



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 7LKZ / pdb_00007lkz
EMDB ID : EMD-23410
Title : Structure of ATP-bound human ABCA4
Authors : Liu, F.; Lee, J.; Chen, J.
Deposited on : 2021-02-03
Resolution : 3.27 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

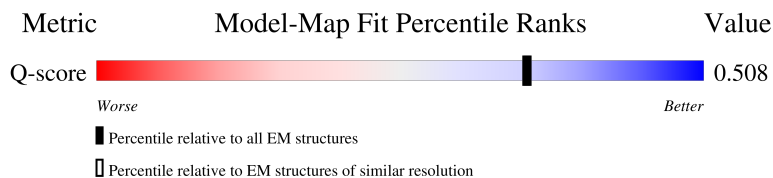
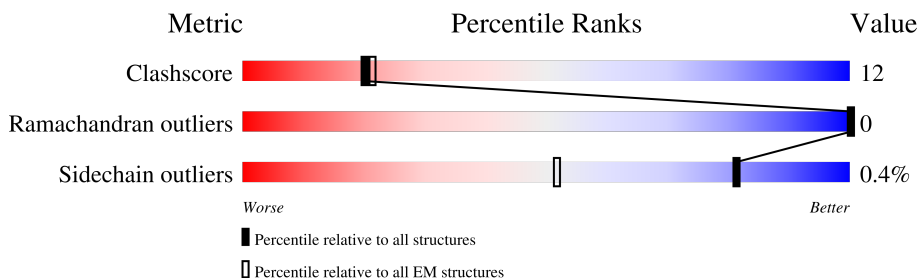
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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	14508 (2.77 - 3.77)

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	2273	
2	B	3	
3	C	5	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15515 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.

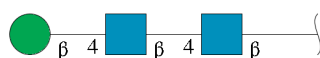
- Molecule 1 is a protein called Retinal-specific phospholipid-transporting ATPase ABCA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1920	Total	C	N	O	S	0	0
			15117	9777	2528	2727	85		

There are 2 discrepancies between the modelled and reference sequences:

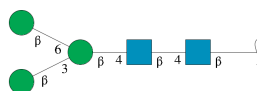
Chain	Residue	Modelled	Actual	Comment	Reference
A	1087	GLN	GLU	engineered mutation	UNP P78363
A	2096	GLN	GLU	engineered mutation	UNP P78363

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



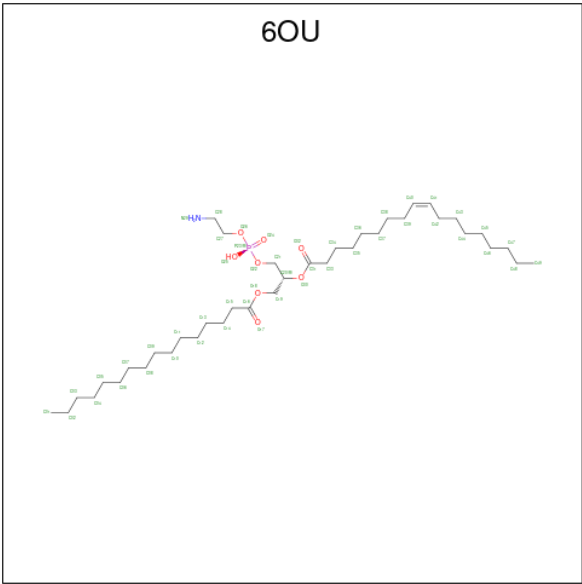
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



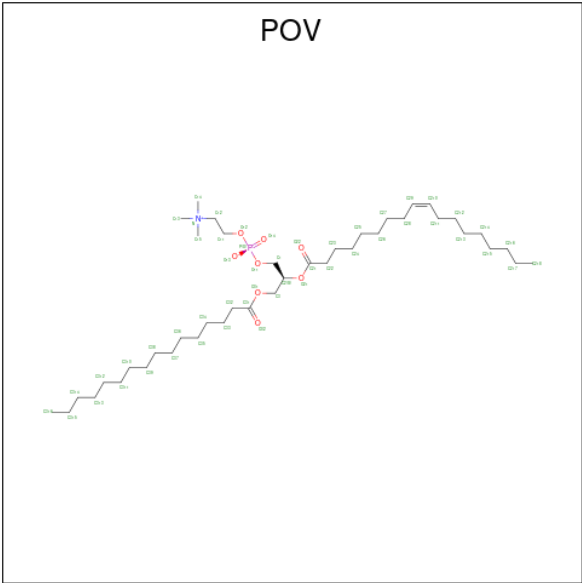
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



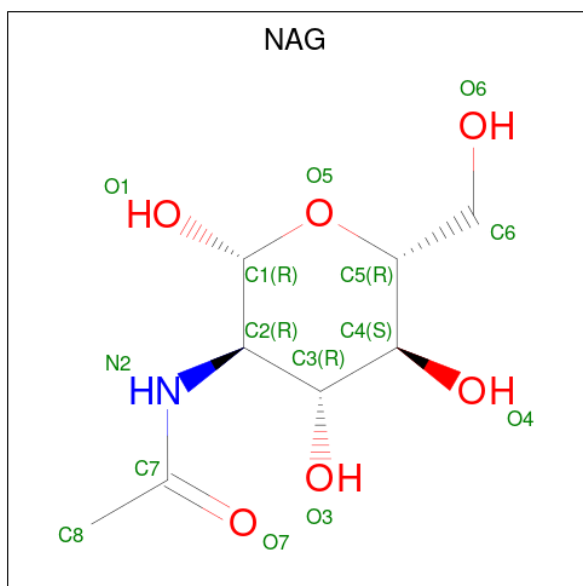
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
4	A	1	Total	C	N	O	P	0
			26	16	1	8	1	
4	A	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			11	11	
5	A	1	Total	C	0
			9	9	
5	A	1	Total	C	0
			15	15	
5	A	1	Total	C	0
			18	18	
5	A	1	Total	C	0
			11	11	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

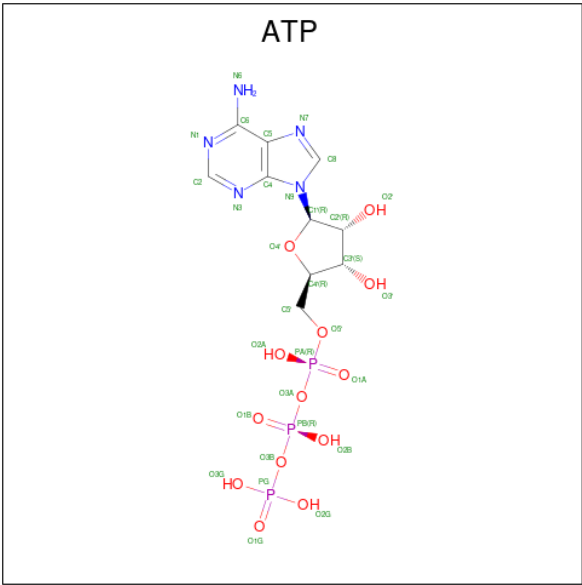


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Mg	0
			2	2	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

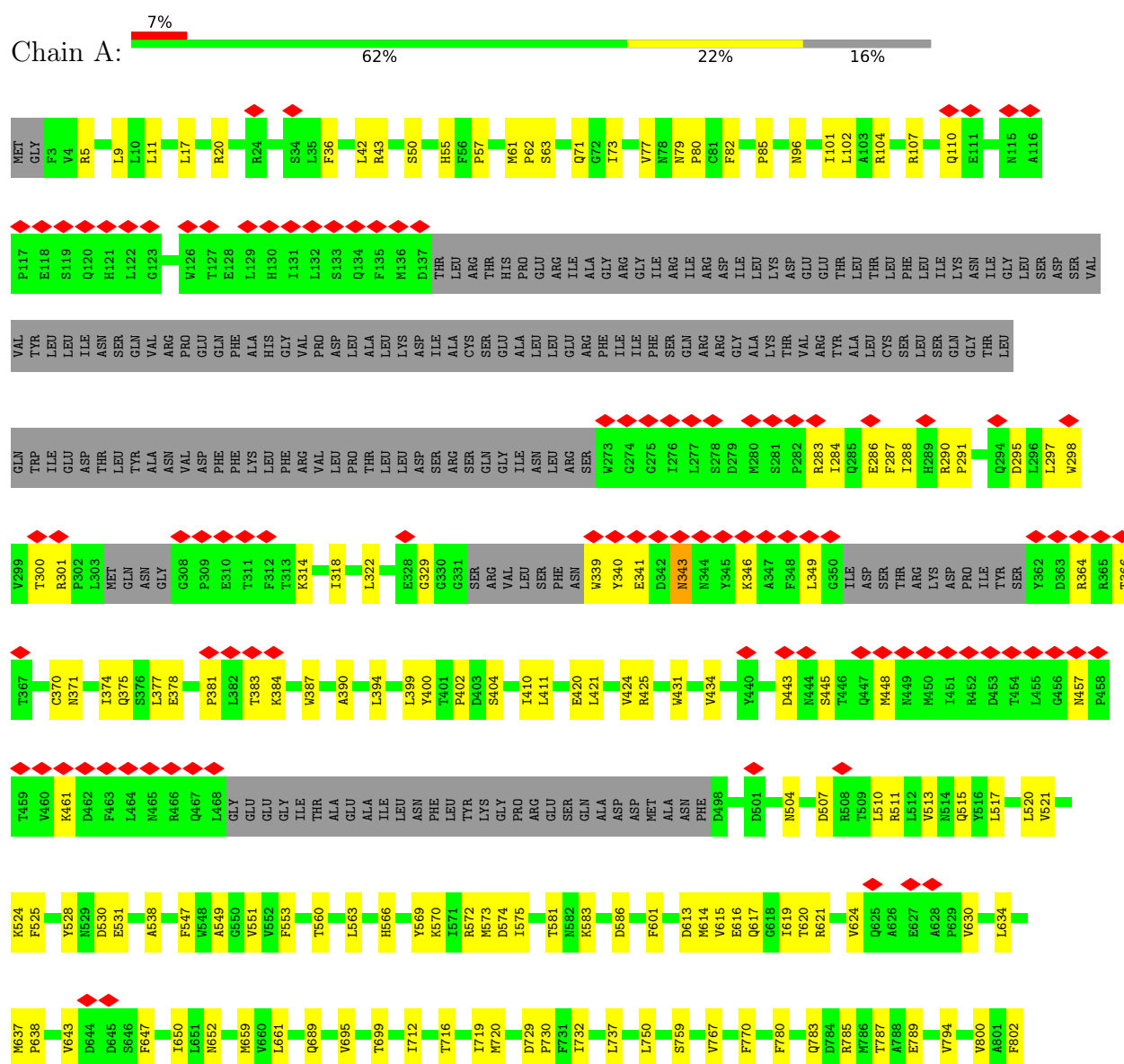


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

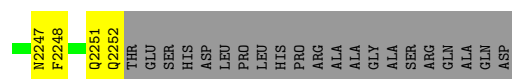
3 Residue-property plots

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: Retinal-specific phospholipid-transporting ATPase ABCA4



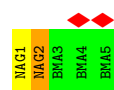
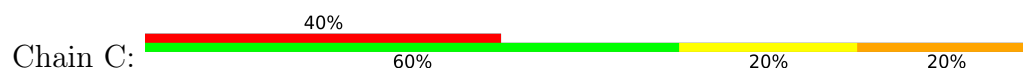




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	333731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.51	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	3.159	Depositor
Minimum map value	-1.828	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.461	Depositor
Map size ($\text{\AA}$)	360.5, 360.5, 360.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	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: 6OU, BMA, POV, NAG, ATP, MG

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	0.34	0/15489	0.55	2/21046 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1719	SER	CA-C-N	5.02	125.04	119.32
1	A	1719	SER	C-N-CA	5.02	125.04	119.32

