



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 03:11 PM JST

PDB ID : 7WLI
EMDB ID : EMD-32584
Title : CryoEM structure of human low-voltage activated T-type calcium channel CaV3.3 (apo)
Authors : He, L.; Yu, Z.; Dong, Y.; Chen, Q.; Zhao, Y.
Deposited on : 2022-01-13
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

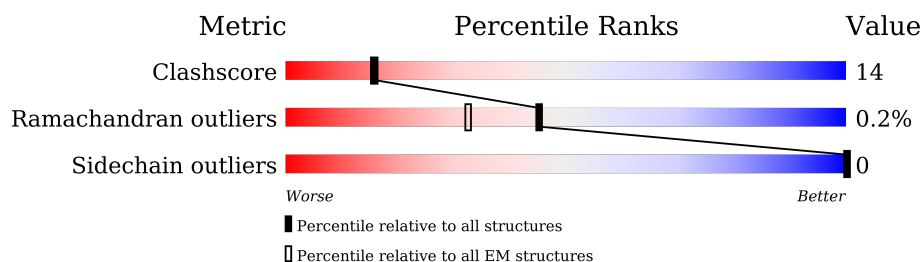
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2223	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9493 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.

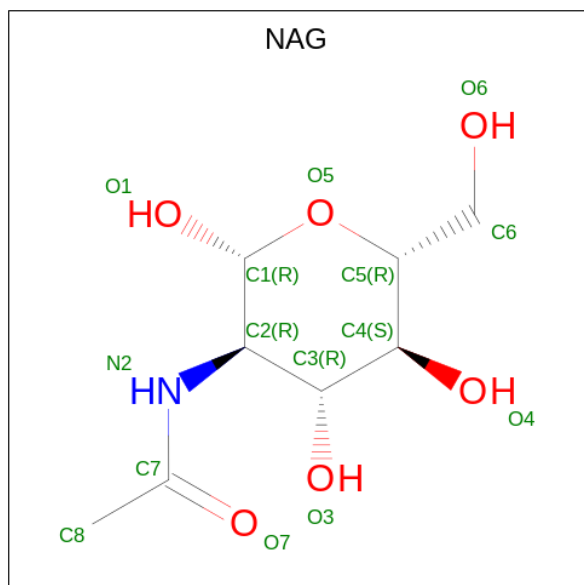
- Molecule 1 is a protein called Voltage-dependent T-type calcium channel subunit alpha-1I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1135	9111	5979	1499	1555	78	1	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

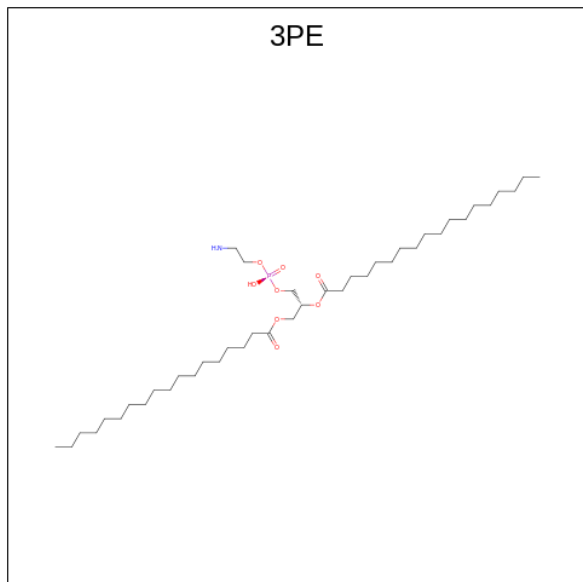
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



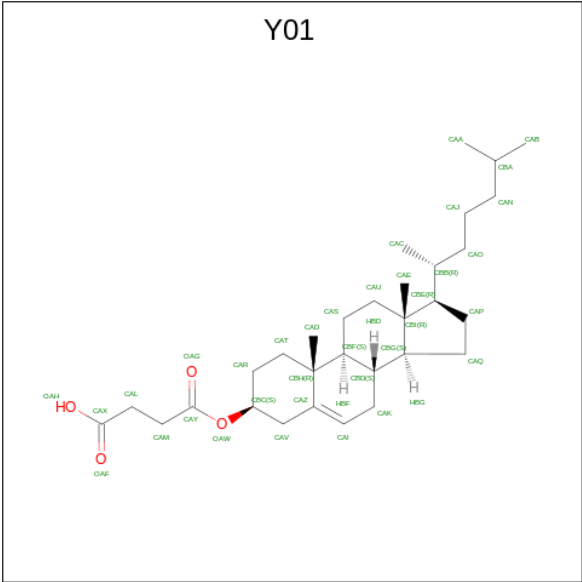
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			32	23	8	1	
4	A	1	Total	C			0
			11	11			
4	A	1	Total	C			0
			12	12			
4	A	1	Total	C			0
			12	12			
4	A	1	Total	C			0
			12	12			
4	A	1	Total	C			0
			13	13			
4	A	1	Total	C			0
			10	10			
4	A	1	Total	C			0
			13	13			
4	A	1	Total	C			0
			16	16			
4	A	1	Total	C			0
			10	10			
4	A	1	Total	C			0
			15	15			

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).

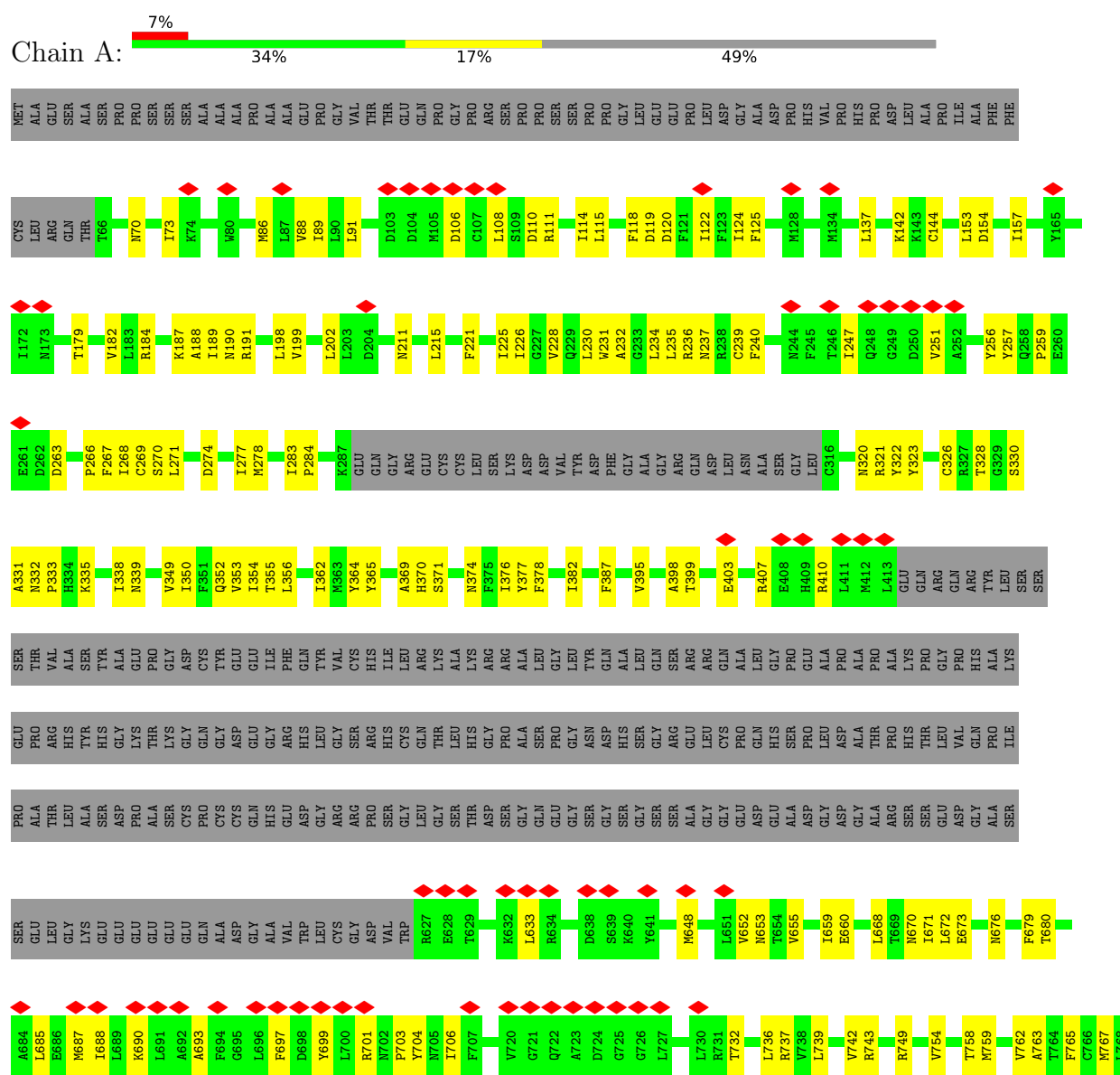


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			31	29	2	
5	A	1	Total	C	O	0
			31	29	2	
5	A	1	Total	C	O	0
			35	31	4	
5	A	1	Total	C	O	0
			35	31	4	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			35	31	4	

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 T-type calcium channel subunit alpha-1I





	MET	PHE	SER	SER	PRO
	GLY	CYS	LEU	LEU	LEU
	LEU	PRO	ARG	ASP	LEU
	PRO	PRO	LEU	ALA	PRO
	PRO	PRO	GLY	SER	MET
	LEU	PRO	ARG	PRO	PRO
	ALA	PRO	ALA	SER	ALA
	PRO	PRO	HIS	SER	GLU
	PRO	PRO	HIS	SER	PHE
	PRO	ALA	GLN	SER	GLY
	PRO	ALA	ARG	ALA	PHE
	PRO	PRO	ARG	SER	GLY
	GLN	LEU	SER	GLY	HIS
	PRO	THR	SER	LEU	PRO
	LEU	PRO	SER	LEU	ALA
	PRO	ALA	SER	GLN	VAL
	PRO	ALA	GLY	THR	SER
	GLY	ALA	GLY	THR	ALA
	LEU	LYS	SER	LEU	SER
	LEU	PHE	THR	GLU	GLN
	GLU	SER	ASP	ASP	LYS
	PRO	SER	PRO	SER	GLY
	GLY	THR	GLY	LEU	PRO
	ASP	ALA	SER	THR	GLU
	ALA	SER	CYS	THR	LYS
	ALA	SER	THR	LEU	GLY
	ALA	SEU	HIS	SER	GLY
	SEU	ALA	HIS	ASP	THR
	LYS	ALA	HIS	SER	GLY
	ARG	ALA	ASP	SER	THR
	LYS	PRO	SER	PRO	GLY
	ARG	GLY	MET	ARG	GLY
		ARG	ASP	ARG	THR
		PRO	PRO	ALA	LEU
		HIS	SER	LEU	PRO
		ALA	ASP	GLY	LYS
		ALA	GLU	PRO	TLE
		ALA	GLU	PRO	ALA
		LEU	GLY	ALA	LEU
		ALA	ARG	PRO	GLN
		HIS	GLY	ALA	GLY
		GLY	GLY	PRO	THR
		LEU	ALA	GLY	TRP
		ALA	GLY	PRO	ALA
		ARG	GLY	ARG	SER
		SER	GLY	ALA	LEU
		PRO	GLY	GLY	ARG
		SER	ALA	LEU	PRO
		TRP	GLY	SER	ARG
		ALA	SER	PRO	VAL
		ASP	GLU	ALA	ASN
		ARG	SER	ARG	CYS
		LYS	THR	ARG	THR
		SER	ASP	LEU	LEU
		PRO	SER	SER	ARG
		PRO	SER	LEU	GLN
		GLY	LEU	ARG	ALA
		ALA	LEU	GLY	THR
		ALA	THR	ARG	GLY
		PRO	THR	GLY	SER
		LEU	SER	LEU	THR
		PRO	LEU	THR	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93988	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 ($e^-/\text{\AA}^2$)	9.6	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	3.327	Depositor
Minimum map value	-2.203	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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, 3PE, NAG, Y01

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	0.33	3/9314 (0.0%)	0.48	1/12625 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1443	ALA	C-O	6.69	1.36	1.23
1	A	1459	LYS	C-O	5.31	1.33	1.23
1	A	1439	GLN	C-O	5.21	1.33	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1446	ALA	C-N-CA	-5.03	109.12	121.70

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	9111	0	9291	264	0
2	A	2	0	0	0	0
3	A	28	0	26	2	0
4	A	156	0	245	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	196	0	282	19	0
All	All	9493	0	9844	277	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 14.

