



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:31 AM UTC

PDB ID : 7FBS / pdb_00007fbs
EMDB ID : EMD-31519
Title : structure of a channel
Authors : Jiang, D.J.; Catterall, W.A.
Deposited on : 2021-07-12
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

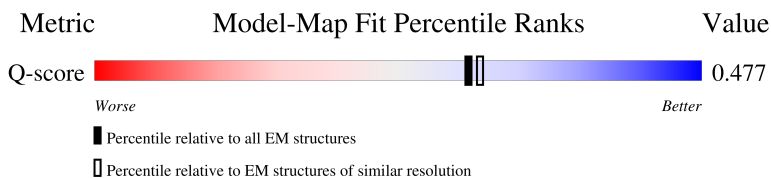
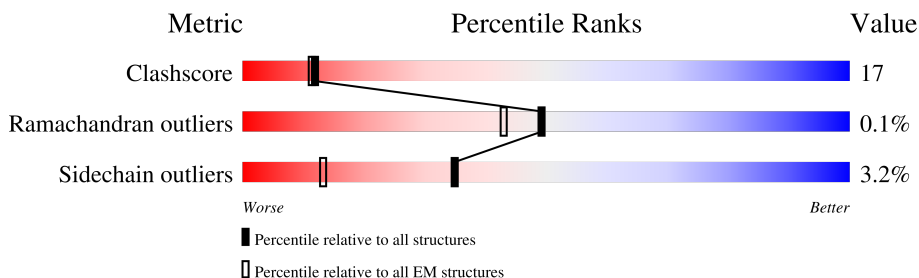
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

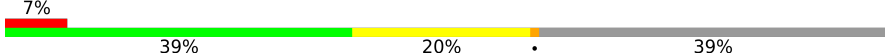
The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1838	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9274 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.

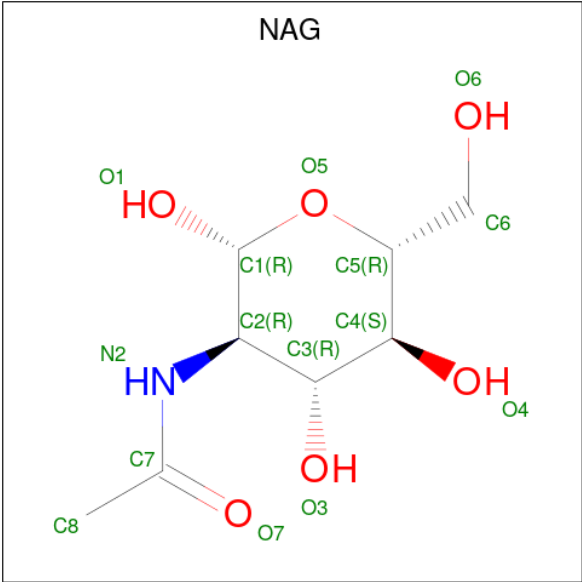
- Molecule 1 is a protein called Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,G protein/GFP fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1118	Total	C	N	O	S	0	0
			8849	5868	1406	1510	65		

There are 22 discrepancies between the modelled and reference sequences:

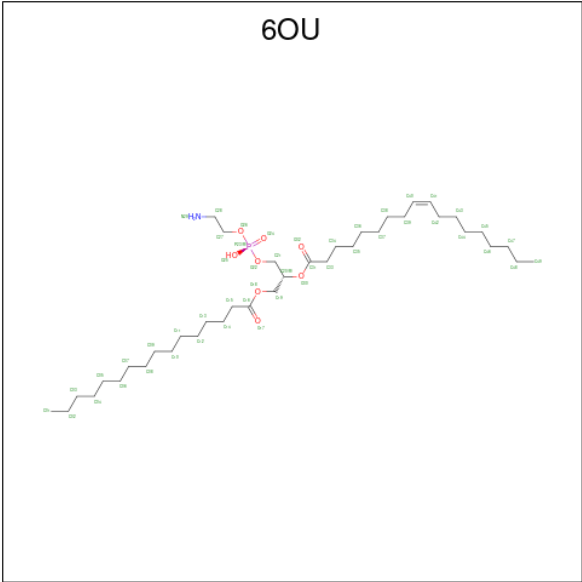
Chain	Residue	Modelled	Actual	Comment	Reference
A	1487	GLN	ILE	engineered mutation	UNP P15389
A	1488	GLN	PHE	engineered mutation	UNP P15389
A	1489	GLN	MET	engineered mutation	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	2147	GLY	-	expression tag	UNP B7UCZ6
A	2148	SER	-	expression tag	UNP B7UCZ6
A	2149	ASP	-	expression tag	UNP B7UCZ6
A	2150	TYR	-	expression tag	UNP B7UCZ6
A	2151	LYS	-	expression tag	UNP B7UCZ6
A	2152	ASP	-	expression tag	UNP B7UCZ6
A	2153	ASP	-	expression tag	UNP B7UCZ6
A	2154	ASP	-	expression tag	UNP B7UCZ6
A	2155	ASP	-	expression tag	UNP B7UCZ6
A	2156	LYS	-	expression tag	UNP B7UCZ6

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



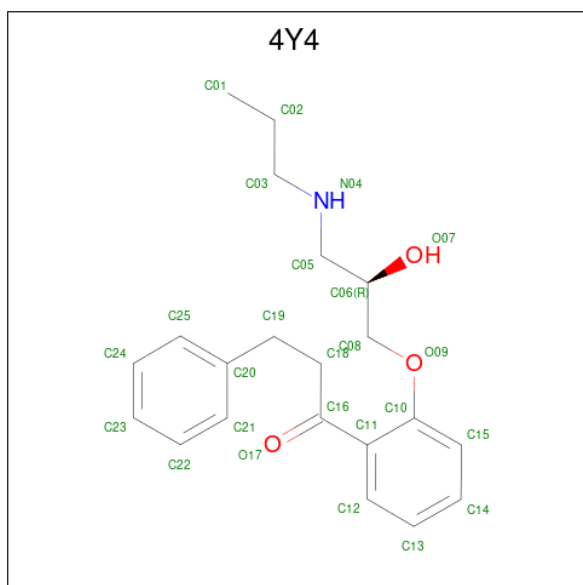
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



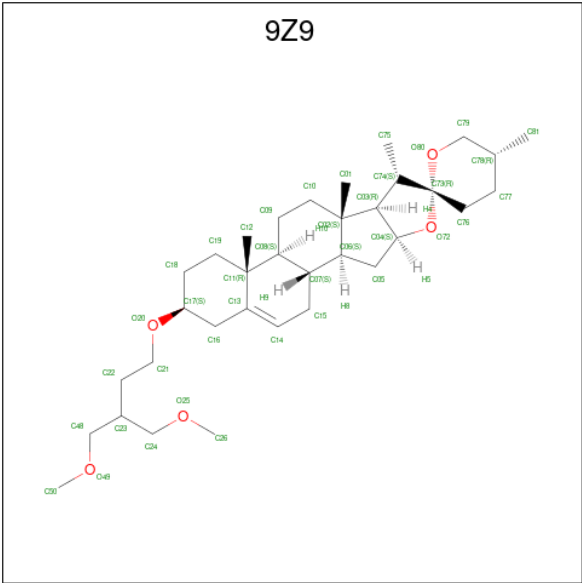
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
3	A	1	Total	C	O			0
			15	12	3			
3	A	1	Total	C	O			0
			26	21	5			
3	A	1	Total	C	O			0
			29	25	4			
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	A	1	Total	C	O			0
			27	23	4			
3	A	1	Total	C	O	P		0
			25	16	8	1		
3	A	1	Total	C	O			0
			17	15	2			
3	A	1	Total	C	O			0
			15	13	2			
3	A	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 4 is 1-[2-[(2R)-2-oxidanyl-3-(propylamino)propoxy]phenyl]-3-phenyl-propan-1-one (CCD ID: 4Y4) (formula: C₂₁H₂₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			25	21	1	3	

- Molecule 5 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).

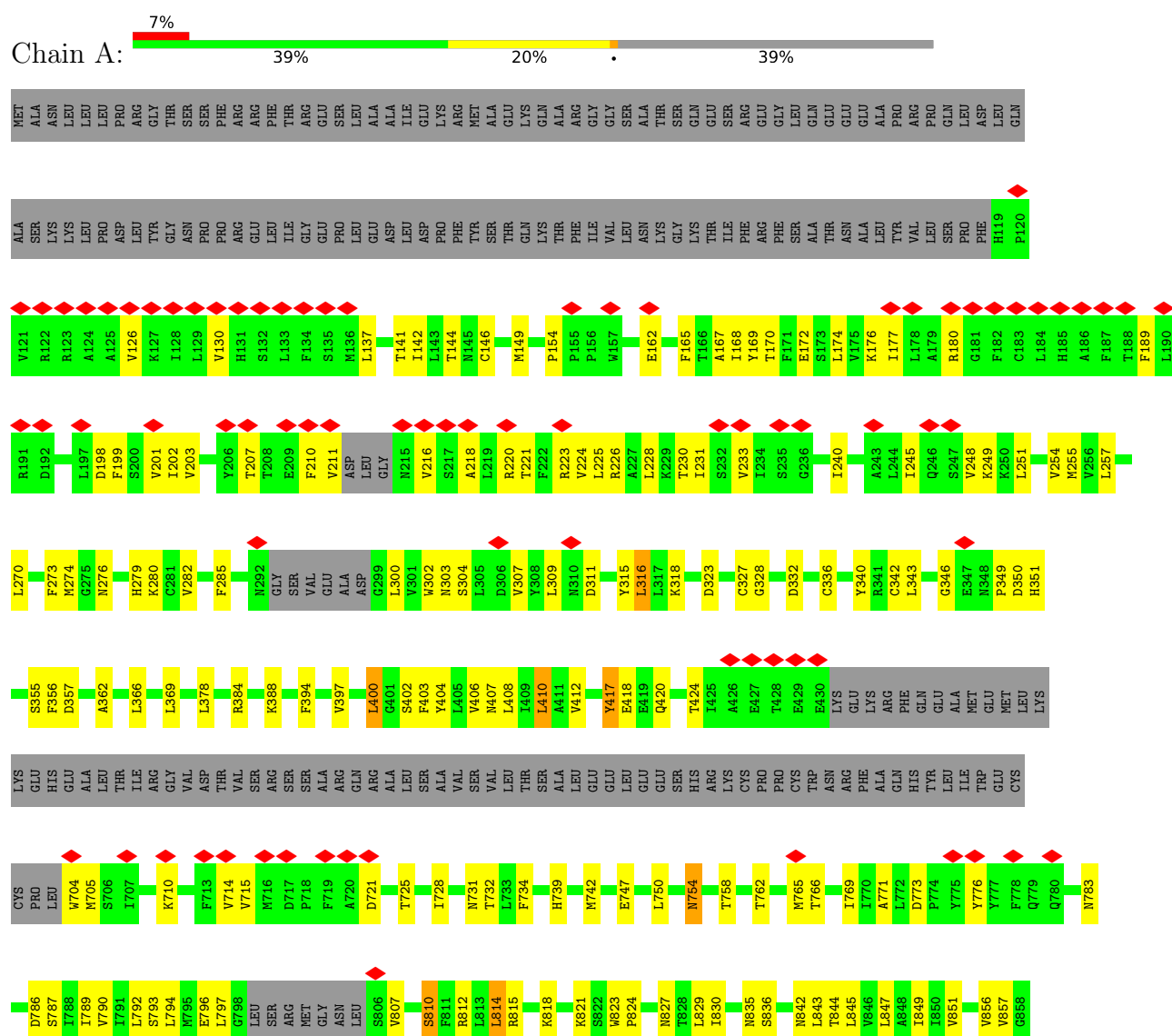


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O		0
			34	31	3		
5	A	1	Total	C	O		0
			30	27	3		

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: Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,G protein/GFP fusion protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	6.486	Depositor
Minimum map value	-3.763	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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: 4Y4, NAG, 9Z9, 6OU

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	0.37	0/9063	0.50	3/12315 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1373	LEU	CA-C-N	6.95	128.53	119.84
1	A	1373	LEU	C-N-CA	6.95	128.53	119.84
1	A	1368	GLN	N-CA-C	5.60	117.38	111.28

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	8849	0	8919	311	0
2	A	42	0	39	8	0
3	A	294	0	0	0	0
4	A	25	0	0	0	0
5	A	64	0	0	13	0
All	All	9274	0	8958	317	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 17.