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	15117	0	14972	375	0
2	B	39	0	33	0	0
3	C	61	0	52	3	0
4	A	86	0	0	0	0
5	A	64	0	104	4	0
6	A	84	0	76	3	0
7	A	2	0	0	0	0
8	A	62	0	24	0	0
All	All	15515	0	15261	379	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (379) 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:504:ASN:ND2	6:A:2510:NAG:C1	1.68	1.55
1:A:1476:LYS:NZ	1:A:1477:GLN:HG3	1.41	1.36
1:A:1477:GLN:OE1	1:A:1479:TRP:NE1	1.89	1.06
1:A:343:ASN:HA	1:A:346:LYS:HB2	1.43	1.00
1:A:1476:LYS:NZ	1:A:1477:GLN:CG	2.26	0.98
1:A:364:ARG:HA	1:A:364:ARG:NH1	1.83	0.91
1:A:1476:LYS:HZ2	1:A:1477:GLN:HG3	1.10	0.88
1:A:956:ASN:ND2	1:A:1109:SER:O	2.08	0.86
1:A:364:ARG:HA	1:A:364:ARG:HH11	1.36	0.86
1:A:2006:ASN:ND2	1:A:2009:GLU:OE1	2.12	0.82
1:A:2178:LEU:HG	1:A:2180:PRO:HD2	1.61	0.82
1:A:377:LEU:HD13	1:A:387:TRP:CD2	2.17	0.80
1:A:1476:LYS:HZ1	1:A:1477:GLN:HG3	1.41	0.80
1:A:521:VAL:O	1:A:524:LYS:NZ	2.15	0.79
1:A:410:ILE:HD11	1:A:563:LEU:HD21	1.65	0.78
1:A:377:LEU:HD13	1:A:387:TRP:CE3	2.19	0.77
1:A:637:MET:HE2	1:A:1620:ASN:HB2	1.64	0.77
1:A:2028:THR:OG1	1:A:2031:GLU:OE2	2.03	0.75
1:A:1159:LEU:HD12	1:A:1159:LEU:O	1.86	0.75
1:A:1918:ASP:OD1	1:A:1919:ASP:N	2.20	0.74
1:A:549:ALA:HB2	1:A:573:MET:HE2	1.69	0.73
1:A:817:LEU:HD11	1:A:1546:LEU:HD11	1.70	0.73
1:A:1996:ALA:HB3	1:A:2003:ILE:HD12	1.71	0.72
1:A:2150:CYS:HB2	1:A:2157:LEU:HD21	1.71	0.70
1:A:993:ASP:OD1	1:A:994:ILE:N	2.24	0.70
1:A:1159:LEU:HD13	1:A:1259:LEU:HD22	1.74	0.69
1:A:1525:LEU:HD12	1:A:1525:LEU:O	1.92	0.69
1:A:404:SER:OG	1:A:560:THR:O	2.11	0.69
1:A:1260:SER:HB2	1:A:2155:GLN:HG2	1.73	0.69
1:A:61:MET:HG3	1:A:62:PRO:HD2	1.75	0.69
1:A:381:PRO:HA	1:A:384:LYS:HB3	1.75	0.69
1:A:341:GLU:O	1:A:341:GLU:CD	2.34	0.68
1:A:1472:GLN:HA	1:A:1475:GLN:HE21	1.58	0.68
1:A:1817:GLU:OE2	1:A:1817:GLU:HA	1.93	0.67
1:A:1476:LYS:HZ1	1:A:1477:GLN:CG	2.01	0.67
1:A:349:LEU:HA	1:A:1867:ALA:HB2	1.77	0.67
1:A:1718:VAL:HG23	1:A:2039:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:TRP:CD1	1:A:1126:LEU:HD11	2.31	0.66
1:A:1160:VAL:HG22	1:A:1261:SER:HB3	1.78	0.65
1:A:1010:GLN:O	1:A:1068:ARG:NH1	2.30	0.65
1:A:530:ASP:OD1	1:A:531:GLU:N	2.29	0.65
1:A:719:ILE:HG22	1:A:720:MET:HE2	1.79	0.65
1:A:370:CYS:O	1:A:374:ILE:HG13	1.97	0.64
1:A:402:PRO:HG2	1:A:553:PHE:HB2	1.80	0.64
1:A:1416:PHE:CD2	1:A:1525:LEU:HD11	2.32	0.64
1:A:1472:GLN:HA	1:A:1475:GLN:NE2	2.13	0.63
1:A:298:TRP:HD1	1:A:301:ARG:HH21	1.46	0.63
1:A:1403:LEU:HG	1:A:1403:LEU:O	1.97	0.63
1:A:364:ARG:HB3	1:A:366:THR:HG22	1.80	0.63
1:A:695:VAL:O	1:A:699:THR:HG23	1.99	0.63
1:A:650:ILE:HG12	1:A:1812:ILE:HG23	1.80	0.62
1:A:341:GLU:OE2	1:A:346:LYS:HD2	1.99	0.62
1:A:1079:ASP:OD1	1:A:1111:ARG:NH1	2.32	0.62
1:A:2023:ILE:HD12	1:A:2068:ALA:HB1	1.82	0.62
1:A:812:PHE:HE2	1:A:823:ASN:HB3	1.65	0.62
1:A:935:VAL:HB	1:A:984:SER:HB2	1.82	0.62
1:A:1490:CYS:HB2	1:A:1500:PRO:HB3	1.82	0.62
1:A:1545:SER:OG	1:A:1555:GLN:OE1	2.18	0.62
1:A:977:THR:HG22	1:A:978:GLY:H	1.65	0.61
1:A:1636:ASN:HD21	1:A:1654:ILE:H	1.46	0.61
1:A:1010:GLN:HG3	1:A:1087:GLN:HG3	1.82	0.61
1:A:42:LEU:HD11	1:A:1813:LEU:HD21	1.81	0.61
1:A:431:TRP:HA	1:A:434:VAL:HG12	1.83	0.61
1:A:431:TRP:CE3	1:A:510:LEU:HD22	2.35	0.61
1:A:371:ASN:O	1:A:375:GLN:HG2	2.01	0.61
1:A:1442:ASN:ND2	1:A:1654:ILE:O	2.34	0.60
1:A:2019:GLN:O	1:A:2077:ARG:NH2	2.34	0.60
1:A:951:ILE:HD12	1:A:953:PHE:CE1	2.37	0.60
1:A:1477:GLN:OE1	1:A:1479:TRP:CD1	2.54	0.60
1:A:107:ARG:NH2	6:A:2514:NAG:H2	2.16	0.59
1:A:566:HIS:HD2	1:A:1445:LEU:HD11	1.66	0.59
1:A:283:ARG:NH2	1:A:286:GLU:OE1	2.36	0.59
1:A:411:LEU:HD13	1:A:525:PHE:CD2	2.36	0.58
1:A:55:HIS:CD2	1:A:638:PRO:HB3	2.38	0.58
1:A:712:ILE:O	1:A:716:THR:HG23	2.03	0.58
1:A:1788:PRO:O	1:A:1789:SER:OG	2.20	0.58
6:A:2511:NAG:H83	6:A:2511:NAG:H3	1.84	0.58
1:A:431:TRP:CH2	1:A:507:ASP:HA	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:ASP:H	1:A:1974:ASN:HD21	1.49	0.58
1:A:1101:TRP:HE1	1:A:1122:GLU:HG3	1.69	0.58
1:A:1162:LYS:HE3	1:A:1258:GLY:HA2	1.87	0.57
1:A:1156:TYR:CE2	1:A:1271:GLU:HG3	2.39	0.57
1:A:1479:TRP:HE3	1:A:1479:TRP:O	1.88	0.57
1:A:1101:TRP:NE1	1:A:1122:GLU:HG3	2.20	0.57
1:A:318:ILE:O	1:A:322:LEU:HB2	2.05	0.57
1:A:341:GLU:O	1:A:341:GLU:OE1	2.23	0.57
1:A:934:LEU:HD23	1:A:946:VAL:HG11	1.86	0.57
1:A:955:GLU:HA	1:A:1112:THR:HG22	1.85	0.56
1:A:1687:ILE:HD11	1:A:1842:GLY:HA2	1.87	0.56
1:A:2014:MET:O	1:A:2040:ARG:NH2	2.38	0.56
1:A:57:PRO:CB	1:A:96:ASN:HD21	2.19	0.56
1:A:1489:ARG:HG3	1:A:1489:ARG:HH11	1.69	0.56
1:A:377:LEU:HD23	1:A:383:THR:HG21	1.87	0.56
1:A:101:ILE:HA	1:A:104:ARG:HD3	1.88	0.56
1:A:659:MET:HB3	1:A:802:PHE:HE1	1.69	0.56
1:A:829:THR:OG1	1:A:832:ASP:OD2	2.24	0.56
1:A:411:LEU:HD13	1:A:525:PHE:HD2	1.70	0.56
1:A:616:GLU:O	1:A:620:THR:HG23	2.06	0.56
1:A:804:PHE:HB3	1:A:834:PHE:HE2	1.72	0.55
1:A:399:LEU:HD23	1:A:528:TYR:CE2	2.42	0.55
1:A:947:ASP:OD2	1:A:1137:ARG:NH1	2.39	0.55
1:A:1385:PHE:HB2	1:A:1745:ILE:HD13	1.88	0.55
1:A:965:ASN:OD1	1:A:2102:ASP:HB2	2.06	0.55
1:A:457:ASN:O	1:A:461:LYS:N	2.40	0.55
1:A:394:LEU:HD23	1:A:520:LEU:HD21	1.88	0.55
1:A:420:GLU:OE2	1:A:1608:HIS:HB2	2.06	0.55
1:A:1437:LYS:HB2	1:A:1438:PRO:HD3	1.89	0.55
1:A:1019:THR:O	1:A:1023:HIS:ND1	2.31	0.54
1:A:1419:MET:HE1	1:A:1427:PHE:HB3	1.88	0.54
1:A:1636:ASN:HB3	1:A:1640:ARG:HH21	1.72	0.54
1:A:62:PRO:HG2	1:A:614:MET:HE2	1.89	0.54
1:A:659:MET:HB3	1:A:802:PHE:CE1	2.43	0.54
1:A:1651:GLU:HG3	1:A:1652:TYR:CD1	2.43	0.54
1:A:1925:ARG:HH12	1:A:1957:ARG:HB3	1.72	0.54
1:A:1159:LEU:HD13	1:A:1259:LEU:CD2	2.38	0.54
1:A:1159:LEU:HD11	1:A:1229:LEU:CD2	2.37	0.54
1:A:1160:VAL:CG2	1:A:1261:SER:HB3	2.38	0.54
1:A:5:ARG:HH21	1:A:9:LEU:HD21	1.73	0.54
1:A:2094:LEU:HD23	1:A:2097:PRO:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:PHE:CZ	1:A:1508:GLY:HA2	2.43	0.53
1:A:290:ARG:HG2	1:A:291:PRO:HD2	1.90	0.53
1:A:364:ARG:NH1	1:A:364:ARG:CA	2.66	0.53
1:A:617:GLN:OE1	1:A:621:ARG:NH2	2.42	0.53
1:A:920:ARG:HG3	1:A:920:ARG:HH11	1.72	0.53
1:A:1443:ARG:HH11	1:A:1518:SER:HA	1.73	0.53
1:A:1105:LEU:HD13	1:A:2203:TYR:HB3	1.90	0.53
1:A:507:ASP:O	1:A:511:ARG:HG2	2.09	0.53
1:A:1443:ARG:HH21	1:A:1453:TYR:HB3	1.74	0.53
1:A:2023:ILE:HD11	1:A:2076:LYS:HD3	1.91	0.53
1:A:2017:CYS:SG	1:A:2077:ARG:NH1	2.82	0.53
1:A:1224:CYS:O	1:A:1224:CYS:SG	2.67	0.53
1:A:1488:CYS:HB2	1:A:1503:PRO:HD2	1.91	0.52
1:A:20:ARG:HH21	1:A:20:ARG:HG3	1.74	0.52
1:A:431:TRP:HE3	1:A:510:LEU:HD22	1.75	0.52
1:A:1547:LYS:O	1:A:1548:SER:OG	2.24	0.52
1:A:1554:GLU:CD	1:A:1554:GLU:H	2.17	0.52
1:A:377:LEU:HD23	1:A:383:THR:CG2	2.40	0.52
1:A:1416:PHE:HD2	1:A:1525:LEU:HD11	1.75	0.52
1:A:420:GLU:OE1	1:A:1605:PHE:HA	2.10	0.52
1:A:1154:GLY:O	1:A:1267:THR:OG1	2.26	0.52
1:A:390:ALA:O	1:A:394:LEU:HD12	2.10	0.51
1:A:1486:PRO:HD2	1:A:1505:GLY:O	2.10	0.51
1:A:2247:ASN:O	1:A:2251:GLN:HG2	2.10	0.51
1:A:1461:TRP:HZ3	1:A:1514:ARG:HE	1.59	0.51
1:A:85:PRO:HD2	3:C:2:NAG:H2	1.92	0.51
1:A:1159:LEU:HD12	1:A:1159:LEU:C	2.35	0.51
1:A:71:GLN:NE2	5:A:2508:POV:H29	2.24	0.51
1:A:1098:ARG:NE	1:A:2200:GLU:OE1	2.43	0.51
1:A:2237:THR:HG21	1:A:2240:THR:HB	1.93	0.51
1:A:1940:LEU:CD2	1:A:1943:LEU:HD22	2.40	0.51
1:A:1403:LEU:HD21	1:A:1625:HIS:CE1	2.45	0.51
1:A:399:LEU:HD23	1:A:528:TYR:HE2	1.75	0.51
1:A:1161:ARG:NE	1:A:1227:GLN:HA	2.26	0.51
1:A:55:HIS:CE1	1:A:85:PRO:HG3	2.46	0.50
1:A:785:ARG:O	1:A:785:ARG:HG2	2.09	0.50
1:A:378:GLU:O	1:A:384:LYS:HD3	2.11	0.50
1:A:794:VAL:HG12	1:A:800:VAL:HG11	1.93	0.50
1:A:1516:GLN:NE2	1:A:1522:LEU:HD22	2.27	0.50
1:A:1899:HIS:HB3	1:A:1900:PHE:CD1	2.45	0.50
1:A:820:GLN:OE1	1:A:820:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LEU:HD12	1:A:840:MET:HE2	1.94	0.50
1:A:1665:LYS:HG3	1:A:1860:ARG:HH22	1.76	0.50
1:A:1048:ASP:OD2	1:A:1106:LYS:NZ	2.43	0.50
1:A:1860:ARG:HH11	1:A:1860:ARG:HG3	1.77	0.50
1:A:364:ARG:HB2	1:A:371:ASN:OD1	2.11	0.50
1:A:1471:THR:O	1:A:1475:GLN:HG3	2.11	0.50
1:A:581:THR:HG23	1:A:1403:LEU:CB	2.41	0.50
1:A:1525:LEU:HD13	1:A:1530:ILE:HG12	1.93	0.50
1:A:1825:PHE:CD1	1:A:1825:PHE:C	2.90	0.50
1:A:1636:ASN:ND2	1:A:1654:ILE:H	2.08	0.50
1:A:1157:LEU:HD23	1:A:1233:LEU:HD11	1.93	0.49
1:A:297:LEU:HA	1:A:300:THR:HG22	1.93	0.49
1:A:812:PHE:CE2	1:A:823:ASN:HB3	2.46	0.49
1:A:1217:PRO:HG2	1:A:1218:GLU:OE2	2.12	0.49
1:A:1691:SER:HB2	1:A:1799:ASN:HB3	1.94	0.49
1:A:2127:SER:HB2	1:A:2133:CYS:SG	2.52	0.49
1:A:57:PRO:HB3	1:A:96:ASN:HD21	1.78	0.49
1:A:1499:LEU:O	1:A:1543:ARG:NH1	2.45	0.49
1:A:50:SER:HA	1:A:643:VAL:HA	1.95	0.49
1:A:291:PRO:O	1:A:295:ASP:HB2	2.12	0.49
1:A:1576:LEU:O	1:A:1580:LEU:HG	2.12	0.49
1:A:1995:ASP:OD1	1:A:2002:SER:OG	2.31	0.49
1:A:1388:LEU:HB3	1:A:1749:PHE:CD2	2.48	0.49
1:A:2141:ALA:HB1	1:A:2148:PHE:CD1	2.48	0.49
1:A:1813:LEU:O	1:A:1817:GLU:HB2	2.12	0.49
1:A:759:SER:HB2	1:A:1699:LEU:HD13	1.95	0.49
1:A:1089:THR:O	1:A:1089:THR:OG1	2.31	0.48
1:A:1388:LEU:HB3	1:A:1749:PHE:HD2	1.78	0.48
1:A:652:ASN:HA	1:A:810:VAL:HG11	1.96	0.48
1:A:720:MET:HG3	1:A:730:PRO:HB3	1.96	0.48
1:A:1238:PHE:CZ	1:A:2223:LEU:HD11	2.48	0.48
1:A:2160:LYS:HD2	1:A:2161:PHE:CE1	2.48	0.48
1:A:935:VAL:HG22	1:A:947:ASP:O	2.13	0.48
