Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 02:54 AM 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:

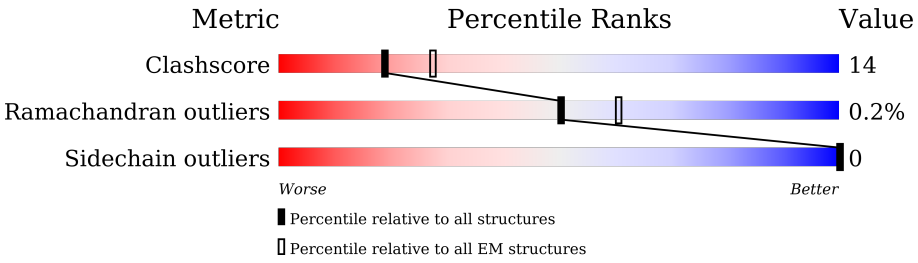
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	7% 34% 17% 49%

2 Entry composition

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.

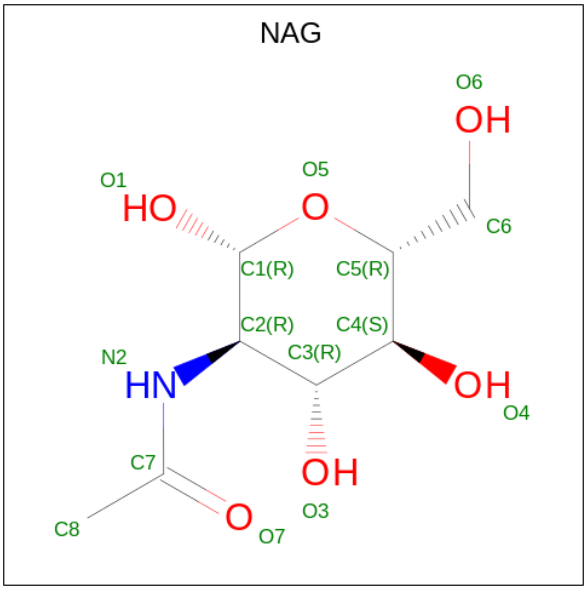
- Molecule 1 is a protein called Voltage-dependent T-type calcium channel subunit alpha-1I.

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).

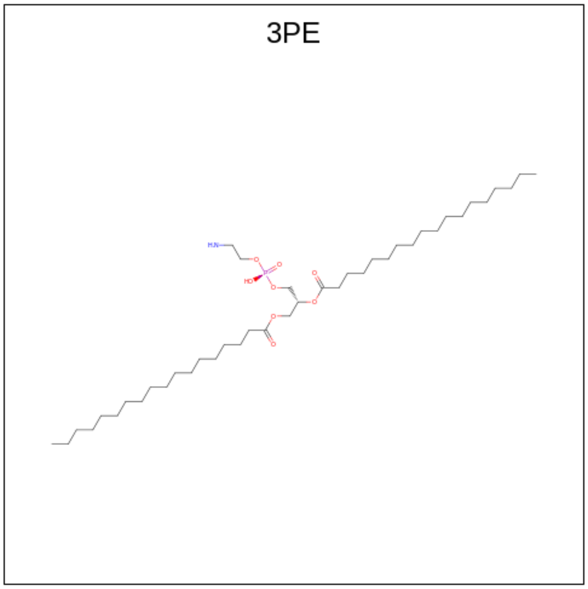
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	2	2	2	0

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



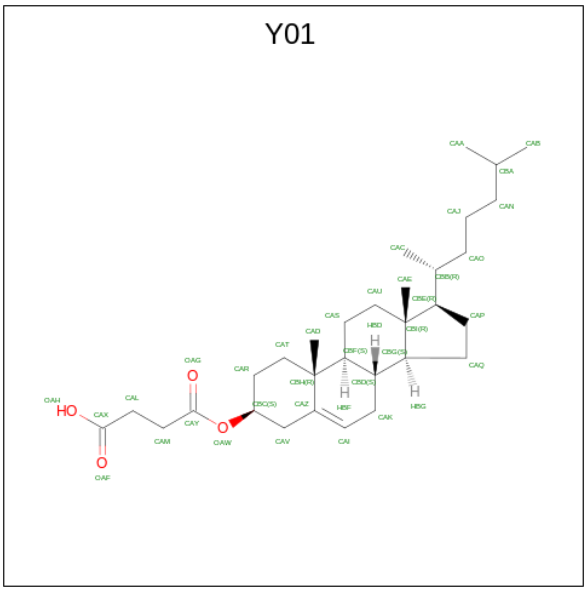
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	28	16	2	10	0
3	A	1	28	16	2	10	0

- 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 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0
4	A	1	Total C O P 156 147 8 1	0

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



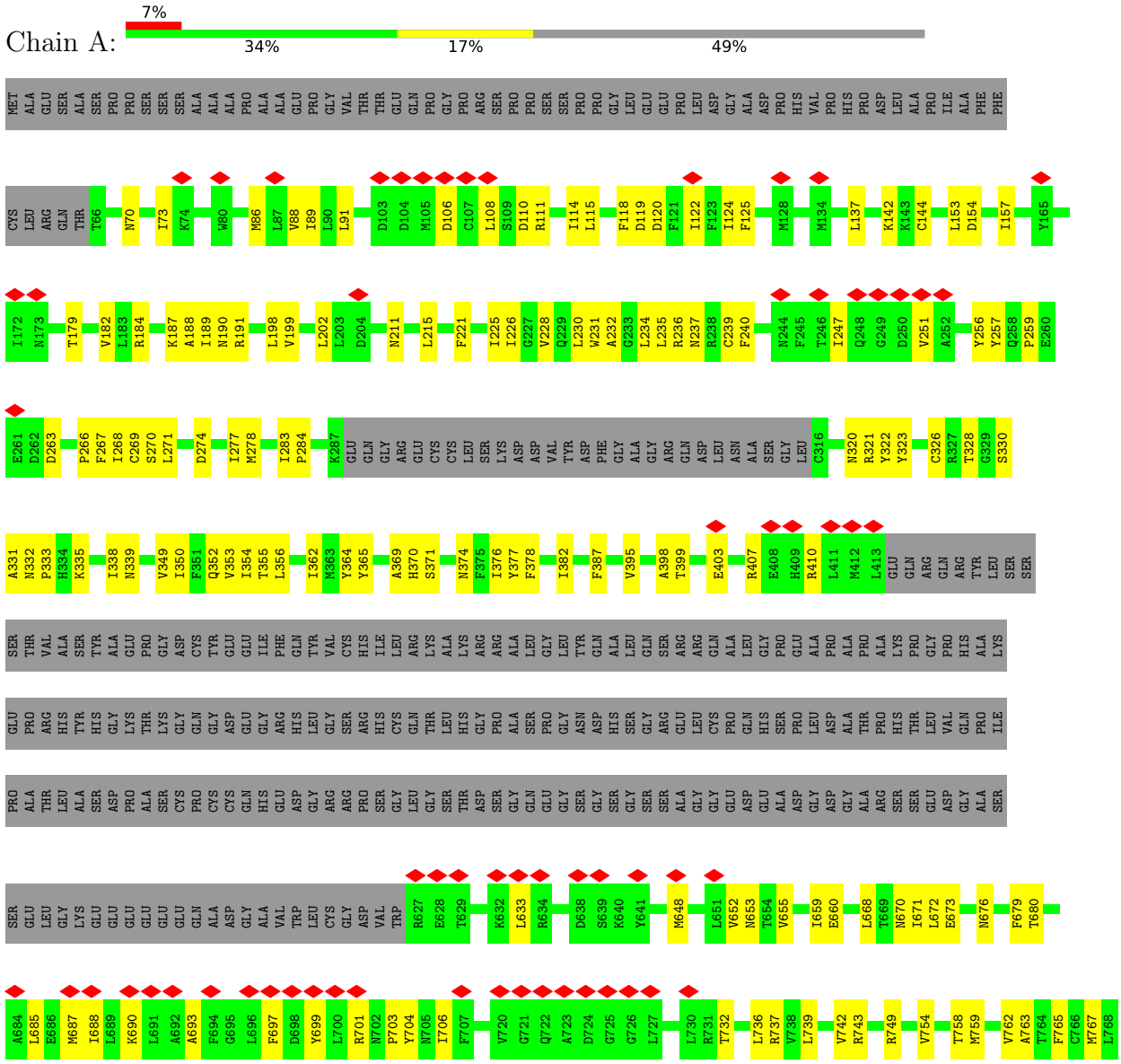
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			196	179	17	
5	A	1	Total	C	O	0
			196	179	17	
5	A	1	Total	C	O	0
			196	179	17	
5	A	1	Total	C	O	0
			196	179	17	
5	A	1	Total	C	O	0
			196	179	17	
5	A	1	Total	C	O	0
			196	179	17	