All (317) 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)
5:A:2216:9Z9:C04	5:A:2216:9Z9:C05	1.77	1.43
5:A:2217:9Z9:C04	5:A:2217:9Z9:C05	1.77	1.40
1:A:403:PHE:HB3	5:A:2217:9Z9:C81	1.61	1.29
1:A:257:LEU:HD12	1:A:1645:ILE:HA	1.33	1.09
1:A:418:GLU:HG2	5:A:2216:9Z9:C22	1.90	1.01
1:A:154:PRO:HG2	1:A:220:ARG:HH22	1.29	0.96
1:A:307:VAL:O	1:A:311:ASP:CB	2.18	0.92
1:A:210:PHE:CD2	1:A:211:VAL:HG13	2.12	0.84
1:A:931:LEU:O	1:A:935:ASN:ND2	2.11	0.82
1:A:162:GLU:HG2	1:A:223:ARG:HH12	1.44	0.81
1:A:316:LEU:HD23	1:A:316:LEU:O	1.80	0.81
1:A:1390:ASN:ND2	2:A:2201:NAG:O7	2.15	0.79
1:A:794:LEU:HA	1:A:797:LEU:HD12	1.66	0.78
1:A:1537:MET:HE1	1:A:1641:GLY:HA3	1.66	0.77
1:A:1273:TRP:CH2	1:A:1316:LEU:HB3	2.20	0.76
1:A:350:ASP:OD1	1:A:351:HIS:N	2.17	0.76
1:A:1670:MET:O	1:A:1674:SER:OG	2.04	0.75
1:A:856:VAL:HA	1:A:859:MET:HG2	1.68	0.74
1:A:282:VAL:HG21	1:A:343:LEU:HD12	1.69	0.74
1:A:223:ARG:HD2	1:A:226:ARG:NH1	2.02	0.74
1:A:1365:CYS:HB3	1:A:1439:GLN:HE22	1.52	0.74
1:A:388:LYS:HE2	1:A:1693:MET:HG3	1.70	0.73
1:A:154:PRO:HG2	1:A:220:ARG:NH2	2.05	0.72
1:A:309:LEU:O	1:A:309:LEU:HD23	1.90	0.70
1:A:257:LEU:HD13	1:A:1648:LEU:HD12	1.72	0.70
1:A:1640:ARG:O	1:A:1646:ARG:NH1	2.24	0.70
1:A:309:LEU:HD23	1:A:309:LEU:C	2.17	0.70
1:A:316:LEU:HD23	1:A:316:LEU:C	2.16	0.69
1:A:154:PRO:CG	1:A:220:ARG:HH22	2.04	0.69
1:A:400:LEU:O	1:A:404:TYR:HB3	1.93	0.69
1:A:1544:MET:HG2	1:A:1548:MET:HE3	1.75	0.68
1:A:1517:ASN:HB2	1:A:1520:GLN:HB2	1.74	0.68
1:A:257:LEU:HD12	1:A:1645:ILE:CA	2.18	0.67
1:A:1365:CYS:HB2	1:A:1397:TRP:CD1	2.31	0.66
1:A:1459:GLY:O	1:A:1463:THR:OG1	2.10	0.66
1:A:332:ASP:HB3	1:A:388:LYS:H	1.62	0.65
1:A:1514:ARG:HG2	1:A:1516:LEU:H	1.61	0.65
1:A:146:CYS:HA	1:A:149:MET:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2201:NAG:O4	2:A:2202:NAG:O7	2.13	0.65
1:A:216:VAL:HG13	1:A:218:ALA:H	1.61	0.65
1:A:384:ARG:NH1	1:A:1692:ASP:OD1	2.30	0.64
1:A:220:ARG:HG3	1:A:223:ARG:HH21	1.62	0.64
1:A:786:ASP:OD1	1:A:789:ILE:HD11	1.97	0.64
1:A:273:PHE:HA	1:A:276:ASN:HD22	1.64	0.63
1:A:873:ILE:HD11	1:A:908:ASP:HB3	1.81	0.63
1:A:280:LYS:HD3	1:A:315:TYR:CE2	2.33	0.63
1:A:1273:TRP:CZ3	1:A:1316:LEU:HB2	2.33	0.62
1:A:165:PHE:HA	1:A:168:ILE:HD12	1.80	0.62
1:A:1365:CYS:HB2	1:A:1397:TRP:HD1	1.63	0.62
1:A:410:LEU:HD23	5:A:2216:9Z9:C76	2.29	0.62
1:A:369:LEU:HD21	1:A:378:LEU:HD23	1.81	0.62
1:A:407:ASN:HD21	1:A:1773:ILE:HD11	1.65	0.61
1:A:766:THR:HA	1:A:769:ILE:HD12	1.82	0.61
1:A:1358:PHE:HA	1:A:1361:LYS:HD2	1.80	0.61
1:A:257:LEU:HD13	1:A:1648:LEU:CD1	2.30	0.61
1:A:1344:LEU:O	1:A:1411:TYR:OH	2.18	0.61
1:A:823:TRP:HZ3	1:A:1345:ILE:HG13	1.66	0.60
1:A:1234:ARG:HB3	1:A:1237:ILE:HG22	1.84	0.60
1:A:231:ILE:HD11	1:A:849:ILE:HD12	1.83	0.60
1:A:1494:LYS:HA	1:A:1497:TYR:CD2	2.37	0.60
1:A:1214:ILE:HG12	1:A:1318:ARG:HG2	1.84	0.59
1:A:1709:ILE:HD11	1:A:1718:LEU:HD13	1.84	0.59
1:A:1361:LYS:NZ	1:A:1435:GLY:O	2.21	0.59
1:A:302:TRP:CD2	1:A:307:VAL:HG11	2.37	0.59
1:A:1443:GLU:OE2	1:A:1446:LEU:HD12	2.02	0.59
1:A:773:ASP:OD2	1:A:776:TYR:N	2.36	0.58
1:A:862:PHE:CZ	1:A:921:VAL:HG11	2.39	0.58
1:A:1376:ASN:HB3	1:A:1379:ILE:HG22	1.85	0.58
1:A:1724:ASN:HD22	1:A:1729:TYR:HB3	1.67	0.58
1:A:302:TRP:CG	1:A:307:VAL:HG11	2.38	0.58
1:A:1273:TRP:CE3	1:A:1276:LEU:HD23	2.38	0.58
1:A:1494:LYS:HA	1:A:1497:TYR:HD2	1.69	0.57
1:A:1526:ILE:HA	1:A:1529:LYS:NZ	2.19	0.57
1:A:875:ASP:OD1	1:A:875:ASP:N	2.36	0.57
1:A:1273:TRP:CZ3	1:A:1316:LEU:CB	2.88	0.57
1:A:180:ARG:HD2	1:A:189:PHE:HB2	1.87	0.57
1:A:366:LEU:HD12	1:A:366:LEU:N	2.18	0.57
1:A:1368:GLN:OE1	1:A:1368:GLN:HA	2.05	0.56
1:A:1220:SER:HB2	1:A:1311:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:CYS:SG	1:A:328:GLY:N	2.78	0.56
1:A:420:GLN:O	1:A:424:THR:HG23	2.06	0.56
1:A:162:GLU:HG2	1:A:223:ARG:NH1	2.19	0.56
1:A:418:GLU:CG	5:A:2216:9Z9:C22	2.74	0.56
1:A:715:VAL:HG21	1:A:771:ALA:HA	1.87	0.56
1:A:1397:TRP:H	2:A:2201:NAG:H82	1.69	0.56
1:A:823:TRP:CZ3	1:A:1345:ILE:HG13	2.40	0.56
1:A:1273:TRP:HH2	1:A:1316:LEU:HD23	1.71	0.56
1:A:1611:SER:HA	1:A:1614:ILE:HD11	1.88	0.56
1:A:257:LEU:CD1	1:A:1645:ILE:HA	2.22	0.56
1:A:327:CYS:SG	1:A:342:CYS:SG	3.01	0.56
1:A:1632:ILE:O	1:A:1635:ILE:HG12	2.06	0.55
1:A:1526:ILE:HA	1:A:1529:LYS:HZ1	1.70	0.55
1:A:734:PHE:CE2	1:A:750:LEU:HA	2.42	0.55
1:A:1676:PHE:O	1:A:1680:ASN:ND2	2.40	0.55
1:A:1363:GLY:HA3	1:A:1397:TRP:CH2	2.42	0.55
1:A:1490:THR:HA	1:A:1493:GLN:HG2	1.87	0.55
1:A:827:ASN:HA	1:A:830:ILE:HG12	1.89	0.55
1:A:315:TYR:CD1	1:A:315:TYR:N	2.71	0.54
1:A:1698:THR:HG22	1:A:1699:PHE:H	1.71	0.54
1:A:786:ASP:O	1:A:790:VAL:HG23	2.07	0.54
1:A:890:ALA:O	1:A:894:ILE:HG12	2.07	0.54
1:A:1394:GLU:HG3	1:A:1395:LEU:HD22	1.89	0.54
5:A:2216:9Z9:C75	5:A:2216:9Z9:C78	2.86	0.54
5:A:2216:9Z9:C75	5:A:2216:9Z9:C77	2.85	0.54
1:A:710:LYS:O	1:A:714:VAL:HG23	2.08	0.53
1:A:792:LEU:O	1:A:796:GLU:HG3	2.08	0.53
1:A:1273:TRP:CH2	1:A:1316:LEU:CB	2.91	0.53
1:A:1545:VAL:O	1:A:1549:VAL:HG23	2.08	0.53
1:A:1628:ARG:CZ	1:A:1631:ARG:HH12	2.21	0.53
1:A:789:ILE:HD13	1:A:815:ARG:HD3	1.90	0.53
1:A:1686:TRP:NE1	1:A:1695:ASN:OD1	2.42	0.53
1:A:721:ASP:O	1:A:725:THR:HG23	2.08	0.53
1:A:223:ARG:HD2	1:A:226:ARG:HH12	1.71	0.53
1:A:280:LYS:HD3	1:A:315:TYR:CD2	2.43	0.53
1:A:845:LEU:O	1:A:849:ILE:HG12	2.07	0.53
1:A:1434:ARG:NH2	1:A:1439:GLN:O	2.42	0.53
1:A:1372:ASP:HB3	1:A:1373:LEU:HD13	1.90	0.53
1:A:1772:ILE:HG21	5:A:2217:9Z9:C75	2.39	0.53
1:A:1417:VAL:HA	1:A:1423:TRP:HB3	1.91	0.52
1:A:254:VAL:HG21	1:A:412:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1595:ILE:O	1:A:1599:VAL:HG23	2.10	0.52
1:A:1601:VAL:O	1:A:1605:ILE:HG13	2.10	0.52
5:A:2216:9Z9:C22	5:A:2216:9Z9:C23	2.88	0.52
1:A:1434:ARG:HA	1:A:1444:ASP:OD2	2.09	0.52
1:A:793:SER:HA	1:A:796:GLU:CD	2.35	0.52
1:A:1347:TRP:O	1:A:1351:SER:OG	2.21	0.52
1:A:355:SER:HB3	1:A:357:ASP:H	1.75	0.51
1:A:1602:ILE:O	1:A:1606:VAL:HG13	2.11	0.51
1:A:1351:SER:O	1:A:1355:VAL:HG23	2.10	0.51
1:A:230:THR:HA	1:A:233:VAL:HB	1.93	0.51
1:A:829:LEU:HD21	1:A:1346:PHE:CD1	2.46	0.51
1:A:842:ASN:OD1	1:A:843:LEU:HD12	2.11	0.51
1:A:1458:PHE:HA	1:A:1462:PHE:HD2	1.76	0.51
1:A:762:THR:HG21	1:A:794:LEU:HD21	1.92	0.51
1:A:356:PHE:HE1	1:A:366:LEU:HD11	1.75	0.51
1:A:394:PHE:HA	1:A:397:VAL:HG12	1.93	0.50
1:A:1606:VAL:HA	1:A:1609:VAL:HG22	1.93	0.50
1:A:786:ASP:O	1:A:789:ILE:HG13	2.11	0.50
1:A:937:PHE:CE1	1:A:1464:LEU:HD23	2.47	0.50
1:A:202:ILE:HD12	1:A:203:VAL:N	2.27	0.50
1:A:894:ILE:O	1:A:898:LEU:HG	2.12	0.50
1:A:704:TRP:HB3	1:A:705:MET:HE2	1.93	0.49
1:A:1390:ASN:HD21	2:A:2201:NAG:C1	2.26	0.49
1:A:248:VAL:HG23	1:A:249:LYS:HD2	1.94	0.49
1:A:937:PHE:HZ	1:A:1464:LEU:HG	1.78	0.49
1:A:1219:LEU:HG	1:A:1248:PHE:HZ	1.76	0.49
1:A:1537:MET:HA	1:A:1540:ILE:HG22	1.94	0.49
1:A:198:ASP:HA	1:A:201:VAL:HB	1.94	0.49
1:A:765:MET:O	1:A:769:ILE:HG13	2.13	0.49
1:A:1338:ASN:OD1	1:A:1339:VAL:N	2.45	0.49
1:A:228:LEU:HA	1:A:231:ILE:HD13	1.93	0.49
1:A:824:PRO:HA	1:A:827:ASN:ND2	2.27	0.48
1:A:1410:GLY:O	1:A:1414:LEU:HG	2.13	0.48
1:A:1540:ILE:HD11	1:A:1634:ARG:HB3	1.95	0.48
1:A:316:LEU:HB2	1:A:340:TYR:CE1	2.48	0.48
1:A:1373:LEU:CD1	1:A:1373:LEU:N	2.76	0.48
1:A:315:TYR:OH	1:A:346:GLY:HA2	2.13	0.48
1:A:1593:TRP:HB3	1:A:1640:ARG:HD3	1.96	0.48
1:A:835:ASN:HD22	1:A:943:SER:HB3	1.79	0.48
1:A:1727:PRO:N	1:A:1728:PRO:HD2	2.29	0.48
1:A:1273:TRP:HZ3	1:A:1316:LEU:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:SG	1:A:342:CYS:HB3	2.54	0.48
1:A:836:SER:O	1:A:844:THR:OG1	2.29	0.48
1:A:1722:ILE:HG13	1:A:1754:PHE:HE2	1.78	0.48
1:A:388:LYS:HD3	1:A:1704:LEU:HD11	1.96	0.47
1:A:397:VAL:O	1:A:397:VAL:HG22	2.14	0.47
1:A:309:LEU:C	1:A:309:LEU:CD2	2.85	0.47
1:A:812:ARG:HB3	1:A:815:ARG:NH2	2.28	0.47
1:A:1316:LEU:HD23	1:A:1326:VAL:HG21	1.97	0.47
1:A:199:PHE:O	1:A:203:VAL:HG23	2.13	0.47
1:A:861:LEU:HD22	1:A:917:LEU:HD21	1.96	0.47
1:A:1450:ILE:O	1:A:1454:VAL:HG23	2.14	0.47
1:A:1727:PRO:HG3	2:A:2202:NAG:H2	1.97	0.47
1:A:303:ASN:O	1:A:307:VAL:HB	2.14	0.47
1:A:167:ALA:O	1:A:170:THR:OG1	2.26	0.47
1:A:402:SER:O	1:A:406:VAL:HB	2.15	0.47
1:A:1570:VAL:HG11	1:A:1608:THR:HG21	1.96	0.47
1:A:224:VAL:HG11	1:A:857:VAL:HG22	1.97	0.47
1:A:1221:SER:O	1:A:1224:LEU:HB2	2.15	0.47
1:A:1288:LEU:O	1:A:1292:THR:HG22	2.15	0.47
1:A:1333:ILE:N	1:A:1334:PRO:HD2	2.30	0.47
1:A:1383:LYS:HB3	1:A:1437:GLU:HB3	1.96	0.47
1:A:248:VAL:HA	1:A:251:LEU:HD12	1.97	0.47
1:A:897:ILE:HD11	1:A:922:PHE:CD2	2.50	0.47
1:A:1358:PHE:HZ	1:A:1451:TYR:CD2	2.33	0.47
1:A:270:LEU:O	1:A:274:MET:HB2	2.15	0.46
1:A:1253:VAL:O	1:A:1257:LEU:HG	2.15	0.46
1:A:174:LEU:HA	1:A:177:ILE:HG22	1.97	0.46
1:A:1561:ILE:O	1:A:1565:ILE:HG13	2.14	0.46
1:A:1297:GLU:HA	1:A:1302:LYS:HB2	1.97	0.46
1:A:404:TYR:CE1	1:A:1652:LEU:HB2	2.51	0.46
1:A:417:TYR:HE2	1:A:935:ASN:OD1	1.98	0.46
1:A:1281:VAL:O	1:A:1285:LEU:HG	2.15	0.46
1:A:1675:ILE:HA	1:A:1678:MET:HE3	1.98	0.46
1:A:1523:ILE:HA	1:A:1526:ILE:HG13	1.98	0.46
1:A:1368:GLN:N	1:A:1394:GLU:O	2.48	0.46
1:A:362:ALA:O	1:A:366:LEU:HD13	2.16	0.46
1:A:303:ASN:OD1	1:A:304:SER:N	2.48	0.45
1:A:257:LEU:CD1	1:A:1645:ILE:HG13	2.46	0.45
1:A:1282:ASP:O	1:A:1286:VAL:HG23	2.16	0.45
1:A:1537:MET:HG3	1:A:1638:LEU:CD2	2.46	0.45
1:A:1457:ILE:O	1:A:1461:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1543:ASN:ND2	1:A:1634:ARG:HD2	2.31	0.45
1:A:1655:SER:O	1:A:1659:LEU:HD12	2.16	0.45
1:A:847:LEU:O	1:A:851:VAL:HG23	2.17	0.45
1:A:1338:ASN:O	1:A:1342:VAL:HG23	2.16	0.45
1:A:1364:ARG:HA	1:A:1364:ARG:HD2	1.88	0.45
1:A:1695:ASN:H	1:A:1701:ASN:HB3	1.82	0.45
1:A:225:LEU:HA	1:A:228:LEU:HD13	1.99	0.45
1:A:1373:LEU:HA	1:A:1374:PRO:HD3	1.77	0.45
1:A:1273:TRP:HH2	1:A:1316:LEU:CD2	2.30	0.45
1:A:169:TYR:O	1:A:172:GLU:HB3	2.17	0.45
1:A:862:PHE:CE2	1:A:921:VAL:HG11	2.52	0.45
1:A:1396:TYR:O	1:A:1398:THR:HG23	2.17	0.45
1:A:177:ILE:HD12	1:A:180:ARG:HB2	1.99	0.45
1:A:915:GLN:O	1:A:919:LEU:HB2	2.16	0.45
1:A:1224:LEU:HD23	1:A:1224:LEU:HA	1.86	0.45
1:A:1445:ASN:O	1:A:1448:MET:HG2	2.17	0.45
1:A:1531:ALA:HA	1:A:1534:VAL:HG22	1.99	0.45
1:A:1520:GLN:O	1:A:1523:ILE:HG13	2.17	0.44
1:A:1727:PRO:CG	2:A:2202:NAG:H82	2.47	0.44
1:A:728:ILE:O	1:A:732:THR:HG23	2.18	0.44
1:A:1543:ASN:ND2	1:A:1634:ARG:HH11	2.15	0.44
1:A:807:VAL:O	1:A:810:SER:OG	2.36	0.44
1:A:1357:LEU:HD22	1:A:1448:MET:HE1	2.00	0.44
1:A:1495:LYS:HE2	1:A:1495:LYS:HB3	1.86	0.44
1:A:1537:MET:CE	1:A:1641:GLY:HA3	2.42	0.44
1:A:418:GLU:OE2	5:A:2216:9Z9:C22	2.66	0.44
1:A:210:PHE:HD2	1:A:211:VAL:HG13	1.76	0.44
1:A:1207:SER:O	1:A:1211:THR:HG23	2.18	0.44
1:A:1375:LEU:HD11	1:A:1395:LEU:HD11	1.99	0.44
1:A:1568:LEU:O	1:A:1572:ILE:HG13	2.18	0.44
1:A:251:LEU:O	1:A:255:MET:HB2	2.17	0.44
1:A:176:LYS:HB2	1:A:176:LYS:HE2	1.75	0.44
1:A:1206:HIS:CE1	1:A:1208:TRP:HD1	2.35	0.44
1:A:1656:LEU:HD12	1:A:1657:PRO:HD3	2.00	0.44
1:A:1734:LEU:O	1:A:1736:ASN:N	2.51	0.44
1:A:937:PHE:HE1	1:A:1464:LEU:HD23	1.82	0.43
1:A:1368:GLN:HB2	1:A:1394:GLU:O	2.18	0.43
1:A:1293:LEU:O	1:A:1293:LEU:HG	2.17	0.43
1:A:1722:ILE:HG13	1:A:1754:PHE:CE2	2.52	0.43
1:A:257:LEU:CD1	1:A:1648:LEU:HD12	2.44	0.43
1:A:862:PHE:HZ	1:A:921:VAL:HG11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:TRP:HE3	1:A:1276:LEU:HD23	1.83	0.43
1:A:1514:ARG:HD2	1:A:1516:LEU:HD22	2.01	0.43
1:A:1624:PHE:O	1:A:1627:ILE:HG13	2.19	0.43
1:A:896:ARG:HG2	1:A:901:GLU:HB2	2.00	0.43
1:A:221:THR:HG21	1:A:861:LEU:HG	2.01	0.43
1:A:280:LYS:HD2	1:A:346:GLY:HA3	2.01	0.43
1:A:126:VAL:O	1:A:130:VAL:HG12	2.19	0.43
1:A:316:LEU:C	1:A:316:LEU:CD2	2.86	0.43
1:A:1443:GLU:OE2	1:A:1446:LEU:CD1	2.66	0.43
1:A:1656:LEU:N	1:A:1657:PRO:HD2	2.34	0.43
1:A:1752:LEU:O	1:A:1756:THR:OG1	2.20	0.43
1:A:366:LEU:N	1:A:366:LEU:CD1	2.81	0.42
1:A:1347:TRP:HB3	1:A:1414:LEU:HD12	2.01	0.42
1:A:821:LYS:HE3	1:A:821:LYS:HB2	1.83	0.42
1:A:882:TRP:CZ2	1:A:1424:MET:HE1	2.53	0.42
1:A:1396:TYR:HA	2:A:2201:NAG:H82	2.01	0.42
1:A:1517:ASN:HD22	1:A:1520:GLN:HG3	1.85	0.42
1:A:285:PHE:HE2	1:A:304:SER:HA	1.84	0.42
1:A:403:PHE:CB	5:A:2217:9Z9:C81	2.58	0.42
1:A:728:ILE:HD11	1:A:818:LYS:CE	2.49	0.42
1:A:1195:ARG:O	1:A:1199:THR:OG1	2.32	0.42
1:A:1531:ALA:O	1:A:1535:THR:HG22	2.20	0.42
1:A:203:VAL:O	1:A:207:THR:HG23	2.20	0.42
1:A:245:ILE:HG23	1:A:249:LYS:NZ	2.34	0.42
1:A:1311:ARG:HG3	1:A:1314:ARG:NH1	2.34	0.42
1:A:762:THR:O	1:A:766:THR:HG22	2.19	0.42
1:A:1361:LYS:HG2	1:A:1436:TYR:HA	2.01	0.42
1:A:1594:ASN:HA	1:A:1597:ASP:OD2	2.20	0.42
1:A:318:LYS:N	1:A:323:ASP:O	2.34	0.42
1:A:1650:PHE:CE2	1:A:1654:MET:HE2	2.55	0.42
1:A:758:THR:HG21	1:A:797:LEU:HD11	2.02	0.42
1:A:812:ARG:HB3	1:A:815:ARG:HH21	1.84	0.42
1:A:1598:PHE:O	1:A:1601:VAL:HG12	2.19	0.42
1:A:1628:ARG:HG3	1:A:1631:ARG:NH1	2.35	0.42
1:A:1681:PHE:HE2	1:A:1753:PHE:CG	2.37	0.42
1:A:754:ASN:ND2	1:A:812:ARG:HD3	2.35	0.41
1:A:1363:GLY:HA3	1:A:1397:TRP:CZ2	2.55	0.41
1:A:1603:LEU:HA	1:A:1606:VAL:HG22	2.02	0.41
1:A:1726:GLY:O	1:A:1730:CYS:N	2.52	0.41
1:A:1204:VAL:HG21	1:A:1263:TYR:HE2	1.85	0.41
1:A:1541:CYS:O	1:A:1545:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:HG3	1:A:189:PHE:HB2	2.02	0.41
1:A:279:HIS:HA	1:A:343:LEU:O	2.20	0.41
1:A:302:TRP:CD1	1:A:307:VAL:HG21	2.56	0.41
1:A:408:LEU:HD21	1:A:1648:LEU:HD22	2.01	0.41
1:A:814:LEU:H	1:A:814:LEU:HD22	1.85	0.41
1:A:1727:PRO:HG3	2:A:2202:NAG:H82	2.02	0.41
1:A:142:ILE:HD13	1:A:169:TYR:OH	2.20	0.41
1:A:1420:PHE:HE1	1:A:1456:ILE:HD13	1.84	0.41
1:A:349:PRO:HG2	1:A:355:SER:OG	2.20	0.41
1:A:1577:CYS:O	1:A:1581:MET:HG2	2.19	0.41
1:A:1695:ASN:HB3	1:A:1697:GLN:HG3	2.02	0.41
1:A:240:ILE:HD13	1:A:240:ILE:HA	1.83	0.41
1:A:773:ASP:OD1	1:A:776:TYR:HB2	2.20	0.41
1:A:783:ASN:O	1:A:787:SER:OG	2.36	0.41
1:A:790:VAL:O	1:A:794:LEU:HG	2.19	0.41
1:A:842:ASN:OD1	1:A:843:LEU:N	2.54	0.41
1:A:942:LEU:HD13	1:A:942:LEU:HA	1.91	0.41
1:A:1455:PHE:CE1	1:A:1459:GLY:HA3	2.56	0.41
1:A:1431:VAL:HG11	1:A:1449:TYR:CD2	2.56	0.41
1:A:1231:LEU:HD23	1:A:1231:LEU:HA	1.80	0.40
1:A:742:MET:HE3	1:A:747:GLU:HG2	2.02	0.40
1:A:864:LYS:O	1:A:868:GLU:HG2	2.21	0.40
1:A:1692:ASP:OD1	1:A:1692:ASP:N	2.54	0.40
1:A:137:LEU:O	1:A:141:THR:OG1	2.35	0.40
1:A:731:ASN:HD21	1:A:815:ARG:HH21	1.70	0.40
1:A:881:ARG:HD2	1:A:1442:TRP:CZ2	2.56	0.40
1:A:888:PHE:HD2	1:A:1446:LEU:HD21	1.86	0.40
1:A:1340:LEU:O	1:A:1344:LEU:HG	2.22	0.40
1:A:1455:PHE:O	1:A:1459:GLY:N	2.39	0.40
1:A:879:LEU:HD13	1:A:879:LEU:HA	1.84	0.40
1:A:1401:LYS:HE3	1:A:1724:ASN:HB3	2.04	0.40
1:A:1662:ILE:CD1	1:A:1768:MET:HB3	2.51	0.40
1:A:1769:TYR:CE2	5:A:2217:9Z9:C81	3.04	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	1104/1838 (60%)	1021 (92%)	82 (7%)	1 (0%)	48 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1374	PRO

