wwPDB EM Validation Summary Report (i)

Nov 23, 2022 – 03:31 AM JST

PDB ID	:	7FBS
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 wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

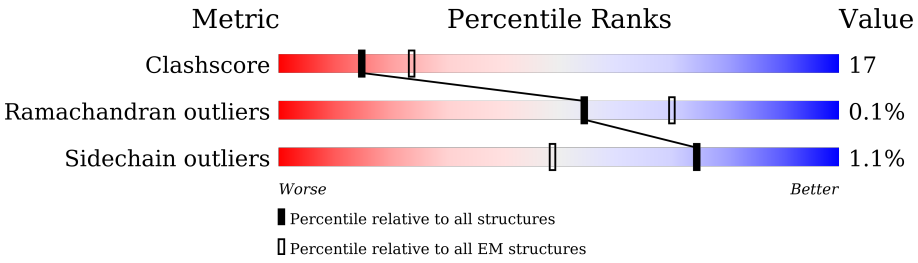
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1838	7% 41% 20% · 39%

2 Entry composition (i)

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.

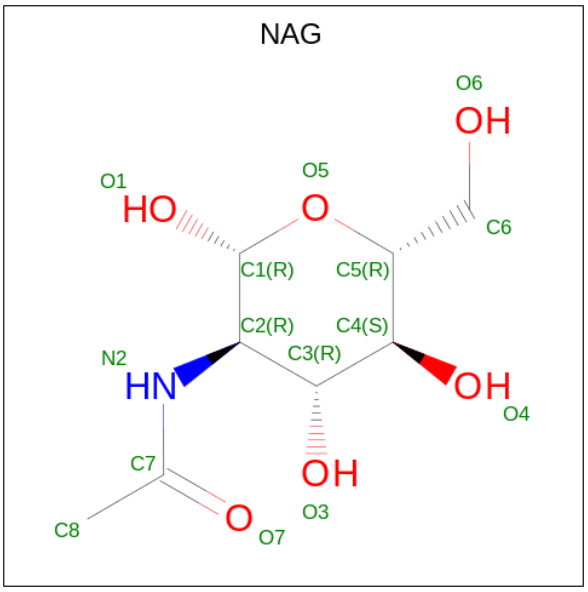
- Molecule 1 is a protein called Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,G protein/GFP fusion protein.

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

There are 22 discrepancies between the modelled and reference sequences:

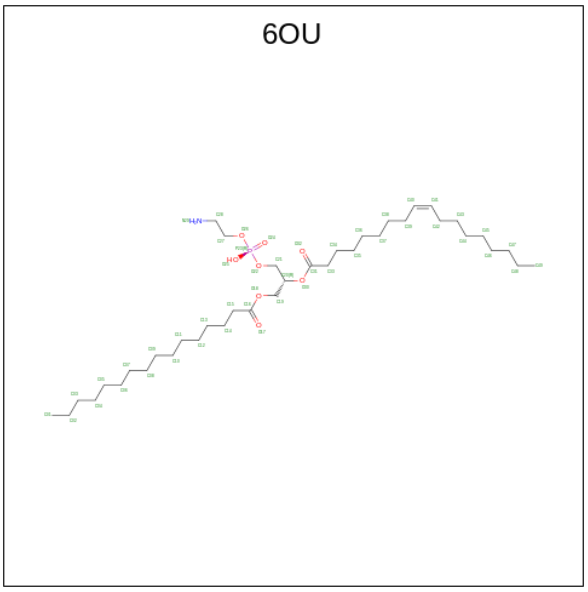
Chain	Residue	Modelled	Actual	Comment	Reference
A	1487	GLN	ILE	engineered mutation	UNP P15389
A	1488	GLN	PHE	engineered mutation	UNP P15389
A	1489	GLN	MET	engineered mutation	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389
A	1902	PHE	-	linker	UNP 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



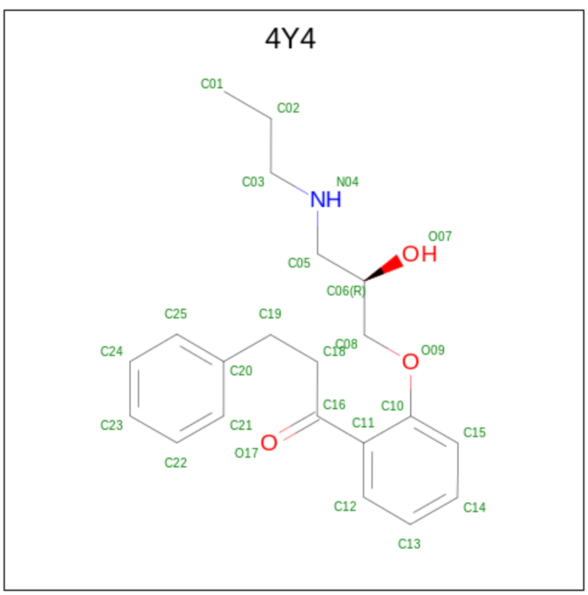
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			42	24	3	15	
2	A	1	Total	C	N	O	0
			42	24	3	15	
2	A	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