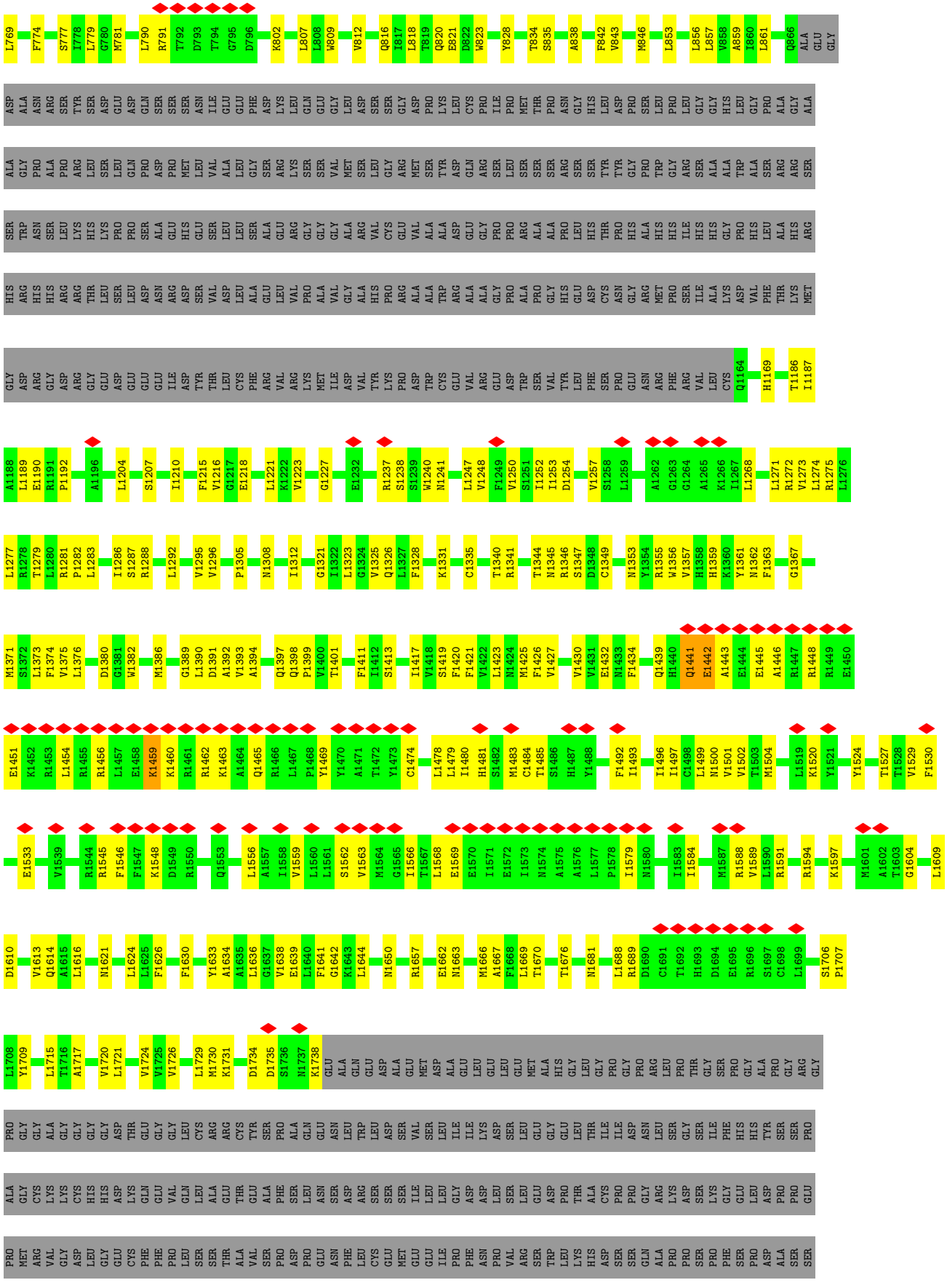
3 Residue-property plots (i)

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

Chain A:





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

SER LEU ASP ALA SER PRO SER SER SER ALA GLY SER LEU GLN THR THR LEU GLU ASP SER LEU THR LEU SER ASP SER PRO ARG ARG ALA LEU GLY PRO PRO ALA PRO ALA PRO GLY PRO ARG ALA GLY LEU SER PRO ALA ALA ARG ARG ARG LEU SER LEU ARG GLY ARG GLY LEU PHE

SER LEU ARG GLY LEU ARG ALA HIS GLN ARG SER HIS SER SER GLY GLY SER THR SER PRO GLY CYS THR HIS HIS ASP SER MET ASP PRO SER ASP GLU GLU GLY ARG GLY GLY ALA GLY GLY GLY GLY ALA GLY SER GLU HIS SER GLU THR LEU SER SER LEU SER LEU THR SER LEU

PHE CYS PRO PRO PRO PRO PRO PRO ALA PRO GLY LEU THR PRO ALA ARG LYS PHE SER SER THR SER SER LEU ALA ALA PRO GLY ARG PRO HIS ALA ALA ALA LEU ALA HIS GLY LEU ALA ARG SER PRO SER TRP ALA ALA ASP ARG SER LYS ASP PRO PRO GLY ARG ALA PRO LEU PRO

MET GLY LEU GLY PRO LEU ALA PRO PRO PRO GLN PRO LEU PRO GLY GLU LEU GLU PRO GLY ASP ALA ALA SER LYS ARG LYS ARG

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: NAG, 3PE, Y01, CA

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(^{o})	Ideal(^{o})
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

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%)	47 77

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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	2307	-	11,11,50	1.52	0	10,10,55	0.88	0
5	Y01	A	2309	-	34,34,38	0.63	0	52,52,57	1.60	8 (15%)
4	3PE	A	2321	-	14,14,50	1.53	0	13,13,55	0.85	0
4	3PE	A	2320	-	9,9,50	1.50	0	8,8,55	0.80	0
5	Y01	A	2315	-	38,38,38	0.67	0	57,57,57	1.62	11 (19%)
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
5	Y01	A	2311	-	38,38,38	0.72	1 (2%)	57,57,57	1.60	9 (15%)
4	3PE	A	2314	-	11,11,50	1.53	0	10,10,55	0.84	0
4	3PE	A	2317	-	9,9,50	1.49	0	8,8,55	0.79	0
4	3PE	A	2316	-	12,12,50	1.53	0	11,11,55	0.83	0
5	Y01	A	2312	-	38,38,38	0.62	0	57,57,57	1.77	12 (21%)
5	Y01	A	2310	-	34,34,38	0.65	1 (2%)	52,52,57	1.68	9 (17%)
3	NAG	A	2303	1	14,14,15	0.38	0	17,19,21	1.24	1 (5%)
4	3PE	A	2308	-	11,11,50	1.51	0	10,10,55	0.88	0
4	3PE	A	2306	-	10,10,50	1.51	0	9,9,55	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	3PE	A	2305	-	31,31,50	2.41	11 (35%)	35,36,55	1.21	2 (5%)
5	Y01	A	2313	-	32,32,38	0.79	2 (6%)	49,49,57	1.51	13 (26%)
4	3PE	A	2319	-	15,15,50	1.54	0	14,14,55	0.85	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	2307	-	-	2/9/9/54	-
5	Y01	A	2309	-	-	5/14/72/77	0/4/4/4
4	3PE	A	2321	-	-	5/12/12/54	-
4	3PE	A	2320	-	-	4/7/7/54	-
5	Y01	A	2315	-	-	5/19/77/77	0/4/4/4
4	3PE	A	2318	-	-	1/10/10/54	-
3	NAG	A	2304	1	-	3/6/23/26	0/1/1/1
5	Y01	A	2311	-	-	11/19/77/77	0/4/4/4
4	3PE	A	2314	-	-	3/9/9/54	-
4	3PE	A	2317	-	-	2/7/7/54	-
4	3PE	A	2316	-	-	1/10/10/54	-
5	Y01	A	2312	-	-	11/19/77/77	0/4/4/4
5	Y01	A	2310	-	-	12/14/72/77	0/4/4/4
3	NAG	A	2303	1	-	5/6/23/26	0/1/1/1
4	3PE	A	2308	-	-	0/9/9/54	-
4	3PE	A	2306	-	-	1/8/8/54	-
4	3PE	A	2305	-	-	12/33/33/54	-
5	Y01	A	2313	-	-	6/12/70/77	0/4/4/4
4	3PE	A	2319	-	-	5/13/13/54	-

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

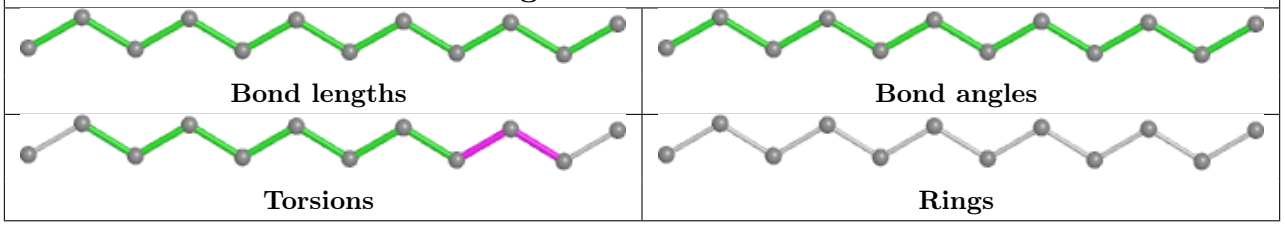
There are no ring outliers.