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	947/1612 (59%)	917 (97%)	30 (3%)	34 58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	THR
1	A	300	LEU
1	A	316	LEU
1	A	400	LEU
1	A	410	LEU
1	A	417	TYR
1	A	739	HIS
1	A	754	ASN
1	A	810	SER
1	A	814	LEU

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Mol	Chain	Res	Type
1	A	875	ASP
1	A	879	LEU
1	A	886	ASP
1	A	931	LEU
1	A	1199	THR
1	A	1320	GLU
1	A	1345	ILE
1	A	1351	SER
1	A	1358	PHE
1	A	1364	ARG
1	A	1372	ASP
1	A	1373	LEU
1	A	1379	ILE
1	A	1502	LYS
1	A	1512	ILE
1	A	1595	ILE
1	A	1611	SER
1	A	1656	LEU
1	A	1730	CYS
1	A	1774	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	152	HIS
1	A	407	ASN
1	A	422	GLN
1	A	739	HIS
1	A	754	ASN
1	A	835	ASN
1	A	871	HIS
1	A	889	HIS
1	A	915	GLN
1	A	1327	ASN
1	A	1356	ASN
1	A	1376	ASN
1	A	1390	ASN
1	A	1439	GLN
1	A	1517	ASN
1	A	1543	ASN
1	A	1560	ASN

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Mol	Chain	Res	Type
1	A	1566	ASN
1	A	1701	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 ⓘ

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	6OU	A	2213	-	14,14,48	1.45	3 (21%)	14,14,53	1.01	1 (7%)
3	6OU	A	2204	-	31,31,48	1.09	4 (12%)	34,36,53	1.29	2 (5%)
3	6OU	A	2211	-	24,24,48	1.28	4 (16%)	27,29,53	1.32	2 (7%)
3	6OU	A	2215	-	33,33,48	1.06	4 (12%)	36,38,53	1.22	2 (5%)
5	9Z9	A	2216	-	38,38,44	8.65	24 (63%)	60,61,68	2.46	27 (45%)
4	4Y4	A	2214	-	26,26,26	1.70	6 (23%)	30,32,32	1.03	1 (3%)
3	6OU	A	2205	-	34,34,48	1.05	2 (5%)	37,39,53	1.17	2 (5%)
3	6OU	A	2206	-	14,14,48	0.94	2 (14%)	14,14,53	1.33	1 (7%)
3	6OU	A	2207	-	25,25,48	1.09	4 (16%)	27,27,53	1.33	2 (7%)
2	NAG	A	2203	-	14,14,15	0.40	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	2202	-	14,14,15	0.25	0	17,19,21	0.73	0
3	6OU	A	2208	-	28,28,48	1.16	4 (14%)	30,30,53	1.38	2 (6%)
3	6OU	A	2212	-	16,16,48	1.36	3 (18%)	16,16,53	1.13	1 (6%)
5	9Z9	A	2217	-	35,35,44	8.46	24 (68%)	58,58,68	2.31	23 (39%)
3	6OU	A	2209	-	38,38,48	0.98	4 (10%)	41,43,53	1.18	3 (7%)
3	6OU	A	2210	-	26,26,48	0.95	2 (7%)	27,27,53	1.29	2 (7%)
2	NAG	A	2201	-	14,14,15	0.36	0	17,19,21	0.44	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
3	6OU	A	2213	-	-	5/13/13/52	-
3	6OU	A	2204	-	-	15/35/35/52	-
3	6OU	A	2211	-	-	13/26/26/52	-
3	6OU	A	2215	-	-	17/37/37/52	-
5	9Z9	A	2216	-	-	2/4/92/100	0/6/6/6
4	4Y4	A	2214	-	-	11/19/19/19	0/2/2/2
3	6OU	A	2205	-	-	22/38/38/52	-
3	6OU	A	2206	-	-	5/13/13/52	-
3	6OU	A	2207	-	-	12/27/27/52	-
2	NAG	A	2203	-	-	4/6/23/26	0/1/1/1
2	NAG	A	2202	-	-	2/6/23/26	0/1/1/1
3	6OU	A	2208	-	-	15/29/29/52	-
3	6OU	A	2212	-	-	4/15/15/52	-
5	9Z9	A	2217	-	-	-	0/6/6/6
3	6OU	A	2209	-	-	24/42/42/52	-
3	6OU	A	2210	-	-	18/26/26/52	-
2	NAG	A	2201	-	-	2/6/23/26	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2216	9Z9	C15-C07	-21.88	1.17	1.53
5	A	2217	9Z9	C15-C07	-21.86	1.17	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2216	9Z9	C07-C06	-20.78	1.14	1.53
5	A	2217	9Z9	C07-C06	-20.54	1.15	1.53
5	A	2216	9Z9	C23-C22	19.35	2.88	1.50
5	A	2217	9Z9	C11-C13	-19.13	1.16	1.52
5	A	2216	9Z9	C11-C13	-19.12	1.16	1.52
5	A	2216	9Z9	C10-C02	-17.86	1.23	1.54
5	A	2217	9Z9	C10-C02	-17.69	1.23	1.54
5	A	2216	9Z9	C10-C09	-11.87	1.29	1.53
5	A	2217	9Z9	C10-C09	-11.73	1.30	1.53
5	A	2217	9Z9	C05-C04	11.60	1.77	1.52
5	A	2216	9Z9	C05-C04	11.57	1.77	1.52
5	A	2217	9Z9	C11-C08	11.31	1.74	1.56
5	A	2216	9Z9	C11-C08	10.79	1.73	1.56
5	A	2217	9Z9	C07-C08	-10.51	1.33	1.53
5	A	2216	9Z9	C07-C08	-10.31	1.34	1.53
5	A	2217	9Z9	C18-C17	-9.08	1.30	1.51
5	A	2217	9Z9	C19-C11	9.02	1.70	1.54
5	A	2216	9Z9	C19-C11	8.57	1.69	1.54
5	A	2216	9Z9	C18-C17	-7.69	1.30	1.51
5	A	2217	9Z9	C02-C03	6.33	1.67	1.56
5	A	2216	9Z9	C02-C03	6.06	1.67	1.56
5	A	2216	9Z9	C15-C14	5.95	1.62	1.50
5	A	2217	9Z9	C15-C14	5.93	1.62	1.50
5	A	2216	9Z9	C03-C04	-5.69	1.43	1.54
5	A	2217	9Z9	C03-C04	-5.54	1.44	1.54
5	A	2216	9Z9	C03-C74	-5.20	1.39	1.54
5	A	2217	9Z9	C03-C74	-4.91	1.40	1.54
5	A	2217	9Z9	O72-C73	-4.60	1.32	1.42
5	A	2216	9Z9	O72-C73	-4.51	1.33	1.42
5	A	2217	9Z9	C16-C13	4.44	1.60	1.51
5	A	2216	9Z9	C16-C13	4.25	1.60	1.51
5	A	2217	9Z9	C16-C17	4.02	1.59	1.52
3	A	2212	6OU	C08-C07	-3.99	1.31	1.51
3	A	2213	6OU	C08-C07	-3.98	1.32	1.51
3	A	2208	6OU	O30-C20	-3.87	1.40	1.47
4	A	2214	4Y4	C14-C15	3.63	1.45	1.38
4	A	2214	4Y4	O09-C08	-3.53	1.32	1.44
5	A	2216	9Z9	C76-C77	-3.21	1.47	1.53
5	A	2217	9Z9	C76-C77	-3.17	1.47	1.53
5	A	2216	9Z9	C16-C17	3.01	1.58	1.52
4	A	2214	4Y4	C08-C06	2.90	1.60	1.51
5	A	2217	9Z9	O20-C17	2.89	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2214	4Y4	C11-C16	2.88	1.54	1.48
3	A	2207	6OU	O30-C20	-2.85	1.39	1.46
5	A	2217	9Z9	O80-C73	2.80	1.46	1.42
4	A	2214	4Y4	O09-C10	2.80	1.43	1.37
3	A	2211	6OU	P23-O26	2.79	1.65	1.54
3	A	2215	6OU	O30-C20	-2.79	1.40	1.46
3	A	2205	6OU	O30-C20	-2.78	1.40	1.46
5	A	2216	9Z9	O80-C73	2.78	1.46	1.42
3	A	2211	6OU	O30-C20	-2.72	1.40	1.46
3	A	2204	6OU	O30-C20	-2.69	1.40	1.46
3	A	2215	6OU	O18-C19	-2.59	1.39	1.45
3	A	2205	6OU	O18-C16	2.53	1.40	1.33
5	A	2217	9Z9	C19-C18	-2.50	1.48	1.53
5	A	2217	9Z9	C05-C06	2.49	1.59	1.54
3	A	2208	6OU	O18-C16	2.49	1.40	1.33
3	A	2209	6OU	O30-C20	-2.48	1.40	1.46
3	A	2210	6OU	O18-C16	2.48	1.40	1.33
3	A	2209	6OU	O18-C16	2.46	1.40	1.33
3	A	2207	6OU	O18-C19	-2.43	1.39	1.45
5	A	2216	9Z9	O20-C17	2.42	1.50	1.43
5	A	2216	9Z9	C19-C18	-2.40	1.48	1.53
3	A	2204	6OU	O18-C16	2.38	1.40	1.33
5	A	2216	9Z9	C05-C06	2.37	1.59	1.54
5	A	2217	9Z9	C76-C73	2.34	1.55	1.51
3	A	2212	6OU	O18-C19	-2.32	1.40	1.45
3	A	2212	6OU	O18-C16	2.32	1.40	1.33
3	A	2213	6OU	O18-C16	2.31	1.40	1.33
3	A	2210	6OU	O30-C31	2.31	1.40	1.33
3	A	2213	6OU	O18-C19	-2.29	1.40	1.45
3	A	2211	6OU	O18-C19	-2.25	1.40	1.45
3	A	2207	6OU	O18-C16	2.16	1.39	1.33
3	A	2206	6OU	O30-C31	2.13	1.39	1.33
3	A	2204	6OU	O18-C19	-2.13	1.40	1.45
3	A	2211	6OU	O18-C16	2.11	1.39	1.33
3	A	2209	6OU	O30-C31	2.11	1.40	1.34
3	A	2204	6OU	O30-C31	2.10	1.40	1.34
3	A	2208	6OU	O30-C31	2.09	1.40	1.34
3	A	2215	6OU	O18-C16	2.08	1.39	1.33
5	A	2217	9Z9	C79-C78	2.07	1.55	1.51
5	A	2216	9Z9	C14-C13	-2.05	1.28	1.33
3	A	2209	6OU	O18-C19	-2.05	1.40	1.45
3	A	2208	6OU	O18-C19	-2.02	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2214	4Y4	C05-N04	-2.01	1.43	1.47
3	A	2206	6OU	O30-C20	-2.01	1.39	1.45
3	A	2207	6OU	O30-C31	2.01	1.39	1.34
3	A	2215	6OU	O30-C31	2.00	1.39	1.34