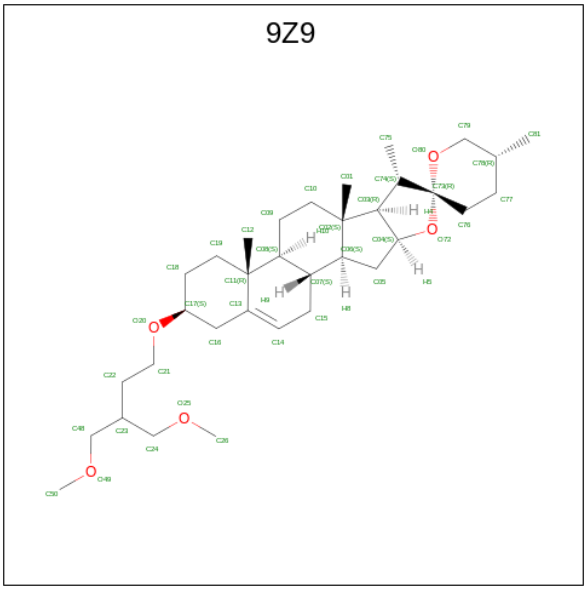
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0
3	A	1	Total 294	C 225	N 4	O 60	P 5	0

- Molecule 4 is 1-[2-[(2R)-2-oxidanyl-3-(propylamino)propoxy]phenyl]-3-phenyl-propan -1-one (three-letter code: 4Y4) (formula: $C_{21}H_{27}NO_3$) (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 (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).



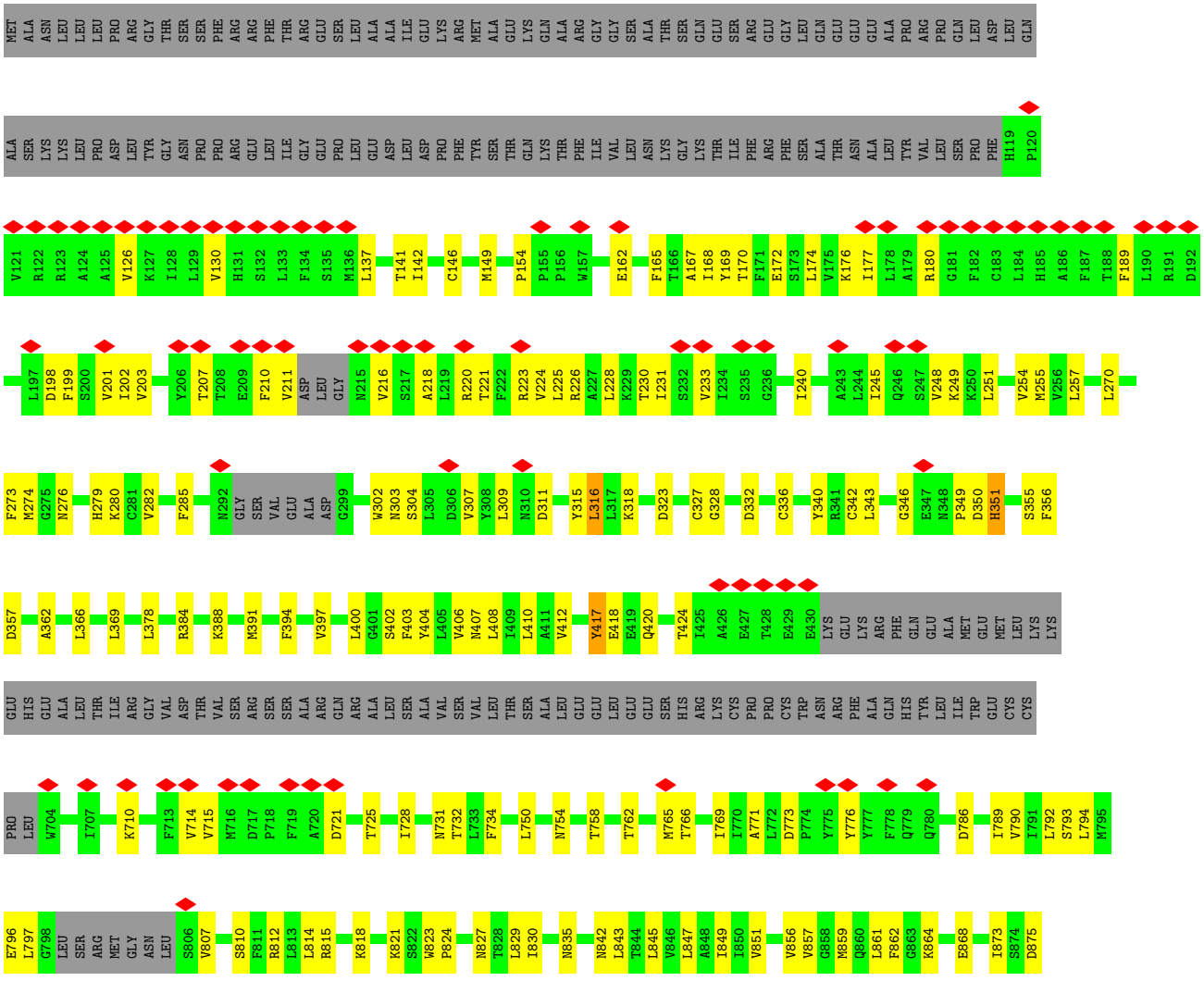
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			64	58	6	
5	A	1	Total	C	O	0
			64	58	6	