14 monomers are involved in 29 short contacts:

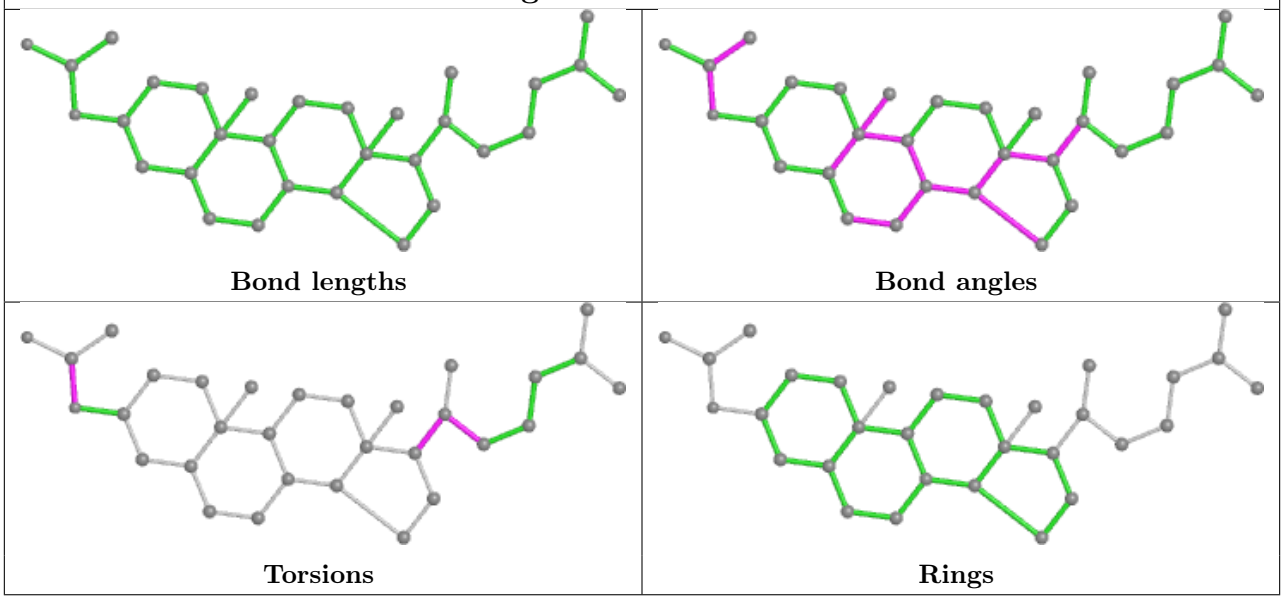
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2309	Y01	1	0
4	A	2321	3PE	1	0
5	A	2315	Y01	2	0
3	A	2304	NAG	1	0
5	A	2311	Y01	8	0
4	A	2314	3PE	1	0
4	A	2317	3PE	1	0
4	A	2316	3PE	2	0
5	A	2312	Y01	4	0
5	A	2310	Y01	1	0
3	A	2303	NAG	1	0
4	A	2308	3PE	2	0
4	A	2305	3PE	1	0
5	A	2313	Y01	4	0