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2216	9Z9	C15-C14-C13	-5.34	116.00	125.02
5	A	2217	9Z9	C16-C13-C11	-5.03	109.99	116.42
5	A	2217	9Z9	C10-C02-C03	4.87	122.29	115.36
5	A	2217	9Z9	C11-C13-C14	-4.86	115.83	122.93
5	A	2216	9Z9	C11-C13-C14	-4.69	116.08	122.93
5	A	2216	9Z9	C10-C02-C03	4.51	121.78	115.36
5	A	2216	9Z9	C05-C06-C02	-4.50	98.51	103.85
3	A	2204	6OU	O30-C31-C33	4.48	121.17	111.48
3	A	2211	6OU	O30-C31-C33	4.37	120.93	111.48
5	A	2216	9Z9	C10-C02-C06	4.33	113.73	107.25
5	A	2216	9Z9	C01-C02-C06	-4.31	103.86	111.68
3	A	2208	6OU	O30-C31-C33	4.25	120.67	111.48
3	A	2209	6OU	O30-C31-C33	4.16	120.48	111.48
5	A	2216	9Z9	C16-C13-C11	-4.16	111.10	116.42
3	A	2215	6OU	O30-C31-C33	4.15	120.46	111.48
5	A	2217	9Z9	C01-C02-C10	-4.07	104.60	110.61
5	A	2217	9Z9	C15-C14-C13	-4.07	118.14	125.02
3	A	2205	6OU	O30-C31-C33	4.07	120.29	111.48
5	A	2217	9Z9	C10-C02-C06	3.95	113.16	107.25
4	A	2214	4Y4	C10-C11-C16	-3.94	119.71	125.26
5	A	2216	9Z9	C03-C02-C06	3.89	105.27	100.18
5	A	2217	9Z9	C03-C02-C06	3.79	105.15	100.18
3	A	2207	6OU	O30-C31-C33	3.76	119.62	111.48
5	A	2216	9Z9	C12-C11-C08	-3.75	107.45	111.66
5	A	2216	9Z9	C01-C02-C10	-3.62	105.27	110.61
5	A	2217	9Z9	C01-C02-C06	-3.59	105.16	111.68
5	A	2217	9Z9	C75-C74-C73	-3.52	109.26	114.94
5	A	2216	9Z9	C15-C07-C08	3.48	113.74	109.72
5	A	2217	9Z9	C08-C11-C13	3.38	114.61	109.65
5	A	2216	9Z9	C02-C03-C74	-3.36	110.56	120.50
5	A	2217	9Z9	C02-C03-C74	-3.34	110.62	120.50
5	A	2217	9Z9	C77-C78-C79	3.31	112.61	108.59
5	A	2216	9Z9	C08-C07-C06	3.28	113.37	109.09
5	A	2216	9Z9	C09-C08-C11	-3.22	109.12	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2216	9Z9	C75-C74-C73	-3.21	109.76	114.94
3	A	2210	6OU	O30-C31-C33	3.07	121.19	111.83
5	A	2216	9Z9	C09-C10-C02	3.06	117.91	112.74
5	A	2217	9Z9	C01-C02-C03	-3.03	105.00	111.58
3	A	2210	6OU	O18-C16-C15	3.02	121.05	111.83
3	A	2206	6OU	O30-C31-C33	2.99	120.94	111.83
5	A	2217	9Z9	C08-C07-C06	2.97	112.96	109.09
5	A	2217	9Z9	C75-C74-C03	-2.93	108.64	114.50
5	A	2217	9Z9	C05-C06-C02	-2.92	100.39	103.85
5	A	2216	9Z9	C01-C02-C03	-2.91	105.25	111.58
3	A	2209	6OU	O18-C16-C15	2.90	120.68	111.83
5	A	2216	9Z9	C02-C03-C04	2.82	107.25	104.20
5	A	2216	9Z9	C08-C11-C13	2.81	113.77	109.65
3	A	2204	6OU	O18-C16-C15	2.80	120.38	111.83
3	A	2207	6OU	O18-C16-C15	2.63	119.87	111.83
3	A	2208	6OU	O18-C16-C15	2.63	119.86	111.83
5	A	2216	9Z9	C05-C06-C07	2.63	124.62	119.53
5	A	2217	9Z9	C02-C03-C04	2.57	106.98	104.20
3	A	2205	6OU	O18-C16-C15	2.56	119.65	111.83
5	A	2217	9Z9	C05-C06-C07	2.55	124.48	119.53
5	A	2217	9Z9	C15-C07-C08	2.51	112.62	109.72
5	A	2216	9Z9	C77-C78-C79	2.51	111.63	108.59
5	A	2217	9Z9	C12-C11-C08	-2.47	108.88	111.66
3	A	2215	6OU	O18-C16-C15	2.47	119.36	111.83
5	A	2216	9Z9	C73-C74-C03	-2.37	99.87	103.37
5	A	2217	9Z9	C79-O80-C73	-2.37	109.60	113.69
3	A	2211	6OU	O18-C16-C15	2.33	118.94	111.83
5	A	2216	9Z9	C75-C74-C03	-2.32	109.87	114.50
5	A	2216	9Z9	C11-C08-C07	-2.31	109.34	112.71
5	A	2216	9Z9	C76-C73-C74	-2.31	111.48	115.66
5	A	2216	9Z9	O72-C73-C74	-2.26	101.56	104.56
5	A	2217	9Z9	C09-C10-C02	2.23	116.50	112.74
5	A	2217	9Z9	C76-C77-C78	2.22	116.11	111.67
3	A	2209	6OU	C21-C20-C19	-2.16	106.74	111.78
3	A	2212	6OU	O18-C16-C15	2.13	120.19	112.14
5	A	2216	9Z9	C18-C17-C16	2.06	113.84	110.97
3	A	2213	6OU	O18-C16-C15	2.04	119.86	112.14

There are no chirality outliers.

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2204	6OU	O26-C27-C28-N29
3	A	2205	6OU	C27-O26-P23-O22
3	A	2205	6OU	C27-O26-P23-O24
3	A	2205	6OU	C27-O26-P23-O25
3	A	2209	6OU	C27-O26-P23-O22
3	A	2209	6OU	C27-O26-P23-O24
3	A	2209	6OU	C27-O26-P23-O25
3	A	2209	6OU	O26-C27-C28-N29
3	A	2210	6OU	C19-C20-O30-C31
3	A	2211	6OU	C21-O22-P23-O25
3	A	2211	6OU	C21-O22-P23-O26
3	A	2211	6OU	C33-C31-O30-C20
3	A	2215	6OU	C27-O26-P23-O22
3	A	2215	6OU	C27-O26-P23-O25
3	A	2215	6OU	O26-C27-C28-N29
3	A	2215	6OU	O32-C31-O30-C20
3	A	2215	6OU	C33-C31-O30-C20
4	A	2214	4Y4	C10-C11-C16-C18
4	A	2214	4Y4	C10-C11-C16-O17
5	A	2216	9Z9	C16-C17-O20-C21
3	A	2204	6OU	O17-C16-O18-C19
2	A	2203	NAG	C4-C5-C6-O6
3	A	2204	6OU	C15-C16-O18-C19
3	A	2208	6OU	O17-C16-O18-C19
3	A	2209	6OU	O17-C16-O18-C19
3	A	2211	6OU	O32-C31-O30-C20
3	A	2209	6OU	C15-C16-O18-C19
2	A	2203	NAG	O5-C5-C6-O6
3	A	2208	6OU	C15-C16-O18-C19
3	A	2212	6OU	C06-C07-C08-C09
3	A	2210	6OU	C15-C16-O18-C19
4	A	2214	4Y4	C02-C03-N04-C05
3	A	2207	6OU	O17-C16-O18-C19
3	A	2210	6OU	O17-C16-O18-C19
3	A	2207	6OU	C15-C16-O18-C19
3	A	2205	6OU	C33-C31-O30-C20
3	A	2205	6OU	C34-C35-C36-C37
3	A	2215	6OU	C31-C33-C34-C35
2	A	2202	NAG	C8-C7-N2-C2
2	A	2202	NAG	O7-C7-N2-C2
2	A	2203	NAG	C8-C7-N2-C2
2	A	2203	NAG	O7-C7-N2-C2
2	A	2201	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	2212	6OU	C04-C05-C06-C07
3	A	2204	6OU	C13-C14-C15-C16
3	A	2205	6OU	C13-C14-C15-C16
3	A	2215	6OU	C13-C14-C15-C16
4	A	2214	4Y4	C05-C06-C08-O09
3	A	2205	6OU	C31-C33-C34-C35
3	A	2207	6OU	C31-C33-C34-C35
3	A	2211	6OU	C31-C33-C34-C35
3	A	2205	6OU	O32-C31-O30-C20
4	A	2214	4Y4	O07-C06-C08-O09
3	A	2206	6OU	O30-C20-C21-O22
3	A	2204	6OU	O32-C31-O30-C20
5	A	2216	9Z9	O20-C21-C22-C23
3	A	2204	6OU	C33-C31-O30-C20
3	A	2209	6OU	C33-C31-O30-C20
2	A	2201	NAG	O5-C5-C6-O6
3	A	2209	6OU	O32-C31-O30-C20
3	A	2208	6OU	C06-C07-C08-C09
3	A	2210	6OU	O18-C19-C20-O30
3	A	2211	6OU	C34-C35-C36-C37
3	A	2209	6OU	C34-C35-C36-C37
3	A	2207	6OU	C33-C34-C35-C36
3	A	2215	6OU	C10-C11-C12-C13
3	A	2207	6OU	C35-C36-C37-C38
3	A	2205	6OU	C10-C11-C12-C13
3	A	2210	6OU	C31-C33-C34-C35
3	A	2210	6OU	C33-C31-O30-C20
3	A	2209	6OU	C35-C36-C37-C38
3	A	2210	6OU	C35-C36-C37-C38
3	A	2205	6OU	C12-C13-C14-C15
3	A	2204	6OU	C12-C13-C14-C15
3	A	2204	6OU	C31-C33-C34-C35
3	A	2210	6OU	C37-C38-C39-C40
3	A	2210	6OU	C41-C42-C43-C44
3	A	2210	6OU	C38-C39-C40-C41
3	A	2204	6OU	C34-C35-C36-C37
3	A	2208	6OU	C33-C34-C35-C36
3	A	2208	6OU	C31-C33-C34-C35
3	A	2212	6OU	C13-C14-C15-C16
3	A	2205	6OU	C37-C38-C39-C40
3	A	2210	6OU	O32-C31-O30-C20
3	A	2213	6OU	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	2206	6OU	C35-C36-C37-C38
4	A	2214	4Y4	C15-C10-O09-C08
3	A	2211	6OU	C21-O22-P23-O24
3	A	2206	6OU	C34-C35-C36-C37
3	A	2206	6OU	C31-C33-C34-C35
3	A	2210	6OU	C11-C12-C13-C14
3	A	2213	6OU	C08-C09-C10-C11
3	A	2215	6OU	C11-C12-C13-C14
3	A	2205	6OU	C07-C08-C09-C10
3	A	2205	6OU	C38-C39-C40-C41
3	A	2215	6OU	C34-C35-C36-C37
4	A	2214	4Y4	C11-C16-C18-C19
3	A	2210	6OU	C42-C43-C44-C45
3	A	2209	6OU	C10-C11-C12-C13
3	A	2204	6OU	C10-C11-C12-C13
3	A	2205	6OU	C15-C16-O18-C19
4	A	2214	4Y4	C11-C10-O09-C08
3	A	2209	6OU	C09-C10-C11-C12
3	A	2207	6OU	O18-C19-C20-C21
3	A	2205	6OU	O18-C19-C20-O30
4	A	2214	4Y4	O17-C16-C18-C19
3	A	2210	6OU	C36-C37-C38-C39
3	A	2205	6OU	O17-C16-O18-C19
3	A	2208	6OU	C34-C35-C36-C37
3	A	2210	6OU	C33-C34-C35-C36
3	A	2205	6OU	O30-C20-C21-O22
3	A	2207	6OU	C12-C13-C14-C15
3	A	2205	6OU	O18-C19-C20-C21
3	A	2207	6OU	O18-C19-C20-O30
3	A	2211	6OU	O18-C19-C20-O30
3	A	2212	6OU	C08-C09-C10-C11
3	A	2205	6OU	C35-C36-C37-C38
3	A	2209	6OU	C11-C12-C13-C14
3	A	2215	6OU	C20-C21-O22-P23
3	A	2215	6OU	C15-C16-O18-C19
3	A	2209	6OU	C37-C38-C39-C40
3	A	2205	6OU	C19-C20-C21-O22
3	A	2215	6OU	C33-C34-C35-C36
3	A	2205	6OU	C09-C10-C11-C12
3	A	2204	6OU	C36-C37-C38-C39
3	A	2215	6OU	O17-C16-O18-C19
3	A	2209	6OU	C21-O22-P23-O24

