1-O11-P-O13
5	A	2311	3PE	C1-O11-P-O14
5	A	2311	3PE	O13-C11-C12-N
5	A	2311	3PE	O21-C2-C3-O31
5	A	2313	3PE	C1-O11-P-O12
5	A	2313	3PE	C1-O11-P-O13
5	A	2313	3PE	C1-O11-P-O14
5	A	2313	3PE	O13-C11-C12-N
5	A	2313	3PE	O22-C21-O21-C2
5	A	2313	3PE	C22-C21-O21-C2
5	A	2315	3PE	C22-C21-O21-C2
6	A	2316	Y01	CAR-CBC-OAW-CAY
6	A	2318	Y01	OAG-CAY-OAW-CBC
5	A	2315	3PE	O32-C31-O31-C3
6	A	2317	Y01	CAR-CBC-OAW-CAY
5	A	2315	3PE	C32-C31-O31-C3
6	A	2318	Y01	CAJ-CAO-CBB-CAC
5	A	2313	3PE	O32-C31-O31-C3
6	A	2318	Y01	CAC-CBB-CBE-CAP
6	A	2318	Y01	CAC-CBB-CBE-CBI
5	A	2308	3PE	O22-C21-O21-C2
5	A	2315	3PE	O22-C21-O21-C2
5	A	2308	3PE	C32-C31-O31-C3
5	A	2313	3PE	C32-C31-O31-C3
5	A	2309	3PE	C22-C21-O21-C2
6	A	2318	Y01	CAM-CAY-OAW-CBC
6	A	2316	Y01	CAJ-CAO-CBB-CAC
6	A	2318	Y01	CAO-CBB-CBE-CBI
3	A	2306	NAG	O5-C5-C6-O6
3	A	2304	NAG	O5-C5-C6-O6
5	A	2308	3PE	O32-C31-O31-C3
5	A	2308	3PE	C22-C21-O21-C2
3	A	2306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	2316	Y01	CAO-CBB-CBE-CAP
6	A	2316	Y01	CAO-CBB-CBE-CBI
6	A	2316	Y01	CAC-CBB-CBE-CAP
6	A	2316	Y01	CAC-CBB-CBE-CBI
6	A	2316	Y01	CAJ-CAO-CBB-CBE
3	A	2304	NAG	C4-C5-C6-O6
6	A	2317	Y01	CAC-CBB-CBE-CBI
3	A	2306	NAG	C8-C7-N2-C2
3	A	2306	NAG	O7-C7-N2-C2
6	A	2318	Y01	CAO-CBB-CBE-CAP
6	A	2318	Y01	CAJ-CAO-CBB-CBE
5	A	2308	3PE	C21-C22-C23-C24
6	A	2317	Y01	CAN-CAJ-CAO-CBB
5	A	2311	3PE	C21-C22-C23-C24
5	A	2313	3PE	C34-C35-C36-C37
6	A	2316	Y01	CAO-CAJ-CAN-CBA
6	A	2318	Y01	CAJ-CAN-CBA-CAB
6	A	2317	Y01	CAO-CBB-CBE-CBI
6	A	2316	Y01	CAJ-CAN-CBA-CAA
6	A	2316	Y01	CAJ-CAN-CBA-CAB
5	A	2313	3PE	C32-C33-C34-C35
6	A	2318	Y01	CAJ-CAN-CBA-CAA
5	A	2314	3PE	C35-C36-C37-C38
5	A	2311	3PE	C23-C24-C25-C26
5	A	2311	3PE	C29-C2A-C2B-C2C
5	A	2314	3PE	C32-C33-C34-C35
5	A	2308	3PE	C23-C24-C25-C26
6	A	2316	Y01	CAM-CAY-OAW-CBC
5	A	2310	3PE	C2E-C2F-C2G-C2H
5	A	2308	3PE	C31-C32-C33-C34
5	A	2310	3PE	C2D-C2E-C2F-C2G
6	A	2316	Y01	OAG-CAY-OAW-CBC
5	A	2313	3PE	C22-C23-C24-C25
5	A	2311	3PE	C1-C2-C3-O31
6	A	2317	Y01	CAV-CBC-OAW-CAY
6	A	2317	Y01	CAC-CBB-CBE-CAP
5	A	2308	3PE	C3-C2-O21-C21
5	A	2313	3PE	C23-C24-C25-C26
5	A	2309	3PE	O11-C1-C2-O21
5	A	2314	3PE	C3A-C3B-C3C-C3D
5	A	2310	3PE	C2B-C2C-C2D-C2E
5	A	2313	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	2315	3PE	O11-C1-C2-C3
5	A	2309	3PE	C1-C2-C3-O31
5	A	2311	3PE	C2C-C2D-C2E-C2F
5	A	2308	3PE	O11-C1-C2-O21
5	A	2314	3PE	C37-C38-C39-C3A
5	A	2313	3PE	C31-C32-C33-C34
5	A	2314	3PE	C3C-C3D-C3E-C3F
5	A	2308	3PE	C22-C23-C24-C25
5	A	2308	3PE	O11-C1-C2-C3
5	A	2313	3PE	C2-C1-O11-P
5	A	2311	3PE	C28-C29-C2A-C2B
5	A	2313	3PE	C3-C2-O21-C21
5	A	2315	3PE	C3-C2-O21-C21
5	A	2313	3PE	O11-C1-C2-O21
5	A	2315	3PE	C12-C11-O13-P
5	A	2311	3PE	C26-C27-C28-C29
5	A	2310	3PE	C2A-C2B-C2C-C2D
5	A	2311	3PE	C27-C28-C29-C2A
6	A	2317	Y01	CAJ-CAO-CBB-CAC
4	A	2307	DZR	C15-C14-N05-C11
6	A	2317	Y01	CAO-CBB-CBE-CAP
5	A	2315	3PE	O11-C1-C2-O21
5	A	2309	3PE	O21-C2-C3-O31
5	A	2313	3PE	O21-C2-C3-O31
5	A	2313	3PE	C1-C2-C3-O31
5	A	2309	3PE	C22-C23-C24-C25
5	A	2312	3PE	C28-C29-C2A-C2B
5	A	2308	3PE	C1-O11-P-O13
5	A	2308	3PE	C11-O13-P-O12
5	A	2315	3PE	C1-C2-O21-C21
6	A	2316	Y01	CAN-CAJ-CAO-CBB
5	A	2309	3PE	O11-C1-C2-C3
5	A	2313	3PE	C33-C34-C35-C36
4	A	2307	DZR	C15-C14-N05-C12
5	A	2312	3PE	C2A-C2B-C2C-C2D
5	A	2309	3PE	C32-C31-O31-C3
5	A	2309	3PE	O32-C31-O31-C3
6	A	2317	Y01	CAM-CAL-CAX-OAH
3	A	2306	NAG	C1-C2-N2-C7
5	A	2308	3PE	C1-C2-C3-O31
6	A	2318	Y01	CAM-CAL-CAX-OAH
3	A	2306	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	A	2317	Y01	CAM-CAL-CAX-OAF
5	A	2309	3PE	C2-C1-O11-P
6	A	2318	Y01	CAM-CAL-CAX-OAF
5	A	2308	3PE	O21-C21-C22-C23
5	A	2309	3PE	C25-C26-C27-C28
5	A	2314	3PE	C3B-C3C-C3D-C3E
5	A	2315	3PE	O31-C31-C32-C33
5	A	2313	3PE	C38-C39-C3A-C3B
5	A	2313	3PE	C36-C37-C38-C39
5	A	2311	3PE	O32-C31-O31-C3
5	A	2313	3PE	C21-C22-C23-C24
5	A	2311	3PE	C2A-C2B-C2C-C2D
5	A	2311	3PE	C32-C31-O31-C3
6	A	2316	Y01	CAL-CAM-CAY-OAW
6	A	2317	Y01	CAO-CAJ-CAN-CBA
6	A	2318	Y01	CAL-CAM-CAY-OAW
6	A	2316	Y01	CAL-CAM-CAY-OAG
5	A	2315	3PE	O32-C31-C32-C33