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

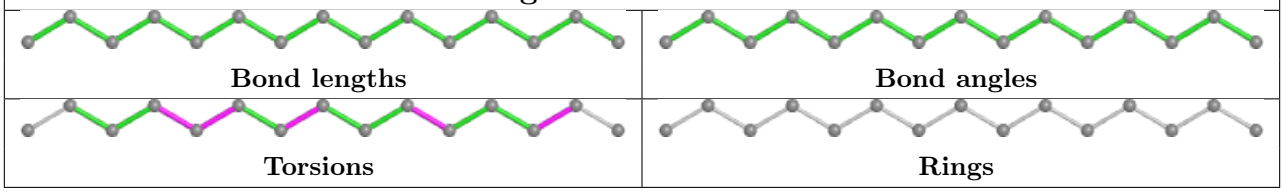
Ligand 3PE A 2307



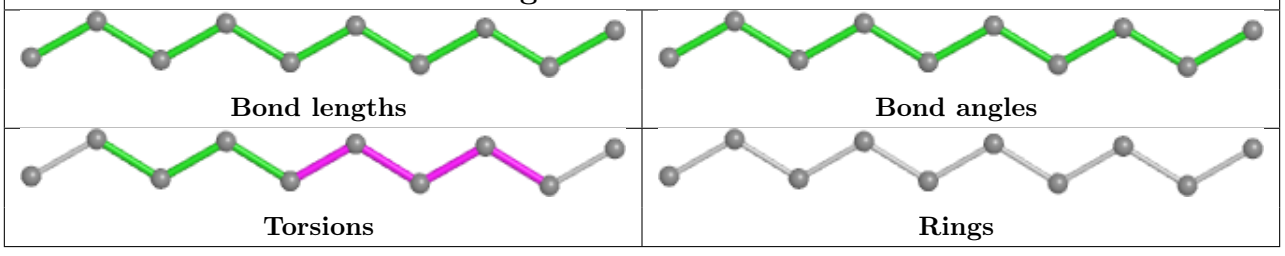
Ligand Y01 A 2309



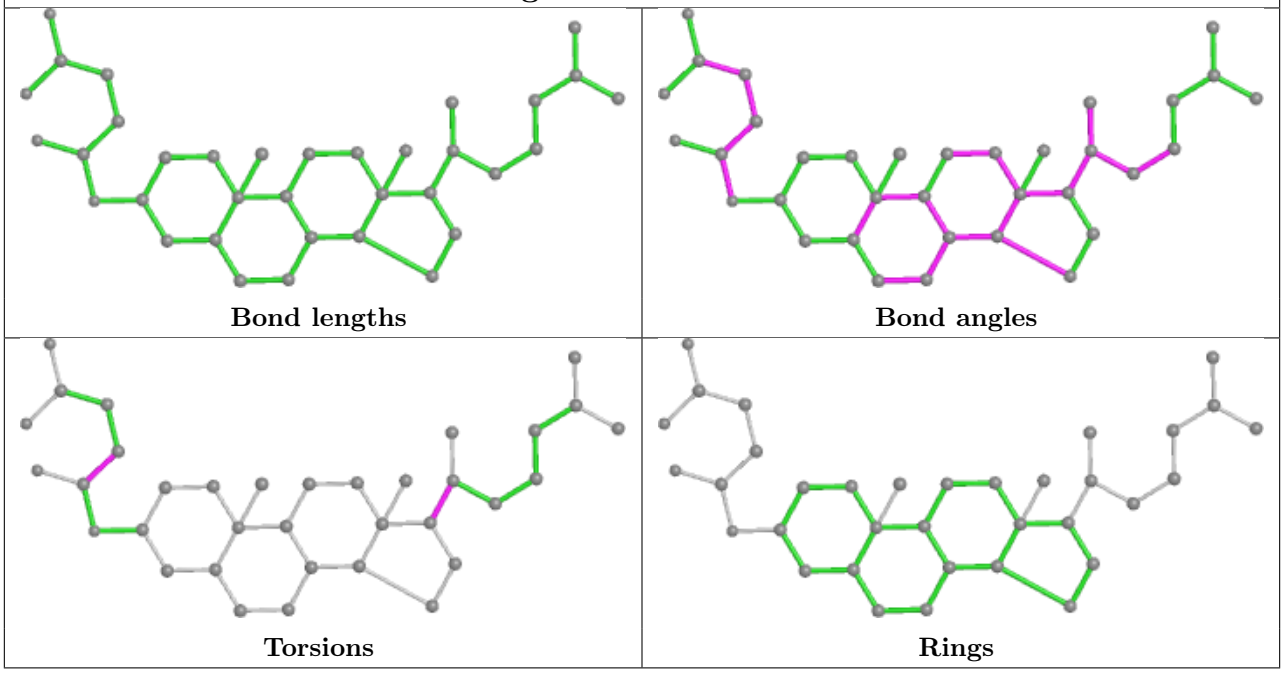
Ligand 3PE A 2321



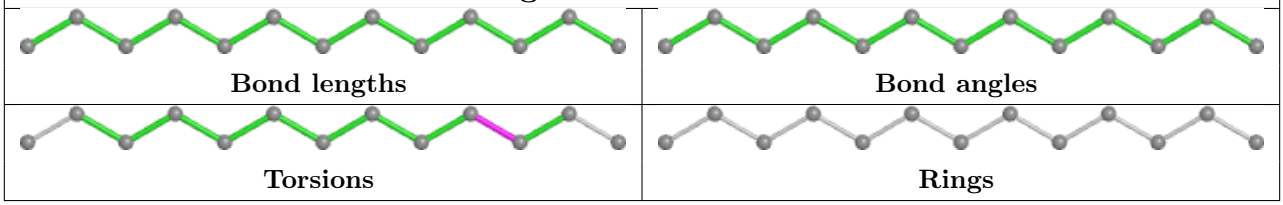
Ligand 3PE A 2320



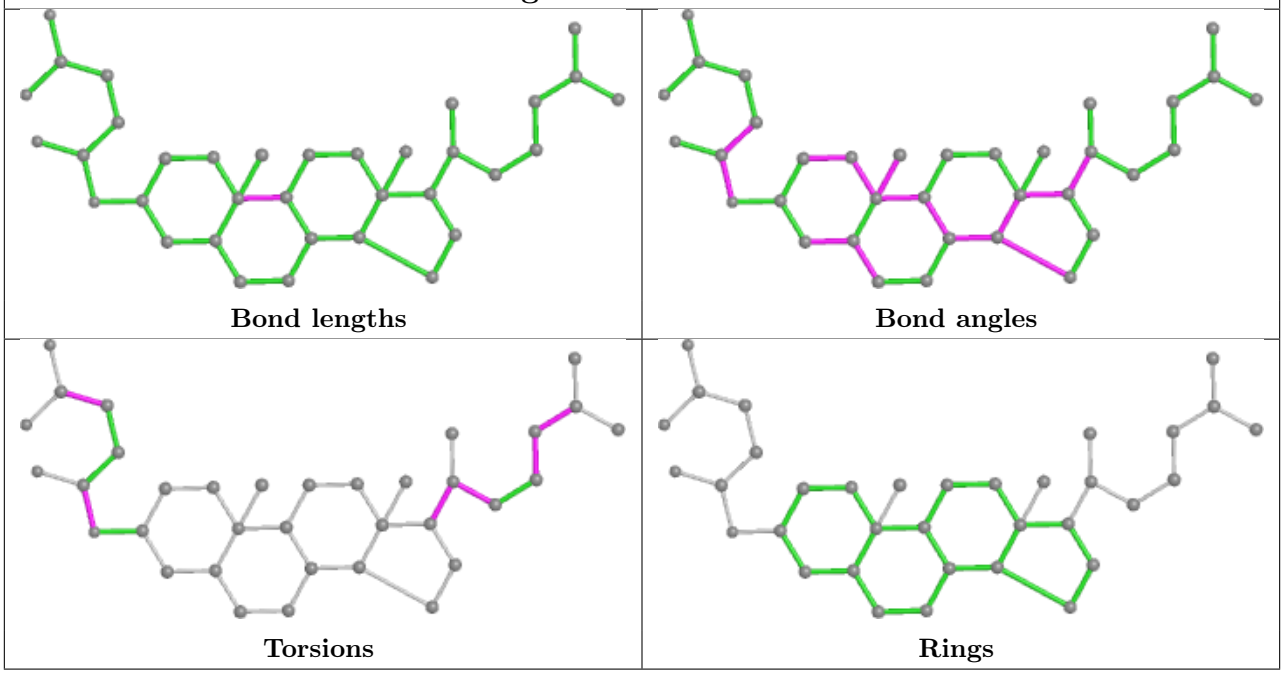
Ligand Y01 A 2315



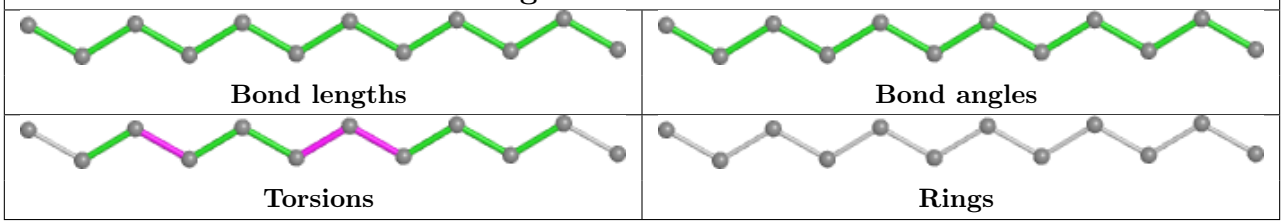
Ligand 3PE A 2318



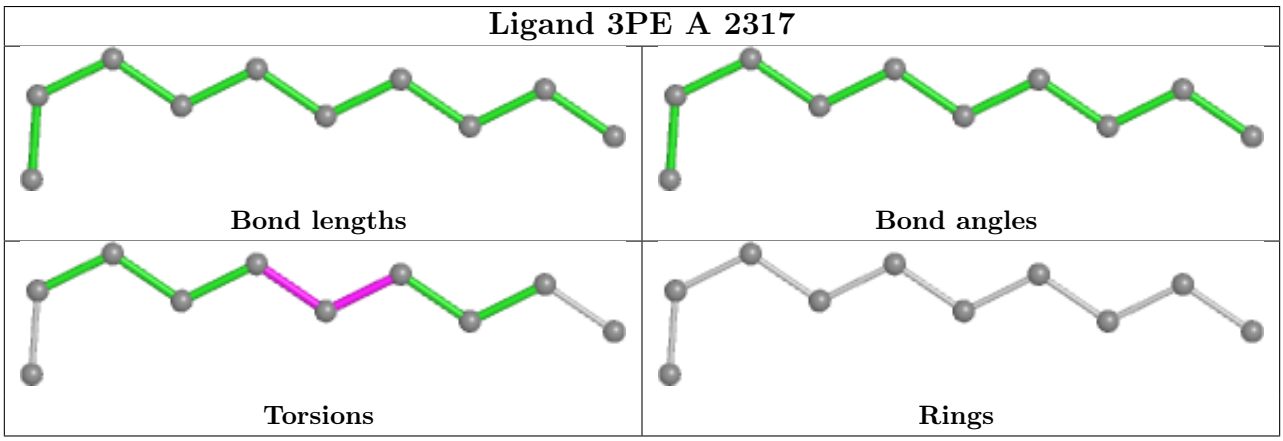
Ligand Y01 A 2311



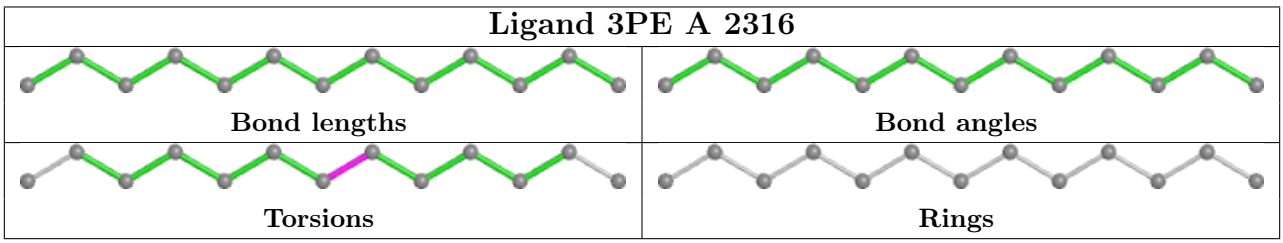
Ligand 3PE A 2314



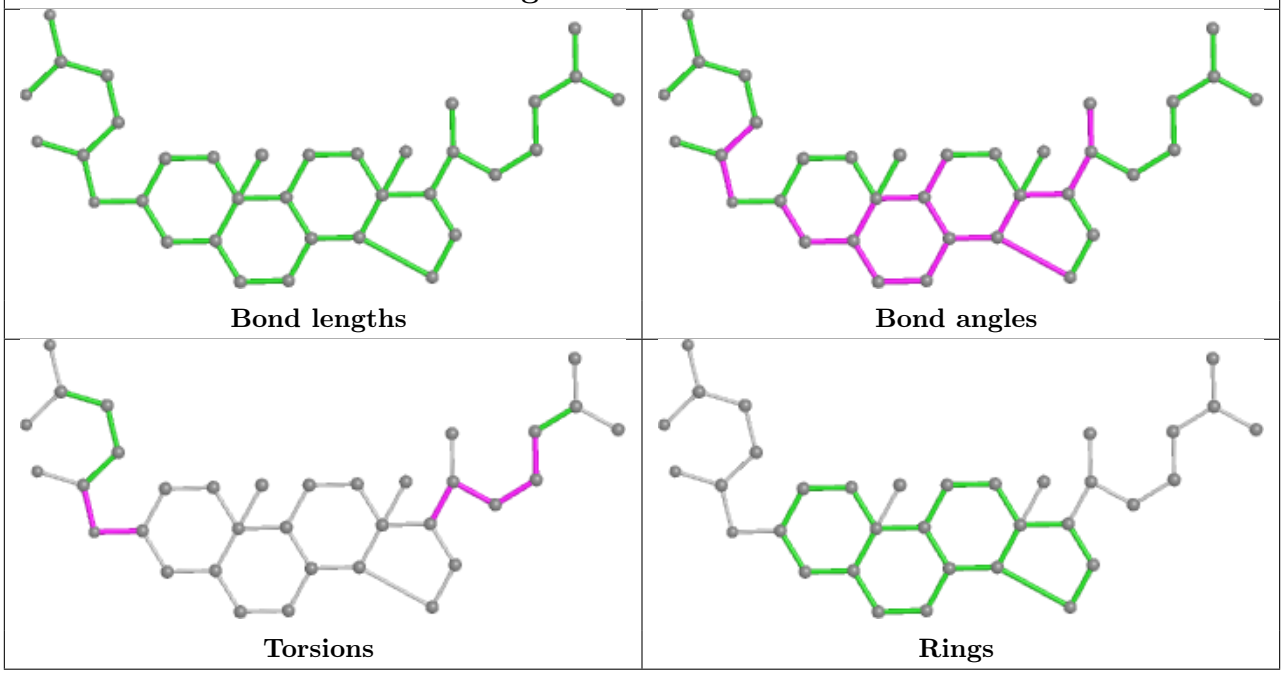
Ligand 3PE A 2317



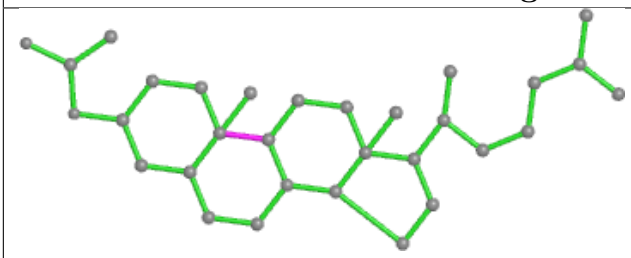
Ligand 3PE A 2316



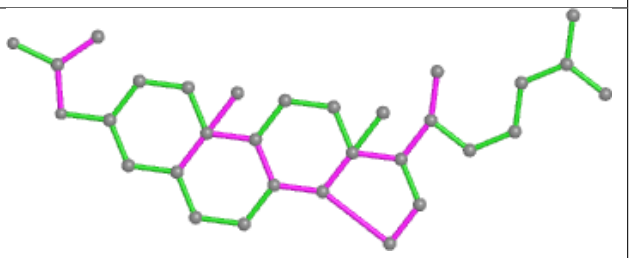
Ligand Y01 A 2312