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Mol	Chain	Res	Type	Atoms
3	A	2209	6OU	C21-O22-P23-O26
3	A	2215	6OU	C21-O22-P23-O24
3	A	2215	6OU	C27-O26-P23-O24
3	A	2209	6OU	C41-C42-C43-C44
3	A	2209	6OU	C19-C20-O30-C31
3	A	2215	6OU	C40-C41-C42-C43
3	A	2208	6OU	C36-C37-C38-C39
3	A	2208	6OU	C37-C38-C39-C40
3	A	2213	6OU	C05-C06-C07-C08
3	A	2208	6OU	C07-C08-C09-C10
3	A	2213	6OU	C10-C11-C12-C13
3	A	2210	6OU	C10-C11-C12-C13
3	A	2208	6OU	O32-C31-O30-C20
3	A	2211	6OU	C20-C21-O22-P23
3	A	2204	6OU	C11-C12-C13-C14
3	A	2211	6OU	O18-C19-C20-C21
3	A	2207	6OU	O30-C20-C21-O22
3	A	2209	6OU	C40-C41-C42-C43
3	A	2204	6OU	C38-C39-C40-C41
3	A	2207	6OU	C38-C39-C40-C41
3	A	2208	6OU	C38-C39-C40-C41
3	A	2213	6OU	C09-C10-C11-C12
3	A	2209	6OU	O30-C20-C21-O22
3	A	2209	6OU	C38-C39-C40-C41
3	A	2205	6OU	C36-C37-C38-C39
3	A	2209	6OU	C19-C20-C21-O22
3	A	2204	6OU	C14-C15-C16-O18
3	A	2207	6OU	C13-C14-C15-C16
3	A	2210	6OU	C14-C15-C16-O18
3	A	2208	6OU	C14-C15-C16-O18
3	A	2209	6OU	C14-C15-C16-O18
3	A	2208	6OU	C33-C31-O30-C20
3	A	2208	6OU	C35-C36-C37-C38
3	A	2211	6OU	C14-C15-C16-O18
3	A	2206	6OU	C38-C39-C40-C41
4	A	2214	4Y4	C18-C19-C20-C21
4	A	2214	4Y4	C18-C19-C20-C25
3	A	2211	6OU	C35-C36-C37-C38
3	A	2204	6OU	C14-C15-C16-O17
3	A	2208	6OU	C14-C15-C16-O17
3	A	2207	6OU	C10-C11-C12-C13
3	A	2210	6OU	C14-C15-C16-O17

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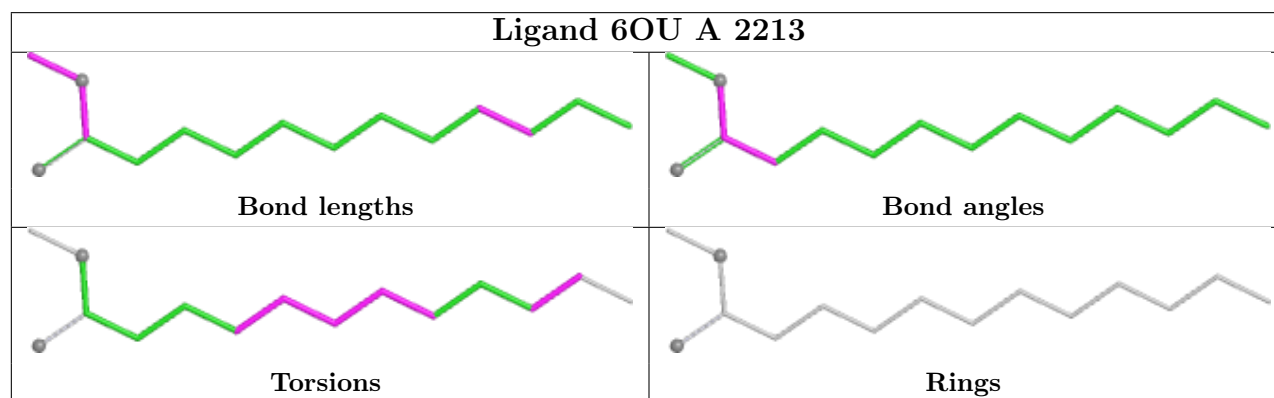
Mol	Chain	Res	Type	Atoms
3	A	2211	6OU	C14-C15-C16-O17
3	A	2209	6OU	C14-C15-C16-O17

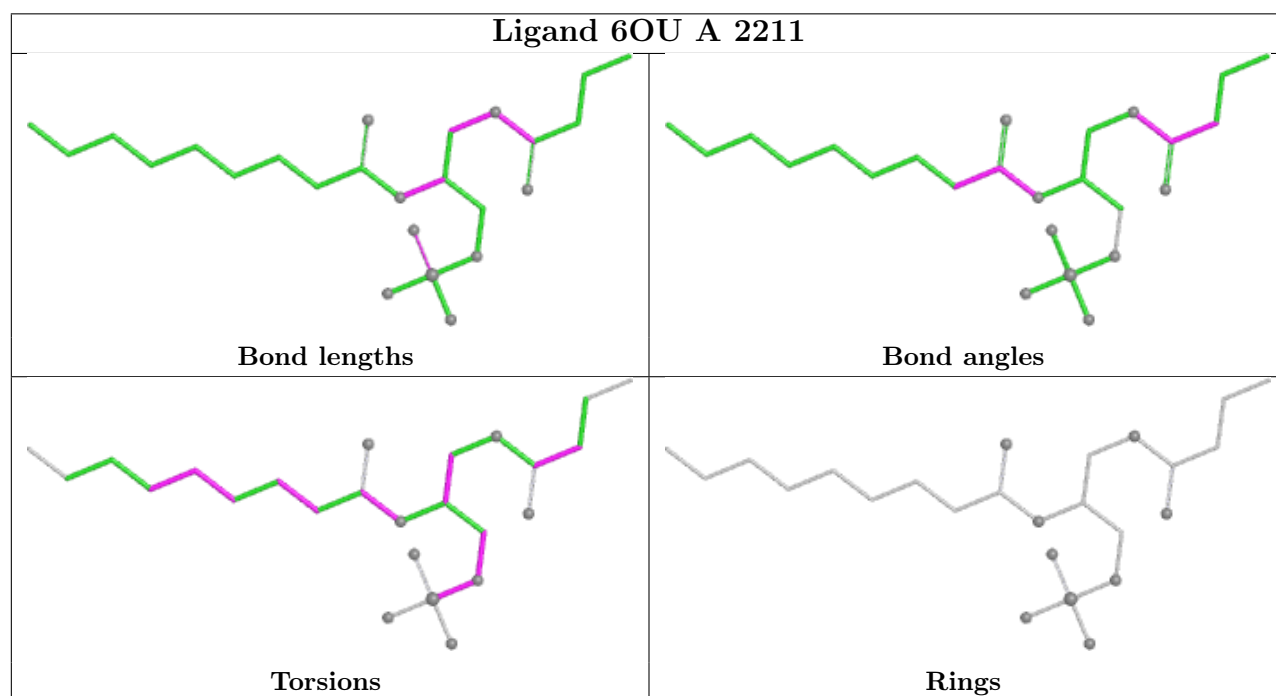
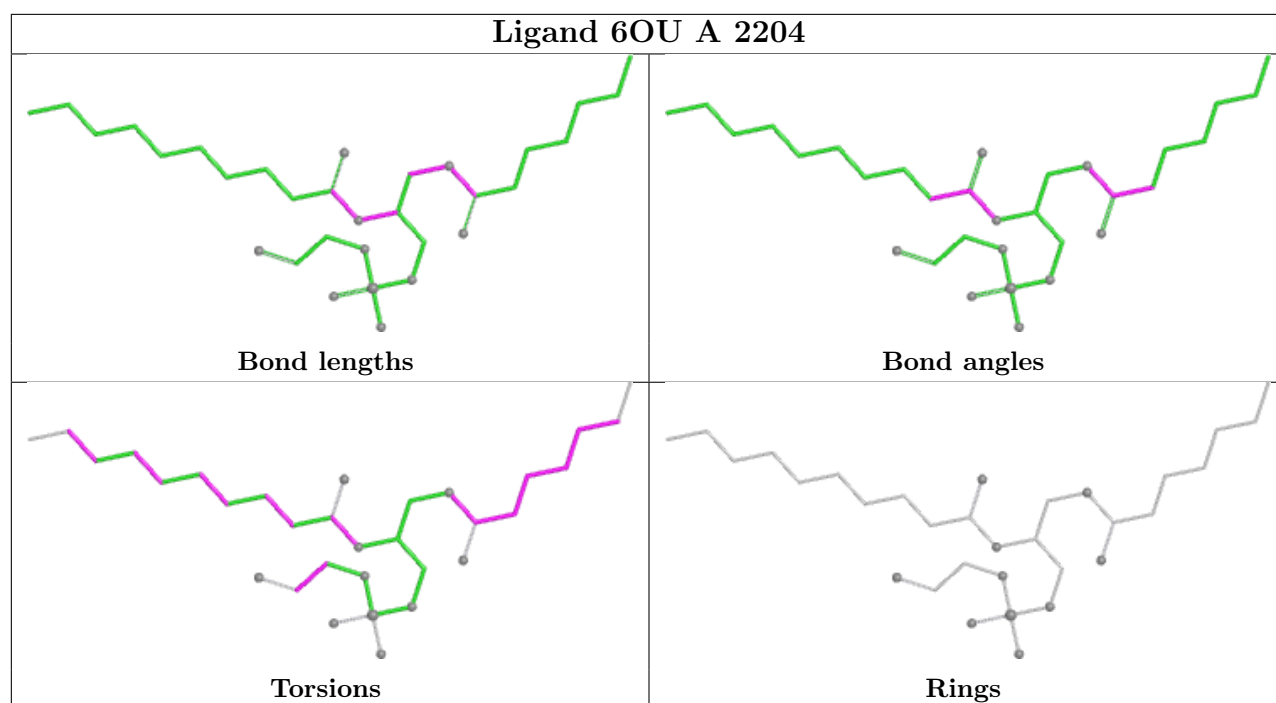
There are no ring outliers.

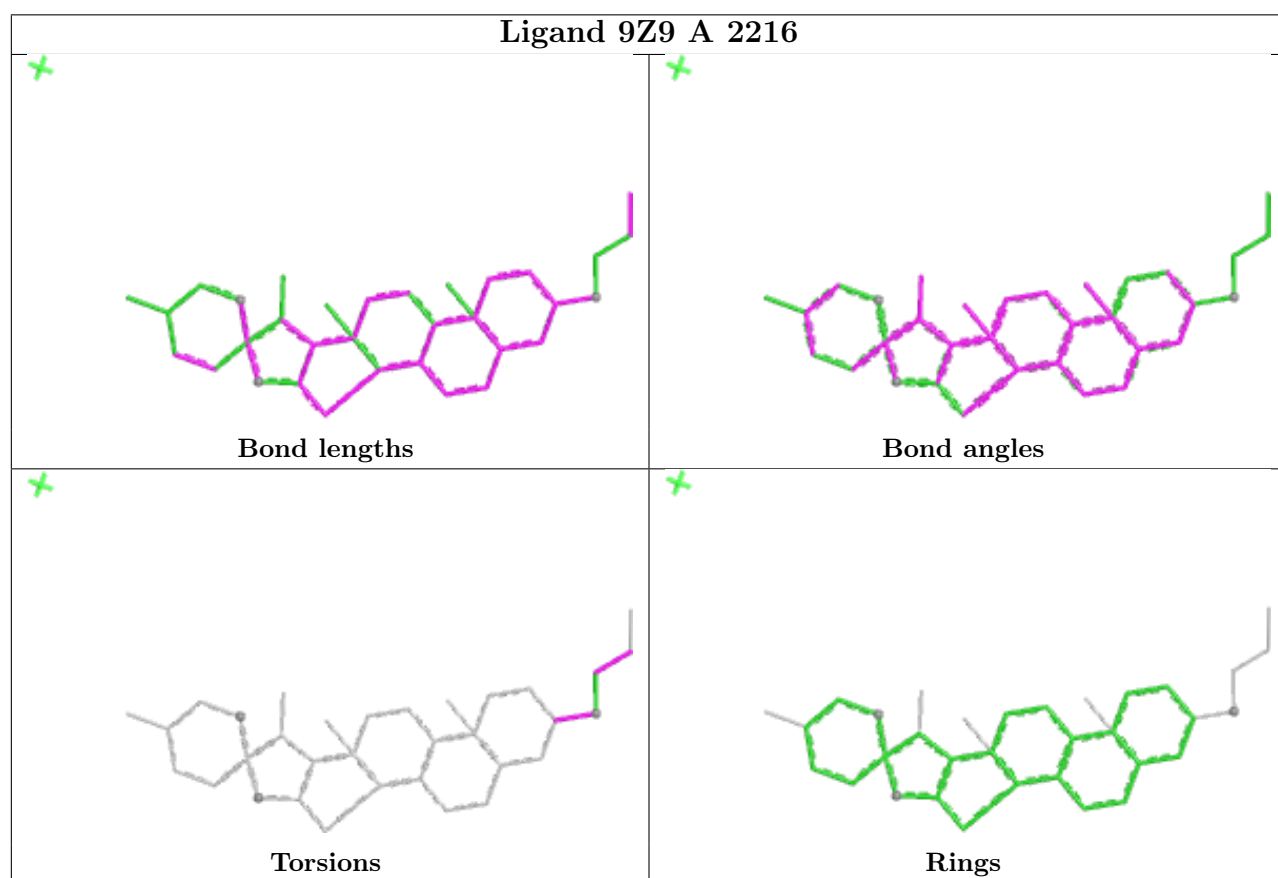
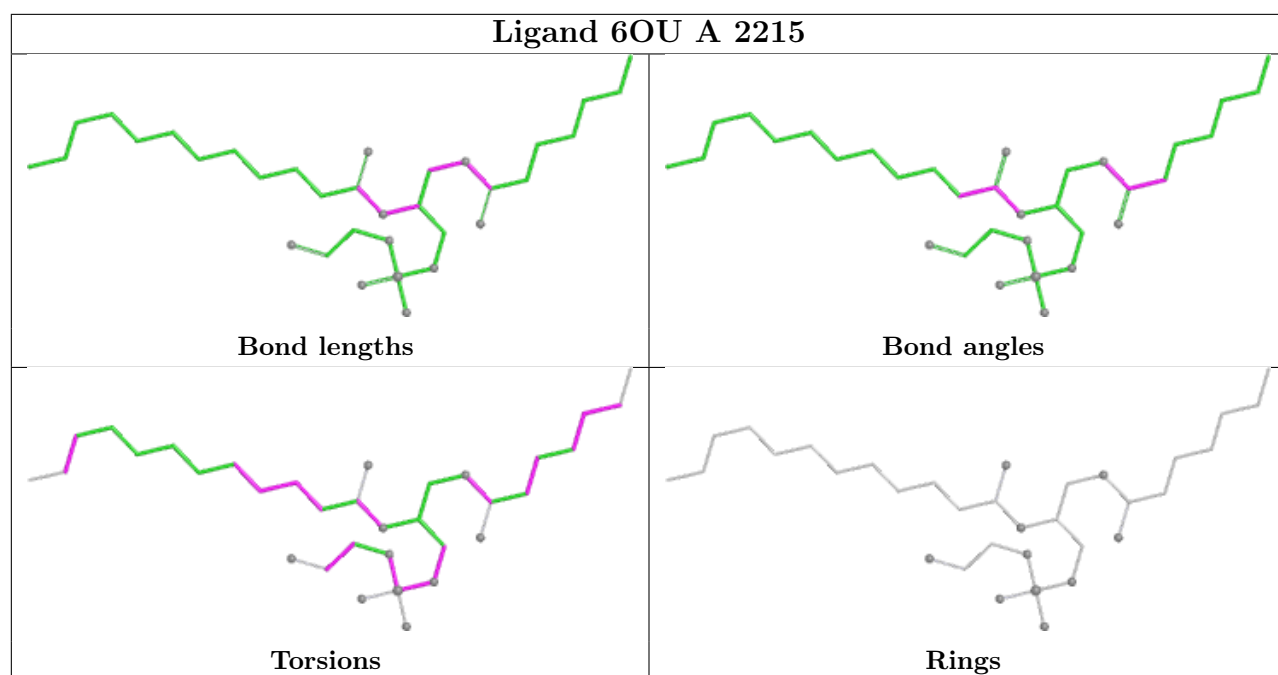
4 monomers are involved in 21 short contacts:

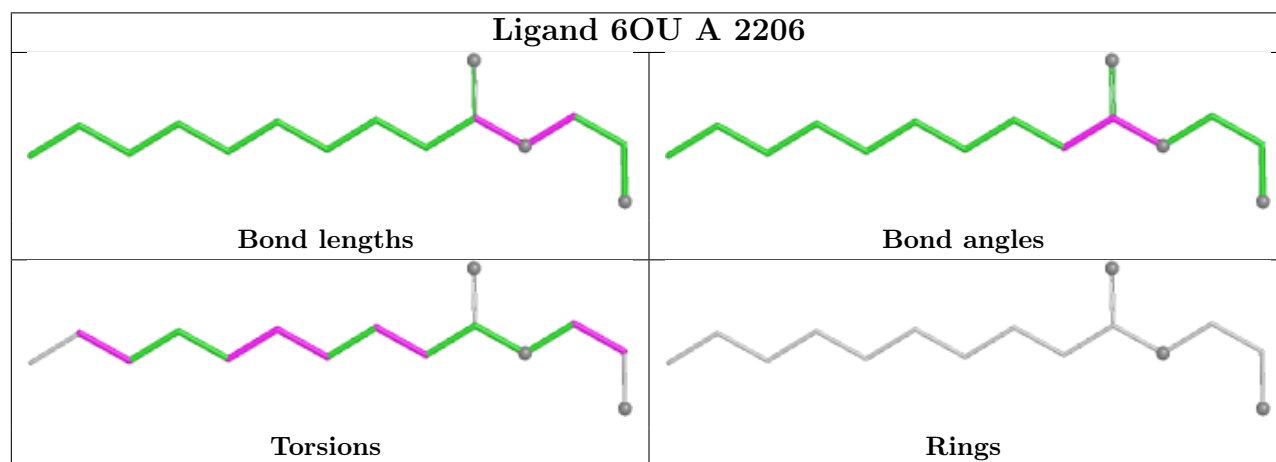
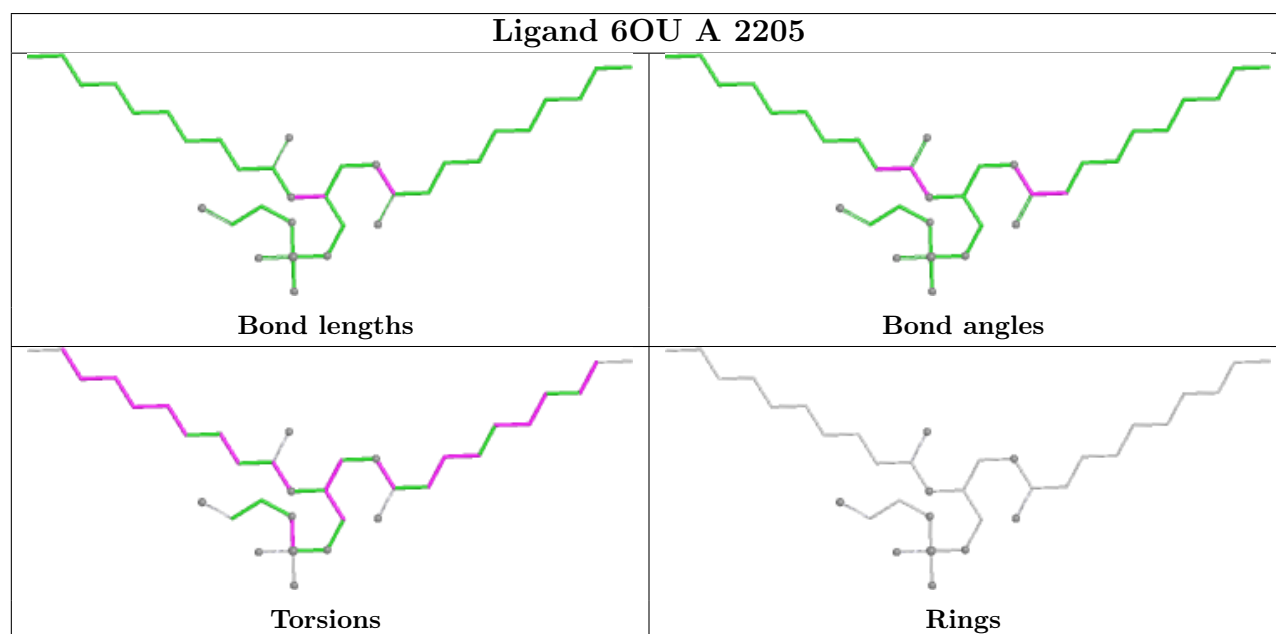
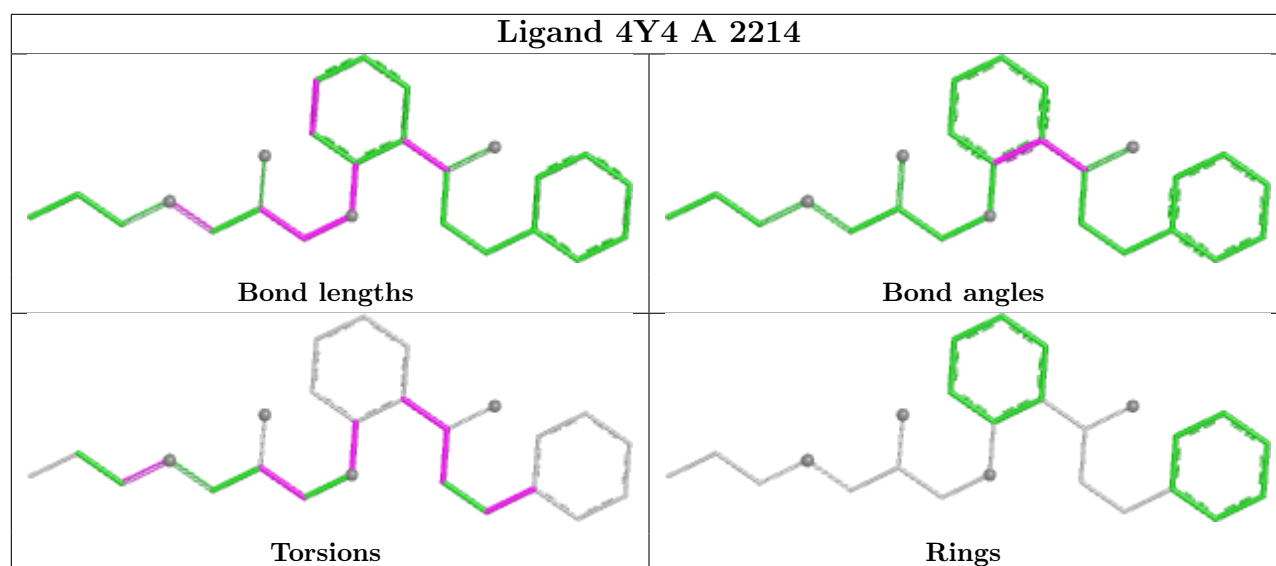
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2216	9Z9	8	0
2	A	2202	NAG	4	0
5	A	2217	9Z9	5	0
2	A	2201	NAG	5	0

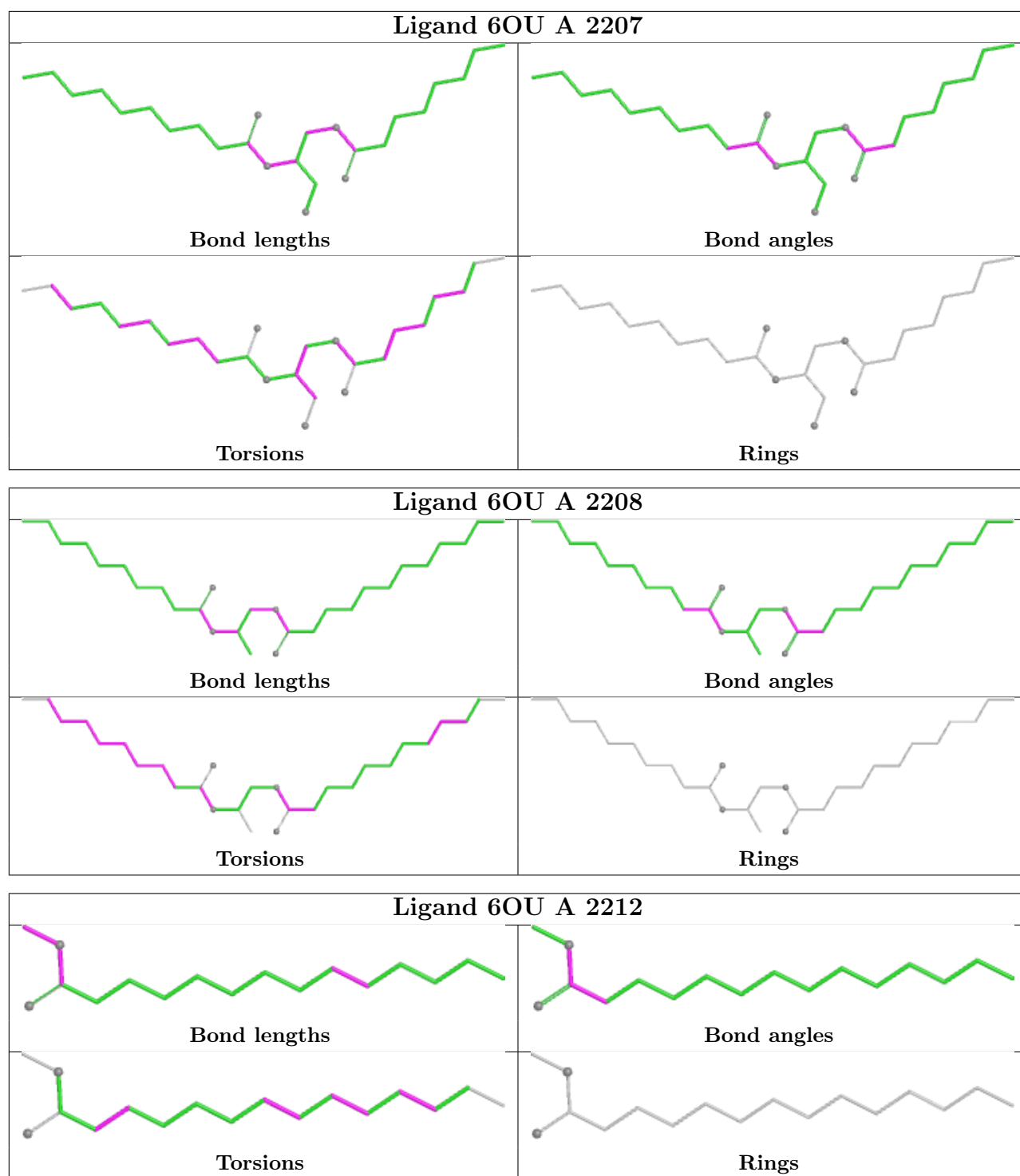
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

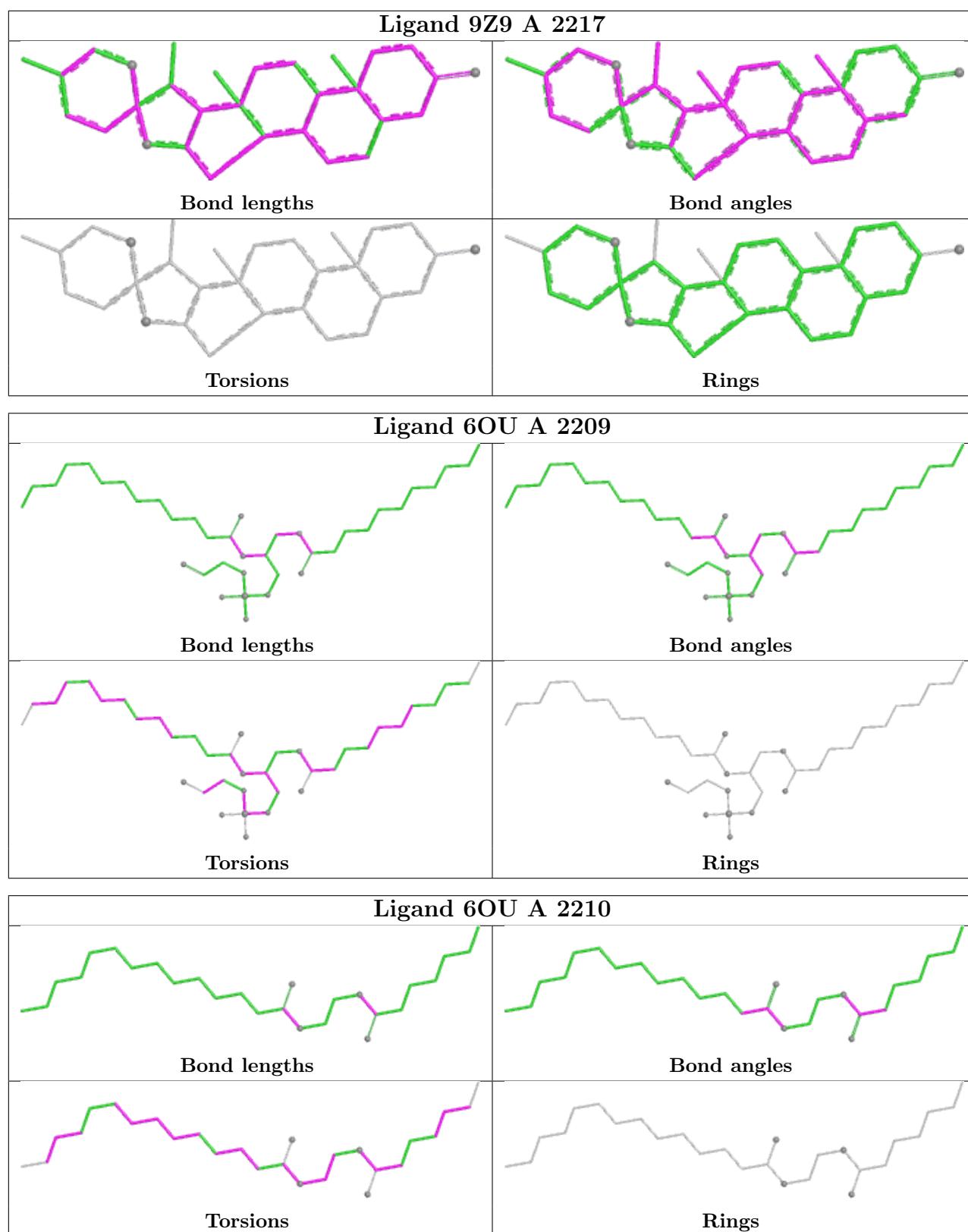












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

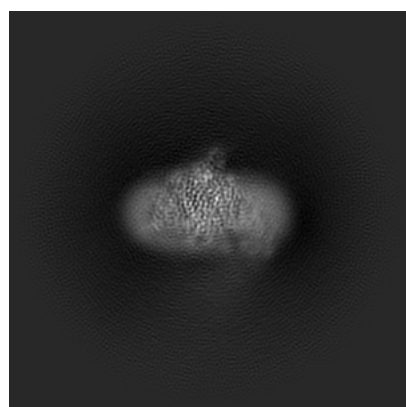
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31519. These allow visual inspection of the internal detail of the map and identification of artifacts.