1:A:1982:PHE:O	1:A:1986:THR:HG23	2.13	0.48
1:A:1205:VAL:O	1:A:1205:VAL:HG12	2.14	0.48
1:A:2136:LEU:H	1:A:2136:LEU:HD23	1.77	0.48
1:A:431:TRP:CG	1:A:510:LEU:HD13	2.49	0.48
1:A:1065:GLY:HA3	1:A:1974:ASN:OD1	2.13	0.48
1:A:1133:ILE:HG22	1:A:1138:LEU:HD12	1.94	0.48
1:A:1644:PRO:HG2	1:A:1647:ARG:HH21	1.79	0.48
1:A:2098:THR:O	1:A:2098:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:VAL:O	1:A:619:ILE:HG13	2.13	0.47
1:A:20:ARG:NH2	1:A:1017:HIS:O	2.47	0.47
1:A:937:ILE:HG12	1:A:944:PRO:HG3	1.96	0.47
1:A:1986:THR:O	1:A:2011:HIS:NE2	2.40	0.47
1:A:314:LYS:HE2	1:A:314:LYS:HA	1.96	0.47
1:A:572:ARG:NH1	1:A:1662:ASN:HB2	2.30	0.47
1:A:920:ARG:HG3	1:A:920:ARG:NH1	2.30	0.47
1:A:79:ASN:ND2	1:A:601:PHE:HE2	2.12	0.47
1:A:400:TYR:CD2	1:A:411:LEU:HD12	2.49	0.47
1:A:110:GLN:OE1	1:A:110:GLN:HA	2.14	0.47
1:A:1525:LEU:O	1:A:1525:LEU:CD1	2.61	0.47
1:A:377:LEU:HD13	1:A:387:TRP:CE2	2.48	0.47
1:A:425:ARG:HD2	1:A:517:LEU:O	2.15	0.47
1:A:586:ASP:N	1:A:586:ASP:OD1	2.45	0.47
1:A:1005:LEU:HD23	1:A:1006:GLY:N	2.30	0.47
1:A:780:PHE:O	1:A:783:GLN:HG3	2.14	0.47
1:A:79:ASN:HD21	1:A:601:PHE:HE2	1.63	0.47
1:A:1466:VAL:HG11	1:A:1509:LEU:HD21	1.97	0.47
1:A:1754:TYR:HB3	1:A:1763:LEU:HD22	1.95	0.47
1:A:377:LEU:HD13	1:A:387:TRP:CZ3	2.50	0.47
1:A:862:PRO:HG3	1:A:869:LEU:HB3	1.95	0.47
1:A:1541:LEU:HD21	1:A:1555:GLN:H	1.80	0.47
1:A:1257:LEU:HB2	1:A:1259:LEU:HG	1.96	0.46
1:A:1718:VAL:HG23	1:A:2039:LEU:CD2	2.45	0.46
1:A:364:ARG:CB	1:A:366:THR:HG22	2.45	0.46
1:A:421:LEU:O	1:A:424:VAL:HG22	2.15	0.46
1:A:2237:THR:HG22	1:A:2238:GLN:H	1.81	0.46
1:A:1218:GLU:OE2	1:A:1218:GLU:N	2.49	0.46
1:A:962:LEU:HD13	1:A:1120:MET:HE1	1.97	0.46
1:A:1648:SER:O	1:A:1651:GLU:HG2	2.16	0.46
1:A:2005:THR:OG1	1:A:2006:ASN:N	2.49	0.46
1:A:947:ASP:O	1:A:948:ARG:HG2	2.16	0.46
1:A:2172:LYS:HB3	1:A:2232:GLU:HB2	1.98	0.46
5:A:2507:POV:H27A	5:A:2507:POV:H210	1.52	0.46
1:A:570:LYS:HB3	1:A:1657:ILE:HB	1.98	0.46
1:A:1743:VAL:O	1:A:1747:ILE:HG12	2.16	0.46
1:A:1978:LYS:HB2	1:A:1978:LYS:HE2	1.76	0.46
1:A:2212:SER:OG	1:A:2213:SER:N	2.47	0.46
1:A:1760:LEU:HB3	1:A:1761:PRO:HD3	1.98	0.46
1:A:1452:GLU:OE1	1:A:1452:GLU:N	2.45	0.45
1:A:1474:PHE:HZ	1:A:1508:GLY:HA2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:PRO:HG2	1:A:1271:GLU:HG2	1.98	0.45
1:A:1158:THR:O	1:A:1158:THR:OG1	2.27	0.45
1:A:1159:LEU:O	1:A:1159:LEU:CD1	2.61	0.45
1:A:977:THR:HG22	1:A:978:GLY:N	2.32	0.45
1:A:1238:PHE:HZ	1:A:2223:LEU:HD11	1.80	0.45
1:A:689:GLN:HG3	1:A:1027:TYR:CE1	2.52	0.45
1:A:1209:MET:O	1:A:1213:LEU:HD13	2.16	0.45
1:A:2089:PRO:HG2	1:A:2092:VAL:HG22	1.98	0.45
1:A:1530:ILE:O	1:A:1534:LEU:HD12	2.17	0.45
1:A:1818:ASN:OD1	1:A:1818:ASN:N	2.49	0.45
1:A:1940:LEU:HD21	1:A:1943:LEU:HD22	1.99	0.45
1:A:2149:ARG:HE	1:A:2252:GLN:HE21	1.64	0.45
1:A:2198:GLN:HG3	1:A:2208:PHE:CZ	2.52	0.45
1:A:951:ILE:HD12	1:A:953:PHE:CZ	2.52	0.45
1:A:1488:CYS:CB	1:A:1503:PRO:HD2	2.46	0.45
1:A:1930:THR:OG1	1:A:1931:GLY:N	2.50	0.45
1:A:812:PHE:CE1	1:A:828:PRO:HB3	2.52	0.45
1:A:1698:VAL:HG11	1:A:1795:LEU:HD12	1.98	0.45
1:A:1869:PRO:HA	1:A:1874:LEU:HD23	1.99	0.45
1:A:1705:ARG:NH1	1:A:1786:ASP:OD1	2.38	0.44
1:A:57:PRO:HB2	1:A:96:ASN:ND2	2.32	0.44
1:A:1971:LEU:HD13	1:A:2130:MET:HE1	1.99	0.44
1:A:2210:VAL:HG12	1:A:2212:SER:H	1.83	0.44
1:A:77:VAL:HG11	5:A:2507:POV:H21F	1.98	0.44
1:A:860:VAL:HG12	1:A:861:PHE:CD1	2.53	0.44
1:A:1464:PRO:HG3	1:A:1513:GLN:HE21	1.82	0.44
1:A:2142:ILE:HG21	1:A:2248:PHE:HD2	1.82	0.44
1:A:1807:SER:HA	1:A:1810:THR:HG22	2.00	0.44
1:A:61:MET:HE1	1:A:634:LEU:CD1	2.48	0.44
1:A:2237:THR:HG22	1:A:2238:GLN:N	2.33	0.44
1:A:448:MET:N	1:A:448:MET:SD	2.89	0.44
1:A:1715:ILE:HD11	1:A:1986:THR:HB	1.99	0.44
1:A:1719:SER:OG	1:A:1720:PRO:HD2	2.18	0.44
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.85	0.44
1:A:574:ASP:OD1	1:A:575:ILE:N	2.46	0.43
1:A:1208:LEU:O	1:A:1212:VAL:HG23	2.17	0.43
1:A:349:LEU:HD21	1:A:1854:VAL:HG12	2.01	0.43
1:A:1581:SER:O	1:A:1585:ARG:HD3	2.19	0.43
1:A:17:LEU:HD11	1:A:1018:LEU:HG	2.01	0.43
1:A:538:ALA:HB1	1:A:1661:LEU:HD21	1.99	0.43
1:A:859:GLN:O	1:A:870:PRO:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:LYS:HG3	1:A:2231:ILE:HB	2.01	0.43
1:A:63:SER:OG	1:A:613:ASP:OD1	2.35	0.43
1:A:996:THR:OG1	1:A:997:SER:N	2.51	0.43
1:A:1163:MET:HG2	1:A:1201:LEU:HA	1.99	0.43
1:A:1924:GLU:OE2	1:A:1927:ARG:NH1	2.51	0.43
1:A:80:PRO:HB2	1:A:82:PHE:CE1	2.54	0.43
1:A:1205:VAL:O	1:A:1209:MET:HB2	2.18	0.43
1:A:1046:LEU:HD21	1:A:1055:ARG:HG3	2.00	0.43
1:A:43:ARG:HB2	1:A:647:PHE:CE2	2.54	0.43
1:A:1489:ARG:HG3	1:A:1489:ARG:NH1	2.32	0.43
1:A:1571:ILE:O	1:A:1572:THR:OG1	2.32	0.43
1:A:1587:MET:HB3	1:A:1589:VAL:HG12	2.01	0.43
1:A:1926:GLN:O	1:A:1930:THR:HG23	2.19	0.43
1:A:1344:LEU:HD23	1:A:1344:LEU:HA	1.87	0.43
1:A:569:TYR:OH	1:A:616:GLU:HG3	2.19	0.43
1:A:102:LEU:HD23	1:A:322:LEU:O	2.18	0.42
1:A:346:LYS:O	1:A:349:LEU:HB2	2.18	0.42
1:A:767:VAL:HG11	1:A:1379:LEU:HD21	2.01	0.42
1:A:1501:GLU:HA	1:A:1543:ARG:HH22	1.84	0.42
1:A:61:MET:HE1	1:A:634:LEU:HD11	2.02	0.42
1:A:82:PHE:CE1	1:A:329:GLY:HA3	2.54	0.42
1:A:343:ASN:N	1:A:343:ASN:OD1	2.51	0.42
1:A:867:THR:HG21	1:A:1002:ARG:HH22	1.83	0.42
1:A:1668:LEU:HD12	1:A:1668:LEU:HA	1.85	0.42
1:A:2151:MET:O	1:A:2151:MET:HG2	2.18	0.42
3:C:1:NAG:H62	3:C:2:NAG:C7	2.49	0.42
1:A:1602:ILE:N	1:A:1603:PRO:HD2	2.34	0.42
1:A:2192:ASN:OD1	1:A:2221:LEU:HD21	2.19	0.42
1:A:853:LEU:HD12	1:A:853:LEU:HA	1.87	0.42
1:A:1643:LEU:HD21	1:A:1652:TYR:HD2	1.83	0.42
1:A:2153:THR:HG22	1:A:2156:HIS:HB3	2.01	0.42
1:A:1434:LEU:O	1:A:1434:LEU:HD23	2.18	0.42
3:C:1:NAG:H62	3:C:2:NAG:N2	2.33	0.42
1:A:965:ASN:ND2	1:A:2074:GLY:HA3	2.35	0.42
1:A:2110:TRP:NE1	1:A:2132:GLU:HG3	2.35	0.42
1:A:445:SER:O	1:A:448:MET:HG2	2.19	0.42
1:A:55:HIS:HD2	1:A:638:PRO:HB3	1.83	0.42
1:A:513:VAL:O	1:A:517:LEU:HD23	2.19	0.42
1:A:661:LEU:HD21	1:A:770:PHE:CE1	2.54	0.42
1:A:787:THR:HG22	1:A:789:GLU:H	1.85	0.42
1:A:1513:GLN:HA	1:A:1522:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ASP:HB3	1:A:732:ILE:HG12	2.01	0.42
1:A:1712:LEU:HD23	1:A:1712:LEU:HA	1.90	0.42
1:A:1874:LEU:HG	1:A:1875:ILE:HG23	2.02	0.42
1:A:2213:SER:OG	1:A:2214:SER:N	2.53	0.42
1:A:1008:CYS:SG	1:A:1068:ARG:NH2	2.93	0.41
1:A:1347:GLY:O	1:A:1351:VAL:HG23	2.20	0.41
1:A:1449:TRP:CE2	1:A:1450:LEU:HD23	2.55	0.41
1:A:1643:LEU:HD21	1:A:1652:TYR:CD2	2.54	0.41
1:A:1708:LYS:HA	1:A:1708:LYS:HD2	1.89	0.41
1:A:1809:ILE:HG22	1:A:1830:ARG:HH12	1.83	0.41
1:A:284:ILE:O	1:A:287:PHE:HB3	2.20	0.41
1:A:624:VAL:HG11	1:A:1642:SER:OG	2.20	0.41
1:A:1405:LEU:HD13	1:A:1628:VAL:CG2	2.50	0.41
1:A:1806:SER:HB3	1:A:1839:PHE:HD1	1.84	0.41
1:A:400:TYR:HA	1:A:551:VAL:O	2.20	0.41
1:A:1361:LYS:HG3	1:A:2035:LEU:HD22	2.02	0.41
1:A:1510:PRO:HA	1:A:1511:PRO:HD3	1.86	0.41
1:A:1576:LEU:HD12	1:A:1576:LEU:HA	1.93	0.41
1:A:73:ILE:HD13	5:A:2506:POV:H27	2.02	0.41
1:A:630:VAL:HG13	1:A:1613:ASP:O	2.21	0.41
1:A:997:SER:O	1:A:997:SER:OG	2.35	0.41
1:A:55:HIS:HE2	1:A:1535:VAL:HG21	1.85	0.41
1:A:339:TRP:O	1:A:340:TYR:HB3	2.21	0.41
1:A:750:LEU:HA	1:A:854:ALA:HB2	2.03	0.41
1:A:1365:HIS:CE1	1:A:2026:LEU:HD12	2.55	0.41
1:A:1417:PHE:CZ	1:A:1435:LEU:HD11	2.55	0.41
1:A:36:PHE:HZ	1:A:659:MET:HG3	1.85	0.41
1:A:860:VAL:HG12	1:A:861:PHE:CE1	2.56	0.41
1:A:1159:LEU:HD11	1:A:1229:LEU:HD23	2.02	0.41
1:A:1731:ASP:OD2	1:A:1779:TYR:OH	2.34	0.41
1:A:431:TRP:CD2	1:A:510:LEU:HD13	2.56	0.41
1:A:2059:GLY:O	1:A:2061:THR:N	2.53	0.41
1:A:650:ILE:HG12	1:A:1812:ILE:CG2	2.50	0.41
1:A:1240:HIS:CE1	1:A:2223:LEU:HD21	2.56	0.41
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.90	0.41
1:A:399:LEU:HD13	1:A:547:PHE:HE1	1.85	0.41
1:A:2040:ARG:HD2	1:A:2086:ILE:O	2.20	0.41
1:A:2092:VAL:HG12	1:A:2094:LEU:CD1	2.51	0.41
1:A:288:ILE:HD12	1:A:288:ILE:H	1.86	0.41
1:A:1958:LEU:HG	1:A:2148:PHE:CE2	2.56	0.41
1:A:443:ASP:C	1:A:448:MET:HE3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:HG23	1:A:1403:LEU:HB2	2.02	0.40
1:A:877:GLU:OE1	1:A:877:GLU:HA	2.22	0.40
1:A:1350:LEU:HA	1:A:1350:LEU:HD12	1.85	0.40
1:A:1443:ARG:NH2	1:A:1453:TYR:HB3	2.35	0.40
1:A:862:PRO:HB2	1:A:866:GLY:HA3	2.03	0.40
1:A:1443:ARG:HG2	1:A:1444:CYS:N	2.37	0.40
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.93	0.40
1:A:1147:LEU:HD23	1:A:1147:LEU:HA	1.78	0.40
1:A:1488:CYS:HB2	1:A:1503:PRO:CD	2.52	0.40
1:A:583:LYS:HB3	1:A:583:LYS:HE3	1.83	0.40
1:A:1130:ILE:HD11	1:A:1147:LEU:HD12	2.03	0.40
1:A:511:ARG:O	1:A:515:GLN:HG3	2.22	0.40
1:A:1417:PHE:CE1	1:A:1435:LEU:HD21	2.56	0.40
1:A:1645:LYS:C	1:A:1647:ARG:H	2.29	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	1898/2273 (84%)	1740 (92%)	158 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	1639/1990 (82%)	1633 (100%)	6 (0%)	84 85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	823	ASN
1	A	1525	LEU
1	A	1718	VAL
1	A	1727	ASN
1	A	1955	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	71	GLN
1	A	78	ASN
1	A	79	ASN
1	A	96	ASN
1	A	566	HIS
1	A	693	ASN
1	A	1017	HIS
1	A	1119	HIS
1	A	1370	HIS
1	A	1406	HIS
1	A	1555	GLN
1	A	1703	GLN
1	A	1799	ASN
1	A	1974	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