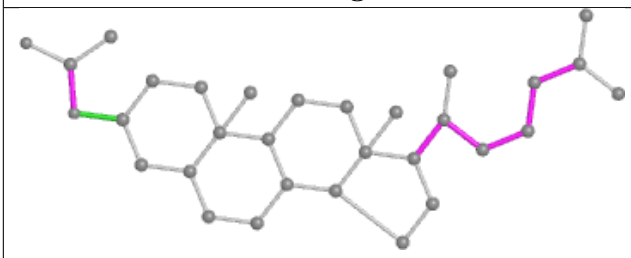
Ligand Y01 A 2310



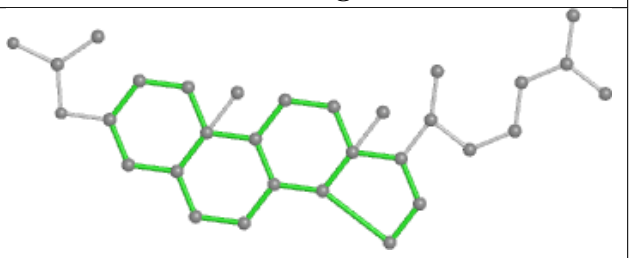
Bond lengths



Bond angles

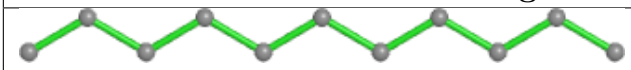


Torsions

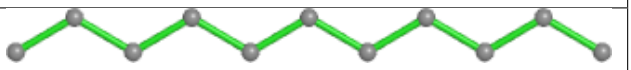


Rings

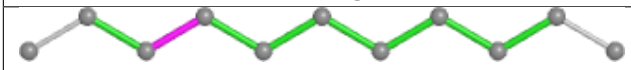
Ligand 3PE A 2306



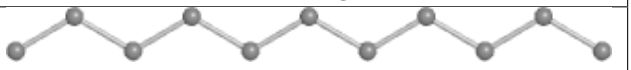
Bond lengths



Bond angles

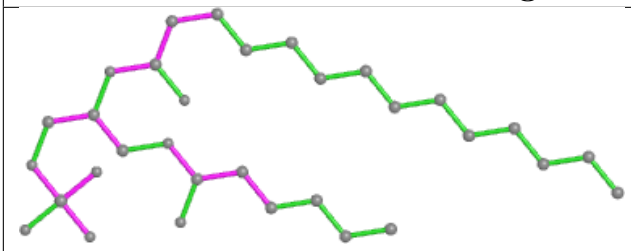


Torsions

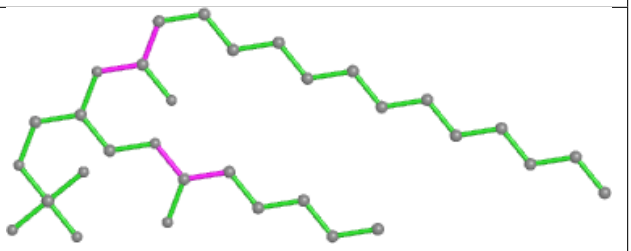


Rings

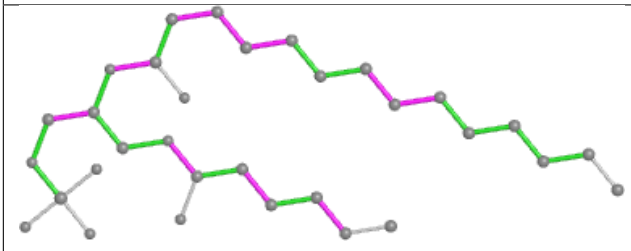
Ligand 3PE A 2305



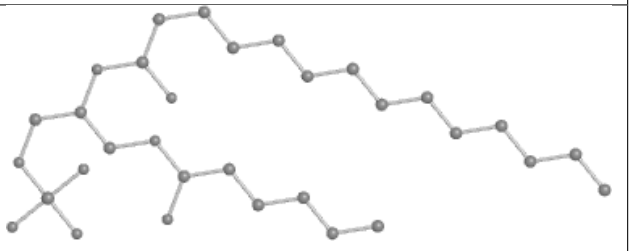
Bond lengths



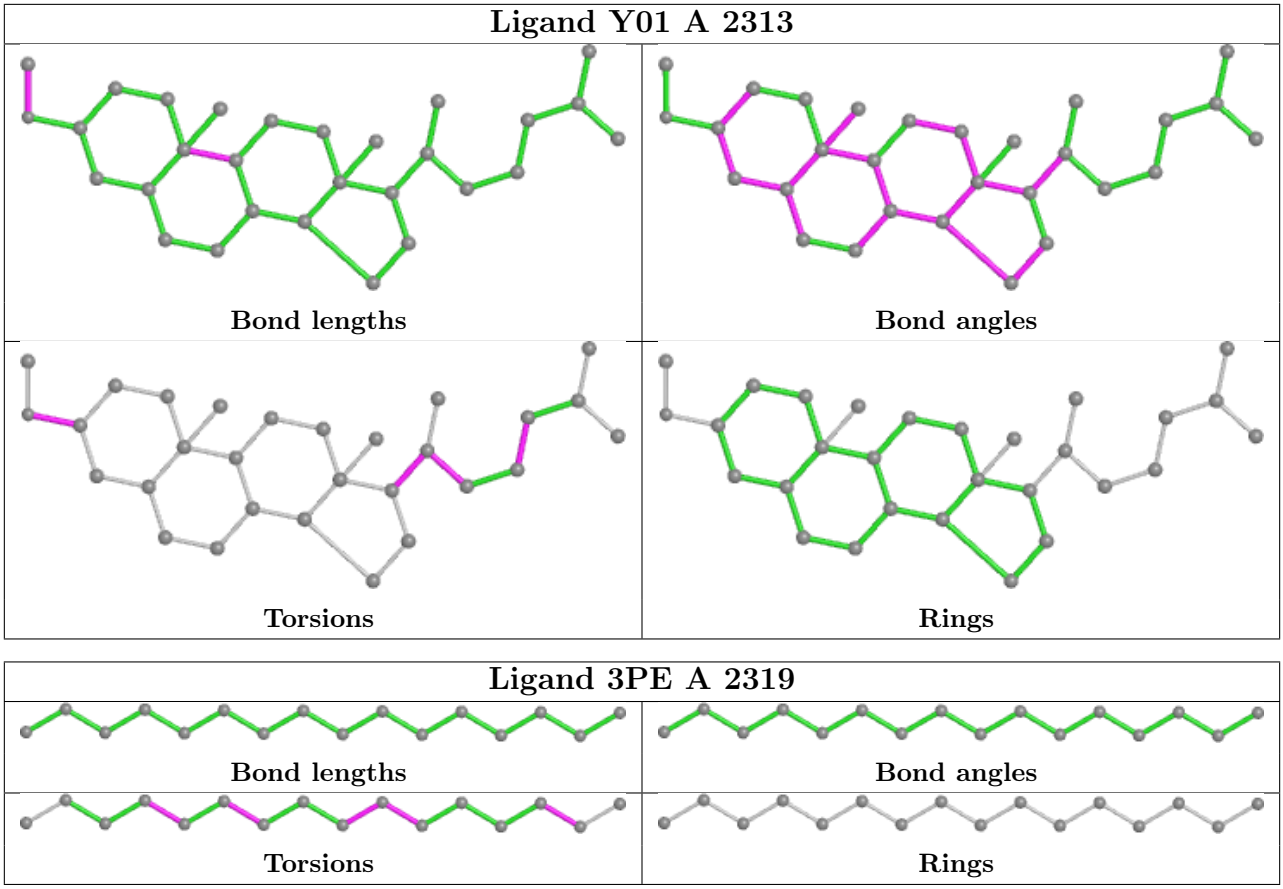
Bond angles



Torsions



Rings



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.