All (277) 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:1460:LYS:O	1:A:1463:LYS:HG3	1.47	1.12
1:A:1441:GLN:OE1	1:A:1734:ASP:OD2	1.89	0.89
1:A:1376:LEU:HD23	1:A:1382:TRP:HB2	1.56	0.87
1:A:1441:GLN:HE21	1:A:1445:GLU:CB	1.93	0.81
1:A:1380:ASP:OD1	1:A:1681:ASN:ND2	2.14	0.79
1:A:1305:PRO:HG2	1:A:1432:GLU:HG3	1.64	0.79
1:A:1441:GLN:OE1	1:A:1734:ASP:CG	2.25	0.75
1:A:660:GLU:OE2	1:A:1326:GLN:NE2	2.20	0.74
1:A:1295:VAL:HG21	1:A:1621:ASN:HB3	1.70	0.74
1:A:1445:GLU:OE1	1:A:1448:ARG:NE	2.24	0.71
1:A:1480:ILE:HA	1:A:1484:CYS:HB2	1.73	0.70
1:A:1527:THR:HG22	1:A:1562:SER:HB3	1.73	0.70
1:A:1663:ASN:ND2	1:A:1666:MET:SD	2.64	0.70
1:A:1441:GLN:NE2	1:A:1445:GLU:CB	2.55	0.70
1:A:1545:ARG:HA	1:A:1548:LYS:HB2	1.72	0.69
1:A:1345:ASN:HA	1:A:1397:GLN:HA	1.75	0.69
1:A:1441:GLN:NE2	1:A:1445:GLU:HB2	2.07	0.69
1:A:371:SER:O	1:A:374:ASN:ND2	2.26	0.68
1:A:1451:GLU:HA	1:A:1454:LEU:HD12	1.75	0.68
1:A:352:GLN:NE2	1:A:828:TYR:OH	2.23	0.67
1:A:349:VAL:HG13	1:A:362:ILE:HD12	1.77	0.66
1:A:820:GLN:HG2	1:A:846:MET:HE3	1.76	0.66
1:A:1237:ARG:HG3	1:A:1237:ARG:O	1.96	0.66
1:A:1481:HIS:O	1:A:1485:THR:OG1	2.14	0.65
1:A:332:ASN:ND2	1:A:339:ASN:HD22	1.94	0.65
1:A:270:SER:OG	1:A:274:ASP:O	2.15	0.64
1:A:1389:GLY:HA3	1:A:1411:PHE:HE2	1.63	0.64
1:A:1445:GLU:HA	1:A:1448:ARG:HB2	1.78	0.64
1:A:231:TRP:HA	1:A:234:LEU:HD12	1.78	0.64
1:A:769:LEU:HD23	1:A:853:LEU:HD23	1.80	0.64
1:A:1335:CYS:H	1:A:1398:GLN:HE22	1.46	0.64
1:A:91:LEU:HD21	1:A:118:PHE:HD2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:HB3	1:A:328:THR:HG22	1.80	0.63
1:A:1268:LEU:HA	1:A:1271:LEU:HD12	1.81	0.63
1:A:1726:VAL:O	1:A:1730:MET:HG2	1.98	0.63
1:A:1474:CYS:H	1:A:1478:LEU:HB3	1.63	0.63
1:A:1441:GLN:O	1:A:1442:GLU:C	2.37	0.62
5:A:2313:Y01:HAR1	5:A:2315:Y01:HAT2	1.79	0.62
1:A:1530:PHE:HB3	1:A:1559:VAL:HG12	1.80	0.62
1:A:236:ARG:HG2	1:A:332:ASN:HB3	1.81	0.62
1:A:1676:THR:HG22	4:A:2316:3PE:H371	1.79	0.62
1:A:1613:VAL:HA	1:A:1616:LEU:HD23	1.82	0.62
1:A:353:VAL:HG13	1:A:362:ILE:HD11	1.81	0.62
1:A:653:ASN:HD21	1:A:737:ARG:HD2	1.64	0.62
1:A:1524:TYR:OH	1:A:1569:GLU:OE1	2.15	0.61
1:A:1169:HIS:HE1	1:A:1221:LEU:HD21	1.64	0.61
1:A:1371:MET:HB2	5:A:2311:Y01:HAQ2	1.83	0.61
1:A:1614:GLN:NE2	1:A:1735:ASP:OD2	2.33	0.61
1:A:215:LEU:HD21	1:A:1609:LEU:HD11	1.82	0.60
1:A:1669:LEU:HD12	5:A:2313:Y01:HAQ2	1.83	0.60
1:A:198:LEU:HD21	1:A:765:PHE:HD1	1.66	0.60
1:A:1247:LEU:HD22	1:A:1281:ARG:HA	1.84	0.60
1:A:1609:LEU:O	1:A:1613:VAL:HG23	2.02	0.59
1:A:1223:VAL:O	1:A:1227:GLY:N	2.36	0.59
1:A:1456:ARG:HA	1:A:1459:LYS:HD2	1.85	0.59
1:A:687:MET:SD	1:A:699:TYR:OH	2.59	0.58
1:A:1391:ASP:HB3	1:A:1399:PRO:HB2	1.84	0.58
1:A:237:ASN:HD22	1:A:271:LEU:HG	1.68	0.58
1:A:652:VAL:HG23	1:A:679:PHE:CZ	2.39	0.58
1:A:1349:CYS:O	1:A:1353:ASN:N	2.37	0.58
1:A:1359:HIS:O	1:A:1362:ASN:ND2	2.37	0.58
1:A:259:PRO:HD3	1:A:267:PHE:HB2	1.86	0.58
1:A:843:VAL:HG21	4:A:2321:3PE:H3D2	1.85	0.58
1:A:802:LYS:HD3	1:A:816:GLN:HE22	1.69	0.57
1:A:1546:PHE:HZ	1:A:1556:LEU:HD22	1.68	0.57
1:A:1389:GLY:HA3	1:A:1411:PHE:CE2	2.39	0.57
1:A:1190:GLU:HG3	1:A:1204:LEU:HD13	1.86	0.57
1:A:86:MET:SD	1:A:191:ARG:HB2	2.45	0.57
1:A:398:ALA:HA	1:A:859:ALA:HB2	1.85	0.57
1:A:1331:LYS:HB3	1:A:1392:ALA:HB1	1.87	0.57
1:A:1434:PHE:HD1	1:A:1730:MET:HE1	1.70	0.57
1:A:89:ILE:HG21	1:A:188:ALA:HB2	1.86	0.57
1:A:332:ASN:HD21	1:A:339:ASN:HD22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:O	1:A:354:ILE:HG12	2.05	0.56
1:A:356:LEU:HD22	1:A:1676:THR:HB	1.88	0.56
1:A:1367:GLY:HA3	5:A:2311:Y01:HBF	1.87	0.56
1:A:1626:PHE:CE2	1:A:1630:PHE:HE2	2.23	0.56
1:A:685:LEU:HD23	1:A:688:ILE:HD11	1.88	0.56
1:A:330:SER:OG	1:A:331:ALA:N	2.39	0.56
1:A:332:ASN:HB2	1:A:333:PRO:HD2	1.88	0.56
1:A:1254:ASP:HA	1:A:1274:LEU:HD13	1.88	0.56
1:A:1496:ILE:HD13	1:A:1529:VAL:HG11	1.88	0.56
1:A:1240:TRP:HB3	1:A:1287:SER:HB3	1.87	0.56
1:A:1610:ASP:O	1:A:1613:VAL:N	2.38	0.55
3:A:2303:NAG:H3	3:A:2303:NAG:H83	1.89	0.55
1:A:1286:ILE:HD13	1:A:1296:VAL:HG21	1.88	0.55
1:A:271:LEU:HB2	1:A:274:ASP:HB2	1.88	0.55
1:A:1279:THR:O	1:A:1282:PRO:HD2	2.07	0.55
1:A:119:ASP:HA	1:A:122:ILE:HD12	1.88	0.54
1:A:1584:ILE:HG22	1:A:1588:ARG:HH11	1.72	0.54
1:A:1634:ALA:O	1:A:1638:VAL:HG23	2.08	0.53
1:A:234:LEU:HD13	1:A:370:HIS:HB2	1.90	0.53
1:A:1430:VAL:HG22	1:A:1726:VAL:HG22	1.90	0.53
1:A:838:ALA:HA	5:A:2312:Y01:HAK1	1.91	0.53
1:A:1563:VAL:HA	1:A:1566:ILE:HG12	1.90	0.53
1:A:1187:ILE:HD11	1:A:1281:ARG:HE	1.73	0.53
1:A:1250:VAL:HG11	1:A:1277:LEU:HB2	1.91	0.53
1:A:1441:GLN:NE2	1:A:1445:GLU:HG2	2.23	0.53
1:A:763:ALA:O	1:A:767:MET:HG2	2.09	0.52
1:A:1279:THR:HG21	1:A:1636:LEU:HA	1.91	0.52
1:A:1273:VAL:O	1:A:1277:LEU:HG	2.08	0.52
1:A:284:PRO:O	1:A:320:ASN:ND2	2.42	0.52
1:A:1344:THR:O	1:A:1398:GLN:N	2.28	0.52
1:A:1419:SER:O	1:A:1423:LEU:HG	2.09	0.52
1:A:1441:GLN:HE21	1:A:1445:GLU:CG	2.23	0.52
1:A:652:VAL:HG23	1:A:679:PHE:HZ	1.75	0.52
1:A:189:ILE:HD13	1:A:199:VAL:HG21	1.92	0.52
1:A:1192:PRO:HG3	1:A:1642:GLY:HA3	1.91	0.52
1:A:226:ILE:HD13	5:A:2309:Y01:HAC2	1.92	0.52
1:A:754:VAL:O	1:A:758:THR:HG23	2.10	0.52
1:A:1345:ASN:OD1	1:A:1347:SER:OG	2.23	0.52
1:A:1441:GLN:OE1	1:A:1734:ASP:OD1	2.27	0.52
1:A:157:ILE:HG21	1:A:184:ARG:HG2	1.92	0.52
1:A:89:ILE:HD11	1:A:187:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ARG:NH2	3:A:2304:NAG:O7	2.44	0.51
1:A:153:LEU:O	1:A:157:ILE:HD12	2.10	0.51
1:A:1731:LYS:HA	1:A:1731:LYS:HE2	1.92	0.51
1:A:653:ASN:ND2	1:A:737:ARG:HD2	2.24	0.50
1:A:1641:PHE:HB3	1:A:1644:LEU:HD12	1.94	0.50
1:A:633:LEU:HD23	1:A:693:ALA:HB2	1.94	0.50
1:A:668:LEU:HA	1:A:671:ILE:HD12	1.94	0.50
1:A:1462:ARG:O	1:A:1465:GLN:NE2	2.39	0.50
1:A:820:GLN:HG2	1:A:846:MET:CE	2.42	0.50
1:A:182:VAL:HG21	1:A:779:LEU:HB2	1.94	0.50
1:A:1328:PHE:HB2	1:A:1363:PHE:HB2	1.94	0.50
1:A:809:TRP:HA	1:A:812:VAL:HG12	1.94	0.50
1:A:1207:SER:HA	1:A:1210:ILE:HG12	1.94	0.50
1:A:690:LYS:HE2	1:A:699:TYR:HE1	1.76	0.49
1:A:1667:ALA:HA	1:A:1670:THR:HG22	1.95	0.49
1:A:739:LEU:O	1:A:742:VAL:HG12	2.12	0.49
1:A:1288:ARG:HD2	1:A:1288:ARG:N	2.27	0.49
1:A:266:PRO:HG3	1:A:333:PRO:HB3	1.94	0.49
1:A:332:ASN:HB2	1:A:333:PRO:CD	2.43	0.49
1:A:1346:ARG:HG3	1:A:1356:TRP:CD2	2.48	0.49
1:A:88:VAL:HG11	1:A:125:PHE:CD2	2.48	0.49
1:A:1441:GLN:NE2	1:A:1445:GLU:CG	2.75	0.48
1:A:765:PHE:HE1	1:A:856:LEU:HD23	1.78	0.48
1:A:861:LEU:HB2	1:A:1427:VAL:HG21	1.94	0.48
1:A:765:PHE:CE2	1:A:857:LEU:HB2	2.47	0.48
1:A:1451:GLU:HG2	1:A:1454:LEU:HD12	1.96	0.48
1:A:221:PHE:CZ	1:A:1501:VAL:HG13	2.48	0.48
1:A:1441:GLN:HE21	1:A:1445:GLU:HG2	1.79	0.48
1:A:1237:ARG:O	1:A:1237:ARG:CG	2.62	0.48
1:A:1445:GLU:HB2	1:A:1448:ARG:HH21	1.78	0.48
1:A:1493:ILE:HD11	1:A:1533:GLU:HG2	1.96	0.48
1:A:1735:ASP:HA	1:A:1738:LYS:HG2	1.95	0.48
1:A:774:PHE:HE1	1:A:807:LEU:HD11	1.78	0.47
1:A:1216:VAL:HG11	1:A:1252:ILE:HD11	1.95	0.47
1:A:1323:LEU:HD21	4:A:2308:3PE:H3B2	1.96	0.47
1:A:137:LEU:O	1:A:144:CYS:HA	2.13	0.47
1:A:179:THR:HG22	1:A:179:THR:O	2.15	0.47
1:A:1321:GLY:O	1:A:1325:VAL:HG23	2.15	0.47
1:A:277:ILE:HG13	1:A:278:MET:H	1.80	0.47
1:A:1281:ARG:O	1:A:1283:LEU:N	2.47	0.47
1:A:668:LEU:O	1:A:672:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:VAL:O	1:A:1252:ILE:HG12	2.15	0.47
1:A:1441:GLN:HE21	1:A:1445:GLU:HB3	1.74	0.47
1:A:1391:ASP:OD1	1:A:1401:THR:HA	2.14	0.47
1:A:1421:PHE:O	1:A:1425:MET:HG3	2.15	0.47
1:A:1500:ASN:O	1:A:1504:MET:HE2	2.15	0.47
1:A:1707:PRO:HB2	5:A:2311:Y01:HAQ1	1.96	0.47
1:A:154:ASP:OD2	1:A:191:ARG:NH2	2.49	0.46
1:A:268:ILE:HD12	1:A:268:ILE:H	1.80	0.46
1:A:1331:LYS:NZ	1:A:1394:ALA:HA	2.30	0.46
1:A:1497:ILE:HD11	1:A:1597:LYS:HE2	1.97	0.46
1:A:1469:TYR:HB3	1:A:1481:HIS:CE1	2.50	0.46
1:A:1520:LYS:HD2	1:A:1569:GLU:HG3	1.97	0.46
1:A:648:MET:O	1:A:652:VAL:HG22	2.16	0.46
1:A:809:TRP:HE3	1:A:812:VAL:HG11	1.81	0.46
1:A:111:ARG:O	1:A:115:LEU:HD23	2.16	0.46
1:A:321:ARG:HG3	1:A:322:TYR:CD1	2.51	0.46
1:A:1238:SER:OG	1:A:1241:ASN:OD1	2.22	0.46
5:A:2311:Y01:HAA1	5:A:2311:Y01:HAJ2	1.67	0.46
1:A:378:PHE:O	1:A:382:ILE:HG12	2.15	0.46
1:A:1715:LEU:HB3	4:A:2305:3PE:H282	1.97	0.46
1:A:110:ASP:O	1:A:114:ILE:HD12	2.16	0.45
1:A:777:SER:O	1:A:781:MET:HG3	2.16	0.45
1:A:235:LEU:HD11	1:A:365:TYR:HB3	1.98	0.45
1:A:1650:ASN:HB3	1:A:1689:ARG:HH12	1.81	0.45
1:A:1268:LEU:O	1:A:1272:ARG:HG3	2.17	0.45
1:A:1434:PHE:CD1	1:A:1730:MET:HE1	2.51	0.45
5:A:2310:Y01:HAP1	5:A:2310:Y01:HAO1	1.49	0.45
1:A:338:ILE:HD12	1:A:349:VAL:HG22	1.98	0.45
1:A:1275:ARG:HG2	1:A:1639:GLU:CD	2.37	0.45
1:A:1420:PHE:HB2	4:A:2317:3PE:H252	1.99	0.45
1:A:818:LEU:HD23	1:A:818:LEU:HA	1.85	0.45
1:A:1386:MET:O	1:A:1390:LEU:HG	2.16	0.45
1:A:228:VAL:O	1:A:232:ALA:HB2	2.17	0.45
1:A:670:ASN:HA	1:A:673:GLU:HG2	1.99	0.45
1:A:1546:PHE:CZ	1:A:1556:LEU:HD22	2.50	0.45
5:A:2312:Y01:HAP1	5:A:2312:Y01:HAO2	1.37	0.45
1:A:257:TYR:HB2	1:A:323:TYR:CD2	2.53	0.44
1:A:736:LEU:HA	1:A:739:LEU:HD12	1.99	0.44
1:A:1556:LEU:HA	1:A:1559:VAL:HG22	1.98	0.44
1:A:106:ASP:HB3	1:A:108:LEU:HD23	1.99	0.44
1:A:1633:TYR:HD1	1:A:1709:TYR:CE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:ILE:O	1:A:1257:VAL:HG23	2.17	0.44
1:A:1335:CYS:H	1:A:1398:GLN:NE2	2.13	0.44
1:A:399:THR:O	1:A:403:GLU:OE2	2.35	0.44
1:A:1413:SER:O	1:A:1417:ILE:HG13	2.17	0.44
1:A:1530:PHE:O	1:A:1533:GLU:HG3	2.18	0.44
1:A:335:LYS:HE2	1:A:335:LYS:HB2	1.78	0.44
1:A:226:ILE:O	1:A:230:LEU:HG	2.17	0.43
1:A:1355:ARG:HD2	1:A:1357:VAL:HG22	2.00	0.43
1:A:1591:ARG:O	1:A:1594:ARG:HG3	2.18	0.43
1:A:1308:ASN:O	1:A:1312:ILE:HG13	2.18	0.43
5:A:2313:Y01:HAC3	5:A:2313:Y01:HAJ1	1.71	0.43
1:A:321:ARG:HG3	1:A:322:TYR:HD1	1.83	0.43
1:A:1588:ARG:HG2	1:A:1591:ARG:HH22	1.83	0.43
1:A:703:PRO:HA	1:A:706:ILE:HG13	1.99	0.43
1:A:704:TYR:CD2	1:A:743:ARG:HG2	2.53	0.43
5:A:2311:Y01:HAD1	5:A:2311:Y01:HAR2	1.86	0.43
1:A:211:ASN:OD1	1:A:1604:GLY:HA3	2.18	0.43
1:A:655:VAL:O	1:A:659:ILE:HG13	2.18	0.43
1:A:356:LEU:HD21	1:A:382:ILE:HG23	2.01	0.43
1:A:407:ARG:HG3	1:A:410:ARG:NH2	2.34	0.43
1:A:1717:ALA:O	1:A:1721:LEU:HG	2.19	0.43
1:A:202:LEU:HD13	1:A:856:LEU:HD22	2.01	0.43
1:A:387:PHE:CD2	4:A:2316:3PE:H332	2.54	0.43
1:A:1426:PHE:O	1:A:1430:VAL:HG23	2.19	0.43
1:A:240:PHE:HA	1:A:256:TYR:HA	2.01	0.42
1:A:256:TYR:OH	1:A:263:ASP:OD2	2.31	0.42
1:A:1192:PRO:HD2	1:A:1662:GLU:O	2.19	0.42
1:A:120:ASP:O	1:A:124:ILE:HG13	2.19	0.42
1:A:697:PHE:O	1:A:701:ARG:N	2.52	0.42
1:A:190:ASN:HB3	1:A:191:ARG:HH11	1.83	0.42
1:A:190:ASN:HB3	1:A:191:ARG:NH1	2.35	0.42
1:A:355:THR:HG1	1:A:823:TRP:HE1	1.68	0.42
1:A:1361:TYR:CE2	1:A:1375:VAL:HG11	2.53	0.42
1:A:376:ILE:HD12	1:A:376:ILE:H	1.85	0.42
5:A:2313:Y01:HAQ1	5:A:2313:Y01:HAE3	1.90	0.42
1:A:364:TYR:CD1	1:A:1657:ARG:HD2	2.53	0.42
1:A:1215:PHE:O	1:A:1218:GLU:HG3	2.20	0.42
1:A:70:ASN:HA	1:A:73:ILE:HG12	2.01	0.42
1:A:247:ILE:HG21	1:A:251:VAL:HG22	2.02	0.42
1:A:1374:PHE:HD2	5:A:2311:Y01:HAB1	1.84	0.42
1:A:1499:LEU:HA	1:A:1502:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD12	1:A:333:PRO:HG3	2.02	0.41
1:A:1626:PHE:HB2	1:A:1720:VAL:HG11	2.01	0.41
1:A:237:ASN:OD1	1:A:268:ILE:HG23	2.20	0.41
1:A:676:ASN:O	1:A:680:THR:HG23	2.20	0.41
1:A:732:THR:HG21	4:A:2314:3PE:H372	2.01	0.41
1:A:1720:VAL:O	1:A:1724:VAL:HG23	2.20	0.41
1:A:790:LEU:HD23	1:A:791:ARG:O	2.20	0.41
1:A:395:VAL:HG22	1:A:1729:LEU:HD13	2.02	0.41
1:A:1374:PHE:CD2	5:A:2311:Y01:HAB1	2.55	0.41
1:A:1434:PHE:HA	1:A:1730:MET:CE	2.51	0.41
1:A:231:TRP:HH2	1:A:377:TYR:CD2	2.39	0.41
1:A:1393:VAL:HG13	1:A:1394:ALA:N	2.35	0.41
5:A:2312:Y01:HAC2	5:A:2312:Y01:HAJ1	1.79	0.41
1:A:1292:LEU:HD11	1:A:1624:LEU:HG	2.01	0.41
1:A:1340:THR:O	1:A:1340:THR:HG22	2.20	0.41
1:A:1568:LEU:HD12	1:A:1579:ILE:HG21	2.01	0.41
1:A:225:ILE:HD12	1:A:1504:MET:HB3	2.02	0.41
1:A:142:LYS:HA	1:A:142:LYS:HD3	1.69	0.41
1:A:267:PHE:CE2	1:A:283:ILE:HG22	2.55	0.41
1:A:816:GLN:NE2	1:A:821:GLU:O	2.49	0.41
1:A:1479:LEU:HD22	1:A:1483:MET:SD	2.61	0.41
5:A:2311:Y01:HAO2	5:A:2311:Y01:HAP1	1.55	0.41
1:A:1186:THR:HA	1:A:1189:LEU:HD12	2.03	0.41
1:A:1492:PHE:CZ	1:A:1496:ILE:HD11	2.55	0.41
1:A:759:MET:HA	1:A:762:VAL:HB	2.03	0.41
1:A:742:VAL:O	1:A:749:ARG:NH1	2.54	0.40
4:A:2308:3PE:H3A1	4:A:2308:3PE:H372	1.95	0.40
1:A:239:CYS:HA	1:A:326:CYS:CB	2.52	0.40
1:A:842:PHE:O	1:A:846:MET:HG3	2.21	0.40
1:A:1373:LEU:HD23	1:A:1376:LEU:HD12	2.04	0.40
5:A:2312:Y01:HAE2	5:A:2312:Y01:HBB	1.65	0.40
5:A:2315:Y01:HBB	5:A:2315:Y01:HAE2	1.65	0.40
1:A:226:ILE:HG12	1:A:1589:VAL:HG22	2.03	0.40
1:A:234:LEU:HB3	1:A:369:ALA:HB1	2.03	0.40
1:A:834:THR:OG1	1:A:835:SER:N	2.55	0.40
1:A:1361:TYR:CE2	1:A:1375:VAL:HG21	2.56	0.40
1:A:269:CYS:HA	1:A:278:MET:HE2	2.04	0.40
1:A:283:ILE:HD12	1:A:320:ASN:HB3	2.03	0.40
1:A:1688:LEU:HD12	1:A:1688:LEU:O	2.22	0.40
1:A:1706:SER:HB3	1:A:1707:PRO:HD3	2.03	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	1128/2223 (51%)	1044 (93%)	82 (7%)	2 (0%)	44 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1442	GLU
1	A	1441	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1006/1879 (54%)	1006 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	339	ASN
1	A	653	ASN
1	A	1441	GLN
1	A	1552	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z > 2$
4	3PE	A	2318	-	12,12,50	1.52	0	11,11,55	0.88	0
3	NAG	A	2304	1	14,14,15	0.21	0	17,19,21	0.54	0
4	3PE	A	2321	-	14,14,50	1.53	0	13,13,55	0.85	0
4	3PE	A	2317	-	9,9,50	1.49	0	8,8,55	0.79	0
4	3PE	A	2307	-	11,11,50	1.52	0	10,10,55	0.88	0
4	3PE	A	2308	-	11,11,50	1.51	0	10,10,55	0.88	0
5	Y01	A	2310	-	34,34,38	0.65	1 (2%)	52,52,57	1.68	9 (17%)
4	3PE	A	2314	-	11,11,50	1.53	0	10,10,55	0.84	0
5	Y01	A	2312	-	38,38,38	0.62	0	57,57,57	1.77	12 (21%)
5	Y01	A	2315	-	38,38,38	0.67	0	57,57,57	1.62	11 (19%)
4	3PE	A	2306	-	10,10,50	1.51	0	9,9,55	0.86	0
4	3PE	A	2320	-	9,9,50	1.50	0	8,8,55	0.80	0
5	Y01	A	2309	-	34,34,38	0.63	0	52,52,57	1.60	8 (15%)
4	3PE	A	2305	-	31,31,50	2.41	11 (35%)	35,36,55	1.21	2 (5%)
3	NAG	A	2303	1	14,14,15	0.38	0	17,19,21	1.24	1 (5%)
4	3PE	A	2319	-	15,15,50	1.54	0	14,14,55	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	Y01	A	2311	-	38,38,38	0.72	1 (2%)	57,57,57	1.60	9 (15%)
5	Y01	A	2313	-	32,32,38	0.79	2 (6%)	49,49,57	1.51	13 (26%)
4	3PE	A	2316	-	12,12,50	1.53	0	11,11,55	0.83	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	3PE	A	2318	-	-	1/10/10/54	-
3	NAG	A	2304	1	-	3/6/23/26	0/1/1/1
4	3PE	A	2321	-	-	5/12/12/54	-
4	3PE	A	2317	-	-	2/7/7/54	-
4	3PE	A	2307	-	-	2/9/9/54	-
4	3PE	A	2308	-	-	0/9/9/54	-
5	Y01	A	2310	-	-	12/14/72/77	0/4/4/4
4	3PE	A	2314	-	-	3/9/9/54	-
5	Y01	A	2312	-	-	11/19/77/77	0/4/4/4
5	Y01	A	2315	-	-	5/19/77/77	0/4/4/4
4	3PE	A	2306	-	-	1/8/8/54	-
4	3PE	A	2320	-	-	4/7/7/54	-
5	Y01	A	2309	-	-	5/14/72/77	0/4/4/4
4	3PE	A	2305	-	-	12/33/33/54	-
3	NAG	A	2303	1	-	5/6/23/26	0/1/1/1
4	3PE	A	2319	-	-	5/13/13/54	-
5	Y01	A	2311	-	-	11/19/77/77	0/4/4/4
5	Y01	A	2313	-	-	6/12/70/77	0/4/4/4
4	3PE	A	2316	-	-	1/10/10/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2305	3PE	P-O13	4.85	1.73	1.54
4	A	2305	3PE	O31-C31	4.68	1.47	1.33
4	A	2305	3PE	O21-C21	4.60	1.47	1.34
4	A	2305	3PE	P-O11	4.10	1.73	1.60
4	A	2305	3PE	C22-C21	3.40	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2305	3PE	C32-C31	3.33	1.60	1.50
4	A	2305	3PE	C3-C2	3.24	1.60	1.50
4	A	2305	3PE	C1-C2	3.24	1.60	1.50
4	A	2305	3PE	P-O14	2.59	1.58	1.50
5	A	2311	Y01	CBH-CBF	-2.38	1.52	1.56
4	A	2305	3PE	C33-C32	2.30	1.60	1.52
4	A	2305	3PE	C23-C22	2.30	1.60	1.52
5	A	2313	Y01	CBH-CBF	-2.19	1.52	1.56
5	A	2313	Y01	OAW-CAY	-2.15	1.34	1.42
5	A	2310	Y01	CBH-CBF	-2.04	1.52	1.56