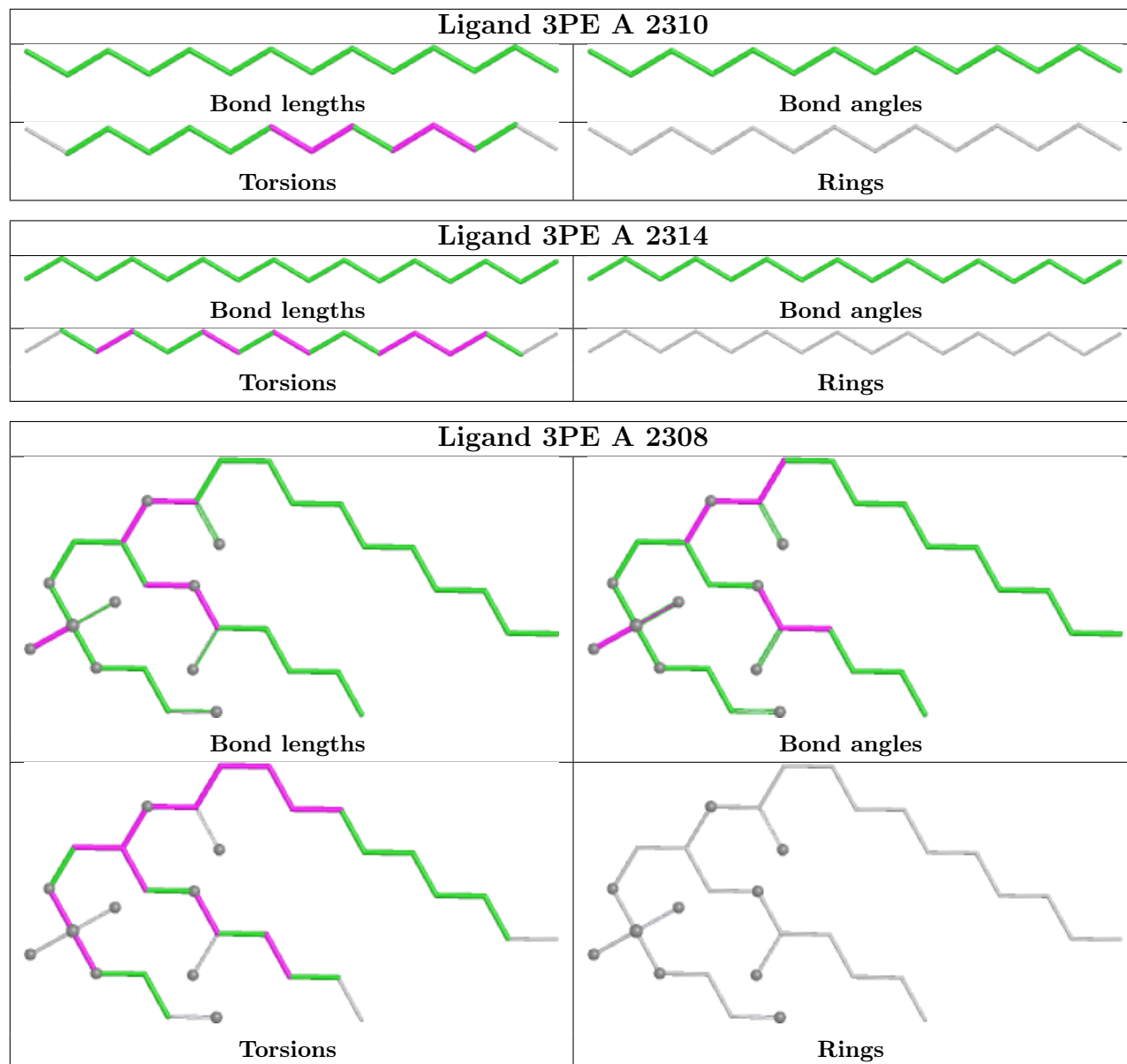
There are no ring outliers.

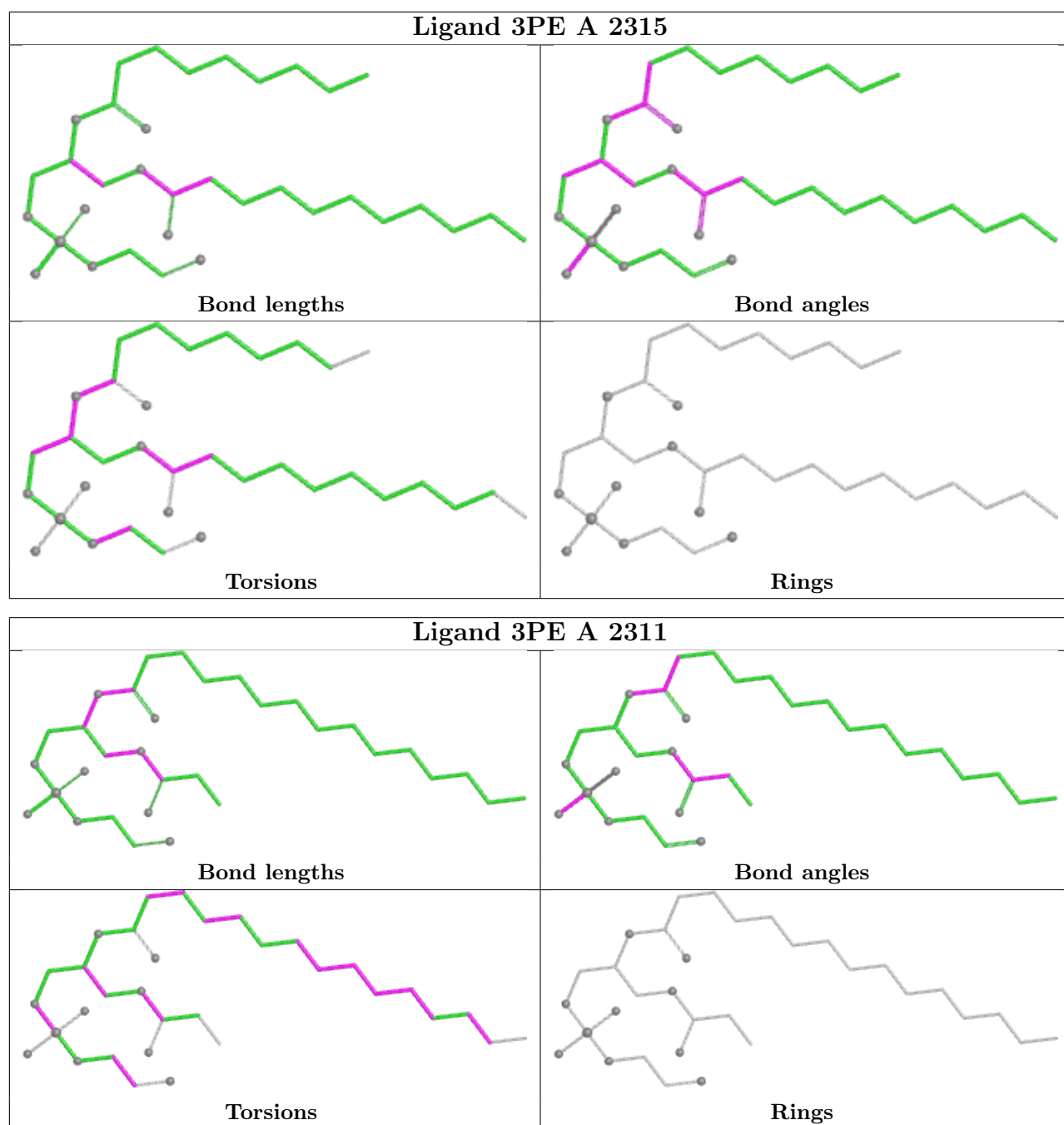
7 monomers are involved in 49 short contacts:

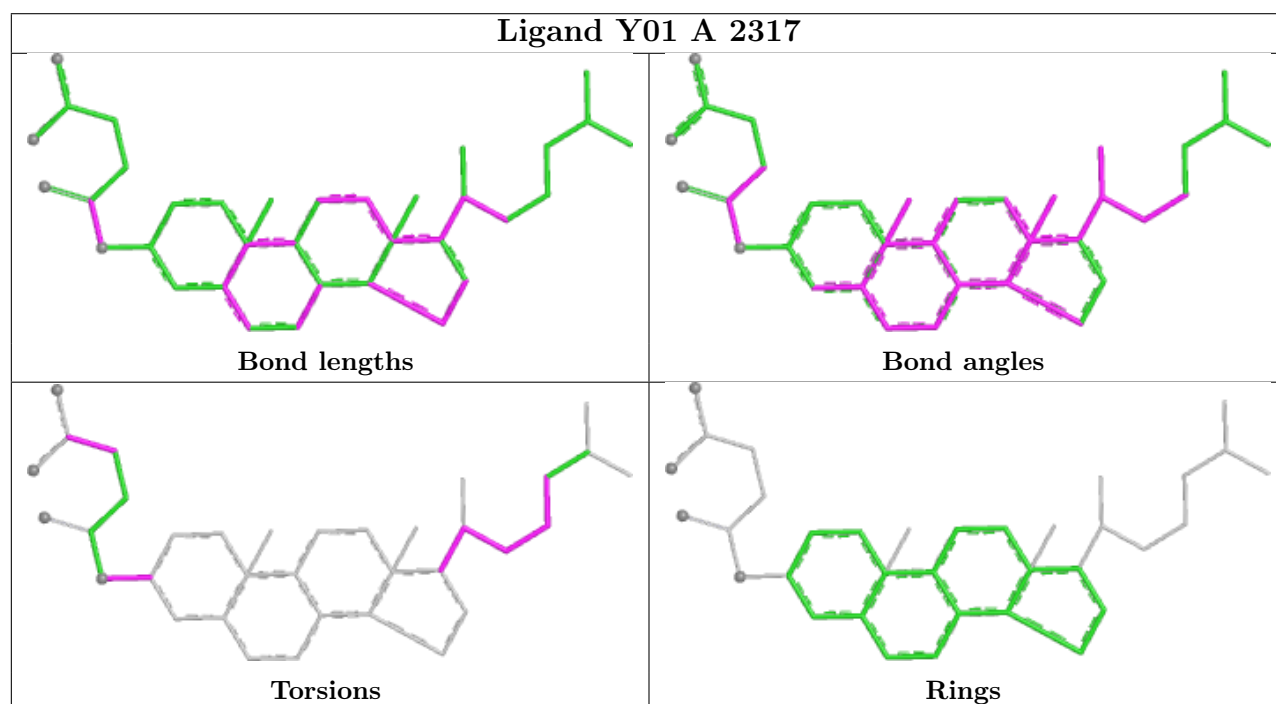
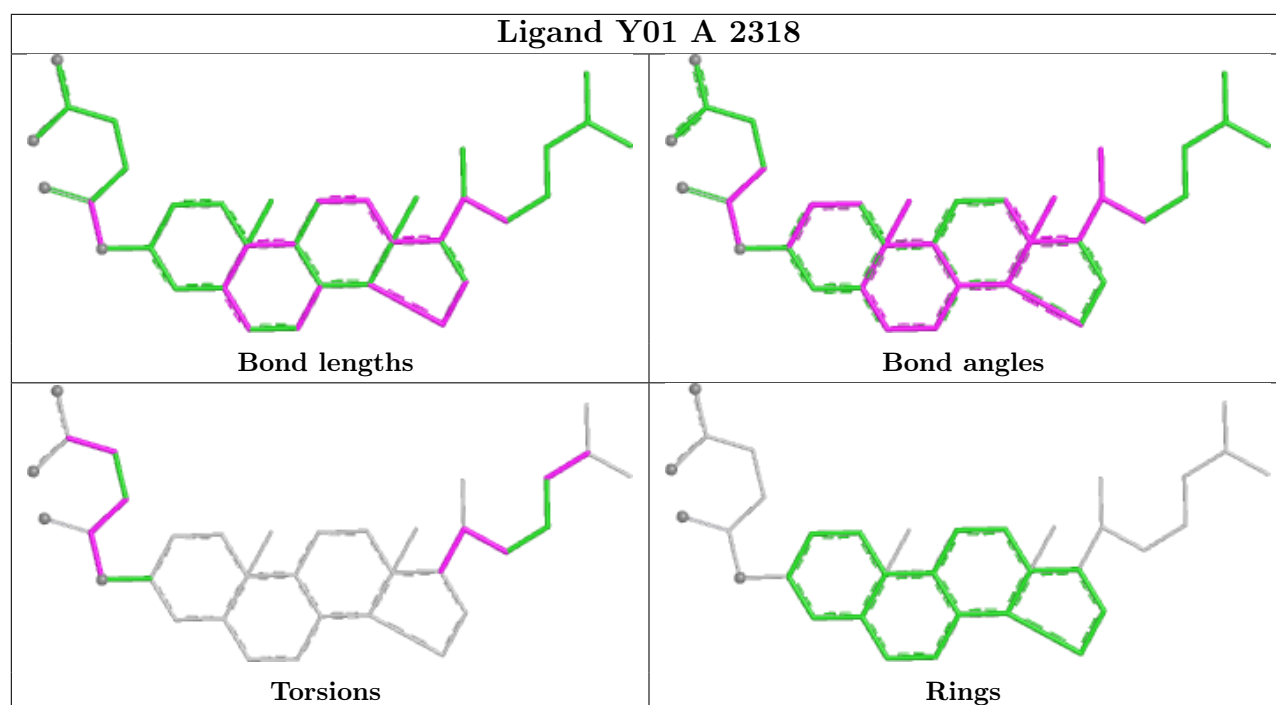
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2310	3PE	1	0
5	A	2315	3PE	9	0
6	A	2318	Y01	3	0
6	A	2317	Y01	23	0
4	A	2307	DZR	1	0
6	A	2316	Y01	8	0
5	A	2313	3PE	5	0