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	B	2	2	14,14,15	0.22	0	17,19,21	0.70	0
2	BMA	B	3	2	11,11,12	0.58	0	15,15,17	0.97	0
3	NAG	C	1	1,3	14,14,15	0.45	0	17,19,21	0.45	0
3	NAG	C	2	3	14,14,15	0.74	1 (7%)	17,19,21	1.36	1 (5%)
3	BMA	C	3	3	11,11,12	0.53	0	15,15,17	0.68	0
3	BMA	C	4	3	11,11,12	0.53	0	15,15,17	0.75	0
3	BMA	C	5	3	11,11,12	0.54	0	15,15,17	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	0/2/19/22	0/1/1/1
3	BMA	C	5	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-3.47	1.37	1.43
3	C	2	NAG	O5-C1	2.64	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	5.09	119.01	112.19
2	B	1	NAG	C3-C4-C5	2.18	114.19	110.23

There are no chirality outliers.

All (10) torsion outliers are listed below:

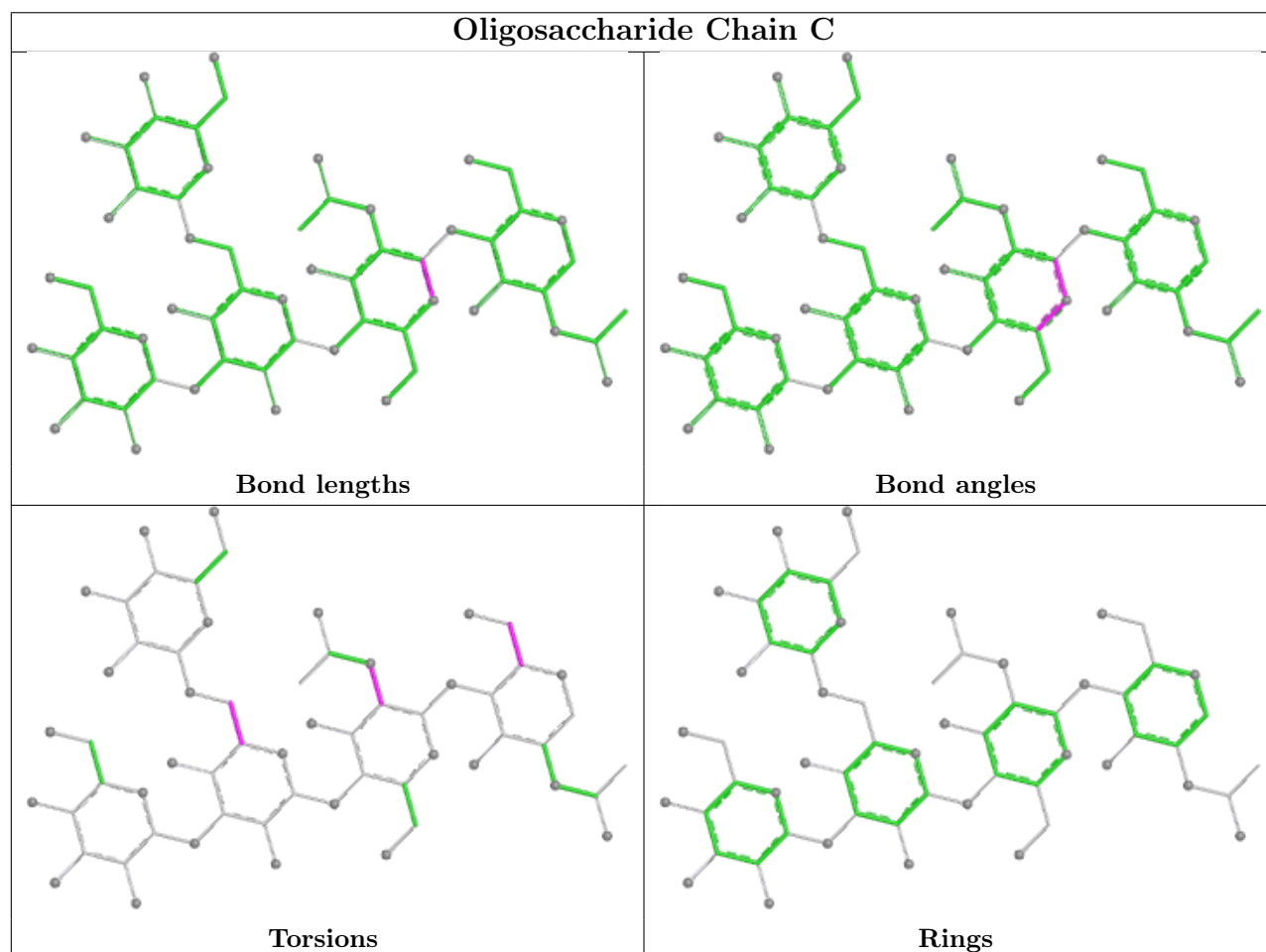
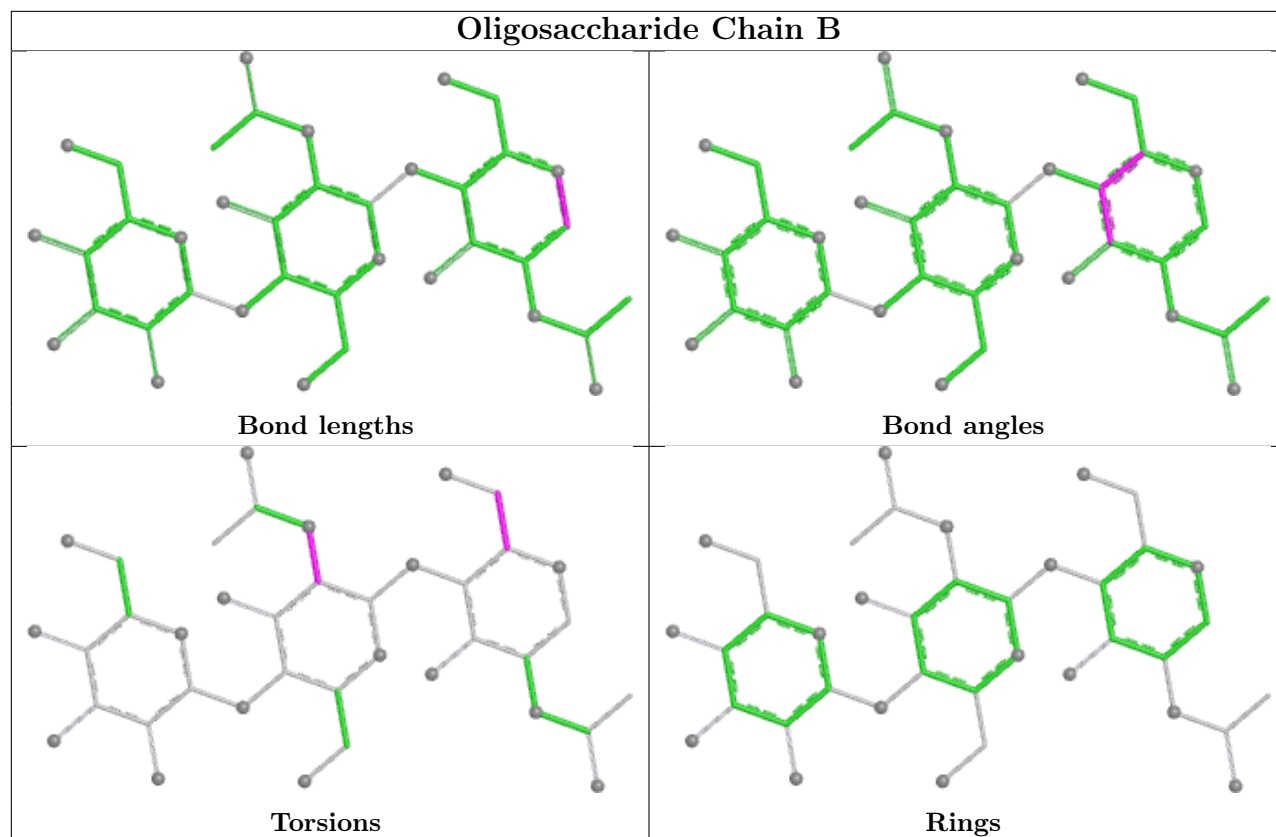
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	2	0
3	C	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	2514	1	14,14,15	0.29	0	17,19,21	0.71	0
6	NAG	A	2512	1	14,14,15	0.19	0	17,19,21	0.53	0
5	POV	A	2505	-	8,8,51	0.29	0	7,7,59	0.78	0
6	NAG	A	2509	1	14,14,15	0.30	0	17,19,21	0.56	0
5	POV	A	2508	-	9,9,51	0.40	0	8,8,59	0.82	0
8	ATP	A	2517	7	32,33,33	1.32	4 (12%)	48,52,52	1.79	9 (18%)
5	POV	A	2504	-	10,10,51	0.30	0	9,9,59	0.80	0
4	6OU	A	2503	-	28,28,48	1.15	4 (14%)	31,33,53	1.21	2 (6%)
5	POV	A	2507	-	17,17,51	0.32	0	16,16,59	0.80	0
6	NAG	A	2510	-	14,14,15	0.86	1 (7%)	17,19,21	1.32	3 (17%)
6	NAG	A	2511	1	14,14,15	0.74	1 (7%)	17,19,21	1.49	2 (11%)
4	6OU	A	2501	-	30,30,48	1.11	3 (10%)	33,35,53	1.16	2 (6%)
5	POV	A	2506	-	14,14,51	1.04	1 (7%)	13,13,59	1.09	2 (15%)
6	NAG	A	2513	1	14,14,15	0.50	0	17,19,21	0.42	0
4	6OU	A	2502	-	25,25,48	1.22	4 (16%)	28,30,53	1.33	3 (10%)
8	ATP	A	2518	7	32,33,33	1.33	5 (15%)	48,52,52	1.77	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	2514	1	-	3/6/23/26	0/1/1/1
6	NAG	A	2512	1	-	4/6/23/26	0/1/1/1
5	POV	A	2505	-	-	2/6/6/55	-
6	NAG	A	2509	1	-	2/6/23/26	0/1/1/1
5	POV	A	2508	-	-	1/7/7/55	-
8	ATP	A	2517	7	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	A	2504	-	-	5/8/8/55	-
4	6OU	A	2503	-	-	13/32/32/52	-
5	POV	A	2507	-	-	5/15/15/55	-
6	NAG	A	2510	-	-	1/6/23/26	0/1/1/1
6	NAG	A	2511	1	-	6/6/23/26	0/1/1/1
4	6OU	A	2501	-	-	13/34/34/52	-
5	POV	A	2506	-	-	6/12/12/55	-
6	NAG	A	2513	1	-	0/6/23/26	0/1/1/1
4	6OU	A	2502	-	-	11/29/29/52	-
8	ATP	A	2518	7	-	5/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2518	ATP	C5-C4	4.46	1.47	1.39
8	A	2517	ATP	C5-C4	4.43	1.47	1.39
5	A	2506	POV	C29-C210	3.72	1.52	1.31
6	A	2510	NAG	O5-C1	-2.87	1.38	1.43
4	A	2501	6OU	O30-C20	-2.84	1.39	1.46
4	A	2503	6OU	O30-C20	-2.73	1.40	1.46
4	A	2502	6OU	O30-C20	-2.69	1.40	1.46
8	A	2518	ATP	C5-C6	2.62	1.48	1.41
8	A	2517	ATP	C5-C6	2.61	1.48	1.41
6	A	2511	NAG	C1-C2	2.47	1.55	1.52
8	A	2518	ATP	C5-N7	-2.39	1.34	1.39
4	A	2502	6OU	O18-C16	2.39	1.40	1.33
4	A	2501	6OU	O18-C16	2.39	1.40	1.33
8	A	2517	ATP	C5-N7	-2.36	1.34	1.39
4	A	2503	6OU	O18-C16	2.35	1.40	1.33
8	A	2518	ATP	C8-N7	2.24	1.36	1.31
4	A	2502	6OU	O30-C31	2.18	1.40	1.34
4	A	2502	6OU	O18-C19	-2.16	1.40	1.45
8	A	2517	ATP	C8-N7	2.14	1.35	1.31
4	A	2503	6OU	O18-C19	-2.14	1.40	1.45
4	A	2501	6OU	O18-C19	-2.14	1.40	1.45
4	A	2503	6OU	O30-C31	2.11	1.40	1.34
8	A	2518	ATP	C4-N9	-2.04	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2517	ATP	C5-C4-N3	-5.82	118.70	126.72
8	A	2518	ATP	C5-C4-N3	-5.65	118.94	126.72
8	A	2517	ATP	N3-C4-N9	4.72	135.19	127.17
8	A	2518	ATP	N3-C4-N9	4.50	134.82	127.17
6	A	2511	NAG	C2-N2-C7	4.41	128.81	122.90
4	A	2502	6OU	O30-C31-C33	4.33	120.85	111.48
4	A	2503	6OU	O30-C31-C33	4.12	120.38	111.48
8	A	2517	ATP	C2-N3-C4	3.79	121.08	111.83
8	A	2518	ATP	C2-N3-C4	3.71	120.88	111.83
4	A	2501	6OU	O30-C31-C33	3.70	119.49	111.48
6	A	2510	NAG	C3-C4-C5	3.47	116.52	110.23
8	A	2517	ATP	N3-C2-N1	-3.46	123.35	128.58
8	A	2518	ATP	C4-C5-N7	-3.37	106.72	110.58
8	A	2517	ATP	C4-C5-N7	-3.35	106.75	110.58
8	A	2518	ATP	N3-C2-N1	-3.34	123.53	128.58
6	A	2511	NAG	C1-O5-C5	3.19	116.46	112.19
6	A	2510	NAG	C1-O5-C5	-3.12	108.00	112.19
8	A	2517	ATP	C4-N9-C8	2.81	108.69	105.74
8	A	2518	ATP	C4-N9-C8	2.77	108.65	105.74
4	A	2501	6OU	O18-C16-C15	2.73	120.16	111.83
4	A	2502	6OU	O18-C16-C15	2.72	120.14	111.83
4	A	2503	6OU	O18-C16-C15	2.69	120.04	111.83
8	A	2518	ATP	C5-N7-C8	2.46	107.32	103.45
8	A	2517	ATP	C5-N7-C8	2.45	107.30	103.45
8	A	2517	ATP	C3'-C2'-C1'	2.31	105.82	101.46
4	A	2502	6OU	C20-O30-C31	-2.17	112.61	117.80
8	A	2518	ATP	C6-C5-N7	2.16	136.25	132.09
5	A	2506	POV	C211-C210-C29	-2.11	108.99	124.83
5	A	2506	POV	C28-C29-C210	-2.09	109.15	124.83
8	A	2517	ATP	C6-C5-N7	2.09	136.11	132.09
6	A	2510	NAG	C4-C3-C2	2.05	114.03	111.02
8	A	2518	ATP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2501	6OU	O26-C27-C28-N29
4	A	2502	6OU	C27-O26-P23-O22
4	A	2502	6OU	C27-O26-P23-O24
4	A	2502	6OU	C27-O26-P23-O25
4	A	2502	6OU	O26-C27-C28-N29
4	A	2503	6OU	O26-C27-C28-N29