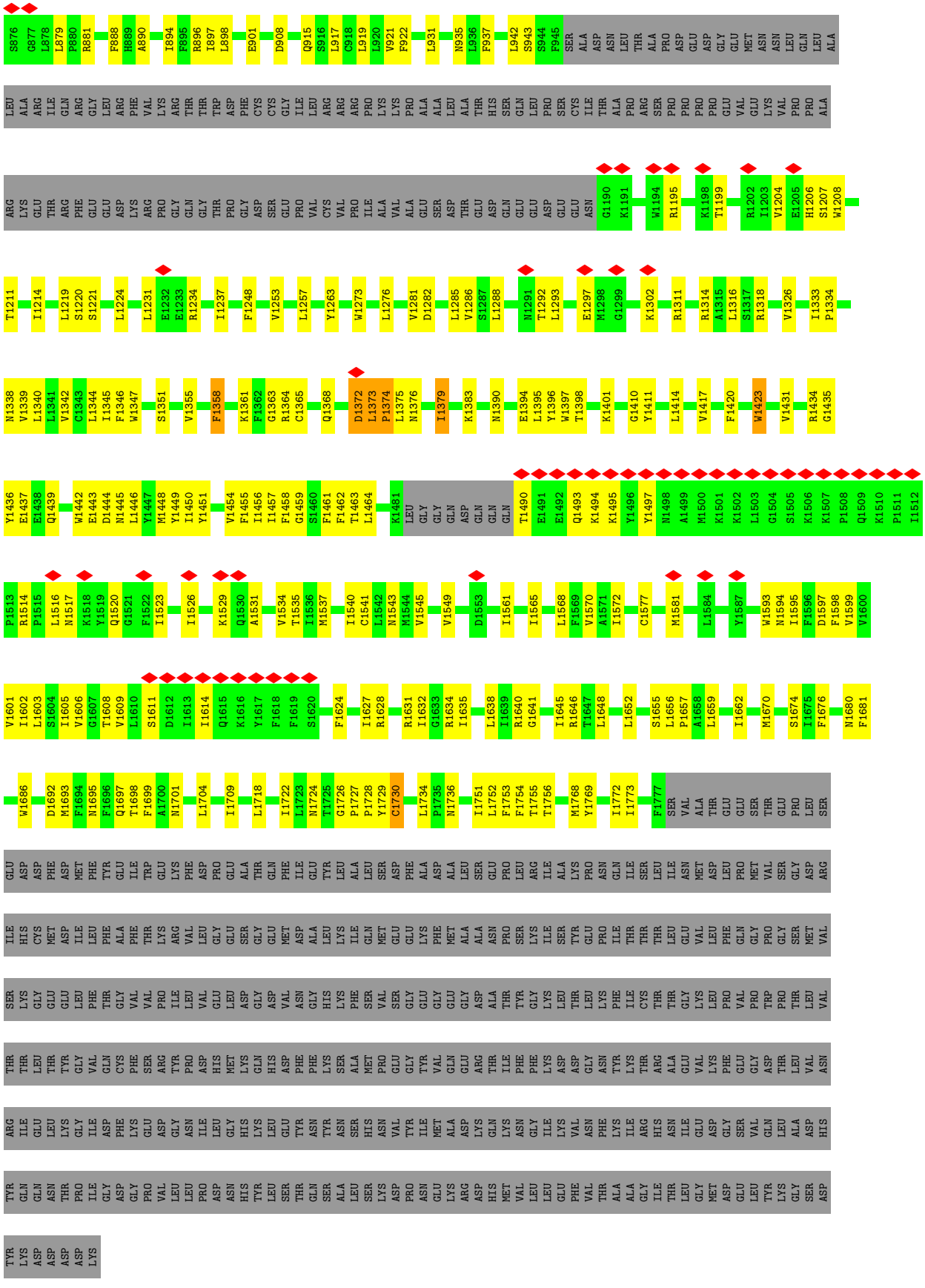
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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