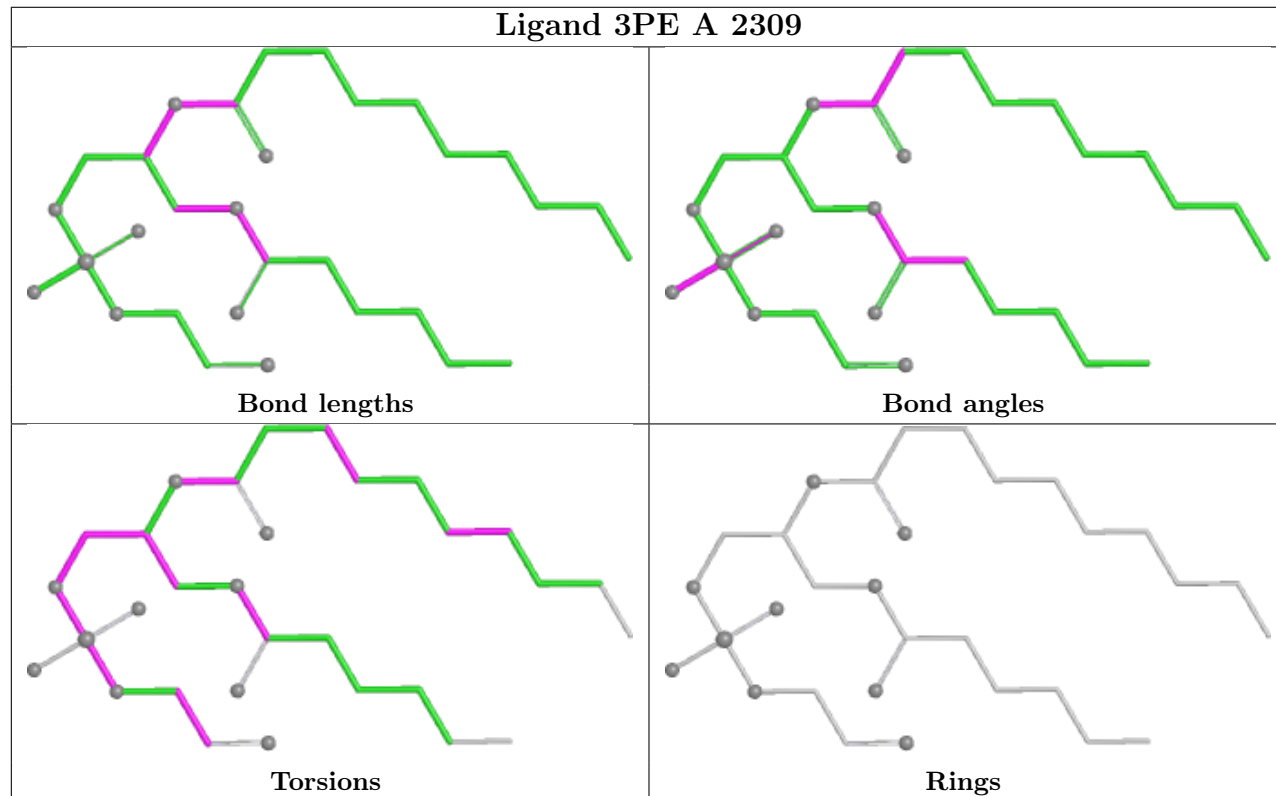
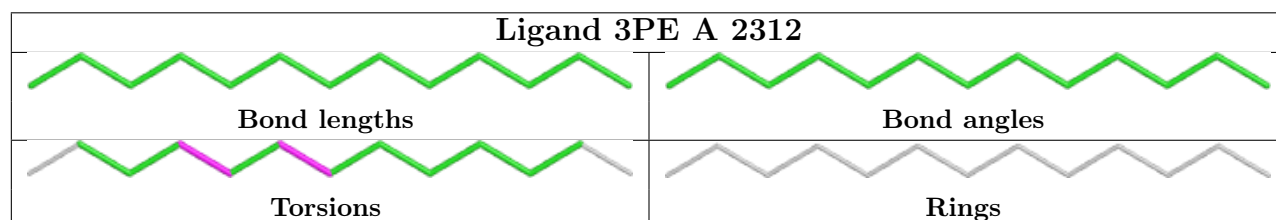
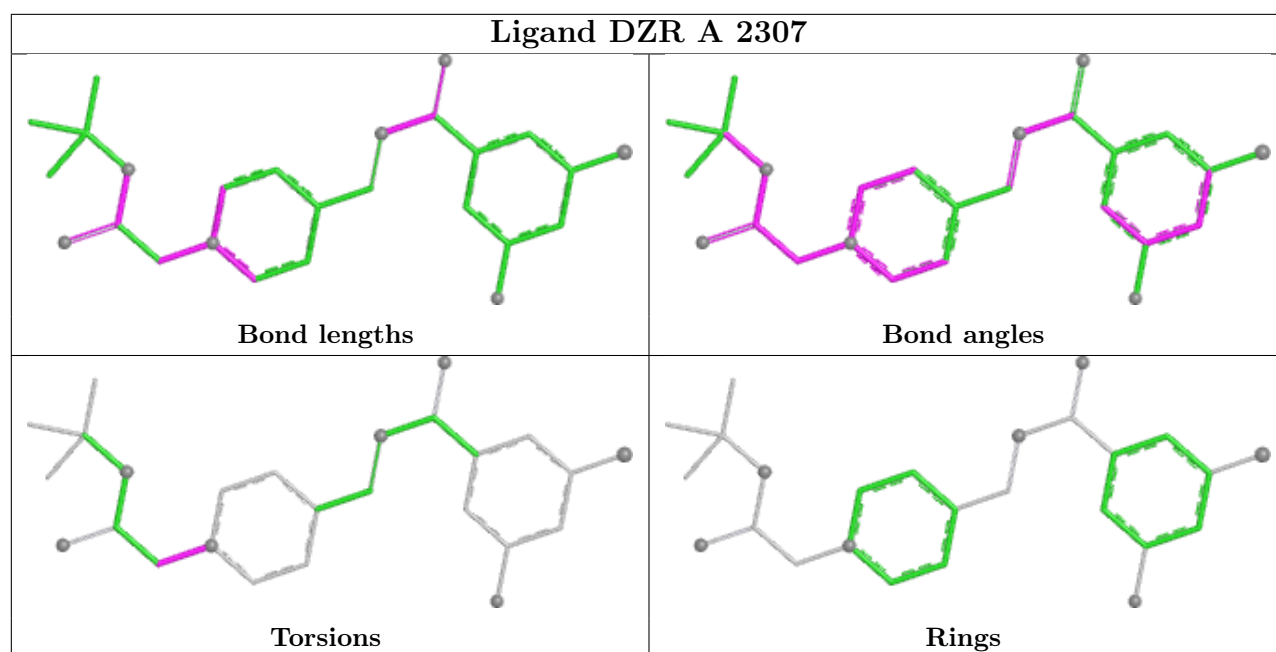
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

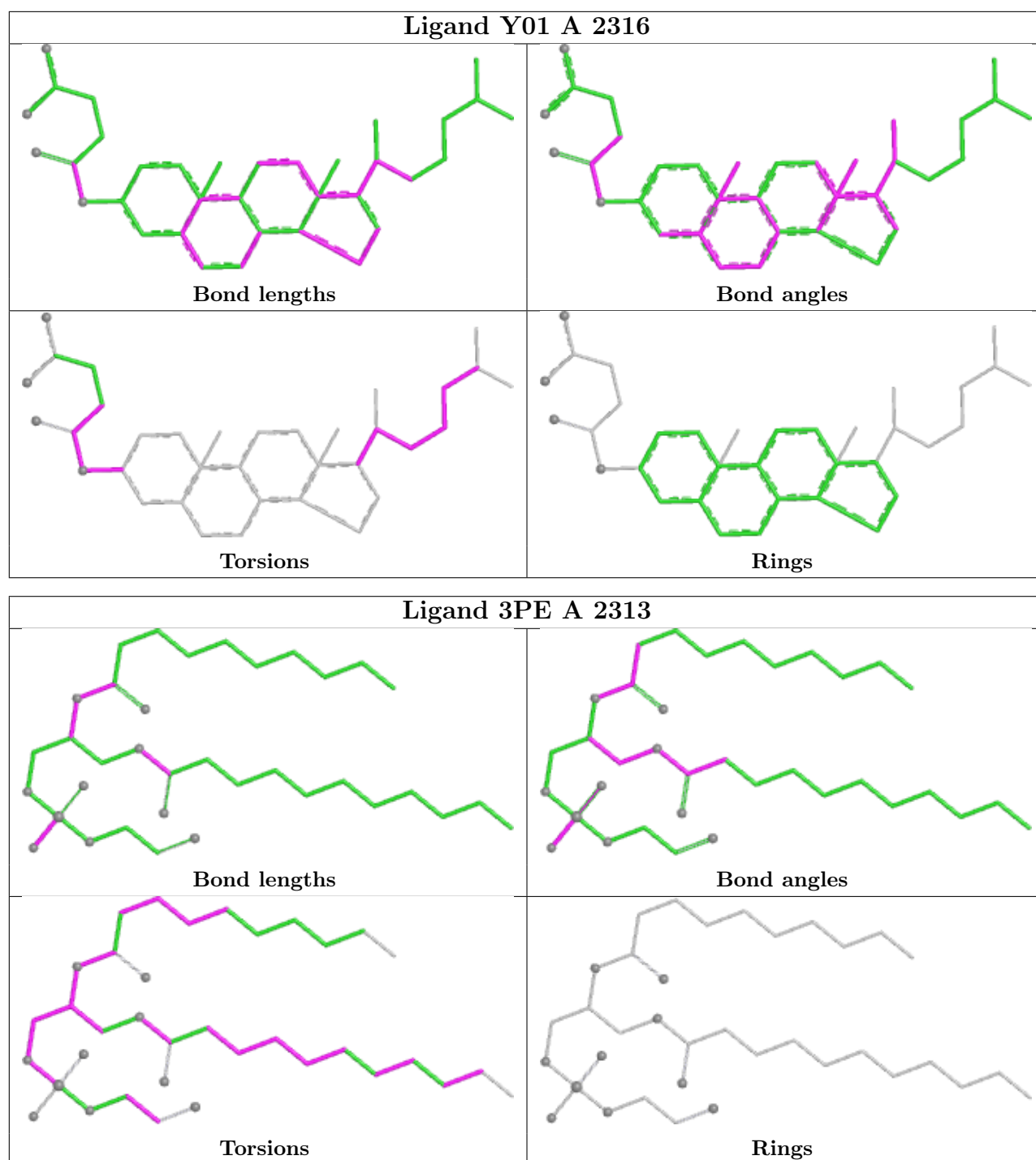
equivalents in the CSD to analyse the geometry.