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Mol	Chain	Res	Type	Atoms
6	A	2509	NAG	C8-C7-N2-C2
6	A	2509	NAG	O7-C7-N2-C2
6	A	2510	NAG	C1-C2-N2-C7
6	A	2514	NAG	O7-C7-N2-C2
8	A	2517	ATP	C5'-O5'-PA-O2A
8	A	2517	ATP	C5'-O5'-PA-O3A
8	A	2518	ATP	C5'-O5'-PA-O2A
8	A	2518	ATP	O4'-C4'-C5'-O5'
6	A	2514	NAG	C8-C7-N2-C2
6	A	2511	NAG	C4-C5-C6-O6
4	A	2501	6OU	C15-C16-O18-C19
4	A	2501	6OU	O17-C16-O18-C19
6	A	2511	NAG	O5-C5-C6-O6
6	A	2511	NAG	C8-C7-N2-C2
6	A	2511	NAG	O7-C7-N2-C2
6	A	2512	NAG	C8-C7-N2-C2
6	A	2512	NAG	O7-C7-N2-C2
6	A	2512	NAG	O5-C5-C6-O6
4	A	2501	6OU	C13-C14-C15-C16
4	A	2503	6OU	C13-C14-C15-C16
8	A	2518	ATP	C3'-C4'-C5'-O5'
4	A	2501	6OU	C33-C31-O30-C20
5	A	2506	POV	C211-C212-C213-C214
4	A	2501	6OU	O32-C31-O30-C20
4	A	2503	6OU	C11-C12-C13-C14
4	A	2501	6OU	C10-C11-C12-C13
5	A	2507	POV	C213-C214-C215-C216
4	A	2503	6OU	C33-C31-O30-C20
4	A	2501	6OU	C12-C13-C14-C15
4	A	2503	6OU	O32-C31-O30-C20
5	A	2506	POV	C26-C27-C28-C29
5	A	2507	POV	C26-C27-C28-C29
4	A	2502	6OU	C31-C33-C34-C35
4	A	2501	6OU	O18-C19-C20-C21
5	A	2506	POV	C212-C213-C214-C215
6	A	2514	NAG	O5-C5-C6-O6
5	A	2506	POV	C213-C214-C215-C216
5	A	2504	POV	C36-C37-C38-C39
4	A	2501	6OU	O18-C19-C20-O30
4	A	2502	6OU	O18-C19-C20-O30
4	A	2503	6OU	O18-C19-C20-O30
4	A	2502	6OU	C33-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
4	A	2503	6OU	C19-C20-C21-O22
6	A	2512	NAG	C4-C5-C6-O6
4	A	2503	6OU	O30-C20-C21-O22
4	A	2502	6OU	C10-C11-C12-C13
4	A	2501	6OU	C35-C36-C37-C38
4	A	2503	6OU	C10-C11-C12-C13
4	A	2502	6OU	O32-C31-O30-C20
4	A	2502	6OU	O18-C19-C20-C21
4	A	2503	6OU	O18-C19-C20-C21
5	A	2504	POV	C39-C310-C311-C312
4	A	2501	6OU	C21-O22-P23-O24
4	A	2503	6OU	C21-O22-P23-O24
8	A	2517	ATP	C5'-O5'-PA-O1A
8	A	2518	ATP	C5'-O5'-PA-O1A
8	A	2518	ATP	C5'-O5'-PA-O3A
5	A	2506	POV	C25-C26-C27-C28
5	A	2507	POV	C24-C25-C26-C27
5	A	2504	POV	C37-C38-C39-C310
5	A	2505	POV	C39-C310-C311-C312
6	A	2511	NAG	C1-C2-N2-C7
6	A	2511	NAG	C3-C2-N2-C7
4	A	2501	6OU	C11-C12-C13-C14
5	A	2506	POV	C29-C210-C211-C212
5	A	2508	POV	C27-C28-C29-C210
4	A	2503	6OU	C14-C15-C16-O18
5	A	2504	POV	C311-C312-C313-C314
5	A	2505	POV	C36-C37-C38-C39
5	A	2507	POV	C23-C24-C25-C26
4	A	2502	6OU	C13-C14-C15-C16
5	A	2507	POV	C27-C28-C29-C210
4	A	2503	6OU	C14-C15-C16-O17
5	A	2504	POV	C34-C35-C36-C37

There are no ring outliers.

6 monomers are involved in 7 short contacts:

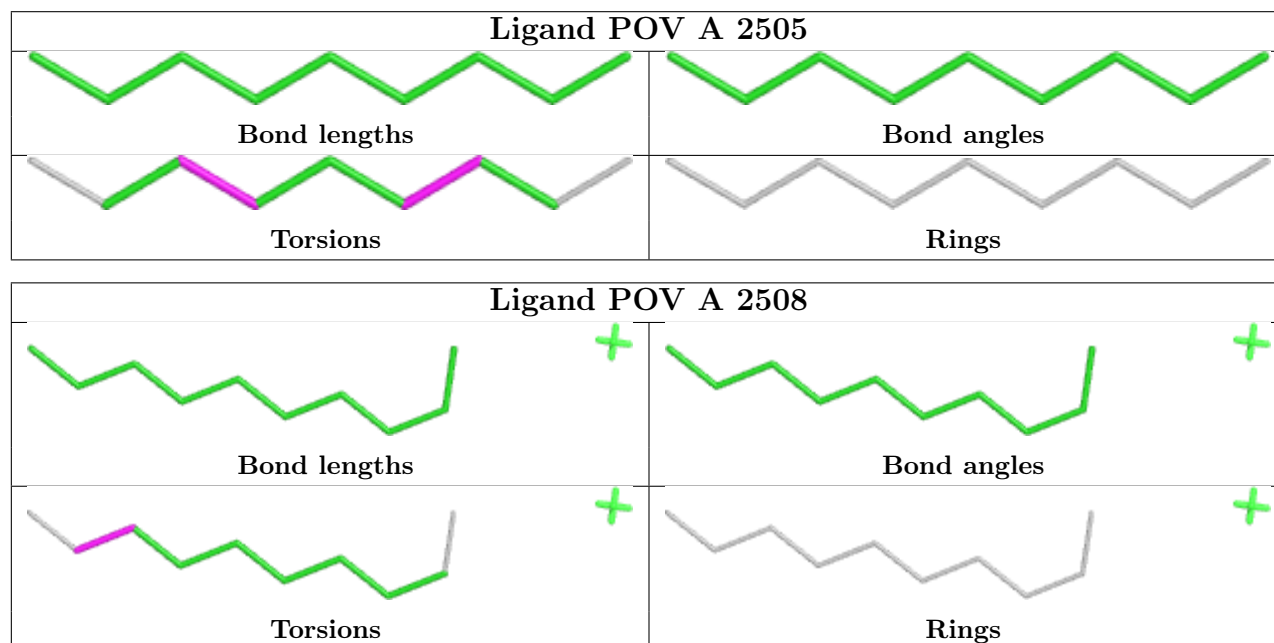
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2514	NAG	1	0
5	A	2508	POV	1	0
5	A	2507	POV	2	0
6	A	2510	NAG	1	0
6	A	2511	NAG	1	0

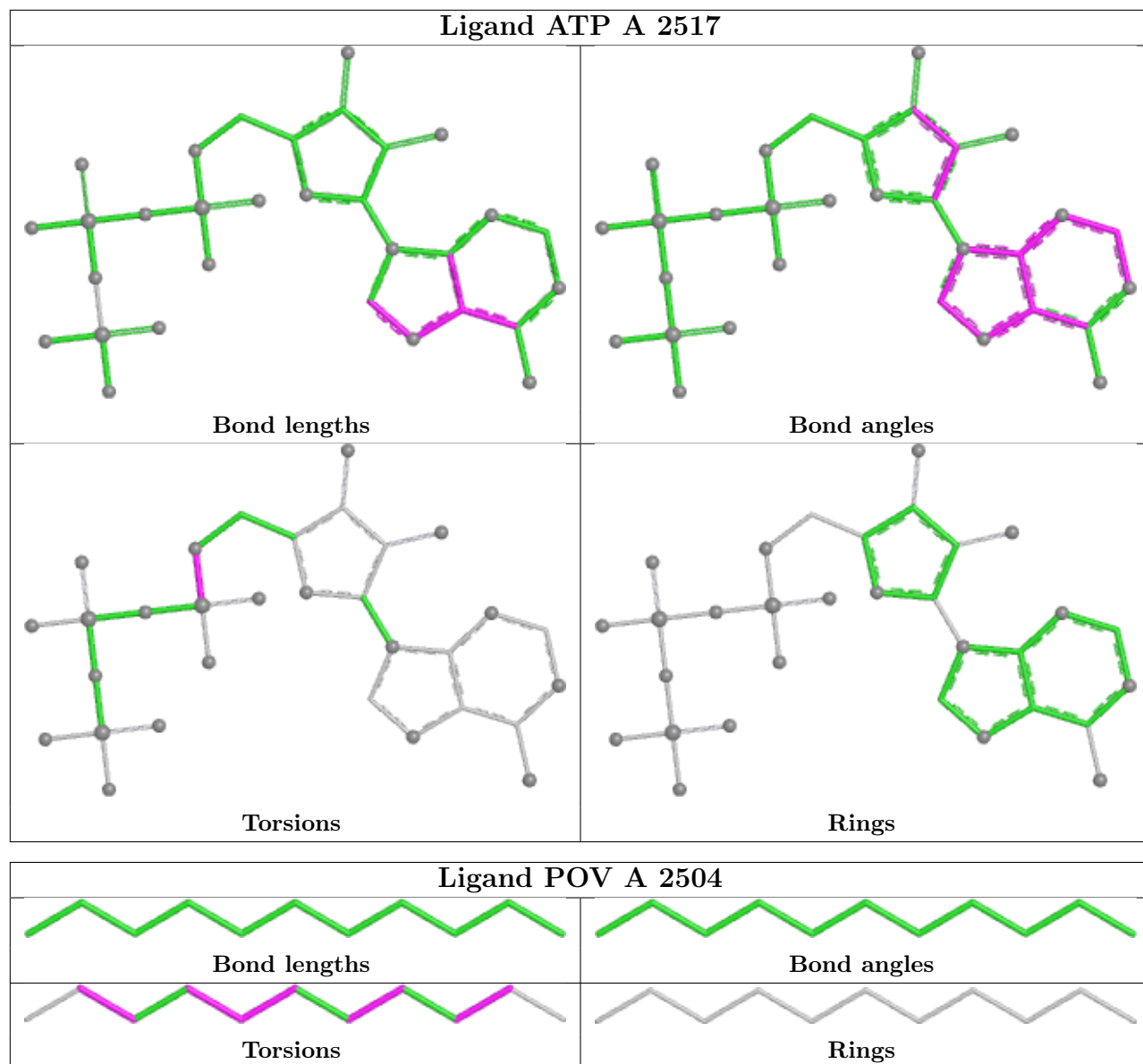
Continued on next page...