Chain A: 7% 41% 20% 39%




S376 G877 L878 L879 P880 R881 F888 H889 A890 I894 F895 R896 I897 L898 E901 D908 Q915 S916 L917 C918 L919 L920 V921 F922 L931 N935 L936 F937 L942 S943 S944 F945 SER ALA ASP ASN LEU THR ALA PRO ARG SER PRO PRO PRO PRO GLU VAL GLU LYS VAL PRO PRO ALA
LEU ALA ARG ILE GLN ARG GLY LEU ARG PHE VAL LYS ARG THR THR TRP ASP PHE CYS CYS GLY ILE LEU ARG ARG PRO LYS LYS PRO ALA ALA LEU ALA THR HIS SER GLN LEU PRO SER CYS ILE THR ALA PRO ARG SER PRO PRO PRO PRO GLU GLU VAL GLU LYS VAL LEU GLN LEU ALA
ARG LYS GLU THR ARG PHE GLU GLU ASP LYS ARG PRO GLY GLN GLY THR PRO GLY ASP SER GLU PRO VAL CYS VAL PRO ILE ALA VAL ALA GLU SER ASP THR GLU ASP GLN GLU GLU ASP GLU GLU ASN G1190 K1191 W1194 R1195 K1198 T1199 R1202 I1203 V1204 E1205 H1206 S1207 W1208
T1211 I1214 L1219 S1220 S1221 L1224 L1231 E1232 E1233 R1234 I1237 F1248 V1253 L1257 Y1263 W1273 L1276 V1281 D1282 L1285 V1286 S1287 L1288 N1291 T1292 L1293 E1297 M1298 G1299 K1302 R1311 R1314 A1315 L1316 S1317 R1318 V1326 I1333 P1334
N1338 V1339 L1340 L1341 V1342 C1343 L1344 I1345 F1346 W1347 S1351 V1355 F1358 K1361 F1362 G1363 R1364 C1365 Q1368 D1372 L1373 P1374 L1375 N1376 I1379 K1383 N1390 E1394 L1395 Y1396 W1397 T1398 K1401 G1410 Y1411 L1414 V1417 F1420 W1423 V1431 R1434 G1435
Y1436 E1437 E1438 Q1439 W1442 E1443 D1444 N1445 L1446 Y1447 M1448 Y1449 I1450 Y1451 V1454 F1455 I1456 I1457 F1458 G1459 S1460 F1461 F1462 T1463 L1464 K1481 LEU GLY GLY GLN ASP GLN GLN GLN T1490 E1491 E1492 Q1493 K1494 K1495 Y1496 Y1497 N1498 A1499 M1500 K1501 K1502 L1503 G1504 S1505 K1506 K1507 P1508 Q1509 K1510 P1511 I1512
P1513 R1514 P1515 L1516 N1517 K1518 Y1519 Q1520 G1521 F1522 I1523 I1526 K1529 Q1530 A1531 V1534 T1535 I1536 M1537 I1540 C1541 L1542 N1543 M1544 V1545 V1549 D1553 I1561 I1565 L1568 F1569 V1570 A1571 I1572 C1577 M1581 L1584 Y1587 W1593 N1594 I1595 F1596 D1597 F1598 V1599 V1600
V1601 I1602 L1603 S1604 I1605 V1606 G1607 T1608 V1609 L1610 S1611 D1612 I1613 I1614 Q1615 K1616 Y1617 F1618 F1619 S1620 F1624 I1627 R1628 R1631 I1632 G1633 R1634 I1635 L1638 I1639 R1640 G1641 I1645 R1646 T1647 L1648 L1652 S1655 L1656 P1657 A1658 L1659 I1662 M1670 S1674 I1675 F1676 N1680 F1681
W1686 D1692 M1693 F1694 N1695 F1696 Q1697 T1698 F1699 A1700 N1701 L1704 I1709 L1718 I1722 L1723 N1724 T1725 G1726 P1727 P1728 Y1729 C1730 L1734 P1735 N1736 I1751 L1752 F1753 F1754 T1755 T1756 M1768 Y1769 I1772 I1773 F1777 SER VAL ALA THR GLU GLU SER THR GLU PRO LEU SER
GLU ASP ASP PHE ASP MET PHE TYR GLU ILE TRP GLU LYS PHE ASP PRO GLU ALA THR GLN PHE ILE GLU TYR LEU ALA LEU LEU SER ASP PHE ALA ASP LEU SER LEU ILE ASN MET ASP LEU PRO MET VAL SER GLY ASP ARG
ILE HIS CYS MET ASP ILE LEU PHE ALA PHE THR LYS ILE ARG VAL LEU GLY GLU SER GLY GLU MET ASP ALA LEU LYS ILE GLN MET GLU LYS PHE MET ALA ALA ASN PRO SER LYS ILE SER TYR GLU PRO ILE THR THR LEU GLU VAL LEU PHE GLN GLY PRO GLY SER MET VAL
SER LYS GLY GLU GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL SER GLY GLU GLY GLU GLY ASP ALA THR TYR GLY LYS LEU THR LEU LYS PHE ILE CYS THR THR LEU GLU GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL
THR THR LEU THR TYR GLY VAL GLN CYS PHE SER ARG TYR PRO ASP HIS MET LYS GLN HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL GLN GLU GLU SER ARG THR ILE PHE PHE LYS ASP ASP ASP LYS GLY ASN TYR LYS THR ARG ALA GLU VAL LYS PHE GLU GLY PRO VAL PRO THR LEU VAL ASN
ARG ILE GLU LEU LYS GLY ILE ASP PHE LYS GLU ASP GLY ASN ILE LEU GLU TYR ASN TYR ASN SER HIS ASN VAL TYR ILE MET ALA ASP LYS GLN LYS ASN GLY ILE LYS VAL ASN PHE LYS ILE ARG HIS ASN ILE GLU ASP GLY SER VAL GLN LEU ALA ASP HIS
TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER ALA LEU SER LYS ASP PRO ASN GLU LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR LEU GLY MET ASP GLU LEU TYR LYS GLY SER ASP
TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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	0.43	0/9063	0.49	0/12315

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8849	0	8919	302	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	308	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.