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.

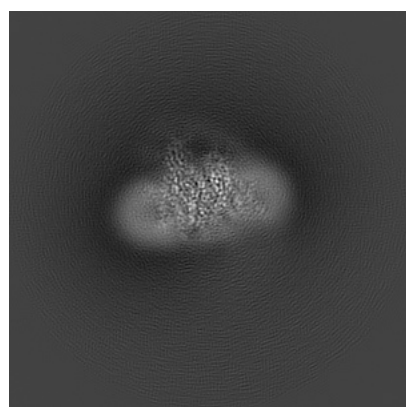
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0792. These allow visual inspection of the internal detail of the map and identification of artifacts.

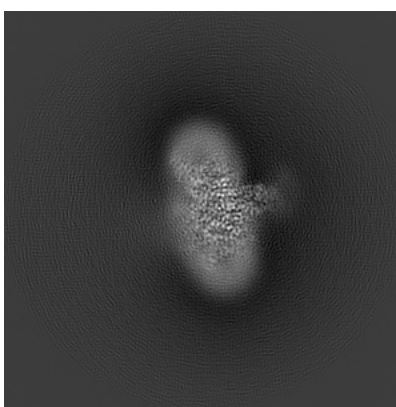
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

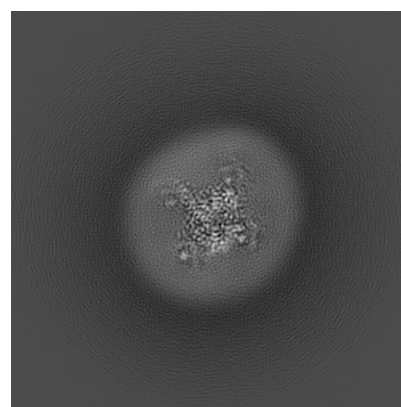
6.1.1 Primary map



X



Y

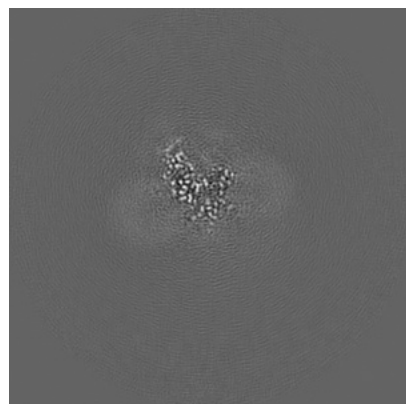


Z

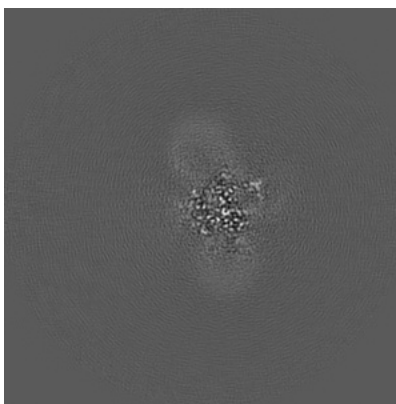
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

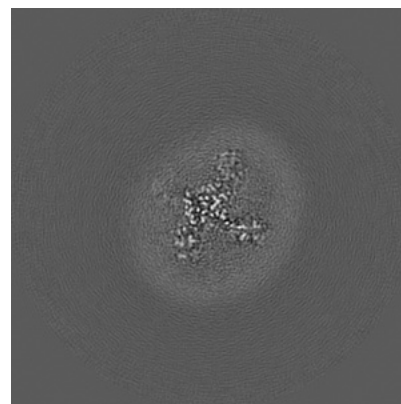
6.2.1 Primary map



X Index: 160



Y Index: 160

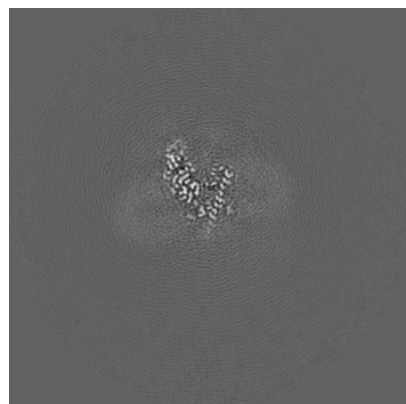


Z Index: 160

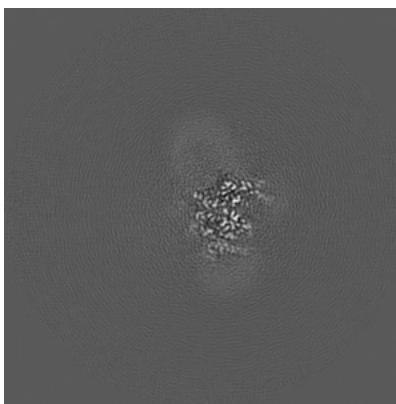
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

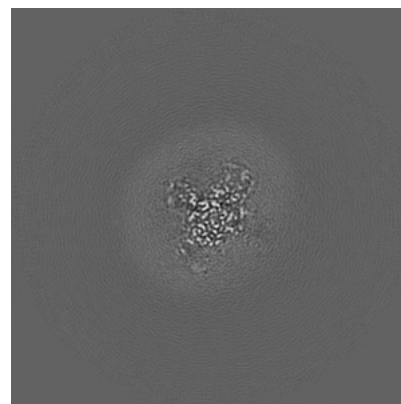
6.3.1 Primary map



X Index: 161



Y Index: 166

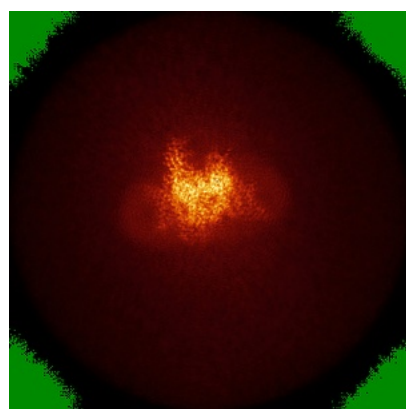


Z Index: 179

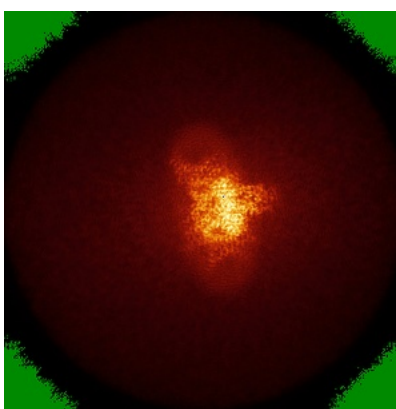
The images above show the largest variance slices of the map in three orthogonal directions.