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2315	Y01	CBI-CBE-CBB	-5.50	110.87	119.49
5	A	2310	Y01	OAW-CAY-CAM	4.96	120.21	111.09
5	A	2309	Y01	OAW-CAY-CAM	4.71	119.75	111.09
5	A	2312	Y01	CBI-CBE-CBB	-4.55	112.36	119.49
3	A	2303	NAG	C2-N2-C7	4.29	129.00	122.90
5	A	2310	Y01	CBI-CBE-CBB	-4.22	112.87	119.49
5	A	2312	Y01	OAW-CAY-CAM	4.18	120.50	111.50
5	A	2312	Y01	CBD-CAK-CAI	-4.10	106.84	112.73
5	A	2309	Y01	CBI-CBG-CBD	-4.01	108.44	114.38
5	A	2311	Y01	OAW-CAY-CAM	3.98	120.08	111.50
4	A	2305	3PE	O21-C21-C22	3.97	120.06	111.50
5	A	2311	Y01	CBI-CBE-CBB	-3.87	113.43	119.49
5	A	2312	Y01	CBI-CBG-CBD	-3.85	108.68	114.38
5	A	2309	Y01	CBI-CBE-CBB	-3.84	113.48	119.49
5	A	2315	Y01	CBI-CBG-CBD	-3.63	109.00	114.38
5	A	2310	Y01	CBI-CBG-CBD	-3.62	109.02	114.38
5	A	2315	Y01	OAW-CAY-CAM	3.56	119.18	111.50
5	A	2312	Y01	CAV-CAZ-CAI	-3.54	115.51	120.61
5	A	2313	Y01	CBI-CBE-CBB	-3.45	114.08	119.49
5	A	2310	Y01	CBF-CBD-CBG	-3.43	104.50	109.09
5	A	2311	Y01	CBF-CBD-CBG	-3.35	104.61	109.09
5	A	2312	Y01	CBC-CAV-CAZ	-3.26	106.45	111.52
5	A	2311	Y01	CAV-CAZ-CAI	-3.16	116.06	120.61
5	A	2311	Y01	CBI-CBG-CBD	-3.13	109.75	114.38
5	A	2315	Y01	CBF-CBH-CAZ	3.12	114.54	109.65
5	A	2313	Y01	CAK-CBD-CBG	-3.05	106.48	110.91
5	A	2309	Y01	CBF-CBH-CAZ	3.01	114.38	109.65
5	A	2310	Y01	CAP-CAQ-CBG	-2.80	99.59	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2311	Y01	CAD-CBH-CBF	-2.78	108.37	111.68
4	A	2305	3PE	O31-C31-C32	2.73	120.49	111.91
5	A	2312	Y01	CBF-CBH-CAZ	2.70	113.89	109.65
5	A	2313	Y01	CAV-CAZ-CAI	-2.68	116.74	120.61
5	A	2310	Y01	CBF-CBH-CAZ	2.66	113.82	109.65
5	A	2315	Y01	CBD-CAK-CAI	-2.62	108.97	112.73
5	A	2315	Y01	CAS-CAU-CBI	-2.58	108.35	112.78
5	A	2310	Y01	CAD-CBH-CBF	-2.57	108.62	111.68
5	A	2310	Y01	CAC-CBB-CBE	-2.54	109.03	112.92
5	A	2313	Y01	CAD-CBH-CBF	-2.53	108.67	111.68
5	A	2315	Y01	CAC-CBB-CBE	-2.47	109.14	112.92
5	A	2311	Y01	CAQ-CBG-CBI	-2.47	100.87	103.84
5	A	2312	Y01	CAQ-CBG-CBD	-2.40	115.14	119.08
5	A	2309	Y01	CBD-CAK-CAI	-2.39	109.30	112.73
5	A	2313	Y01	CAQ-CBG-CBI	-2.39	100.97	103.84
5	A	2309	Y01	CBF-CBD-CBG	-2.37	105.91	109.09
5	A	2315	Y01	CAM-CAL-CAX	-2.37	108.51	113.60
5	A	2313	Y01	CAP-CAQ-CBG	-2.36	100.45	105.13
5	A	2313	Y01	CBI-CBG-CBD	-2.35	110.89	114.38
5	A	2312	Y01	CAC-CBB-CBE	-2.35	109.32	112.92
5	A	2309	Y01	CAQ-CBG-CBI	-2.34	101.02	103.84
5	A	2312	Y01	CAQ-CBG-CBI	-2.33	101.04	103.84
5	A	2313	Y01	CAV-CAZ-CBH	2.32	119.51	116.42
5	A	2311	Y01	CAR-CAT-CBH	-2.31	107.74	112.74
5	A	2313	Y01	CAQ-CBG-CBD	-2.30	115.30	119.08
5	A	2311	Y01	CAQ-CBG-CBD	-2.27	115.34	119.08
5	A	2315	Y01	CAQ-CBG-CBI	-2.26	101.12	103.84
5	A	2313	Y01	CAR-CBC-CAV	-2.23	107.66	110.99
5	A	2315	Y01	CAJ-CAO-CBB	-2.20	108.71	115.03
5	A	2309	Y01	CAD-CBH-CBF	-2.18	109.08	111.68
5	A	2312	Y01	CAS-CBF-CBD	-2.16	108.64	111.75
5	A	2310	Y01	CAQ-CBG-CBI	-2.15	101.25	103.84
5	A	2312	Y01	CAK-CAI-CAZ	-2.13	121.14	125.06
5	A	2315	Y01	CBF-CBD-CBG	-2.13	106.24	109.09
5	A	2313	Y01	CBC-CAV-CAZ	-2.11	108.24	111.52
5	A	2313	Y01	CAS-CAU-CBI	-2.11	109.16	112.78
5	A	2313	Y01	CBF-CBD-CBG	-2.08	106.31	109.09