The worst 5 of 308 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

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%)	51 82

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%)	937 (99%)	10 (1%)	73 86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1379	ILE
1	A	1423	TRP
1	A	1730	CYS
1	A	417	TYR
1	A	1358	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1543	ASN
1	A	1736	ASN
1	A	1701	ASN
1	A	1327	ASN
1	A	1520	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	2207	-	25,25,48	1.07	3 (12%)	27,27,53	1.33	2 (7%)
3	6OU	A	2215	-	33,33,48	1.04	3 (9%)	35,38,53	1.22	2 (5%)
3	6OU	A	2208	-	28,28,48	1.16	3 (10%)	30,30,53	1.40	3 (10%)
3	6OU	A	2206	-	14,14,48	0.94	1 (7%)	14,14,53	1.32	1 (7%)
3	6OU	A	2211	-	24,24,48	1.26	4 (16%)	28,29,53	1.28	2 (7%)
2	NAG	A	2203	-	14,14,15	0.43	0	17,19,21	0.39	0
5	9Z9	A	2217	-	35,35,44	8.14	23 (65%)	58,58,68	2.15	23 (39%)
3	6OU	A	2212	-	16,16,48	1.26	3 (18%)	16,16,53	1.12	1 (6%)
2	NAG	A	2201	-	14,14,15	0.38	0	17,19,21	0.42	0
3	6OU	A	2210	-	26,26,48	0.95	2 (7%)	27,27,53	1.27	2 (7%)
4	4Y4	A	2214	-	26,26,26	1.61	5 (19%)	30,32,32	1.01	1 (3%)
3	6OU	A	2209	-	38,38,48	0.97	3 (7%)	41,43,53	1.17	3 (7%)
5	9Z9	A	2216	-	38,38,44	8.22	23 (60%)	60,61,68	2.28	25 (41%)
3	6OU	A	2204	-	31,31,48	1.08	4 (12%)	34,36,53	1.29	2 (5%)
3	6OU	A	2205	-	34,34,48	1.04	2 (5%)	37,39,53	1.17	2 (5%)
2	NAG	A	2202	-	14,14,15	0.25	0	17,19,21	0.71	0
3	6OU	A	2213	-	14,14,48	1.34	3 (21%)	14,14,53	0.99	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	2207	-	-	12/27/27/52	-
3	6OU	A	2215	-	-	17/37/37/52	-
3	6OU	A	2208	-	-	15/29/29/52	-
3	6OU	A	2206	-	-	5/13/13/52	-
3	6OU	A	2211	-	-	13/26/26/52	-
2	NAG	A	2203	-	-	4/6/23/26	0/1/1/1
5	9Z9	A	2217	-	-	-	0/6/6/6
3	6OU	A	2212	-	-	4/15/15/52	-
2	NAG	A	2201	-	-	2/6/23/26	0/1/1/1
3	6OU	A	2210	-	-	18/26/26/52	-
4	4Y4	A	2214	-	-	11/19/19/19	0/2/2/2
3	6OU	A	2209	-	-	24/42/42/52	-
5	9Z9	A	2216	-	-	2/4/92/100	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	A	2204	-	-	17/35/35/52	-
3	6OU	A	2205	-	-	23/38/38/52	-
2	NAG	A	2202	-	-	2/6/23/26	0/1/1/1
3	6OU	A	2213	-	-	5/13/13/52	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2216	9Z9	C15-C07	-20.91	1.17	1.53
5	A	2217	9Z9	C15-C07	-20.88	1.17	1.53
5	A	2216	9Z9	C07-C06	-20.45	1.14	1.53
5	A	2217	9Z9	C07-C06	-20.20	1.15	1.53
5	A	2217	9Z9	C11-C13	-18.40	1.16	1.52

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2216	9Z9	C15-C14-C13	-4.91	116.00	125.06
5	A	2217	9Z9	C16-C13-C11	-4.84	109.99	116.42
5	A	2217	9Z9	C11-C13-C14	-4.62	115.83	122.90
3	A	2204	6OU	O30-C31-C33	4.49	121.17	111.50
5	A	2216	9Z9	C11-C13-C14	-4.46	116.08	122.90

There are no chirality outliers.

5 of 174 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-O24

There are no ring outliers.

4 monomers are involved in 21 short contacts:

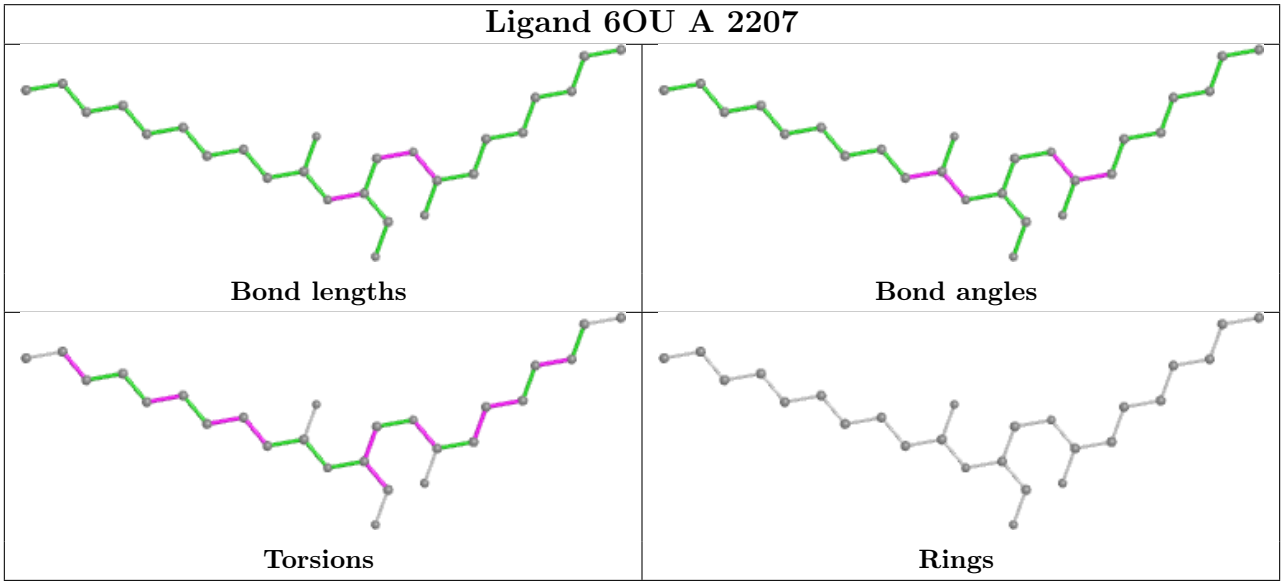
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2217	9Z9	5	0
2	A	2201	NAG	5	0
5	A	2216	9Z9	8	0

Continued on next page...