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

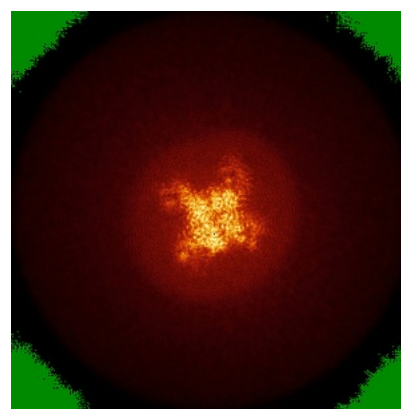
6.4.1 Primary map



X



Y

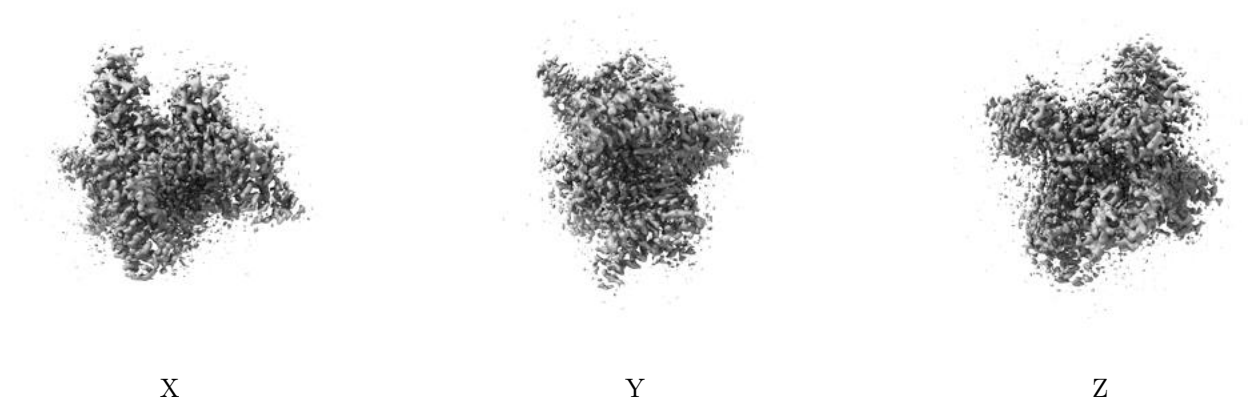


Z

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

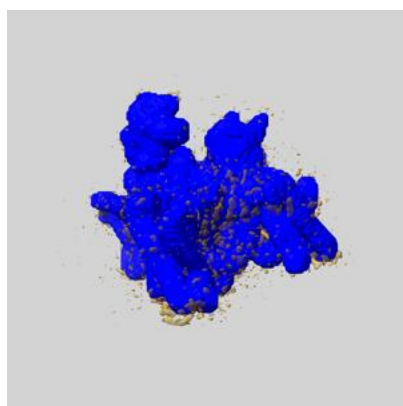
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

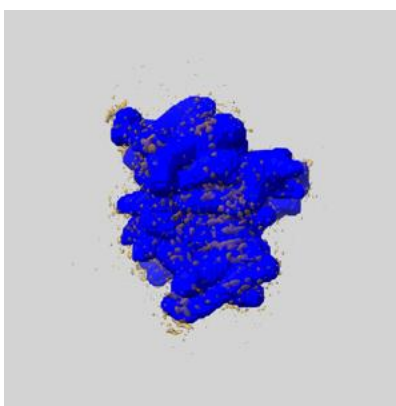
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

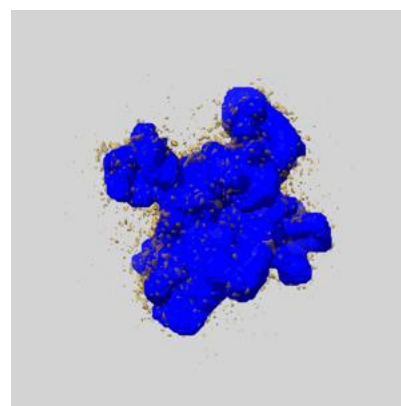
6.6.1 emd_0792_msk_1.map [i](#)