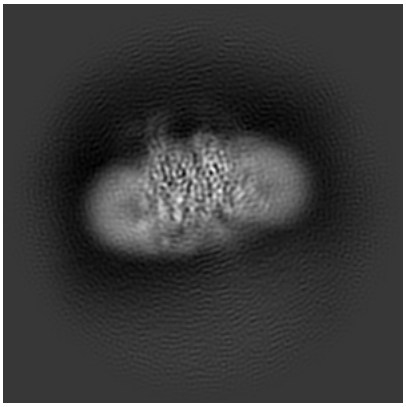
6 Map visualisation

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.

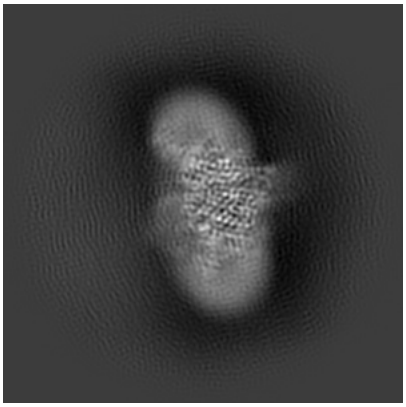
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

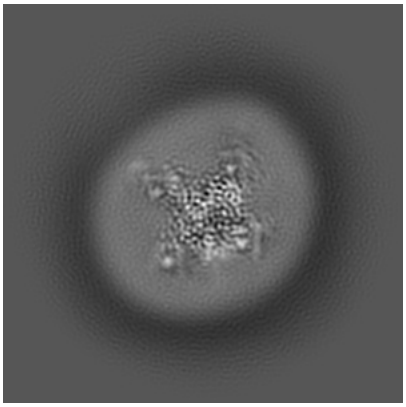
6.1.1 Primary map



X



Y

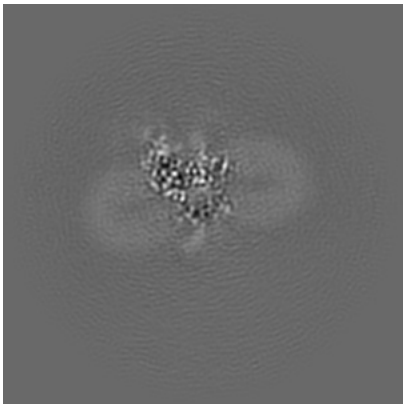


Z

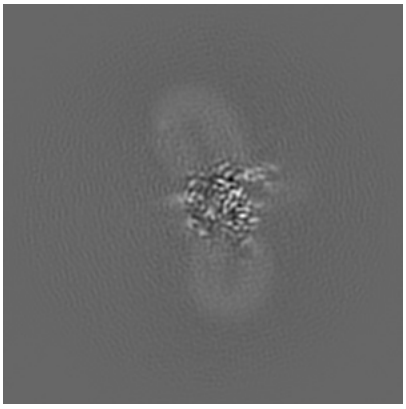
The images above show the map projected in three orthogonal directions.

6.2 Central slices

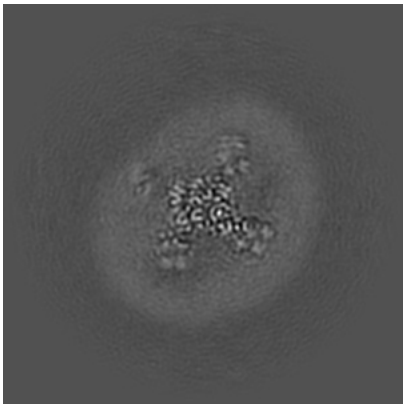
6.2.1 Primary map



X Index: 128



Y Index: 128

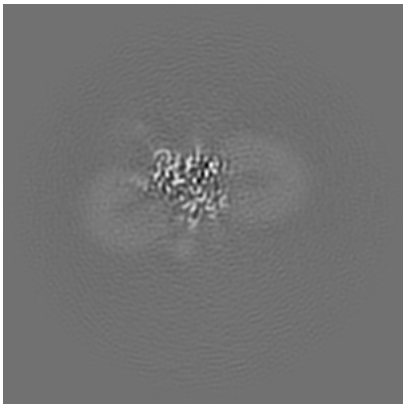


Z Index: 128

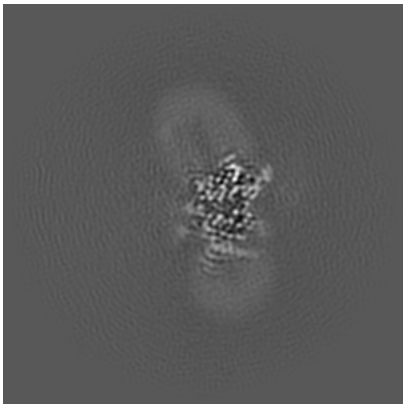
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

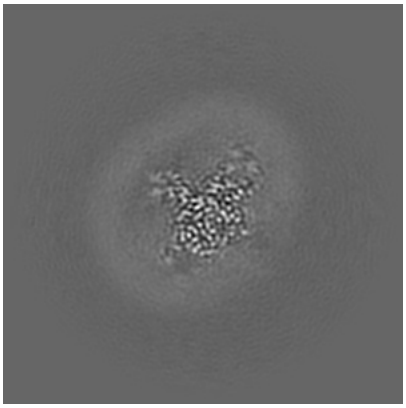
6.3.1 Primary map



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 surface views (i)

6.4.1 Primary map

X

Y

Z

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.

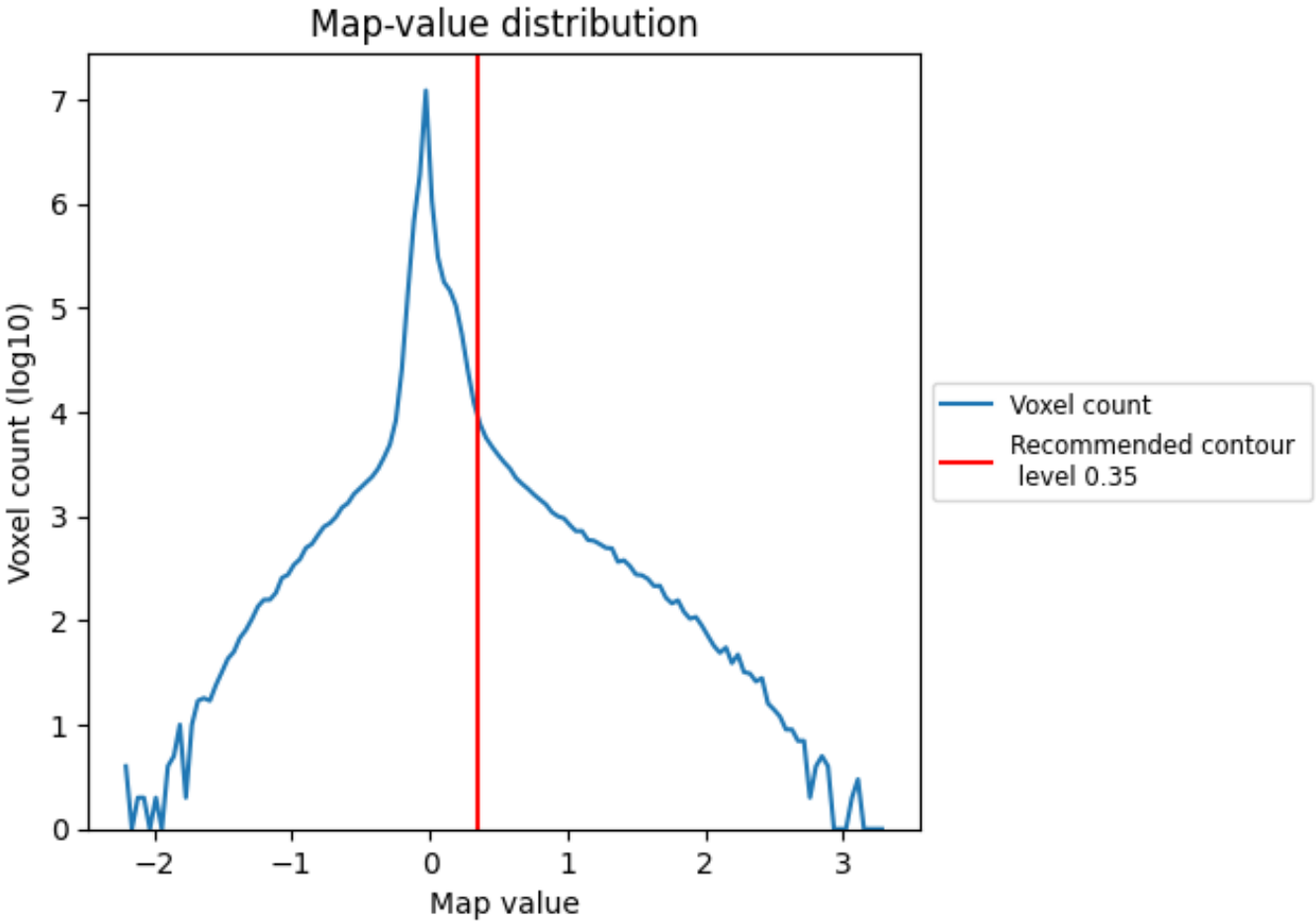
6.5 Mask visualisation (i)