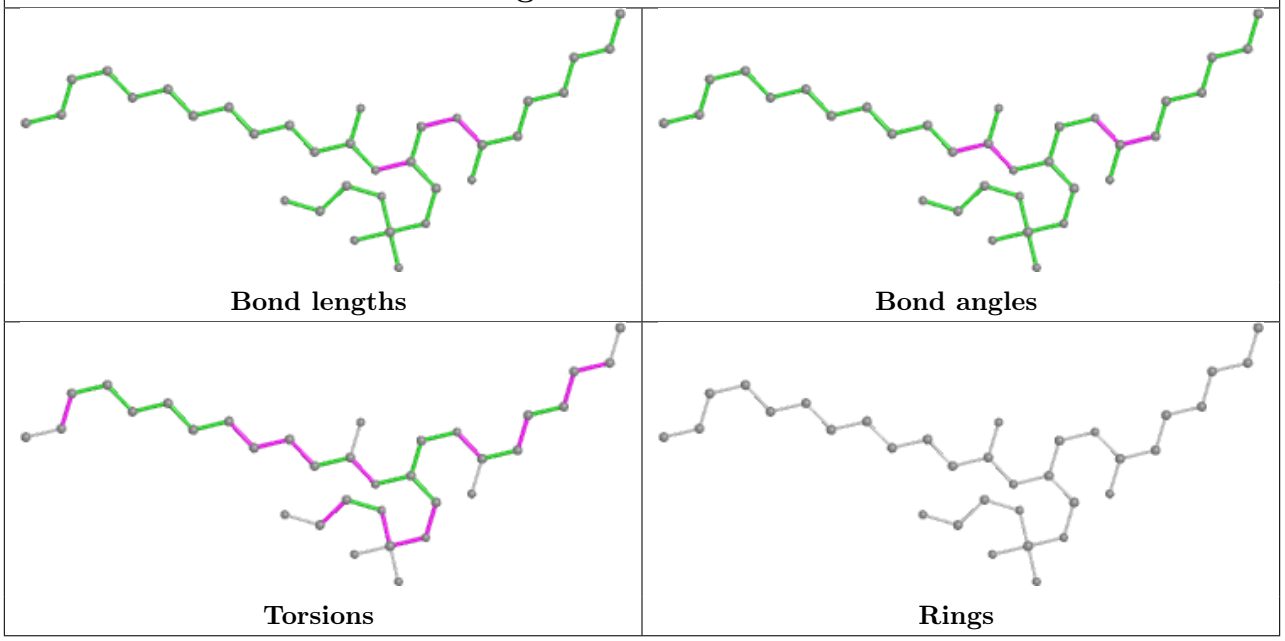
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2202	NAG	4	0

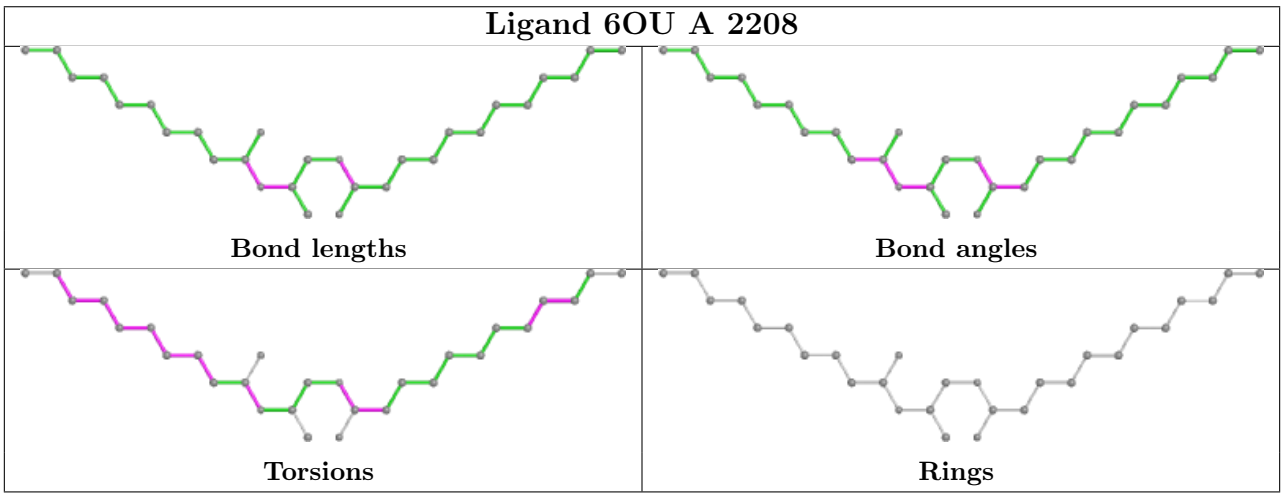
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