X



Y

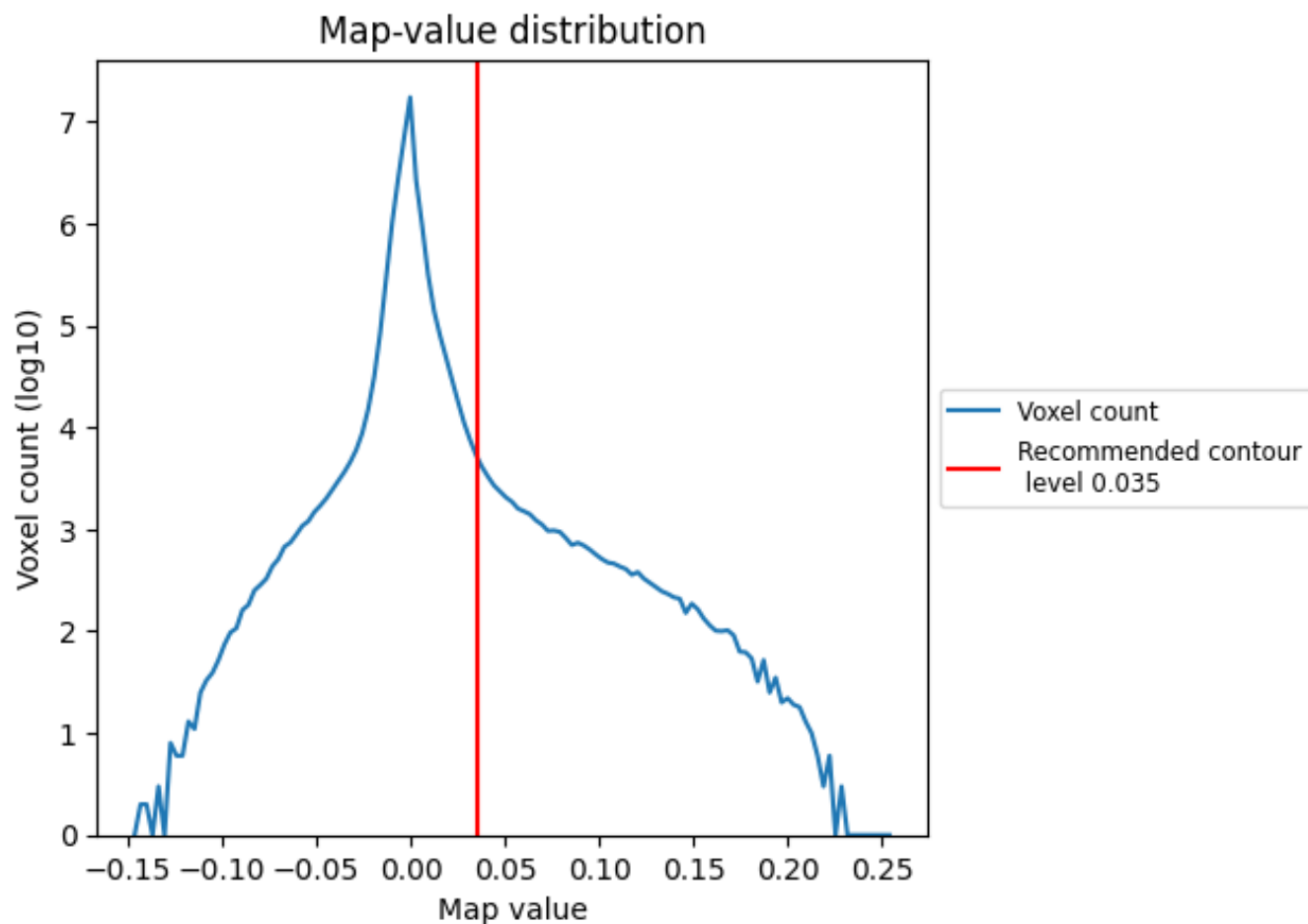


Z

7 Map analysis [i](#)

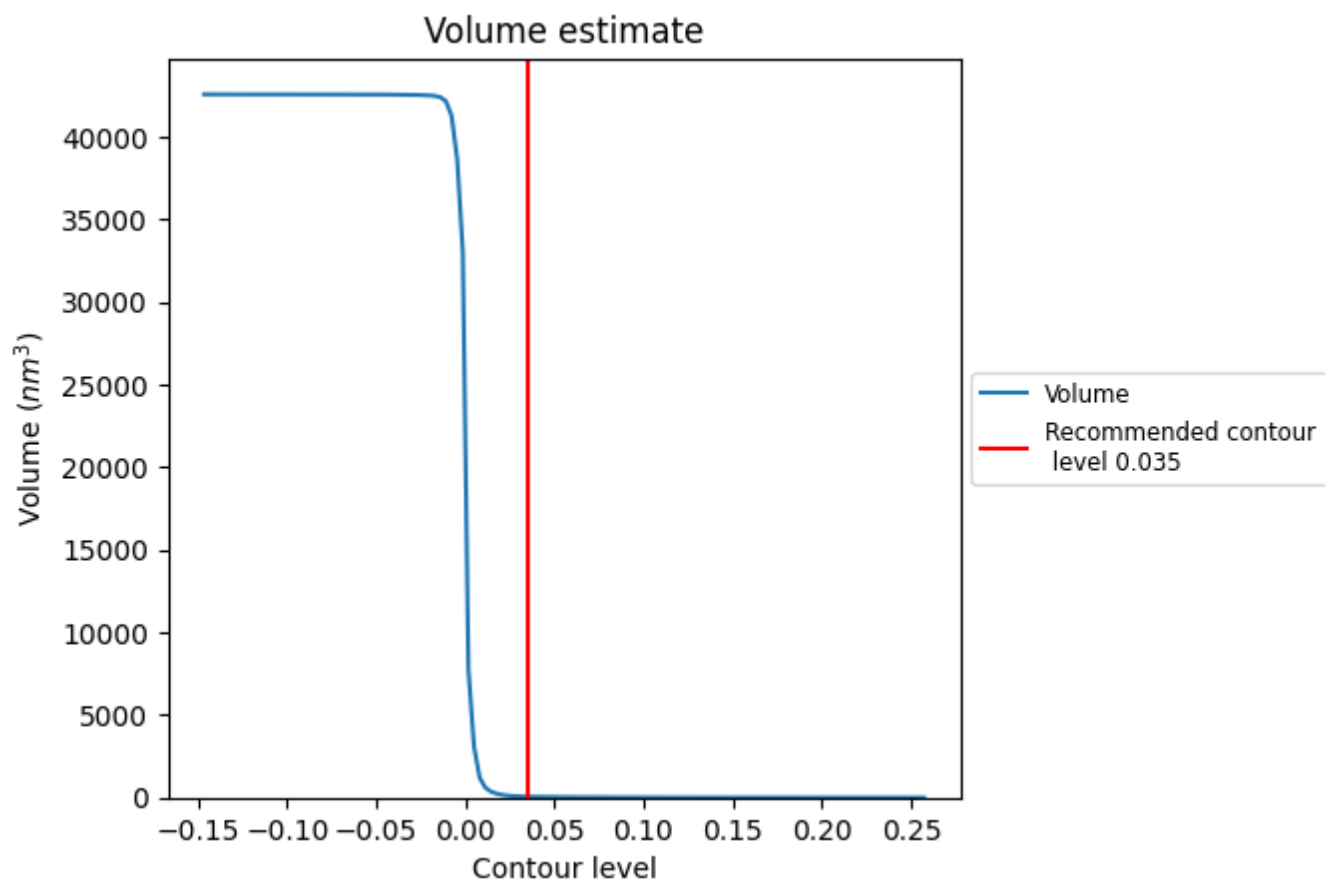
This section contains the results of statistical analysis of the map.

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.

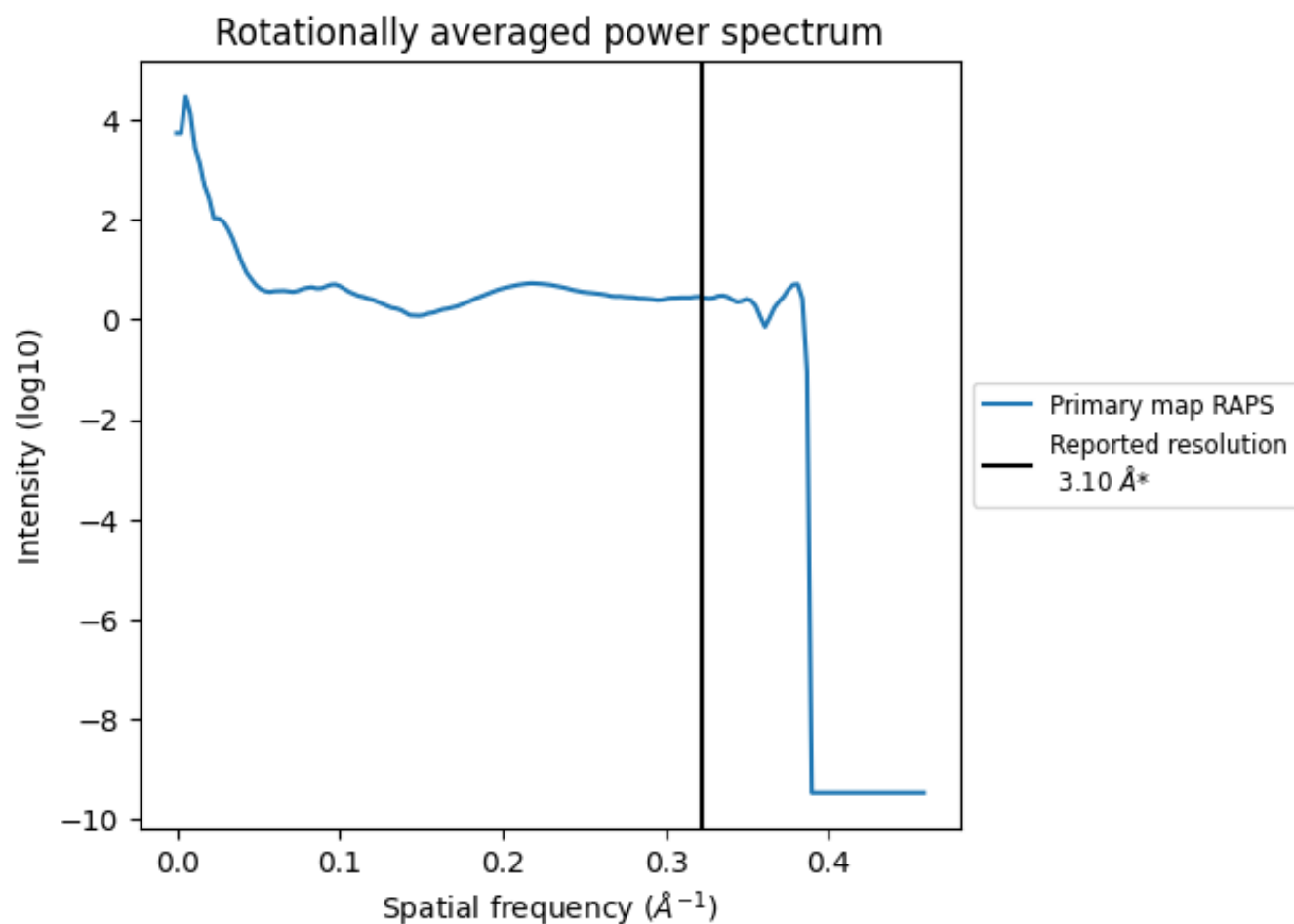
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm^3 ; this corresponds to an approximate mass of 49 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

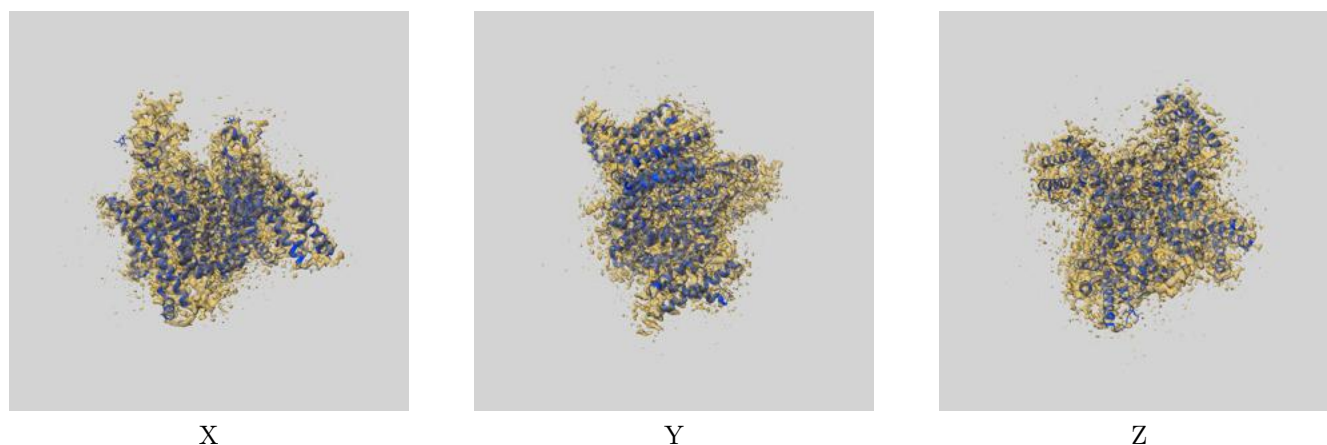
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