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2310	Y01	OAG-CAY-OAW-CBC
5	A	2311	Y01	CAM-CAY-OAW-CBC
5	A	2312	Y01	CAR-CBC-OAW-CAY
5	A	2312	Y01	CAM-CAY-OAW-CBC
5	A	2313	Y01	CAV-CBC-OAW-CAY
5	A	2315	Y01	CAC-CBB-CBE-CBI
5	A	2310	Y01	CAM-CAY-OAW-CBC
5	A	2309	Y01	CAM-CAY-OAW-CBC
5	A	2310	Y01	CAC-CBB-CBE-CBI
5	A	2312	Y01	CAC-CBB-CBE-CBI
5	A	2310	Y01	CAO-CBB-CBE-CBI
5	A	2311	Y01	OAG-CAY-OAW-CBC
5	A	2310	Y01	CAC-CBB-CBE-CAP
5	A	2312	Y01	CAC-CBB-CBE-CAP
5	A	2315	Y01	CAC-CBB-CBE-CAP
5	A	2312	Y01	CAO-CBB-CBE-CBI
5	A	2315	Y01	CAO-CBB-CBE-CBI
5	A	2312	Y01	OAG-CAY-OAW-CBC
5	A	2315	Y01	CAO-CBB-CBE-CAP
3	A	2304	NAG	O5-C5-C6-O6
5	A	2310	Y01	CAJ-CAO-CBB-CBE
5	A	2312	Y01	CAJ-CAO-CBB-CBE
5	A	2309	Y01	OAG-CAY-OAW-CBC
5	A	2312	Y01	CAJ-CAO-CBB-CAC
3	A	2303	NAG	O5-C5-C6-O6
3	A	2303	NAG	C8-C7-N2-C2
3	A	2303	NAG	O7-C7-N2-C2
5	A	2309	Y01	CAJ-CAO-CBB-CAC
5	A	2312	Y01	CAO-CBB-CBE-CAP
4	A	2305	3PE	C31-C32-C33-C34
4	A	2305	3PE	C21-C22-C23-C24
5	A	2310	Y01	CAJ-CAO-CBB-CAC
5	A	2310	Y01	CAO-CBB-CBE-CAP
5	A	2310	Y01	CAN-CAJ-CAO-CBB
5	A	2310	Y01	CAJ-CAN-CBA-CAB
4	A	2305	3PE	C22-C21-O21-C2
4	A	2320	3PE	C34-C35-C36-C37
4	A	2317	3PE	C25-C26-C27-C28
4	A	2305	3PE	O22-C21-O21-C2
5	A	2312	Y01	CAO-CAJ-CAN-CBA
4	A	2316	3PE	C36-C37-C38-C39
4	A	2321	3PE	C36-C37-C38-C39
4	A	2319	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
5	A	2313	Y01	CAO-CAJ-CAN-CBA
4	A	2317	3PE	C24-C25-C26-C27
3	A	2304	NAG	C4-C5-C6-O6
4	A	2305	3PE	C26-C27-C28-C29
4	A	2321	3PE	C33-C34-C35-C36
5	A	2310	Y01	CAJ-CAN-CBA-CAA
4	A	2305	3PE	C32-C31-O31-C3
4	A	2305	3PE	C27-C28-C29-C2A
5	A	2313	Y01	CAJ-CAO-CBB-CAC
4	A	2305	3PE	O32-C31-O31-C3
4	A	2321	3PE	C3C-C3D-C3E-C3F
5	A	2311	Y01	CAC-CBB-CBE-CBI
4	A	2305	3PE	C22-C23-C24-C25
4	A	2314	3PE	C35-C36-C37-C38
5	A	2313	Y01	CAC-CBB-CBE-CBI
3	A	2303	NAG	C4-C5-C6-O6
4	A	2319	3PE	C39-C3A-C3B-C3C
5	A	2311	Y01	CAO-CBB-CBE-CBI
4	A	2318	3PE	C39-C3A-C3B-C3C
4	A	2305	3PE	C23-C24-C25-C26
4	A	2314	3PE	C39-C3A-C3B-C3C
5	A	2312	Y01	CAN-CAJ-CAO-CBB
4	A	2320	3PE	C36-C37-C38-C39
4	A	2319	3PE	C35-C36-C37-C38
4	A	2320	3PE	C37-C38-C39-C3A
5	A	2310	Y01	CAO-CAJ-CAN-CBA
4	A	2314	3PE	C38-C39-C3A-C3B
5	A	2309	Y01	CAC-CBB-CBE-CBI
5	A	2311	Y01	CAJ-CAO-CBB-CBE
5	A	2313	Y01	CAO-CBB-CBE-CBI
5	A	2311	Y01	CAJ-CAN-CBA-CAA
5	A	2311	Y01	CAC-CBB-CBE-CAP
4	A	2305	3PE	C33-C34-C35-C36
3	A	2304	NAG	C3-C2-N2-C7
4	A	2321	3PE	C34-C35-C36-C37
5	A	2311	Y01	CAM-CAL-CAX-OAF
4	A	2321	3PE	C39-C3A-C3B-C3C
5	A	2311	Y01	CAM-CAL-CAX-OAH
4	A	2320	3PE	C35-C36-C37-C38
5	A	2311	Y01	CAO-CBB-CBE-CAP
5	A	2311	Y01	CAO-CAJ-CAN-CBA
4	A	2306	3PE	C32-C33-C34-C35