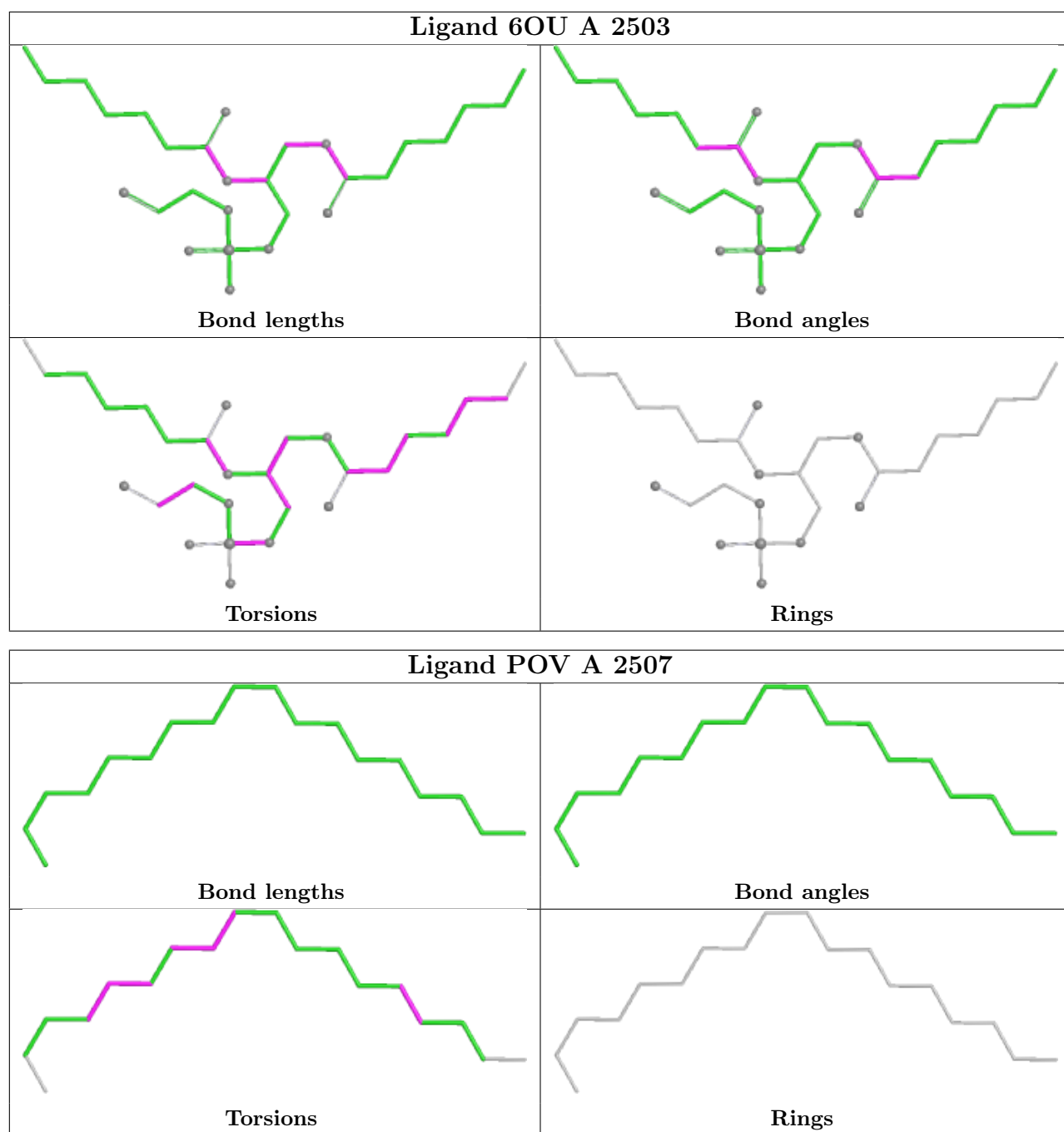
Continued from previous page...

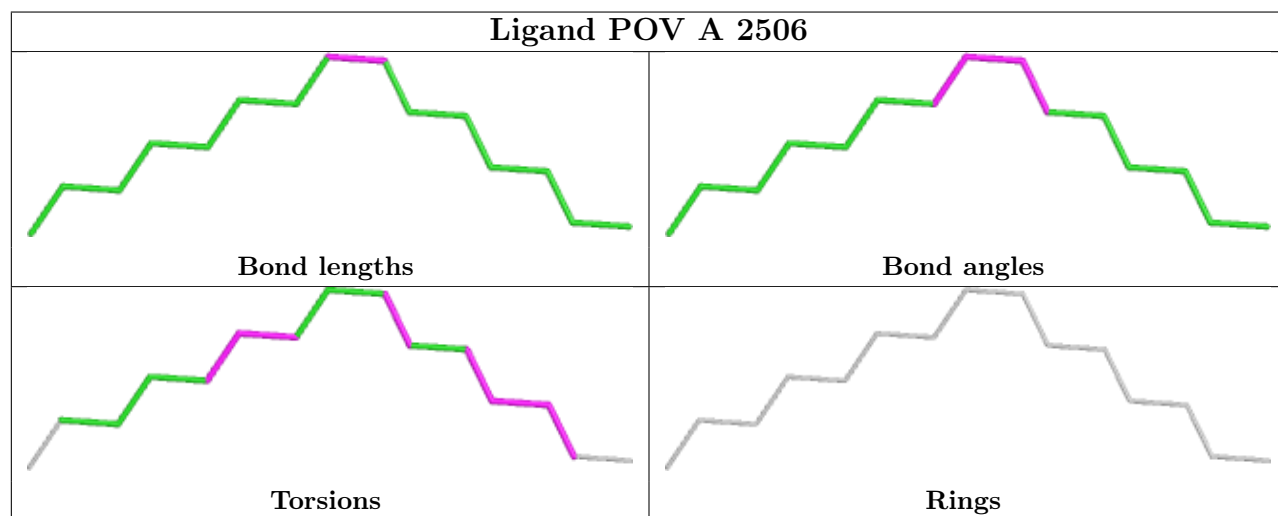
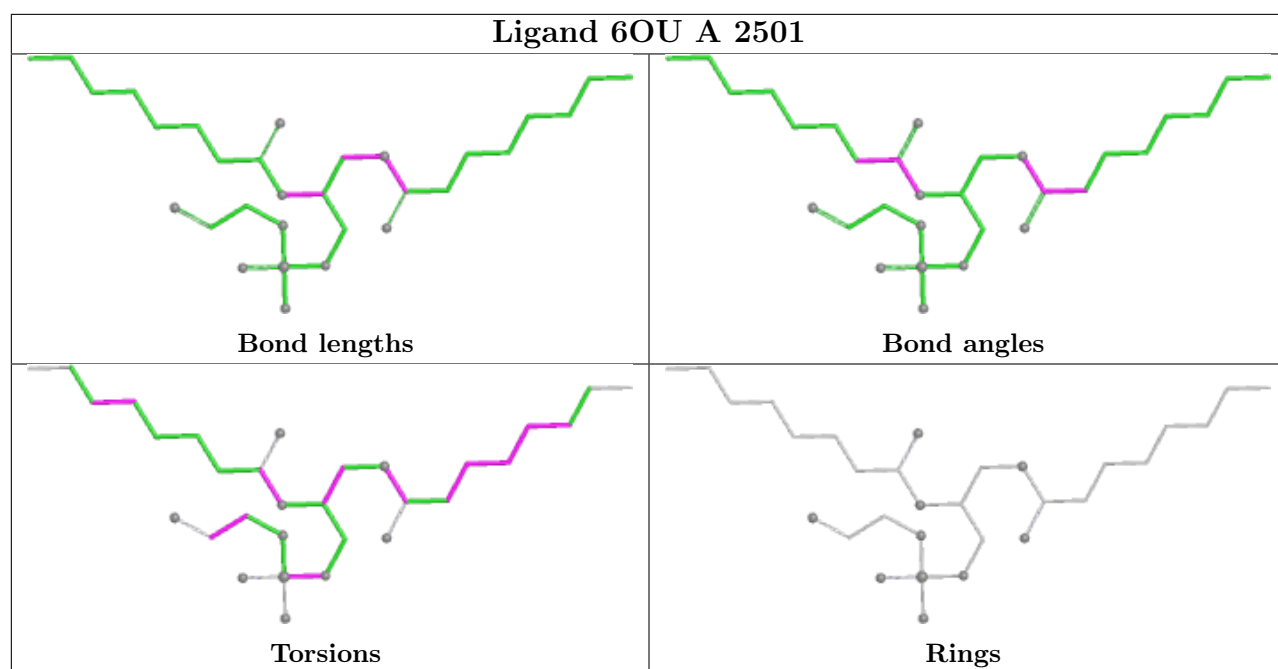
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2506	POV	1	0

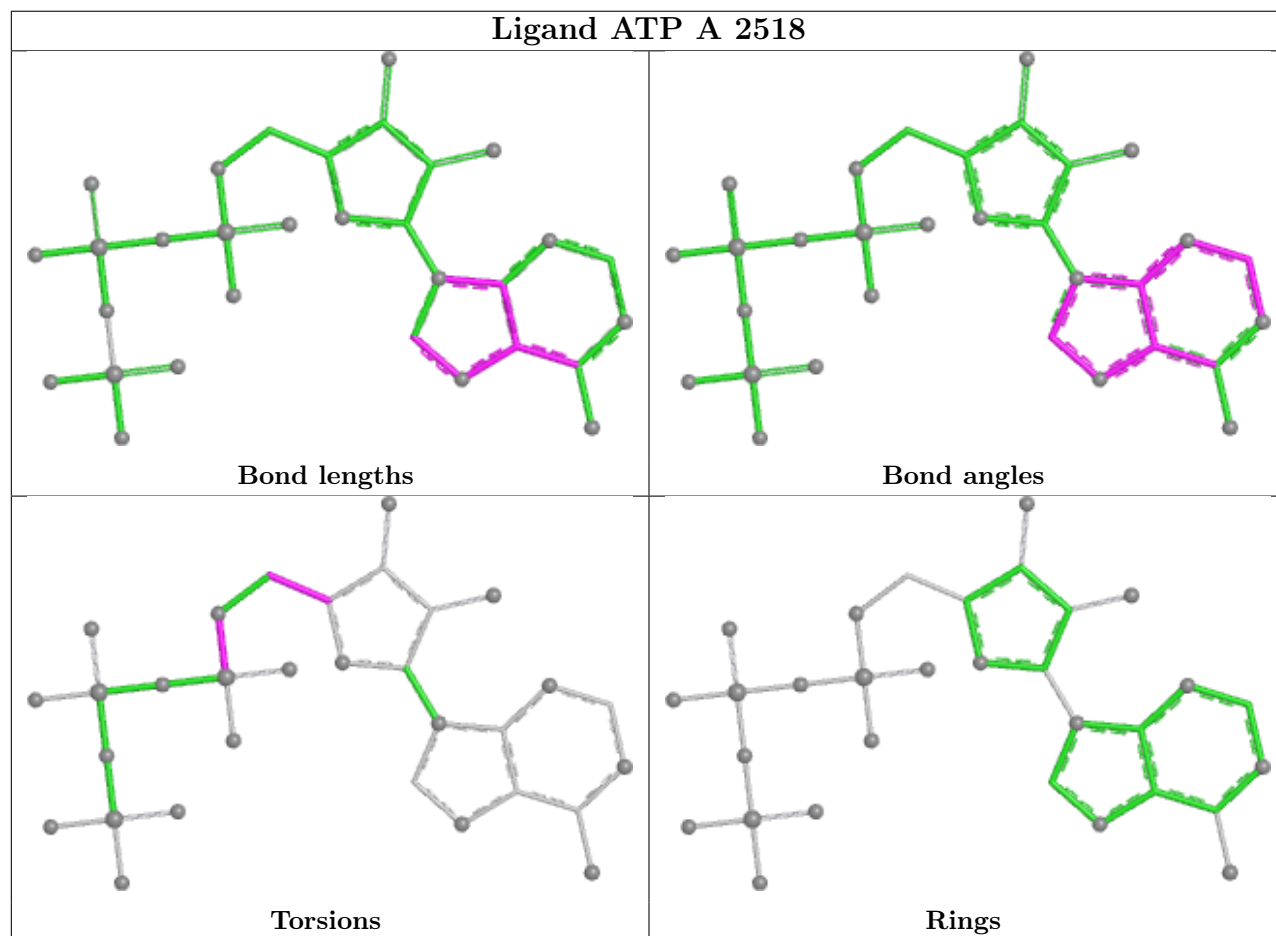
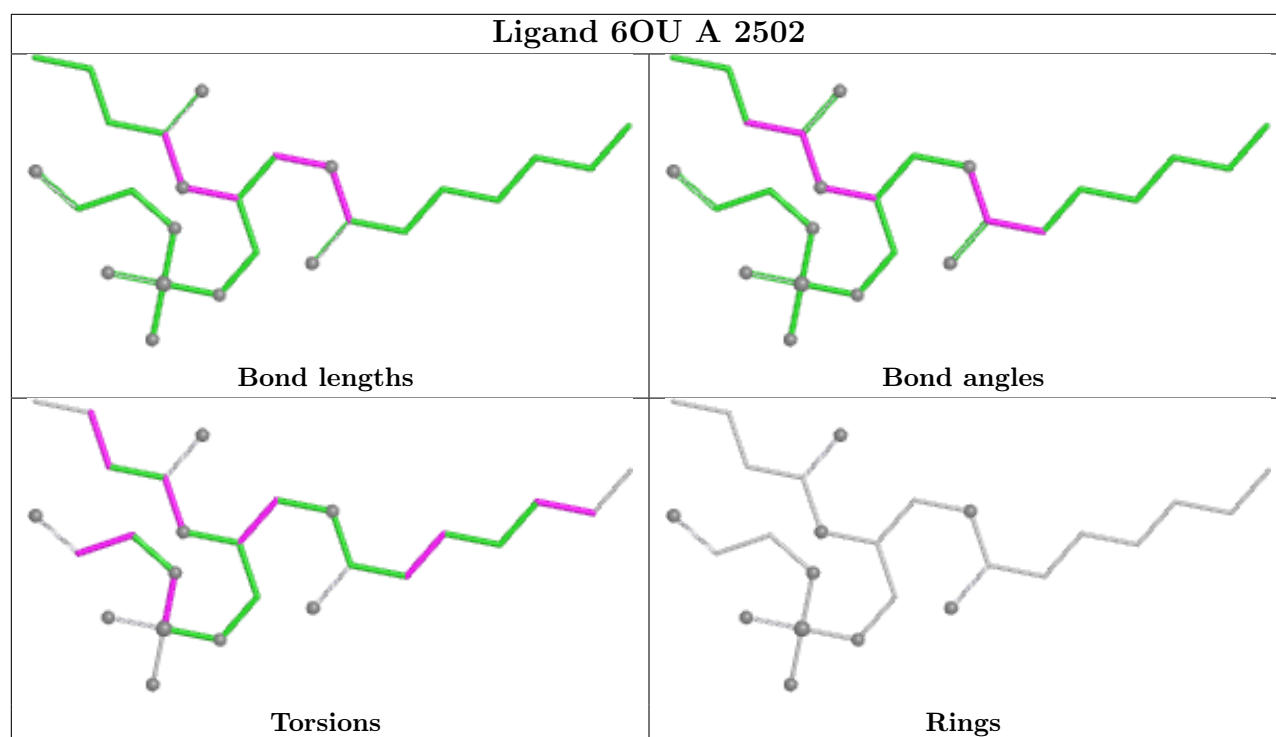
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

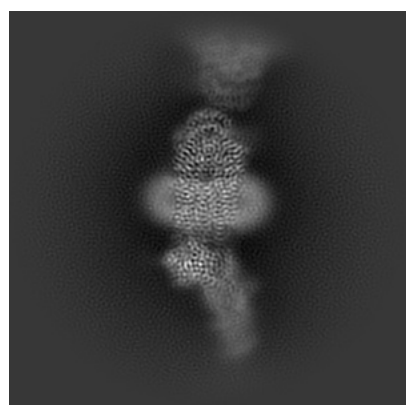
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23410. These allow visual inspection of the internal detail of the map and identification of artifacts.