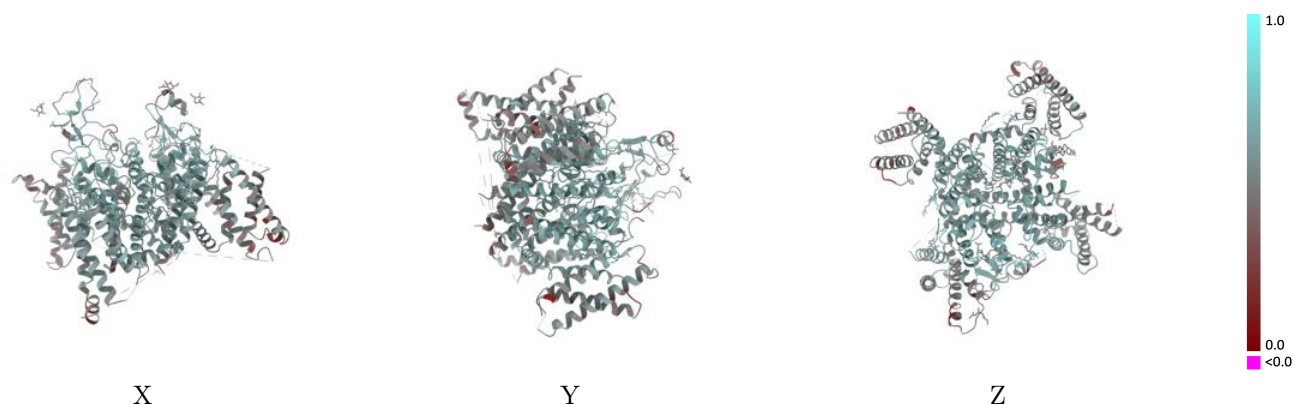
This section contains information regarding the fit between EMDB map EMD-0792 and PDB model 6KZP. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



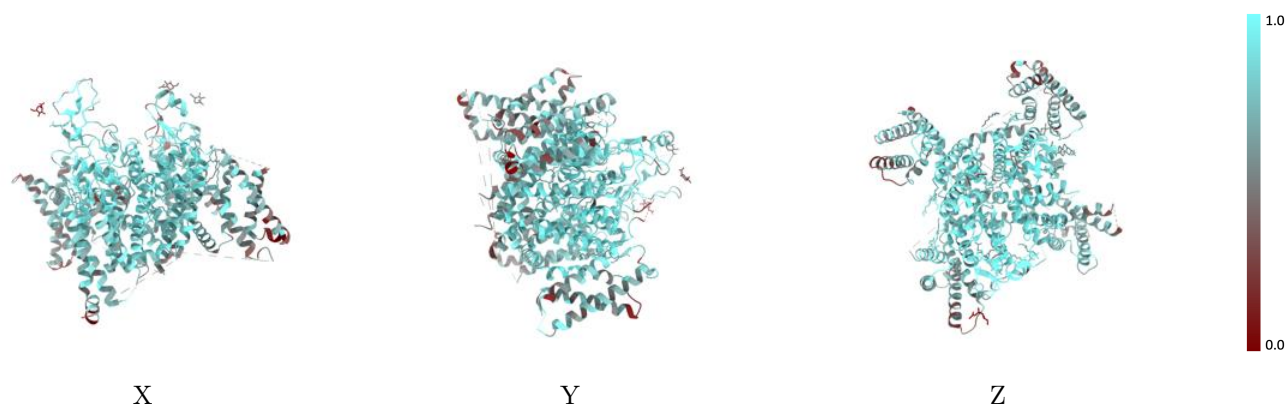
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



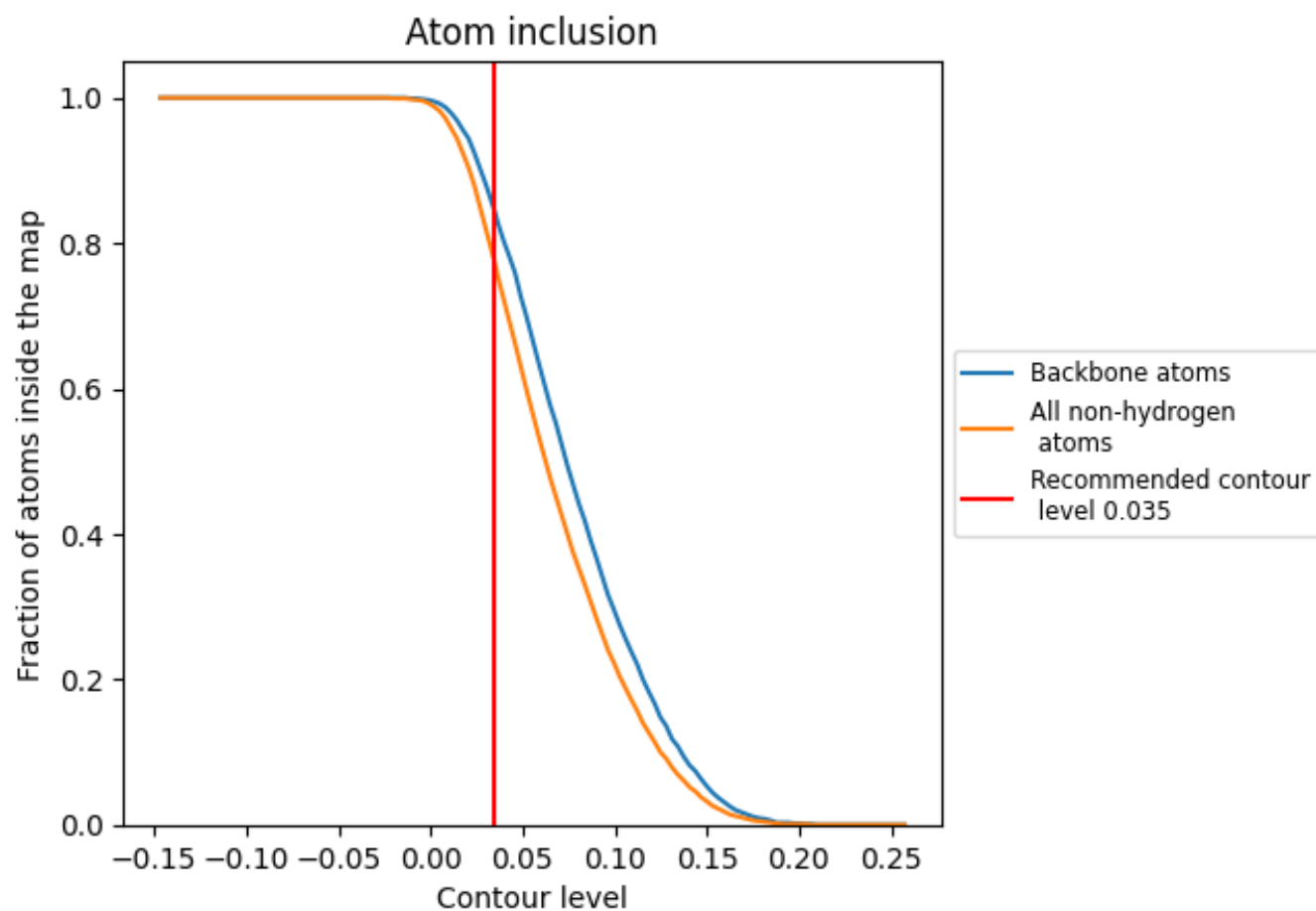
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5480
A	0.7720	0.5480