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

7 Map analysis

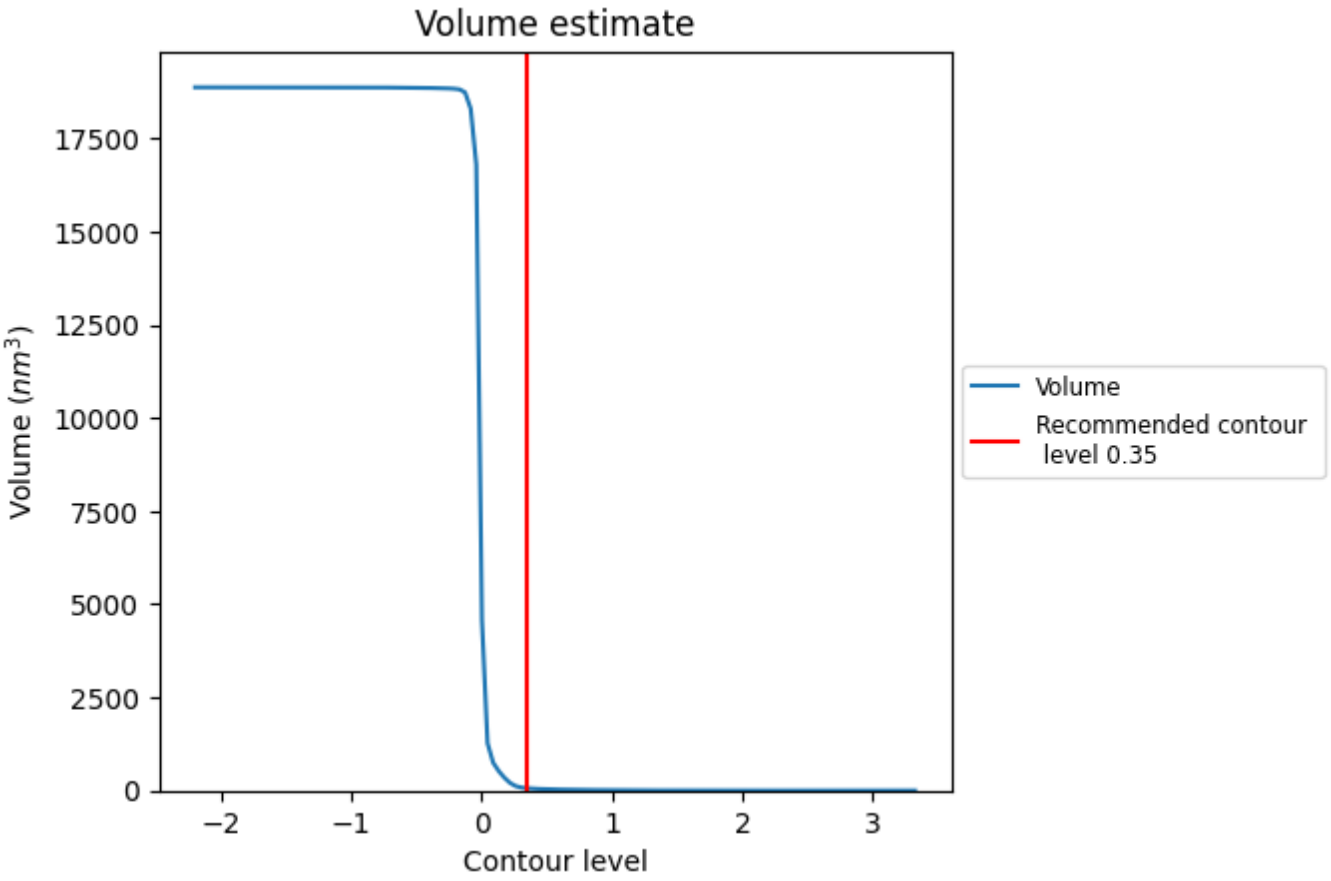
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

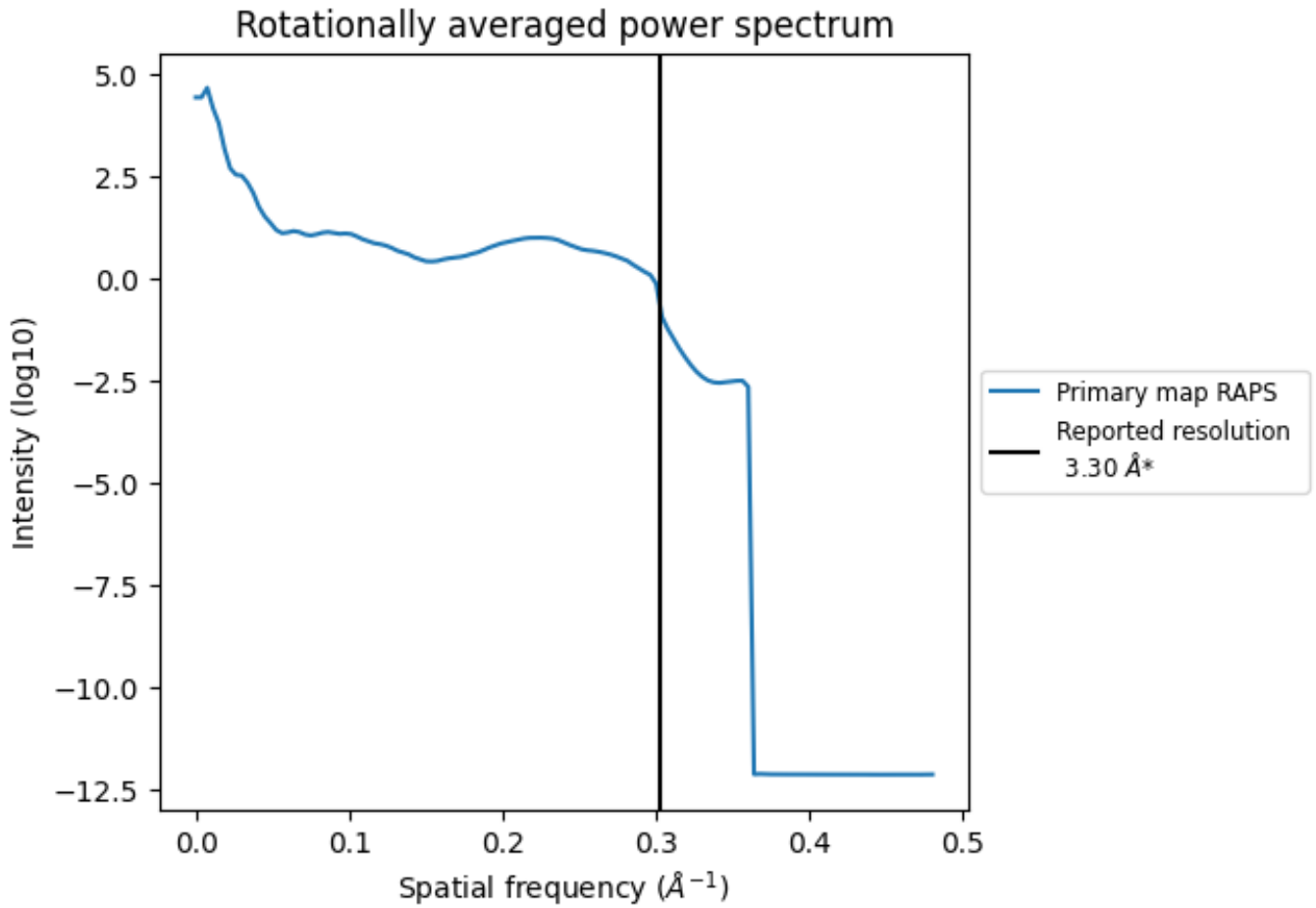
7.2 Volume estimate



The volume at the recommended contour level is 61 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

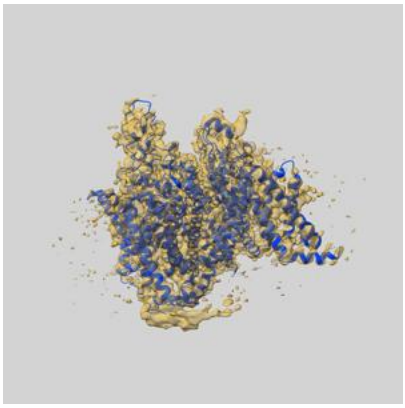
8 Fourier-Shell correlation

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

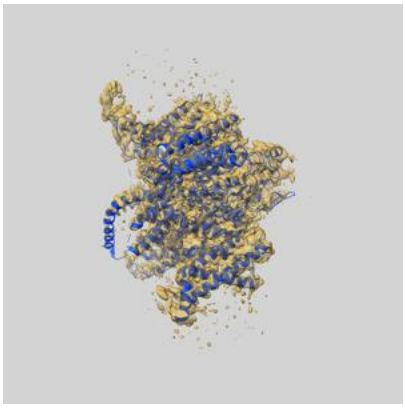
9 Map-model fit

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.