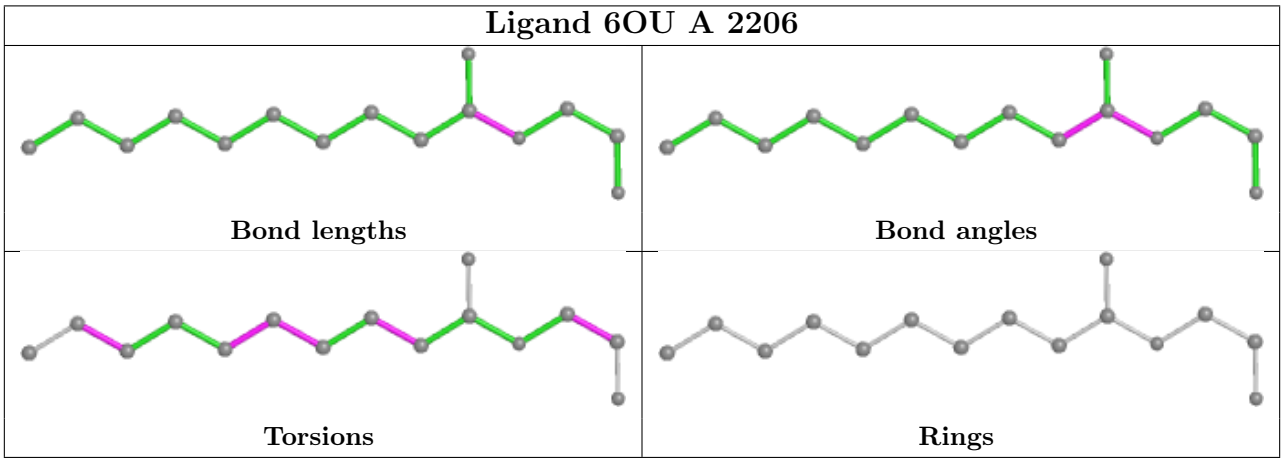
Ligand 6OU A 2215



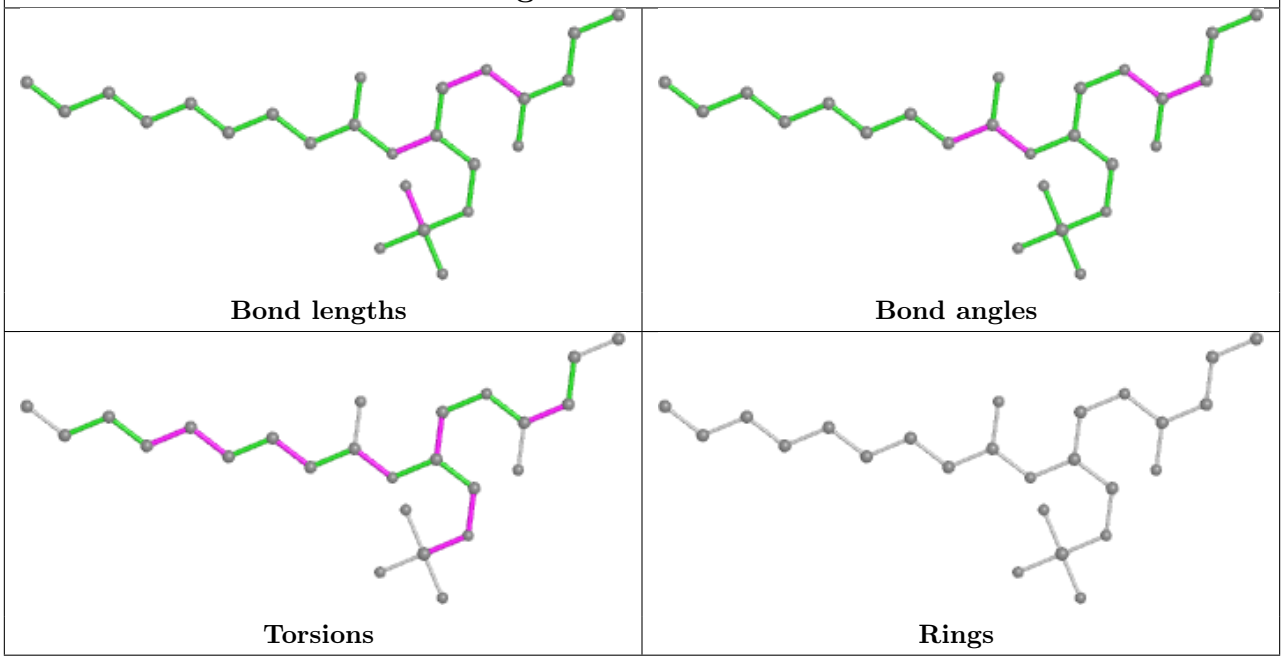
Ligand 6OU A 2208



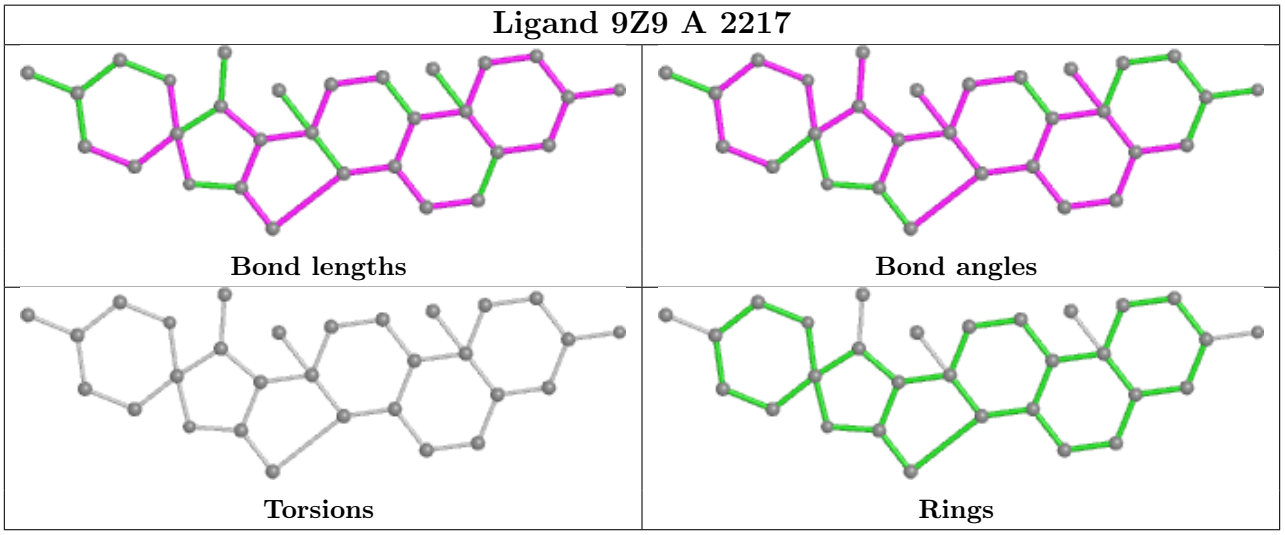