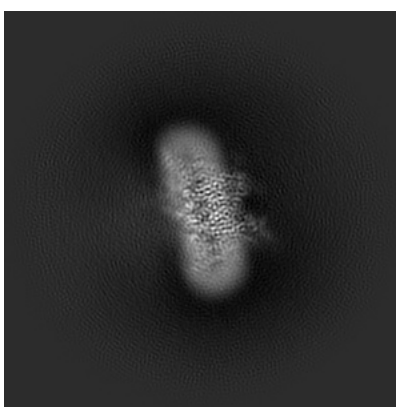
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

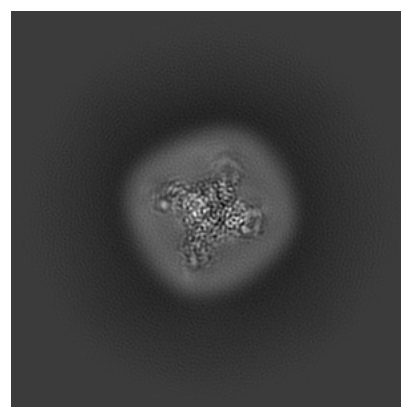
6.1.1 Primary map



X



Y

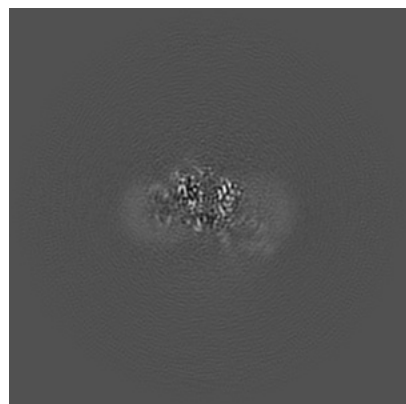


Z

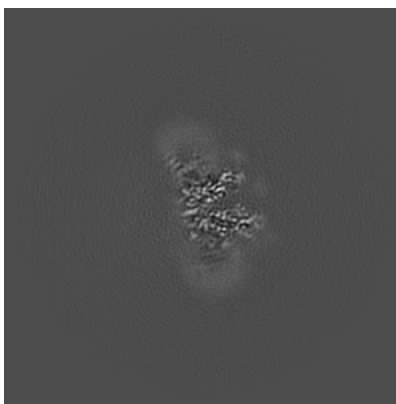
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

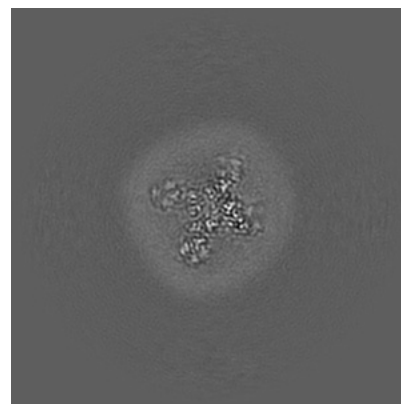
6.2.1 Primary map



X Index: 160



Y Index: 160

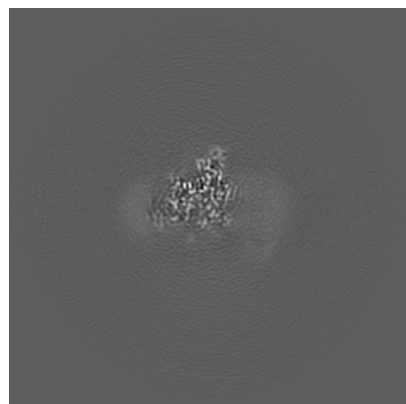


Z Index: 160

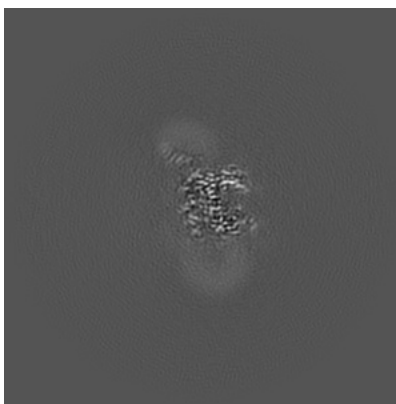
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

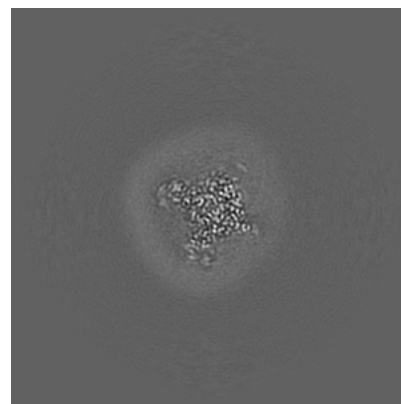
6.3.1 Primary map



X Index: 150



Y Index: 153

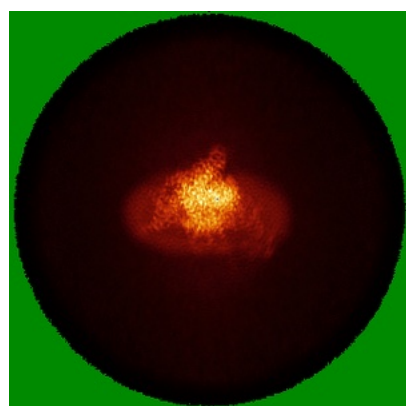


Z Index: 168

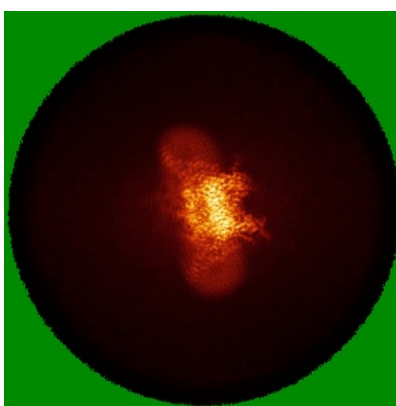
The images above show the largest variance slices of the map in three orthogonal directions.

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

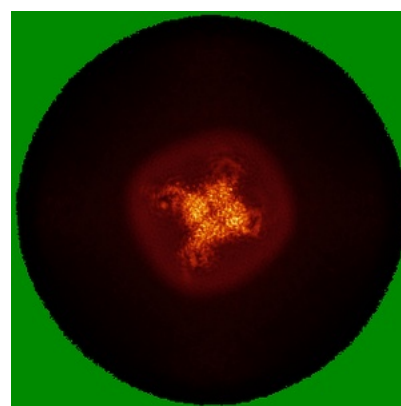
6.4.1 Primary map



X



Y

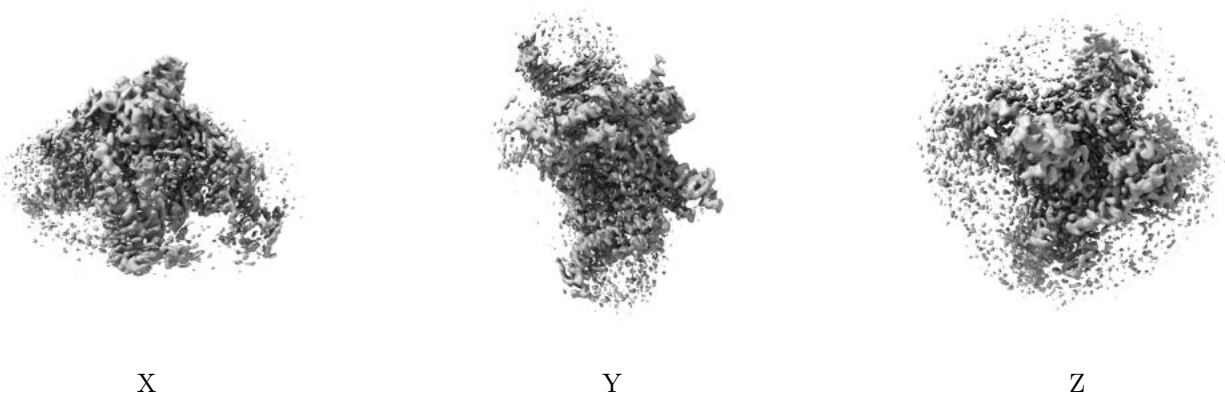


Z

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

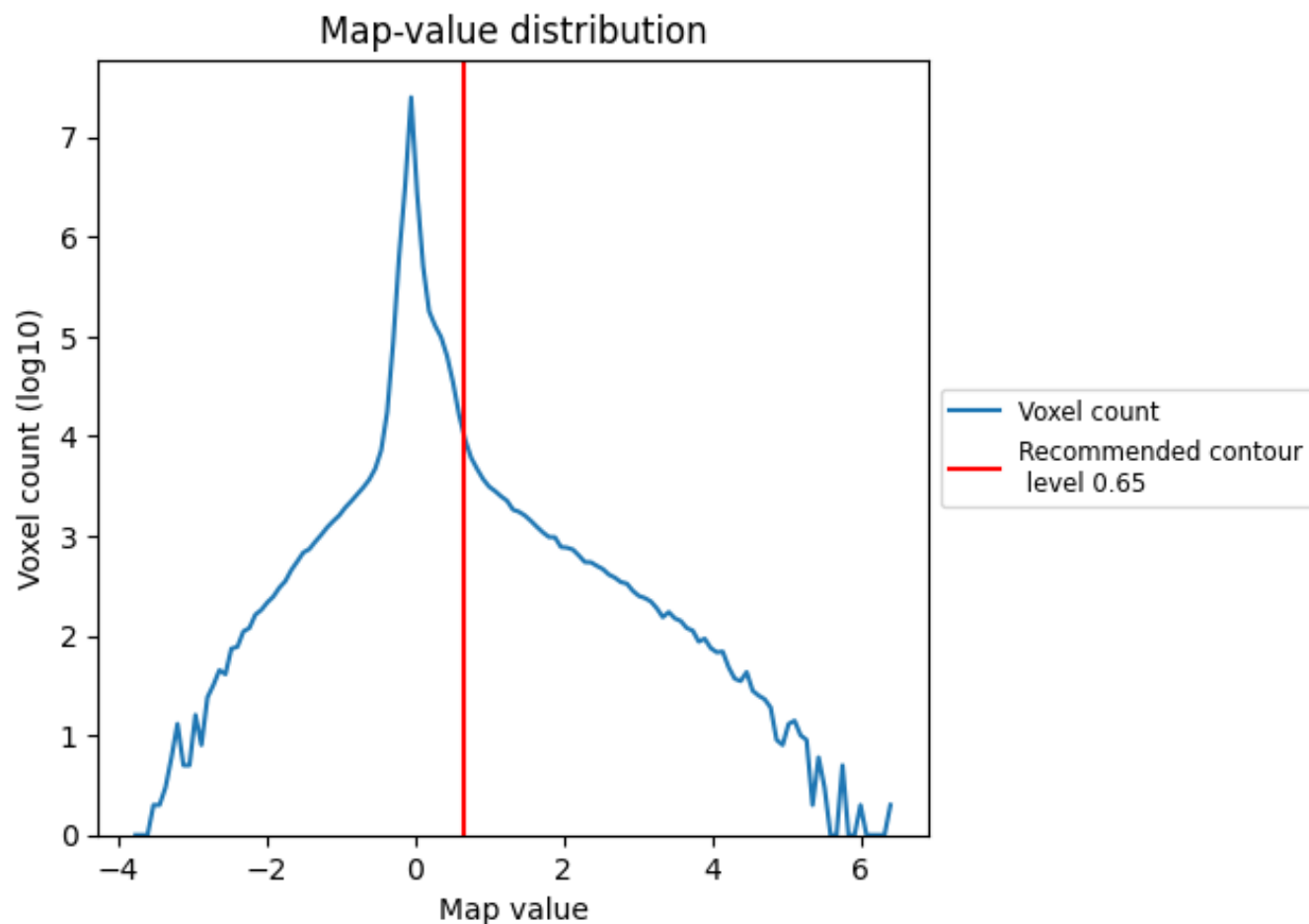
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

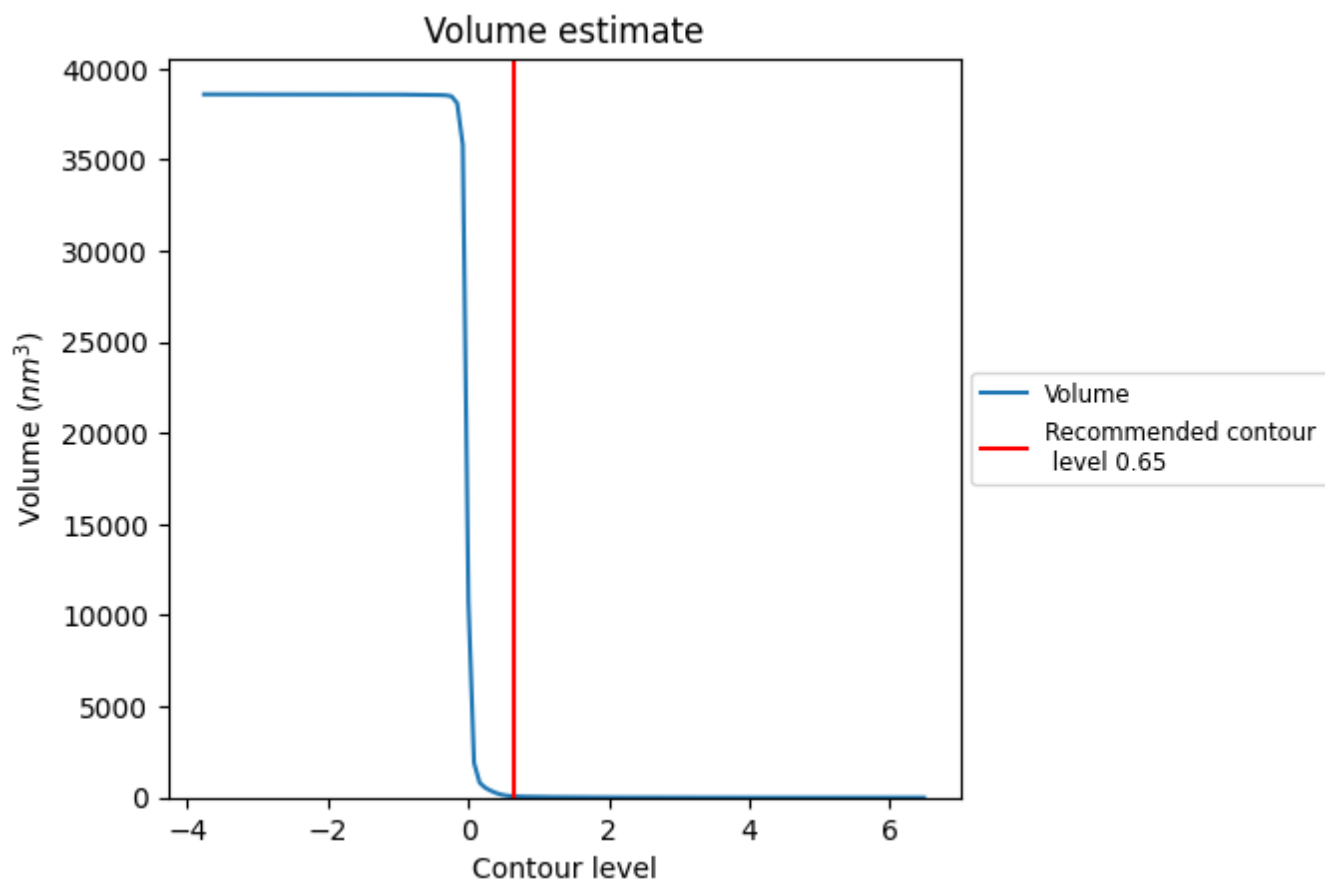
This section contains the results of statistical analysis of the map.

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.