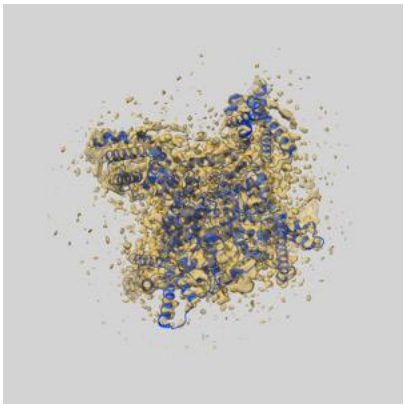
9.1 Map-model overlay



X



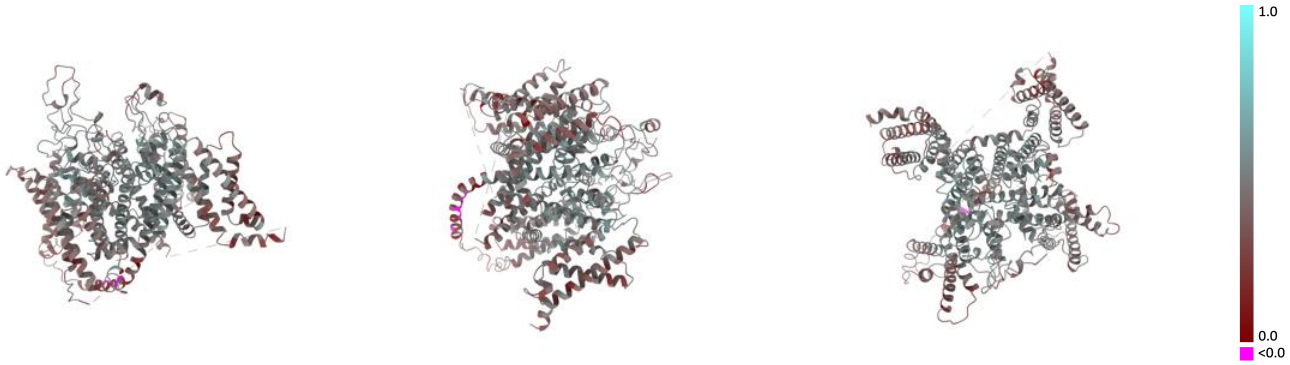
Y



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.

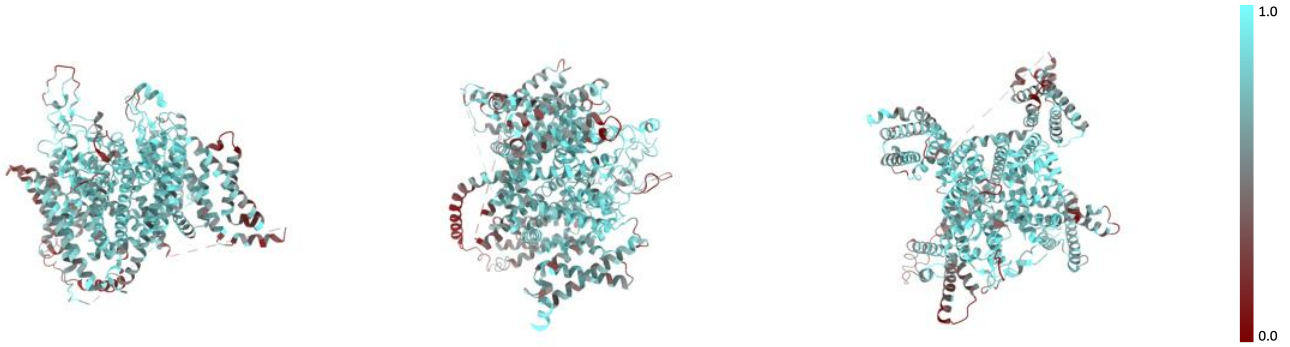
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

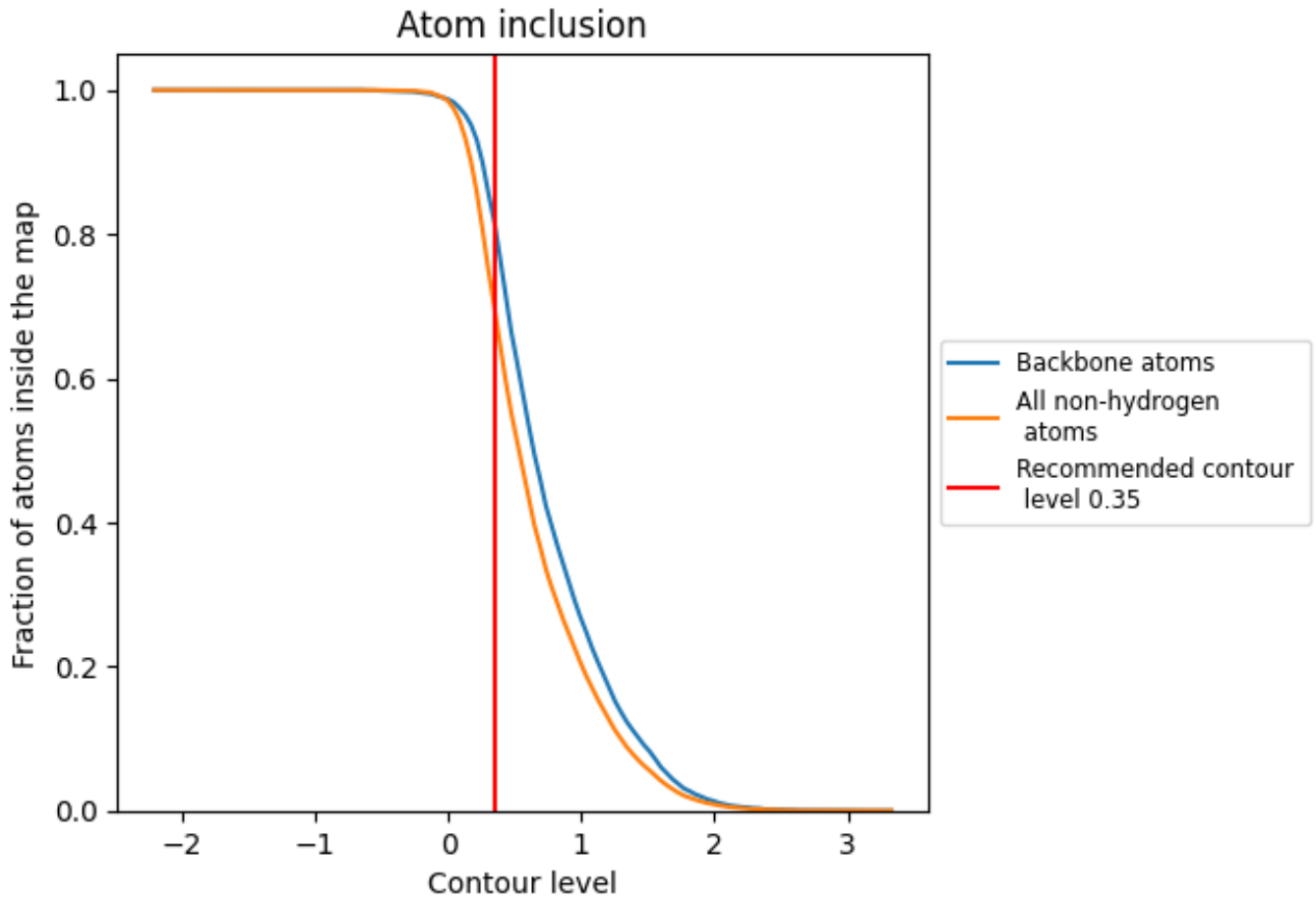
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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	0.6966	0.4430
A	0.6966	0.4430