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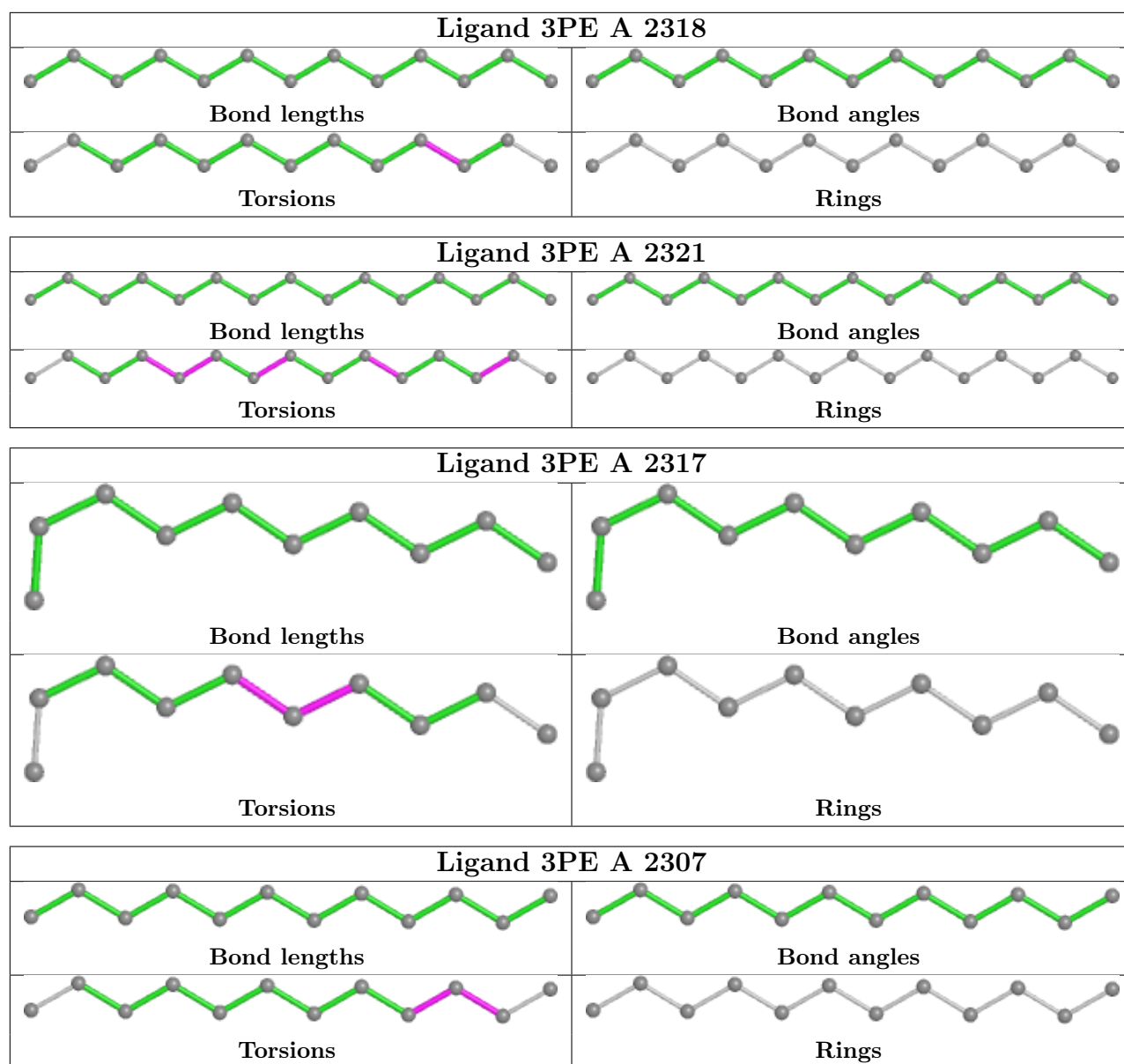
Mol	Chain	Res	Type	Atoms
5	A	2313	Y01	CAC-CBB-CBE-CAP
4	A	2319	3PE	C3D-C3E-C3F-C3G
4	A	2319	3PE	C33-C34-C35-C36
3	A	2303	NAG	C3-C2-N2-C7
4	A	2307	3PE	C38-C39-C3A-C3B
5	A	2315	Y01	CAL-CAM-CAY-OAW
4	A	2305	3PE	O11-C1-C2-O21
4	A	2307	3PE	C39-C3A-C3B-C3C
5	A	2309	Y01	CAO-CBB-CBE-CBI

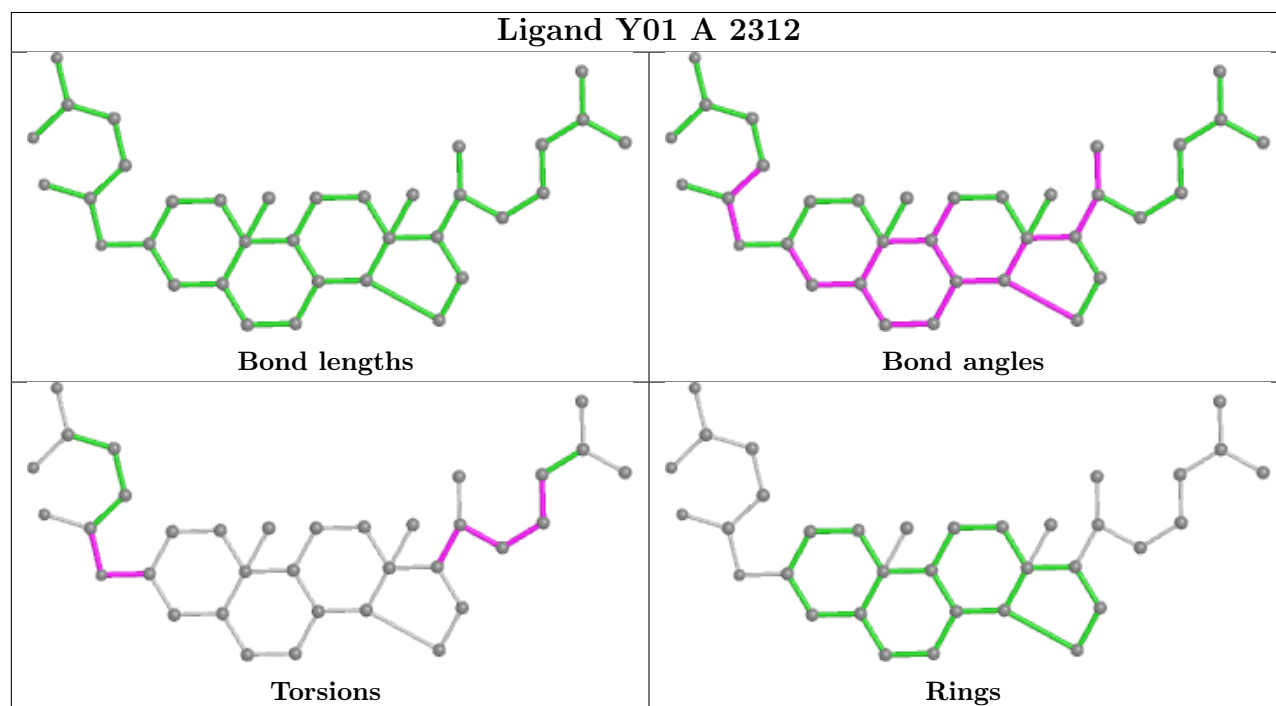
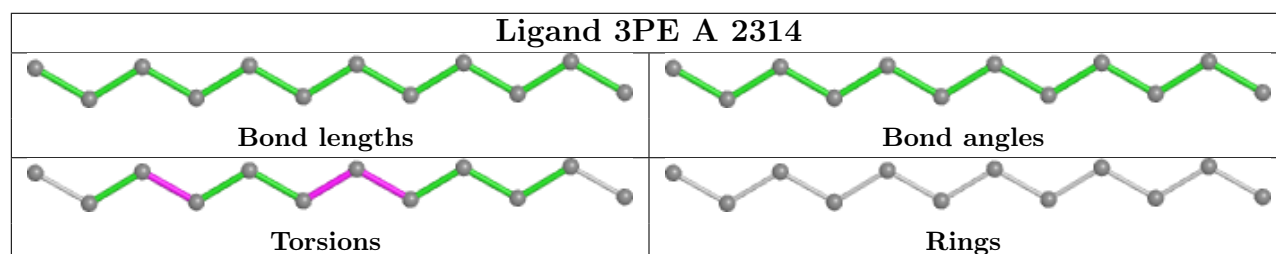
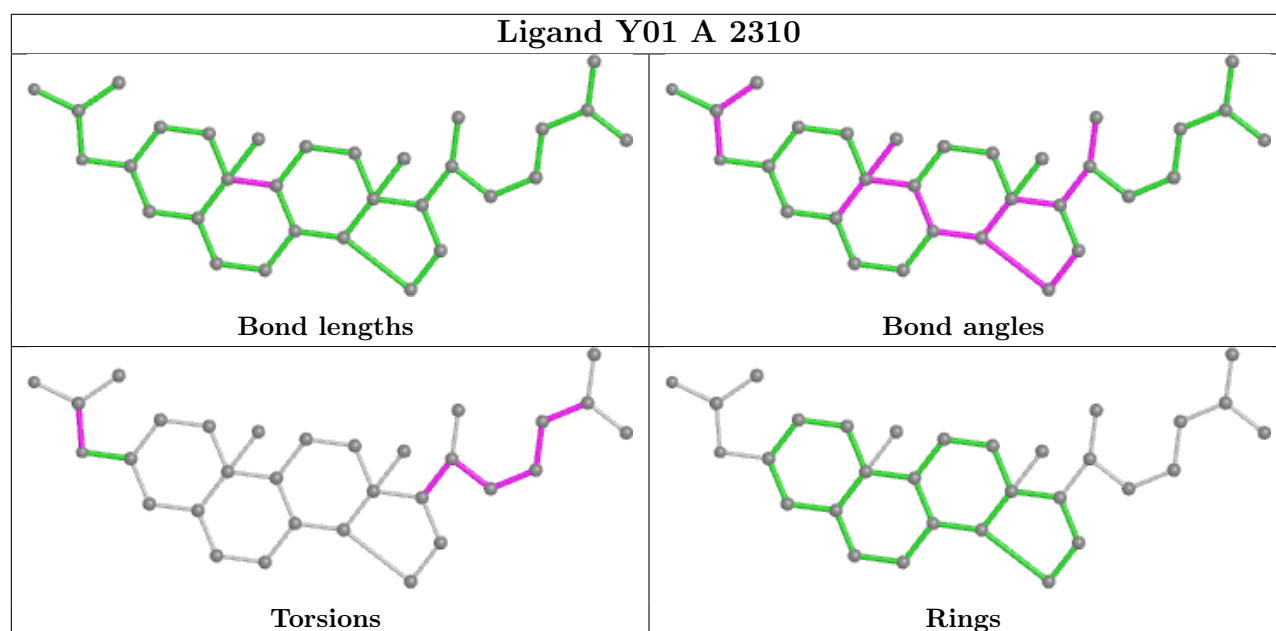
There are no ring outliers.

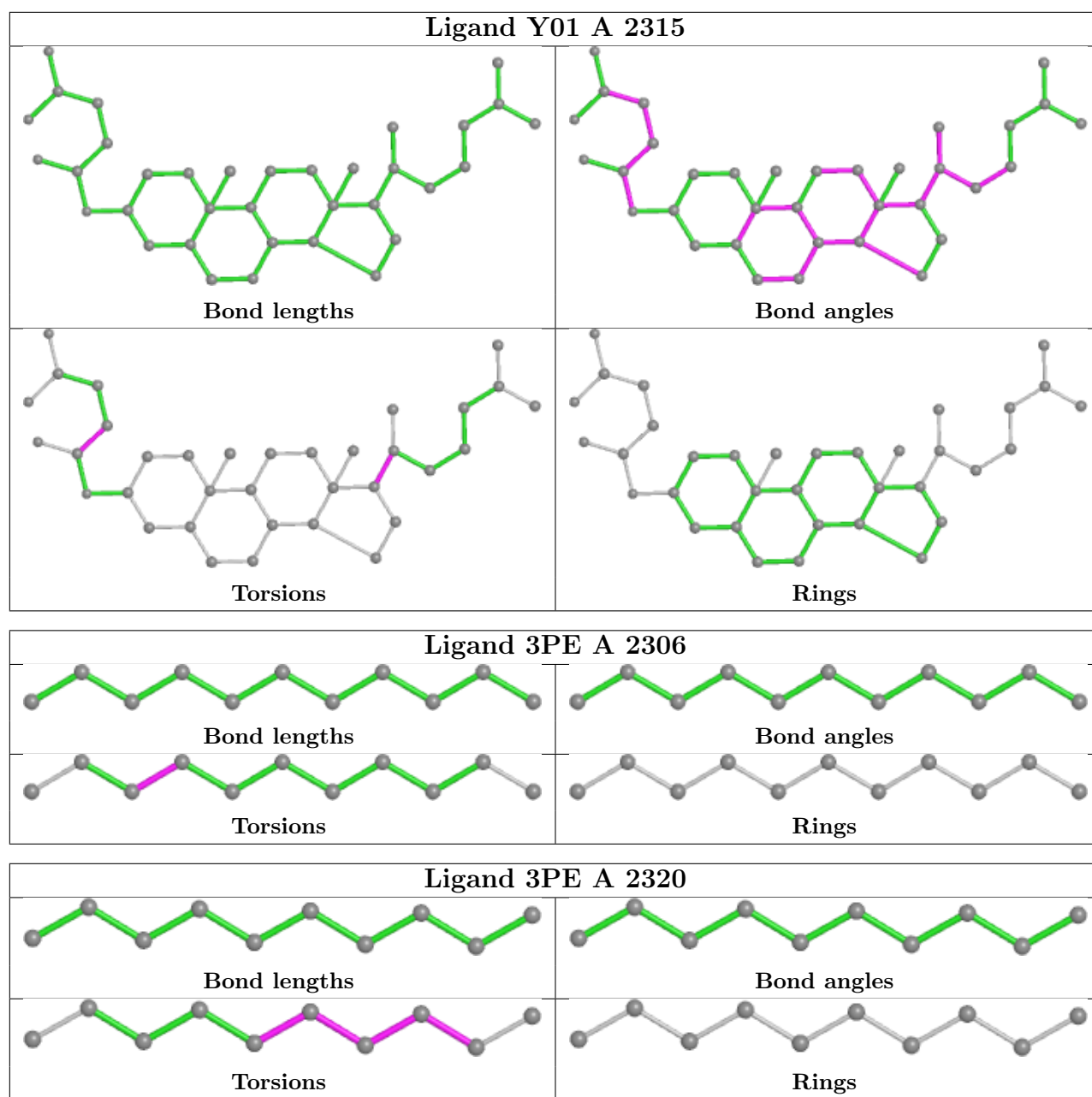
14 monomers are involved in 29 short contacts:

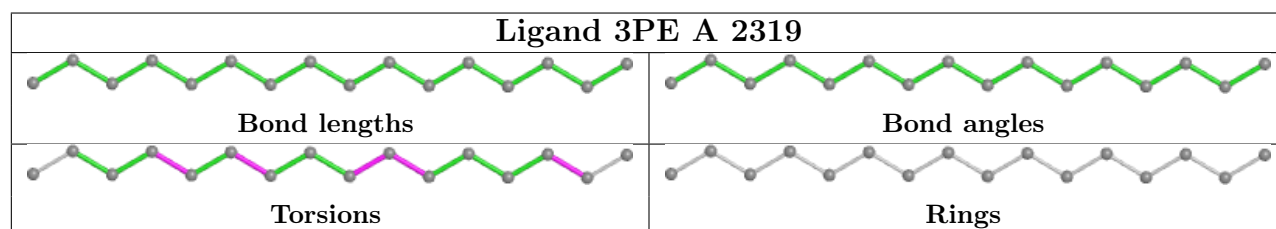
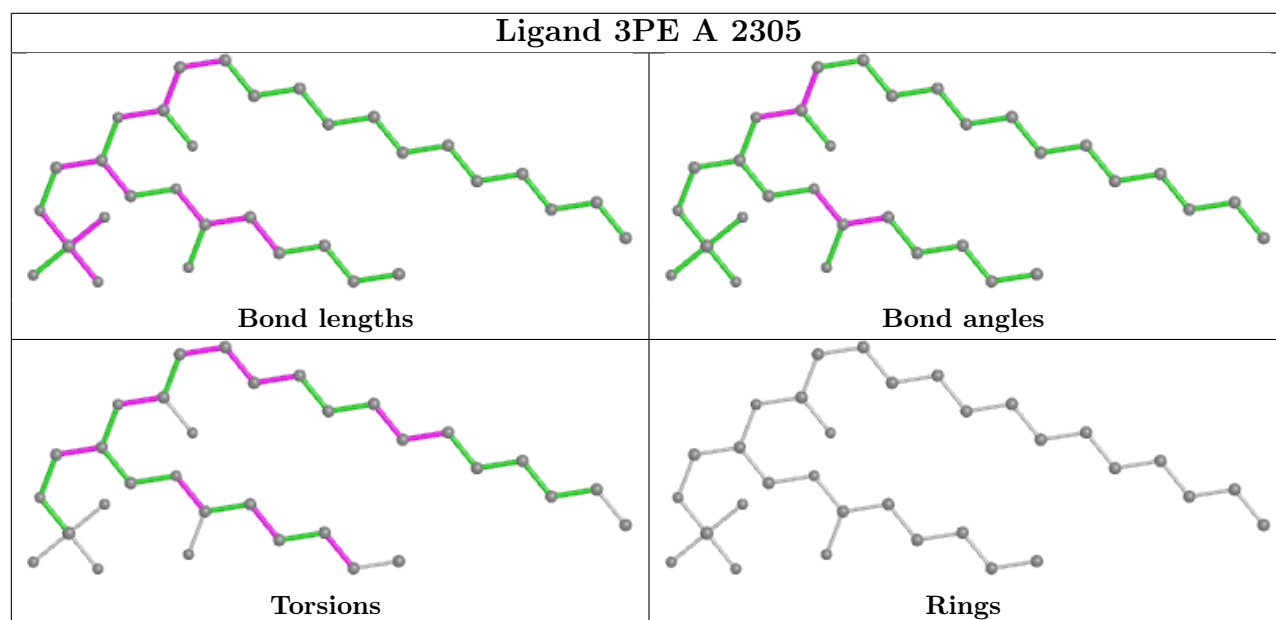
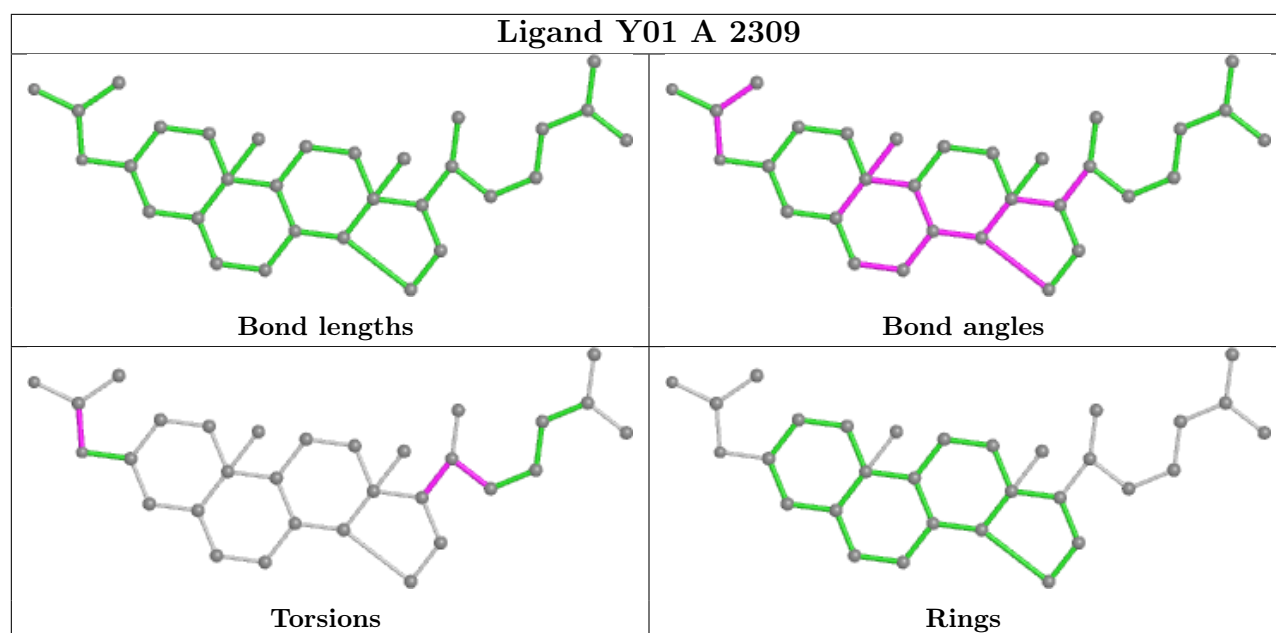
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2304	NAG	1	0
4	A	2321	3PE	1	0
4	A	2317	3PE	1	0
4	A	2308	3PE	2	0
5	A	2310	Y01	1	0
4	A	2314	3PE	1	0
5	A	2312	Y01	4	0
5	A	2315	Y01	2	0
5	A	2309	Y01	1	0
4	A	2305	3PE	1	0
3	A	2303	NAG	1	0
5	A	2311	Y01	8	0
5	A	2313	Y01	4	0
4	A	2316	3PE	2	0

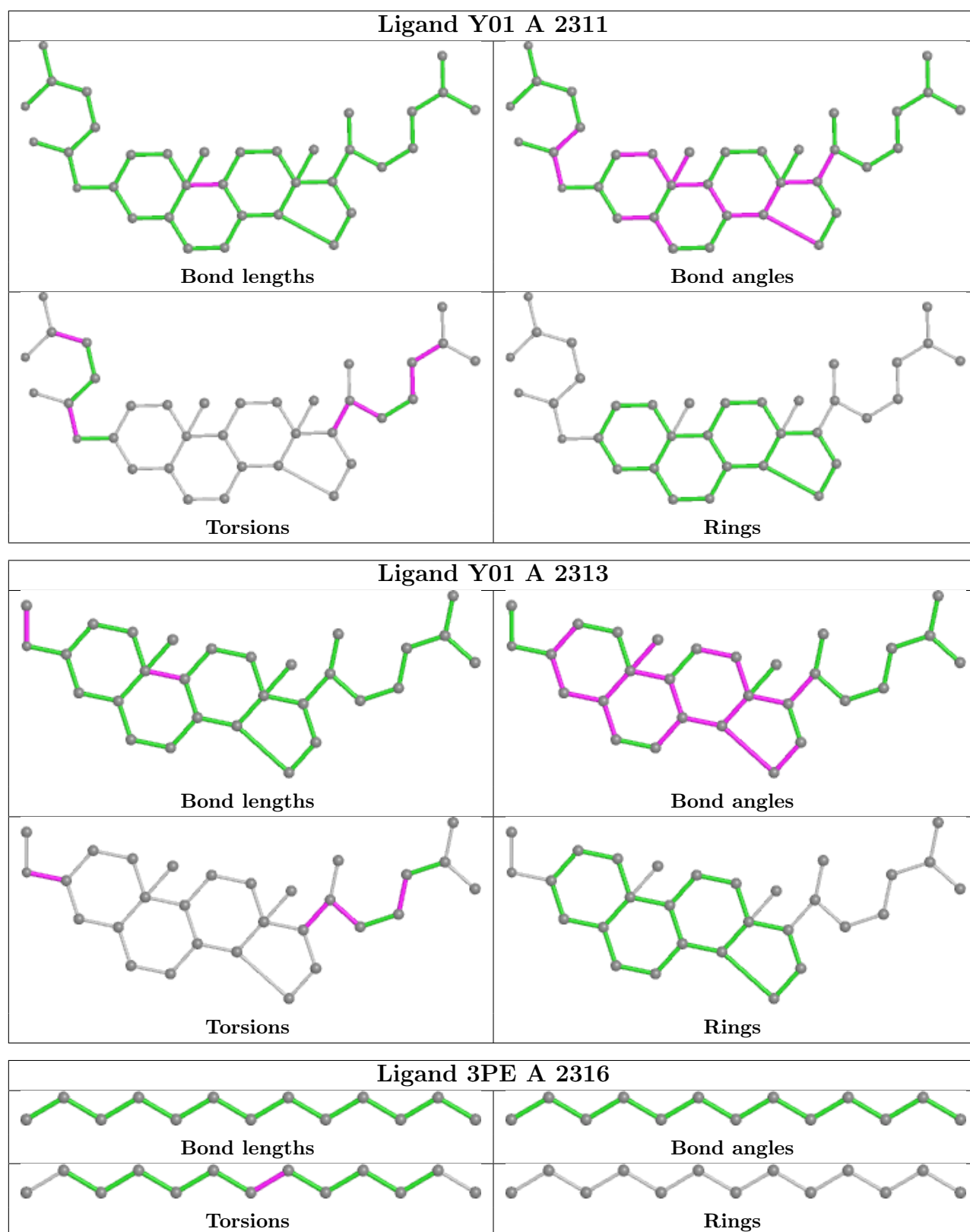
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

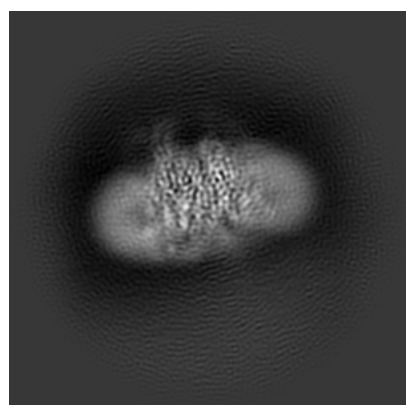
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32584. These allow visual inspection of the internal detail of the map and identification of artifacts.