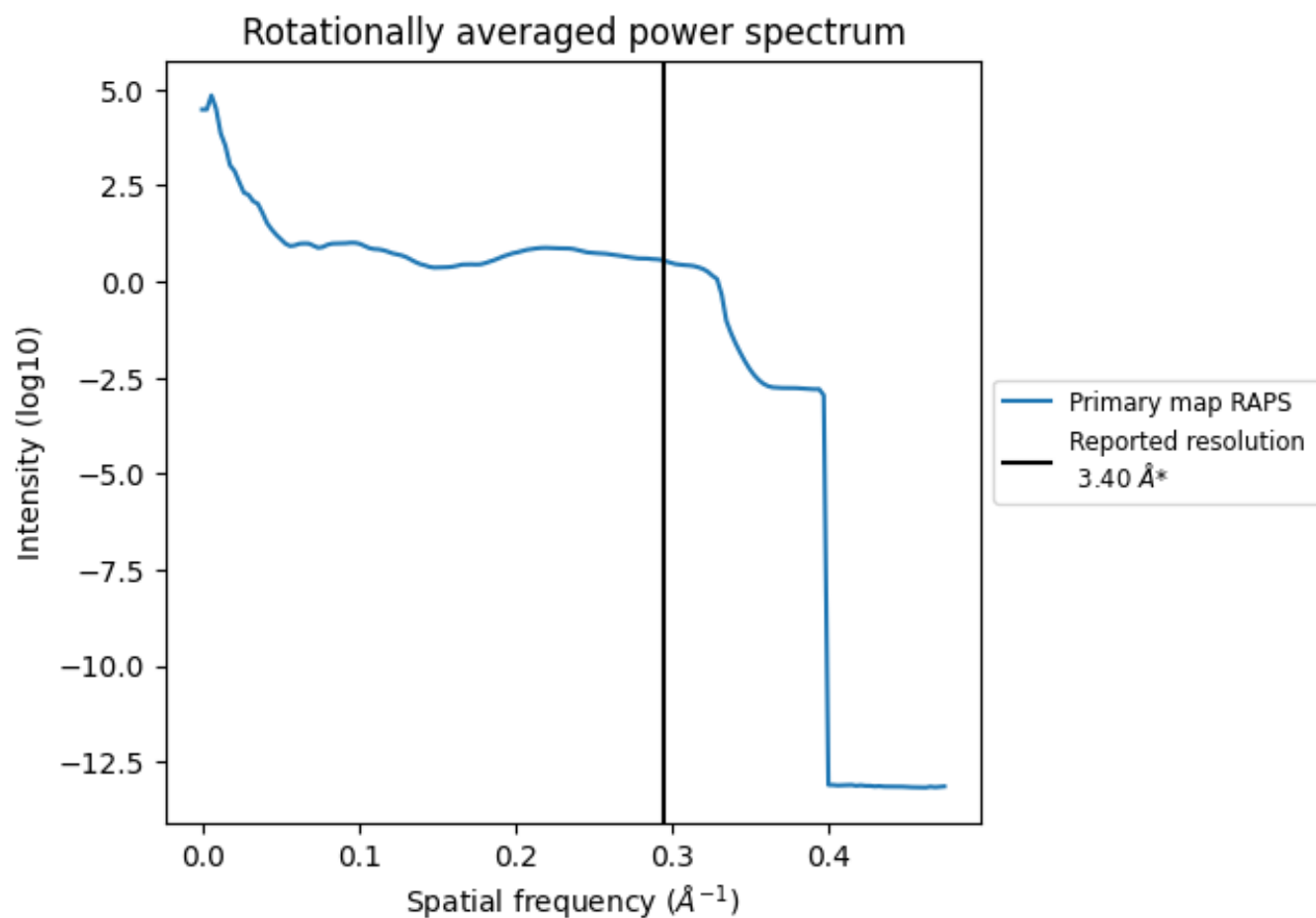
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 63 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 ⓘ

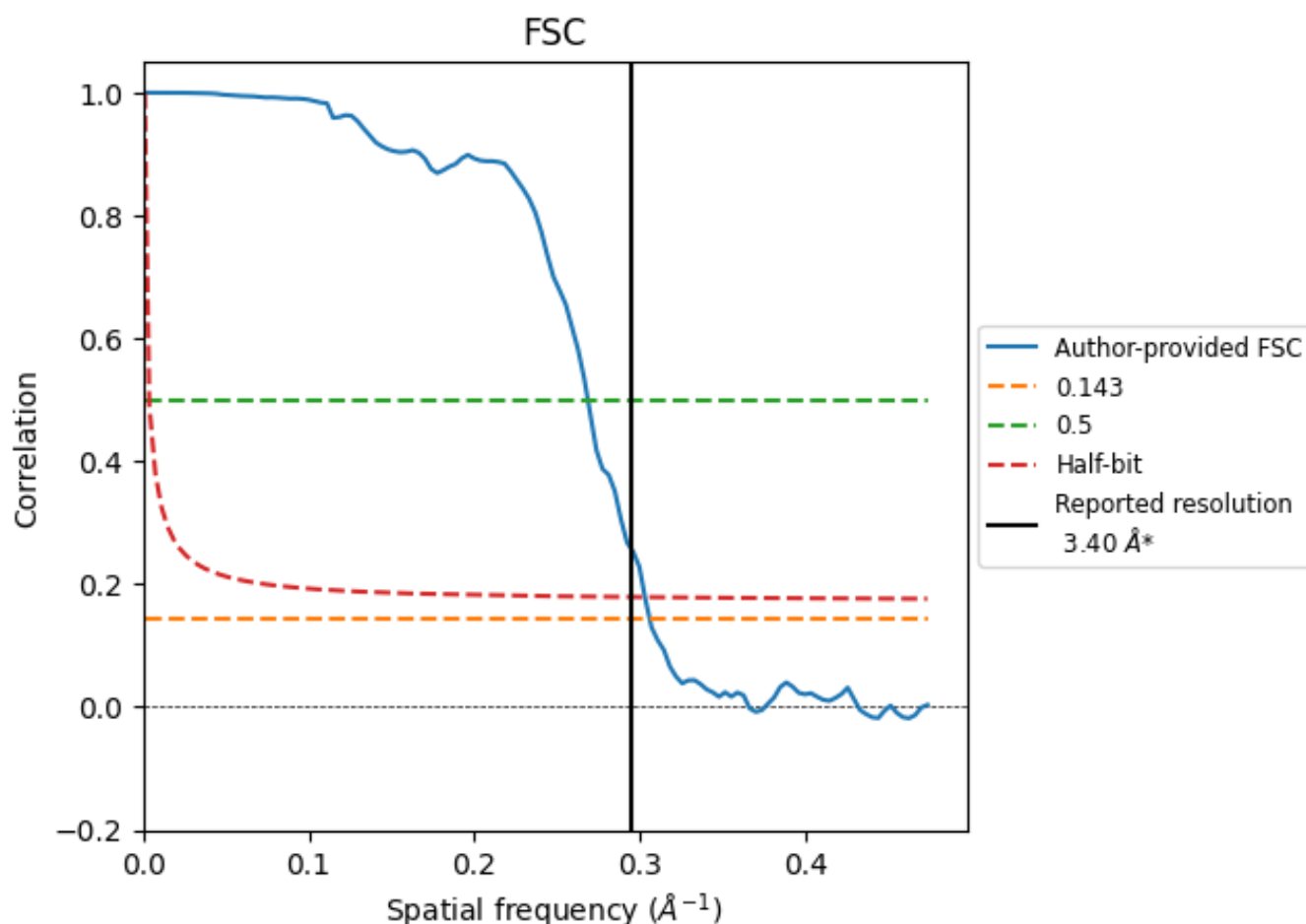


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

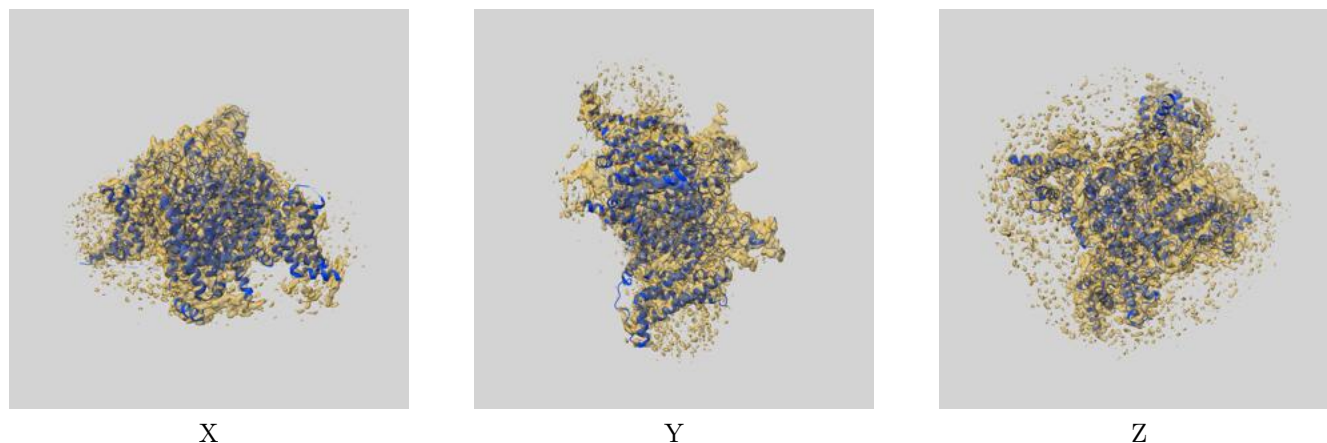
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.27	3.72	3.30
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

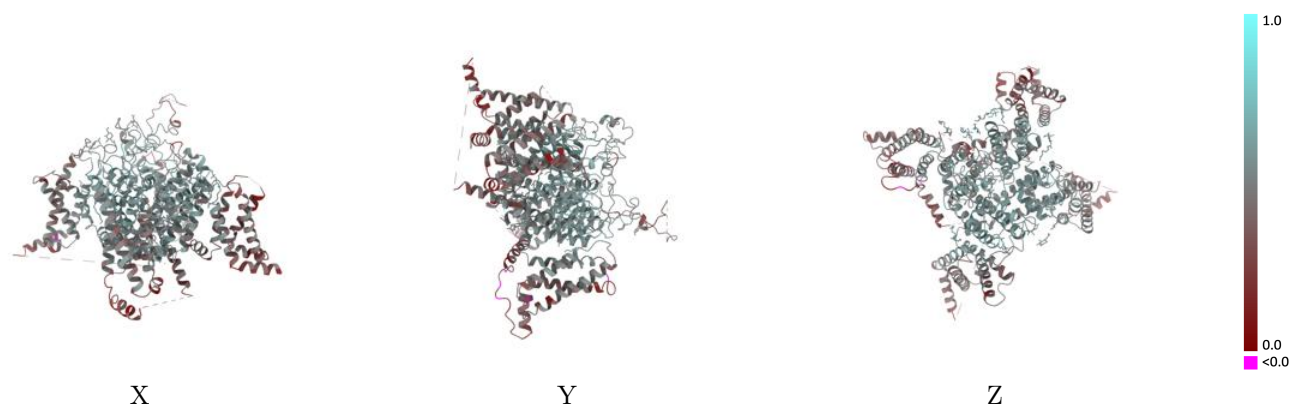
This section contains information regarding the fit between EMDB map EMD-31519 and PDB model 7FBS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



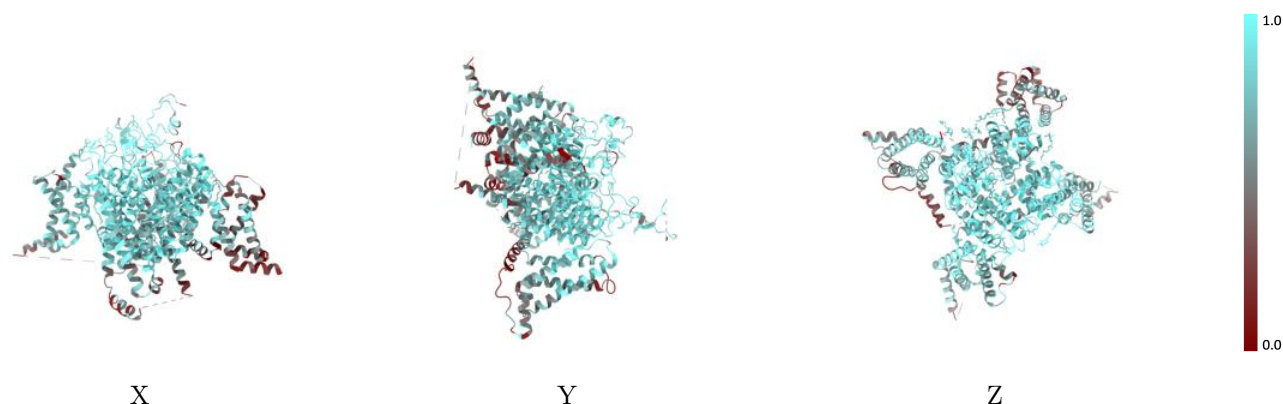
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



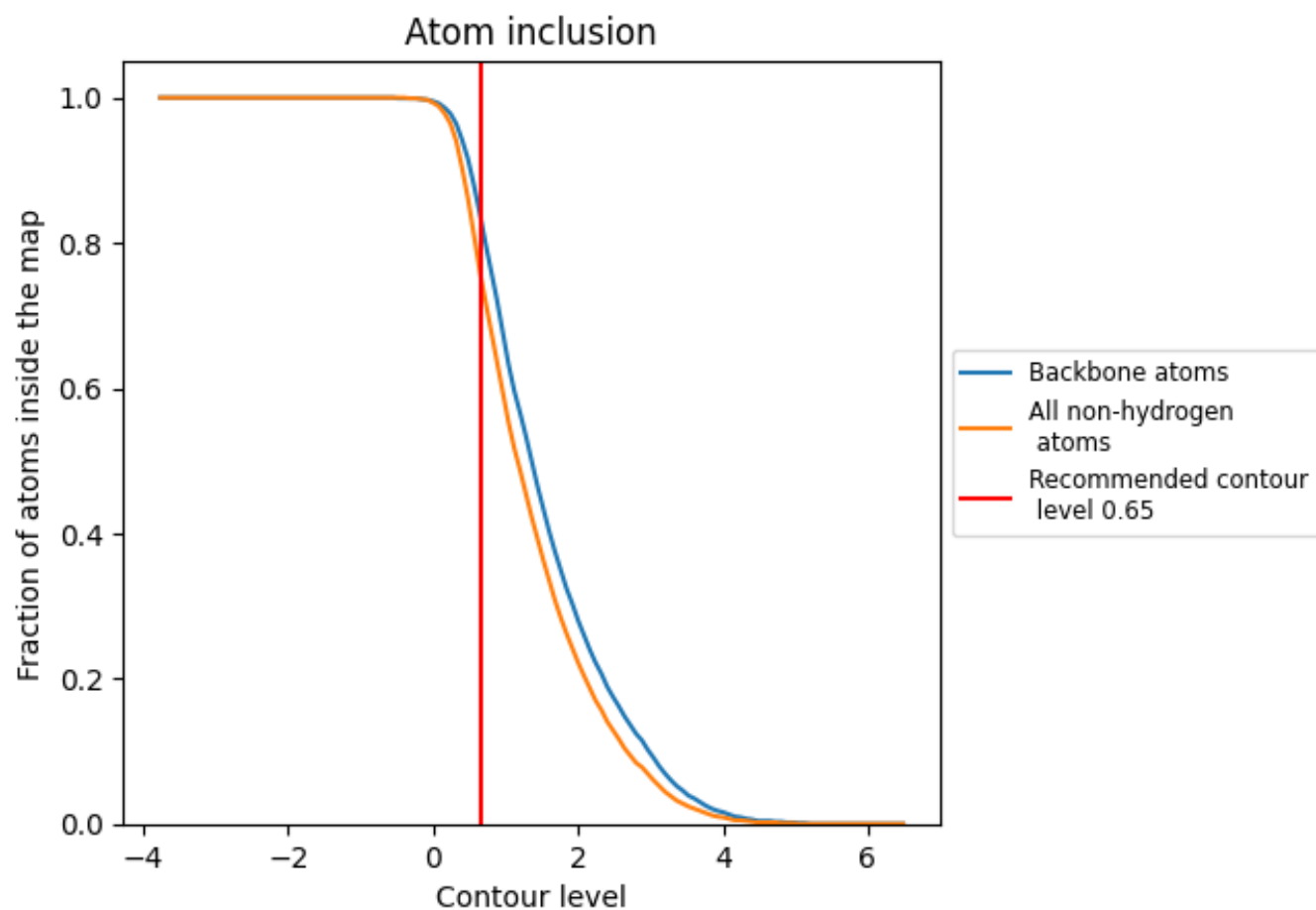
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.4770
A	0.7580	0.4770