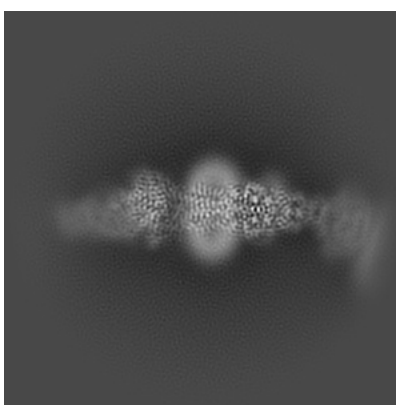
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

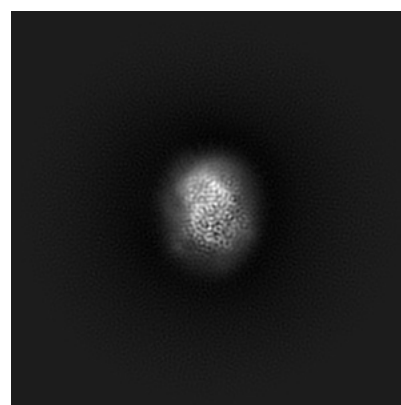
6.1.1 Primary map



X



Y

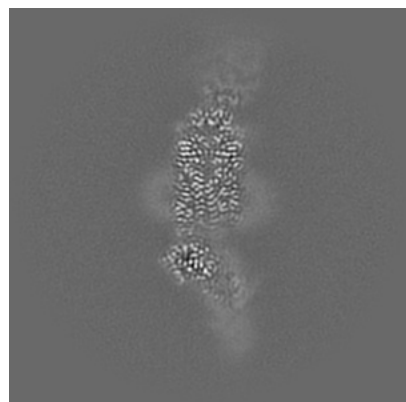


Z

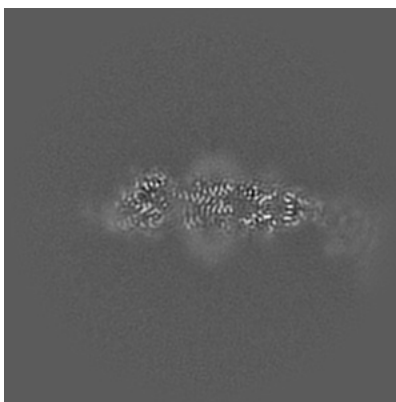
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

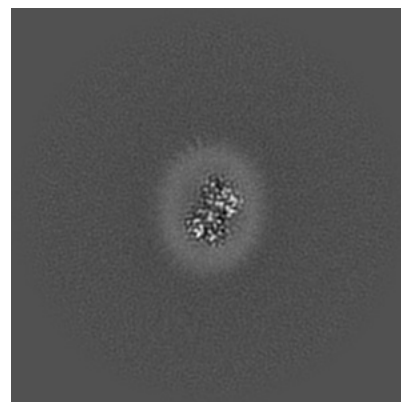
6.2.1 Primary map



X Index: 175



Y Index: 175

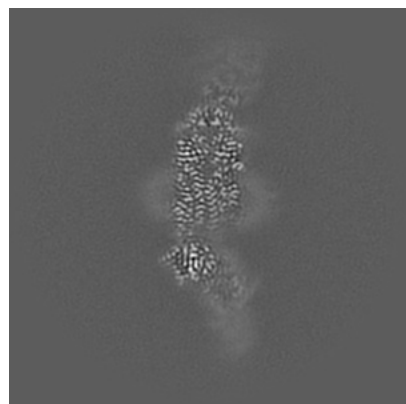


Z Index: 175

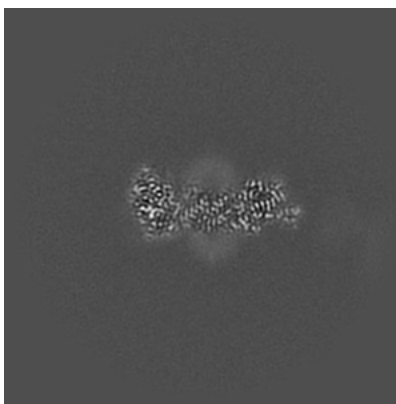
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

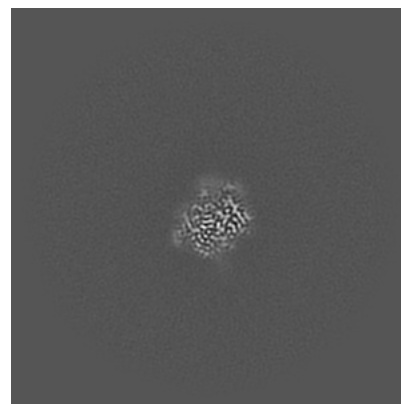
6.3.1 Primary map



X Index: 174



Y Index: 158

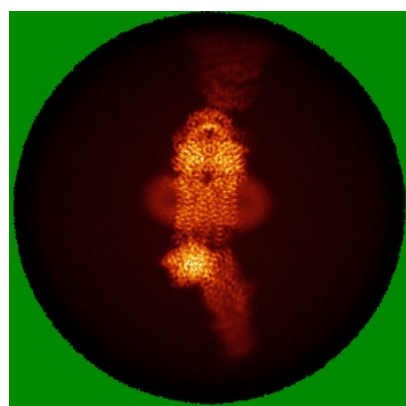


Z Index: 128

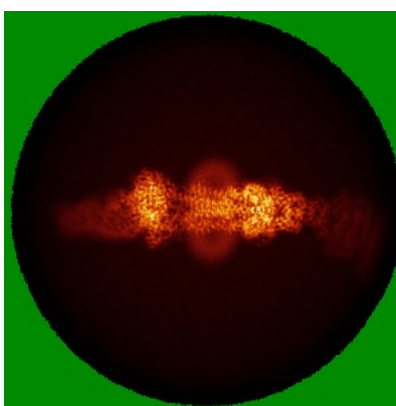
The images above show the largest variance slices of the map in three orthogonal directions.

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

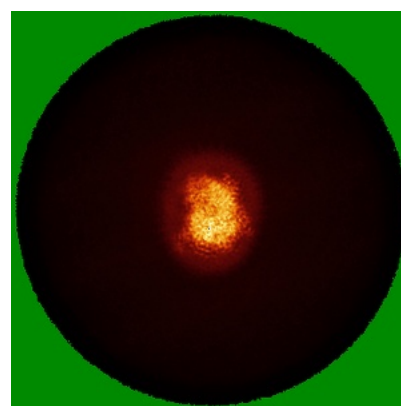
6.4.1 Primary map



X



Y

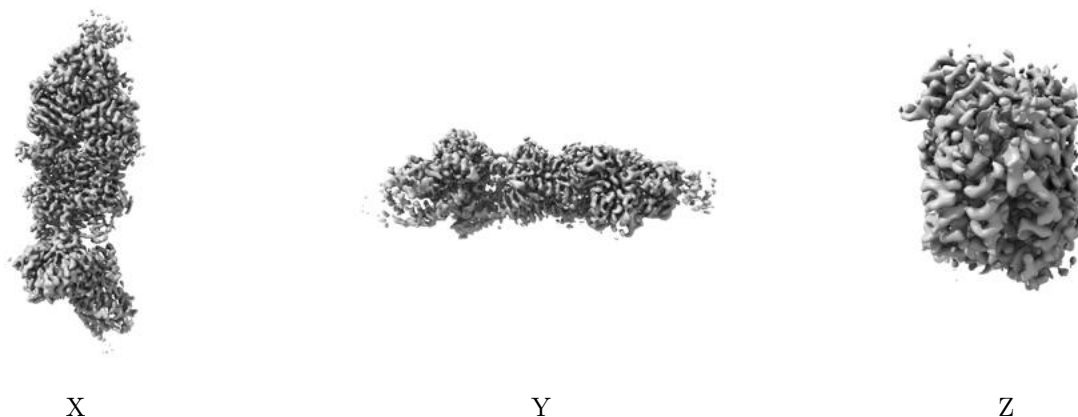


Z

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

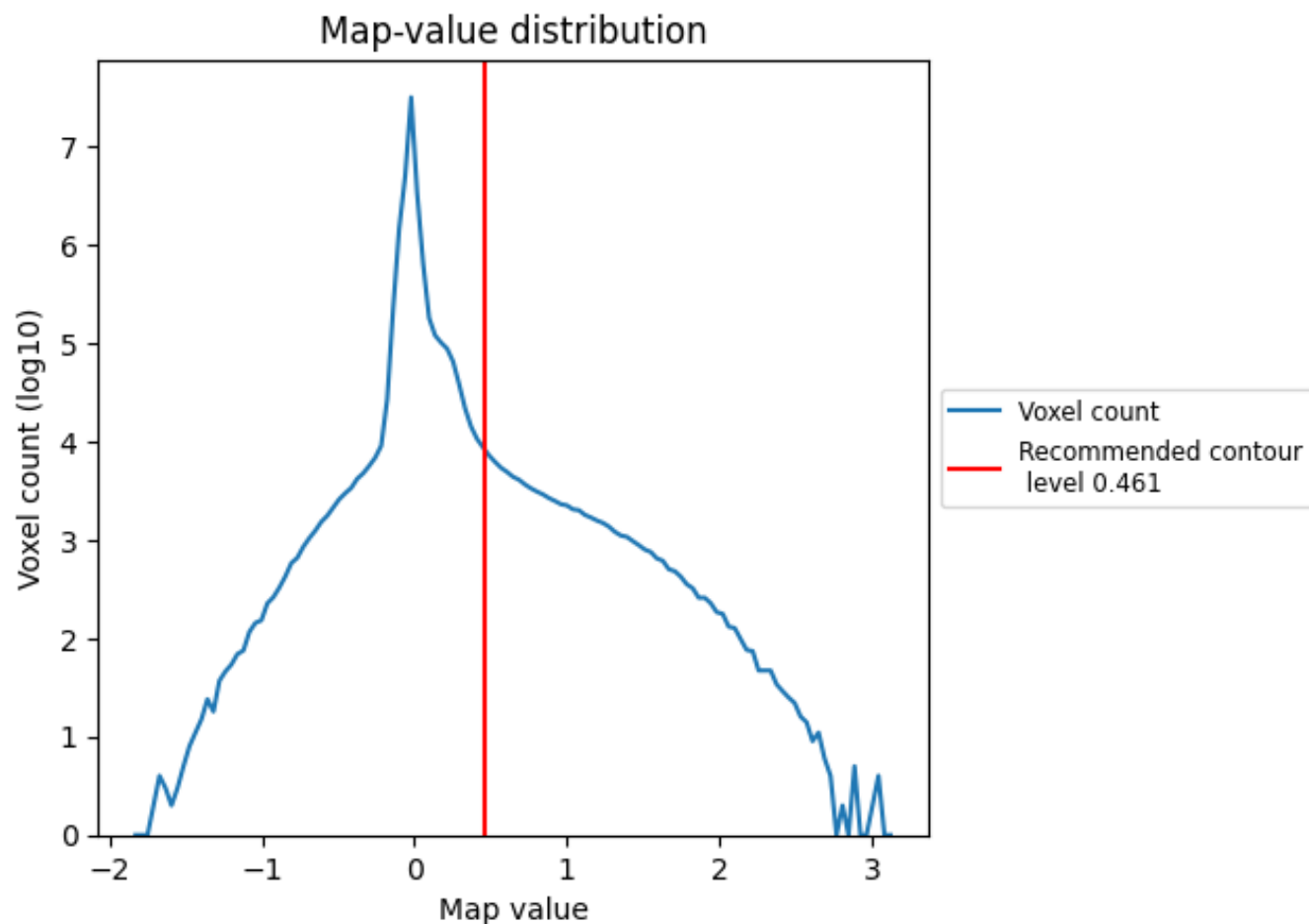
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

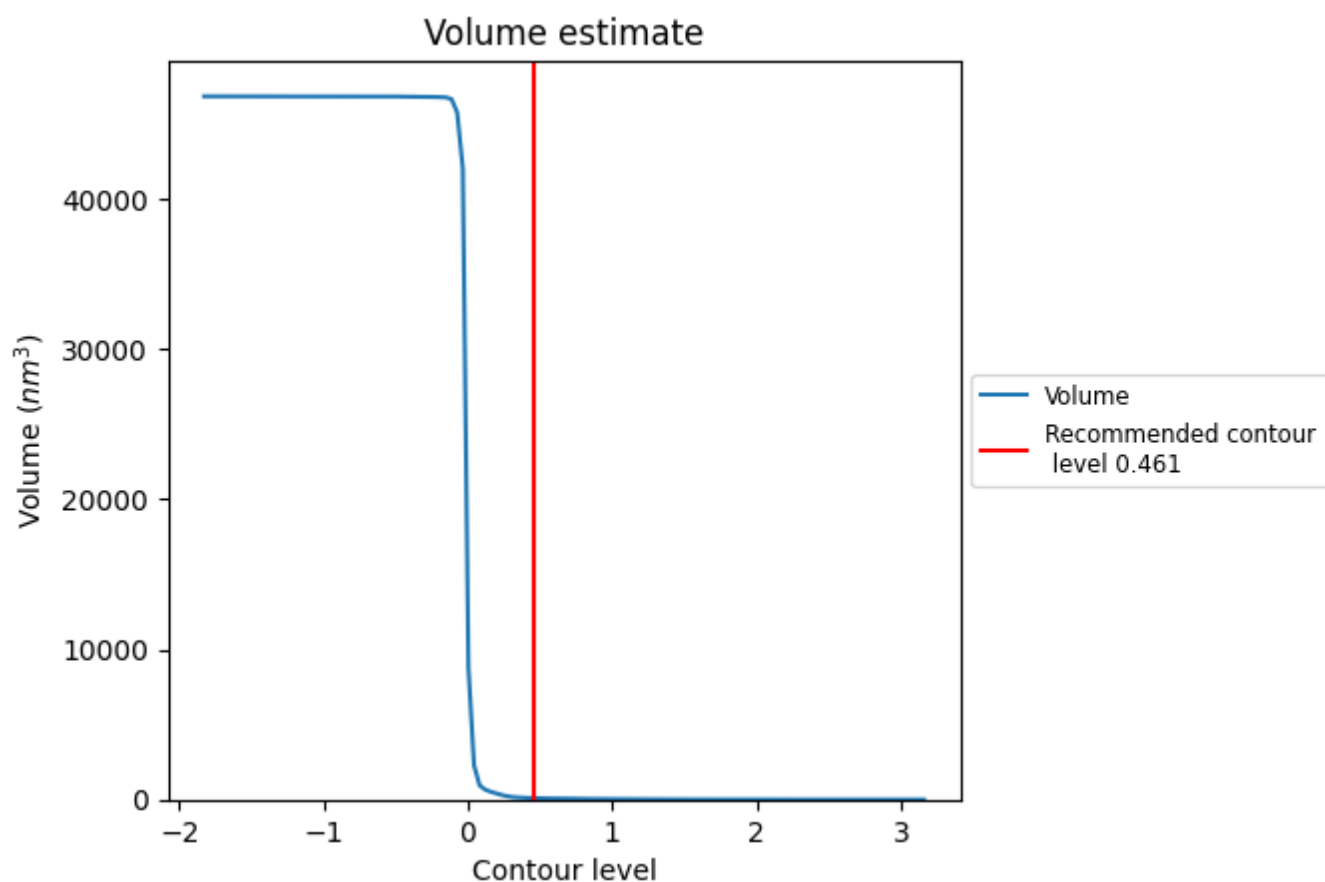
This section contains the results of statistical analysis of the map.