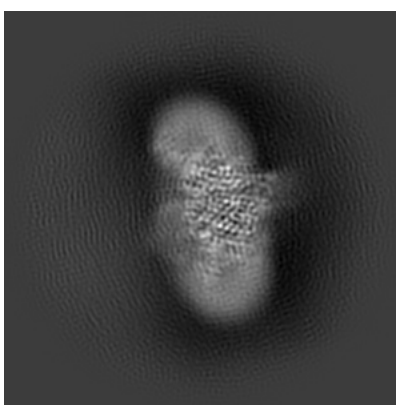
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

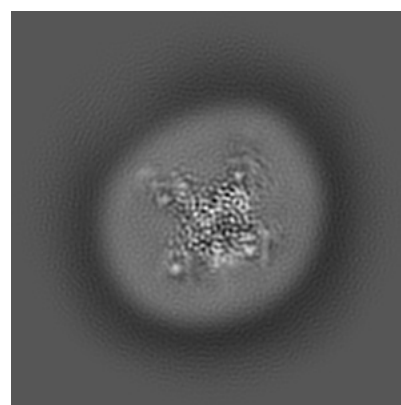
6.1.1 Primary map



X



Y

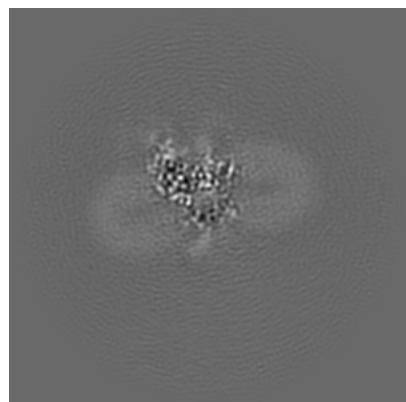


Z

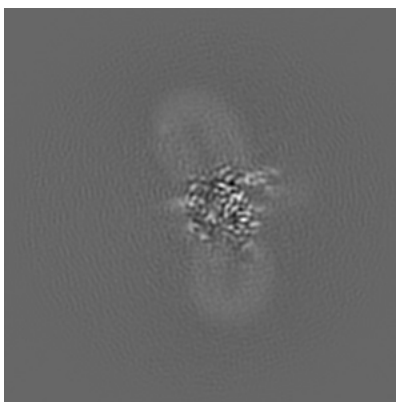
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

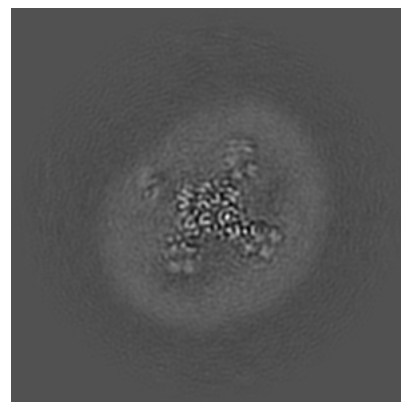
6.2.1 Primary map



X Index: 128



Y Index: 128

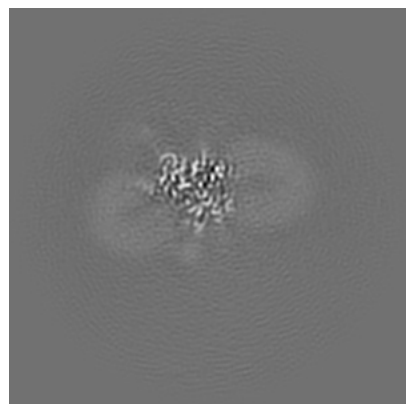


Z Index: 128

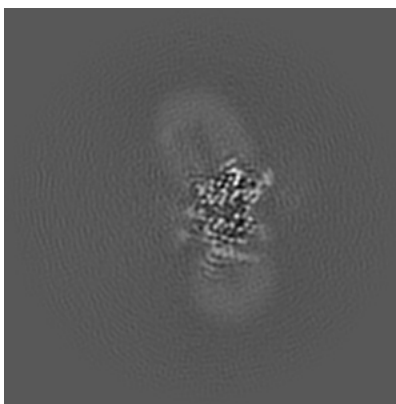
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

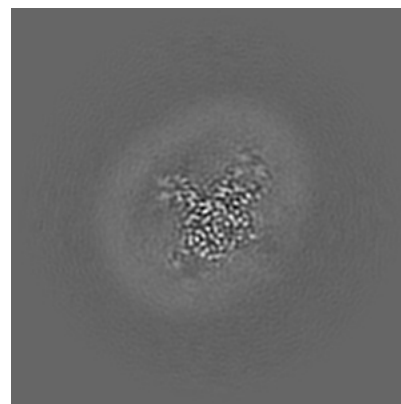
6.3.1 Primary map



X Index: 122



Y Index: 135

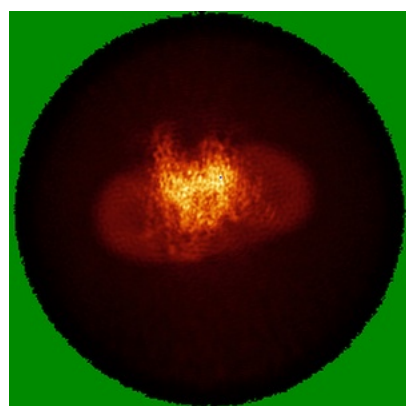


Z Index: 146

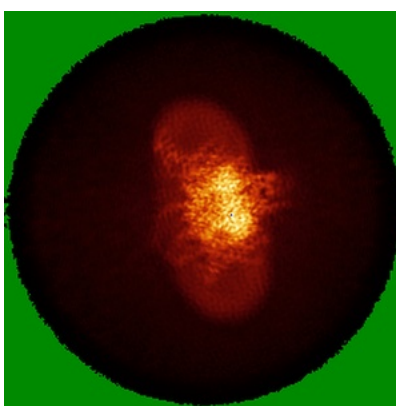
The images above show the largest variance slices of the map in three orthogonal directions.

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

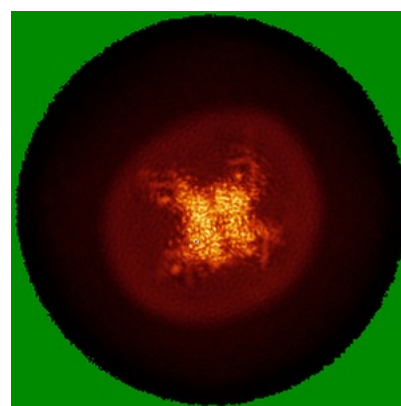
6.4.1 Primary map



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

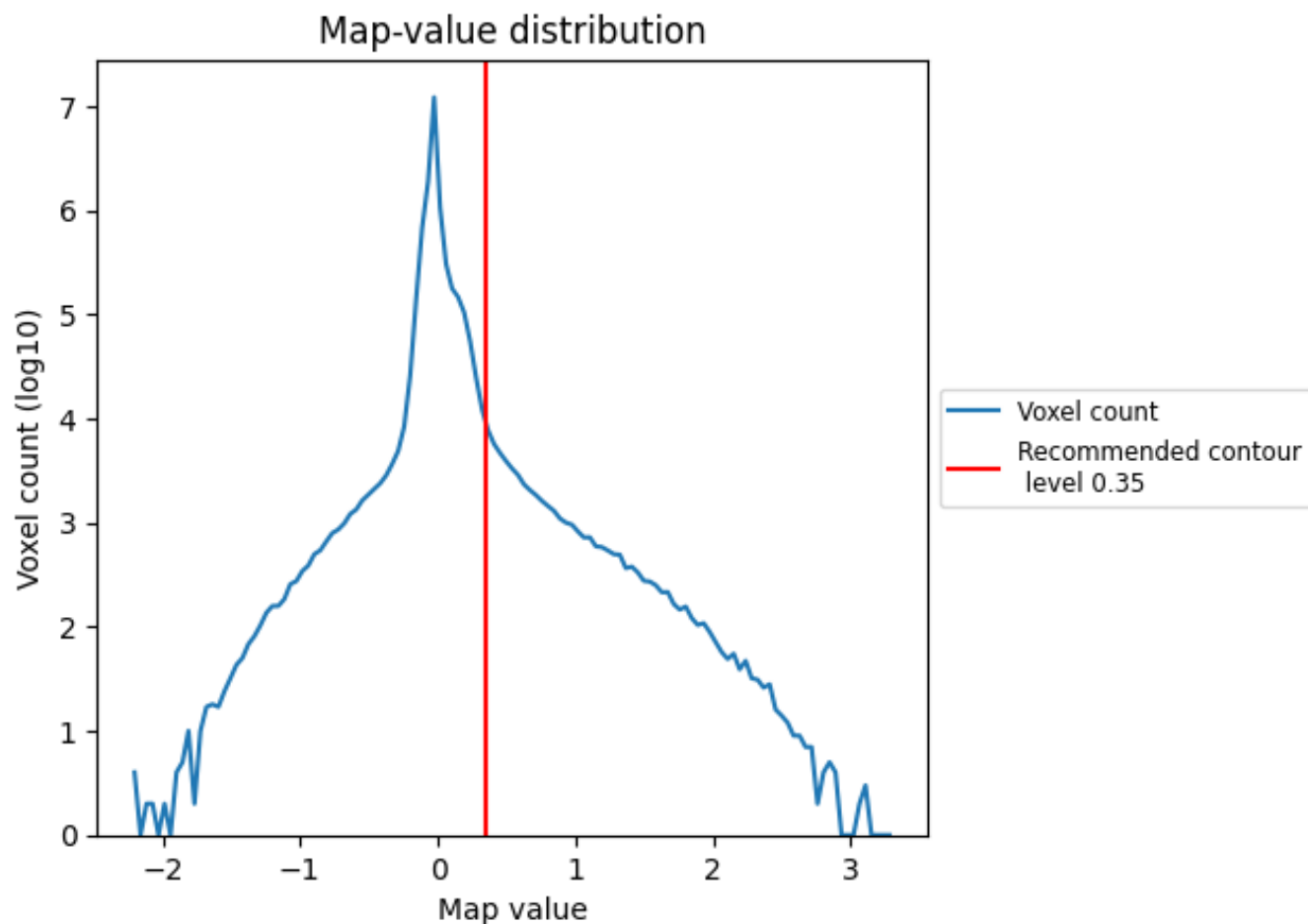
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

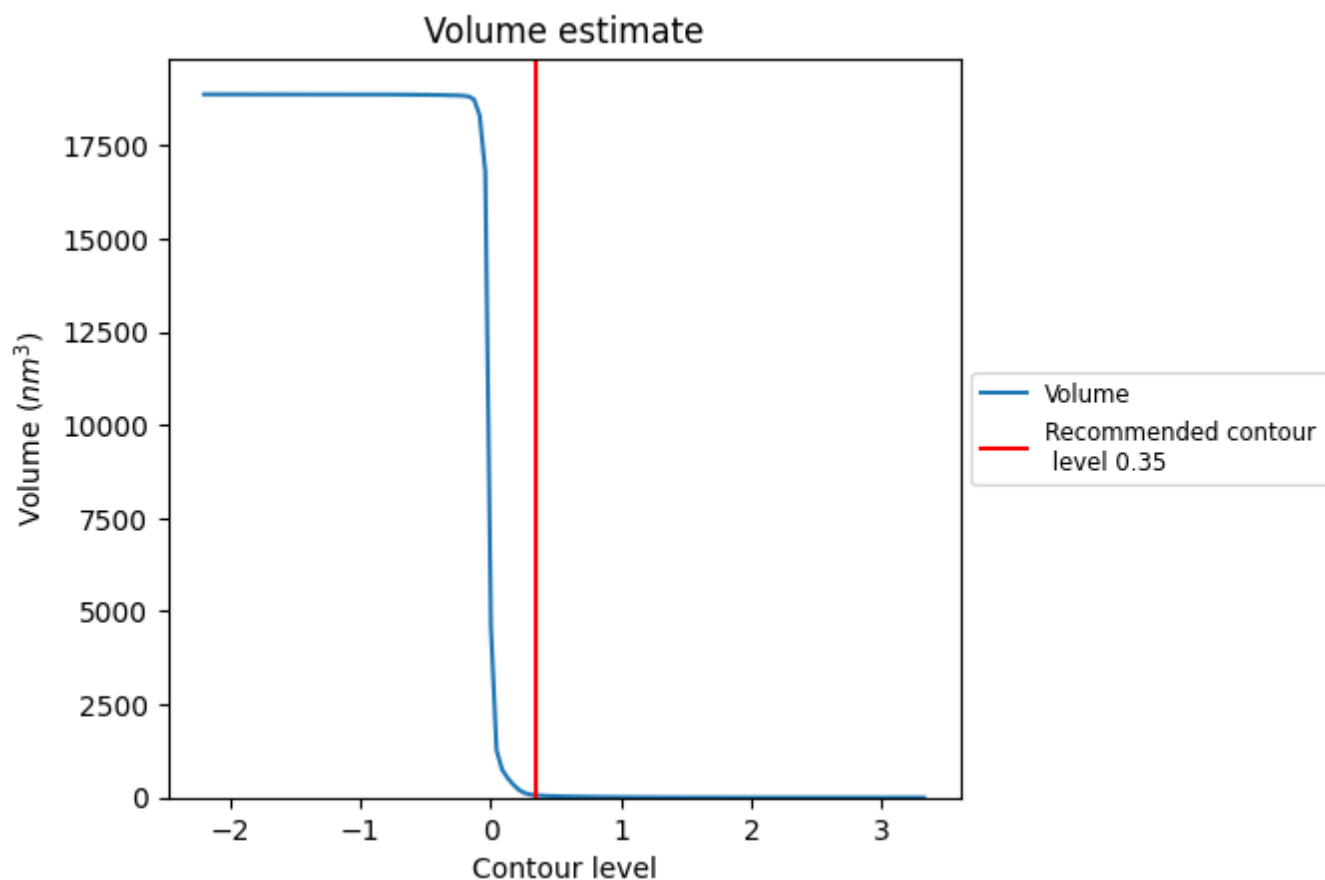
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

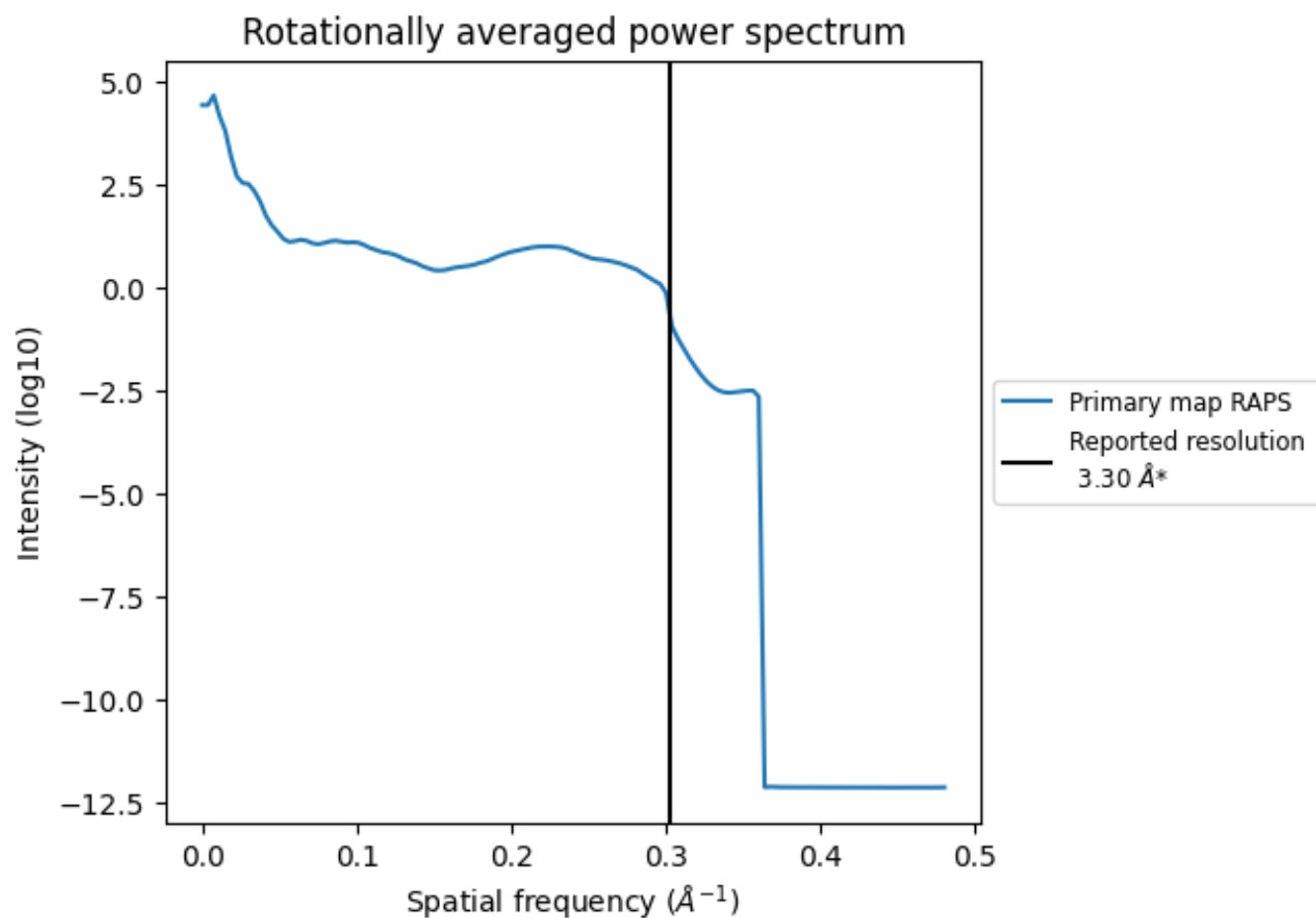
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm³; this corresponds to an approximate mass of 55 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 0.303 Å⁻¹

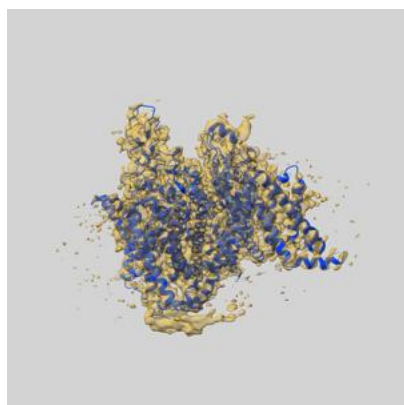
8 Fourier-Shell correlation

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

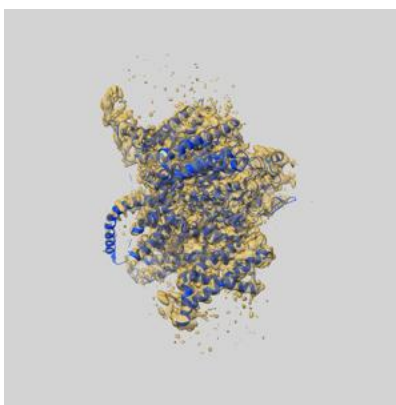
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32584 and PDB model 7WLI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

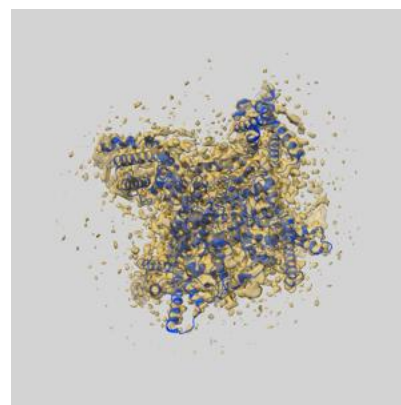
9.1 Map-model overlay [i](#)



X



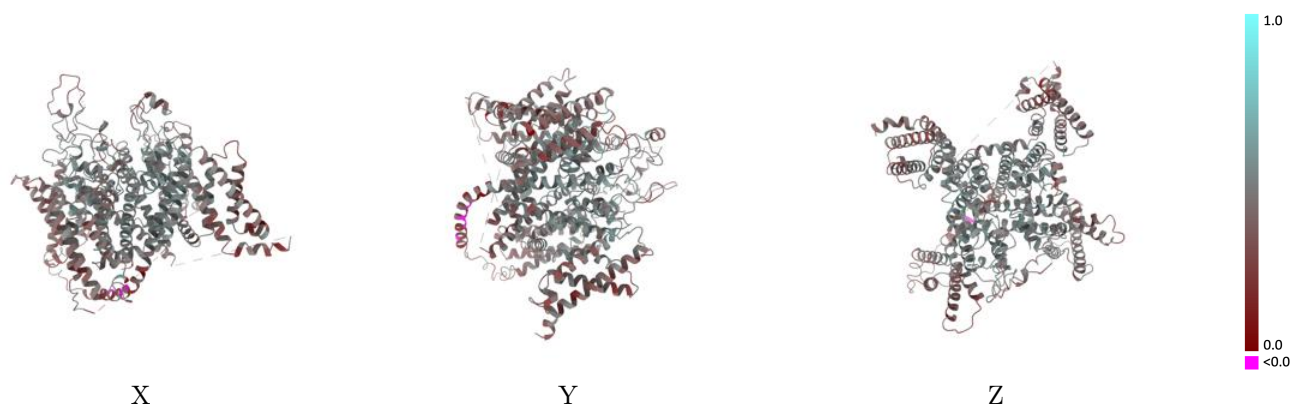
Y



Z

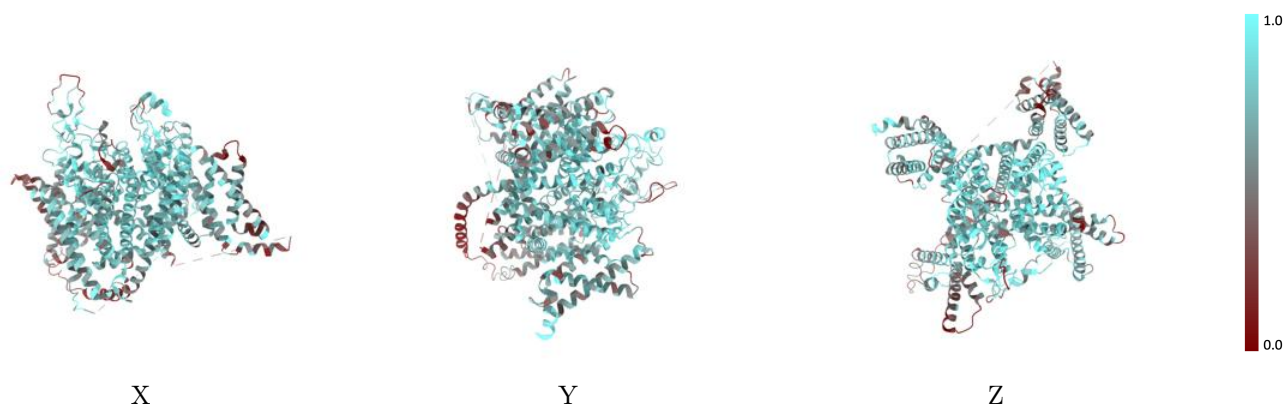
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



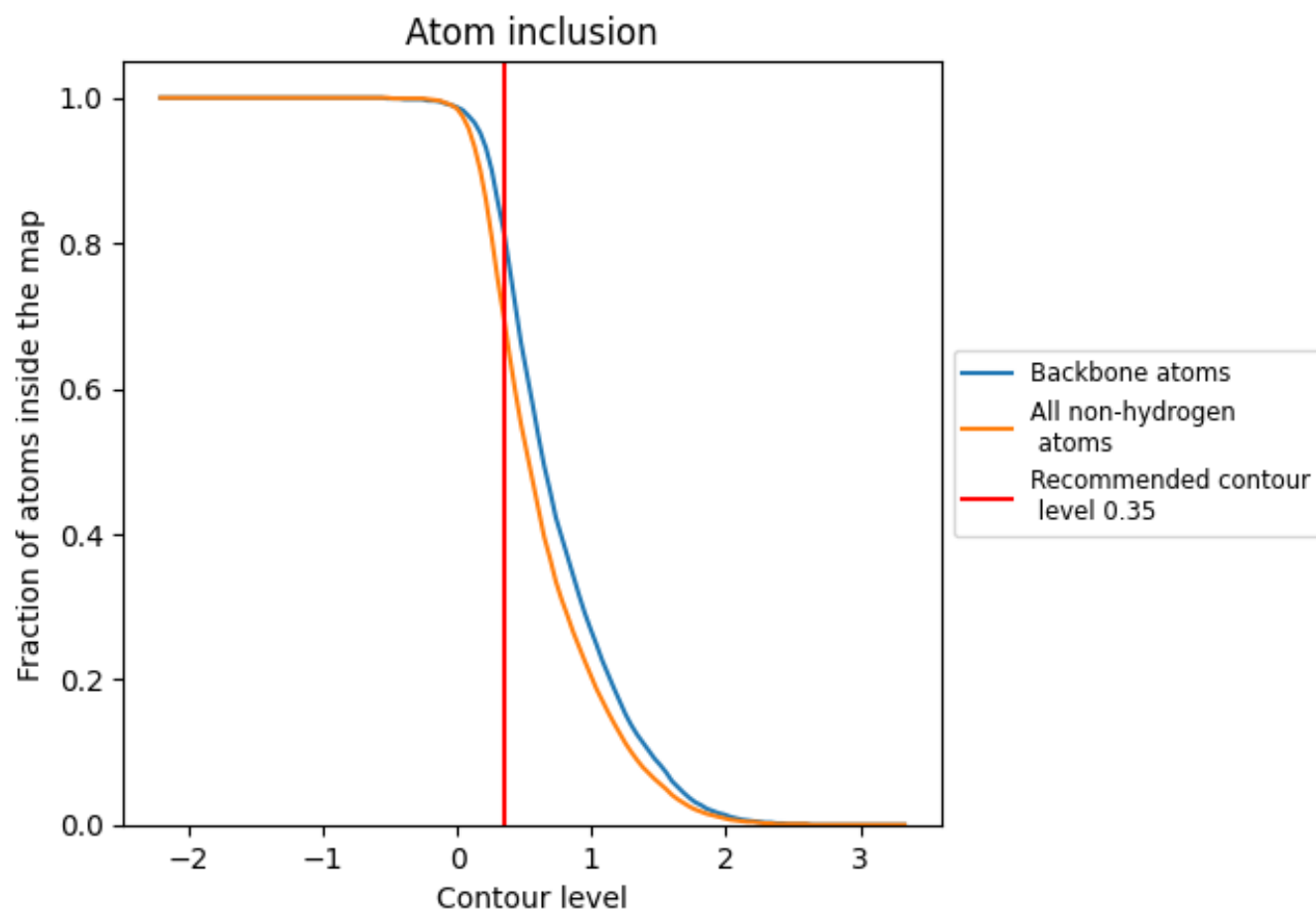
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6970	<div><div></div></div> 0.4430
A	<div><div></div></div> 0.6970	<div><div></div></div> 0.4430