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.

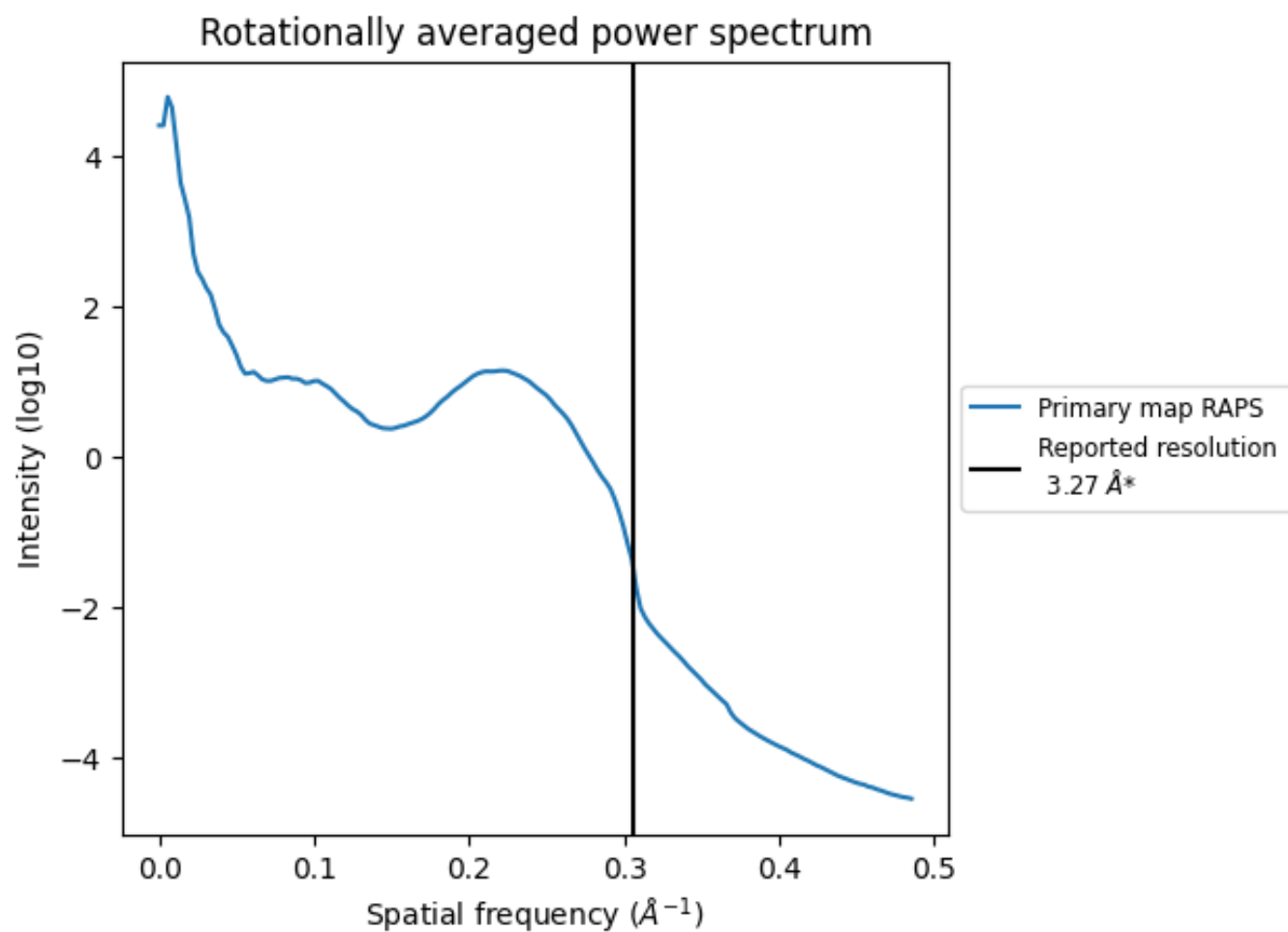
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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 0.306 Å⁻¹

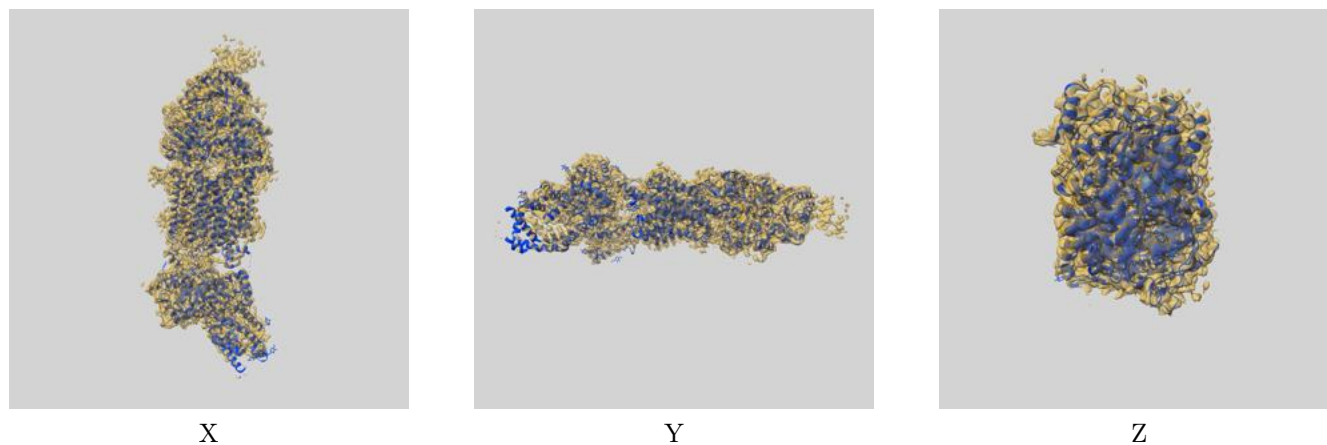
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

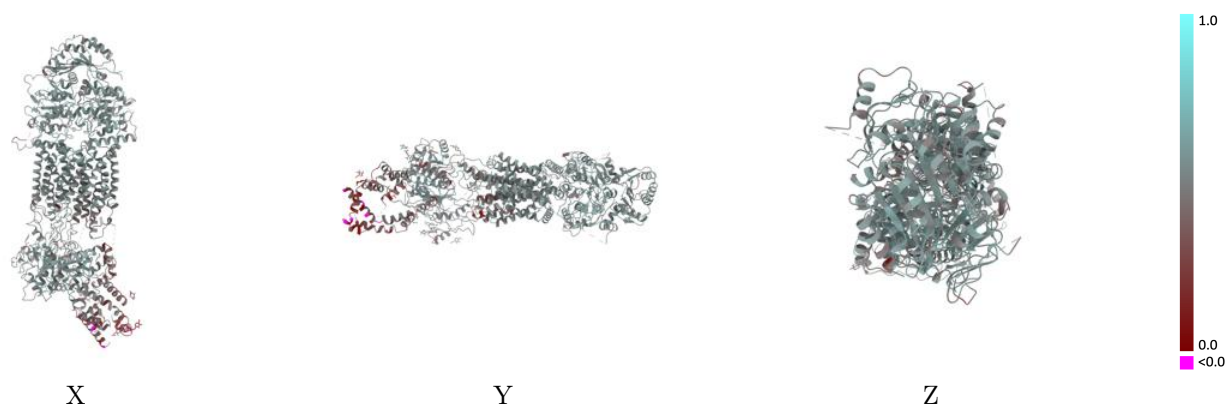
This section contains information regarding the fit between EMDB map EMD-23410 and PDB model 7LKZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



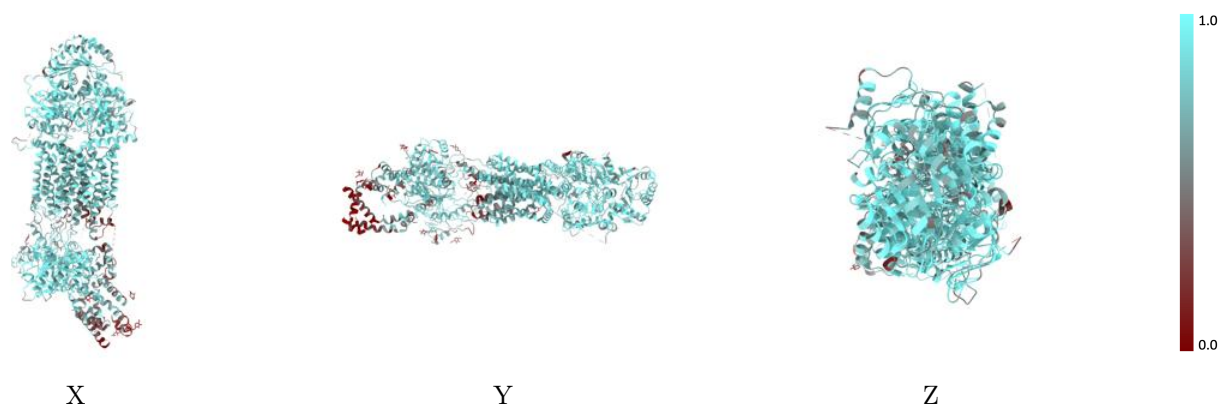
The images above show the 3D surface view of the map at the recommended contour level 0.461 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



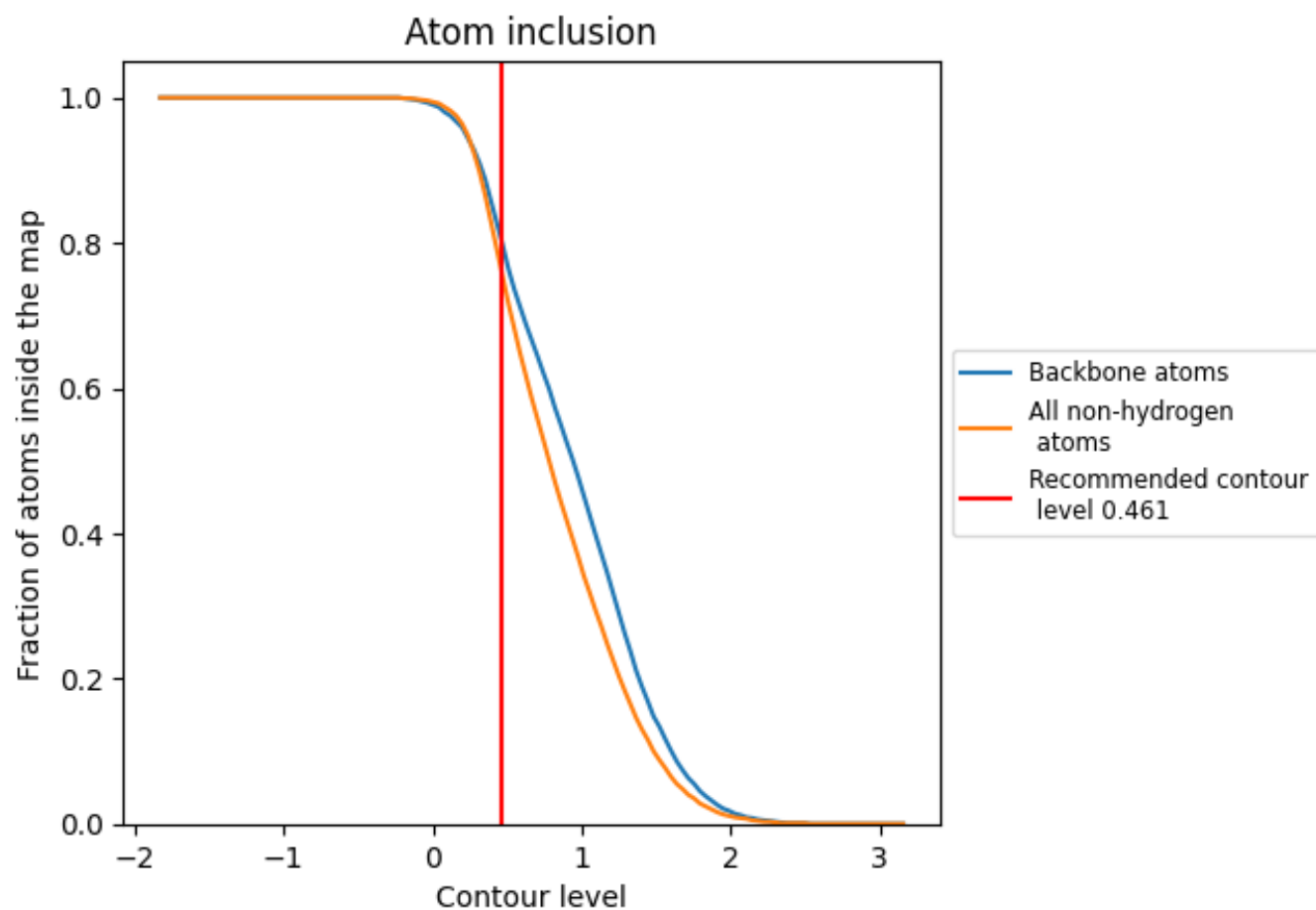
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.461).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (0.461) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5080
A	0.7650	0.5080
B	0.5130	0.4700
C	0.5080	0.4550