Ligand 6OU A 2206



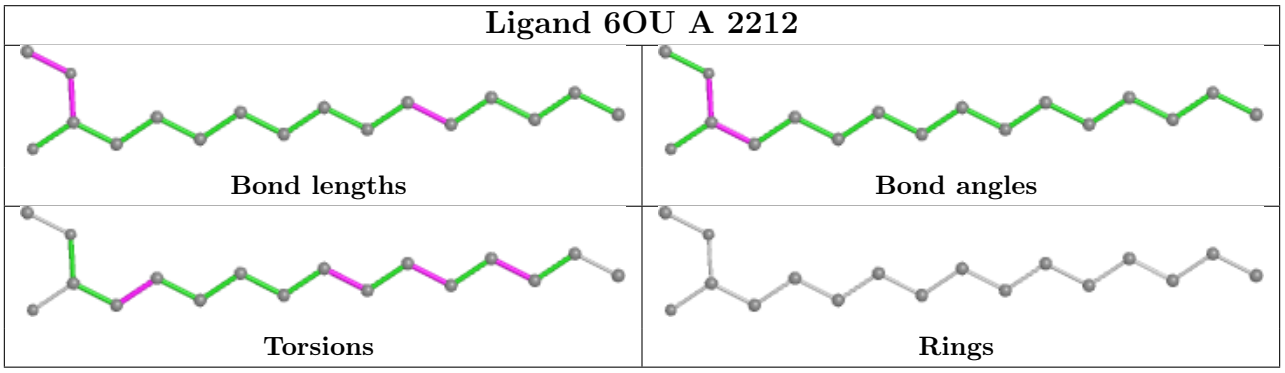
Ligand 6OU A 2211



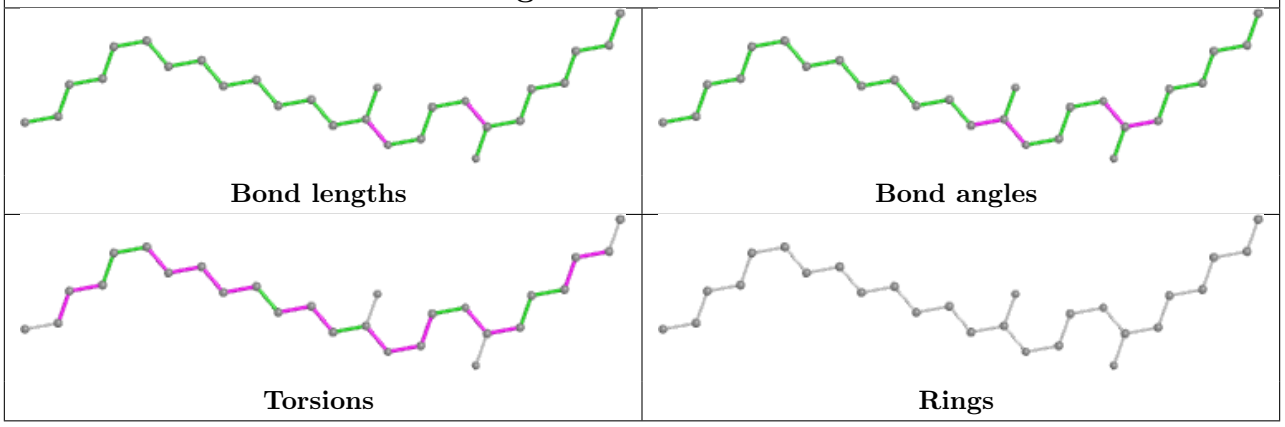
Ligand 9Z9 A 2217



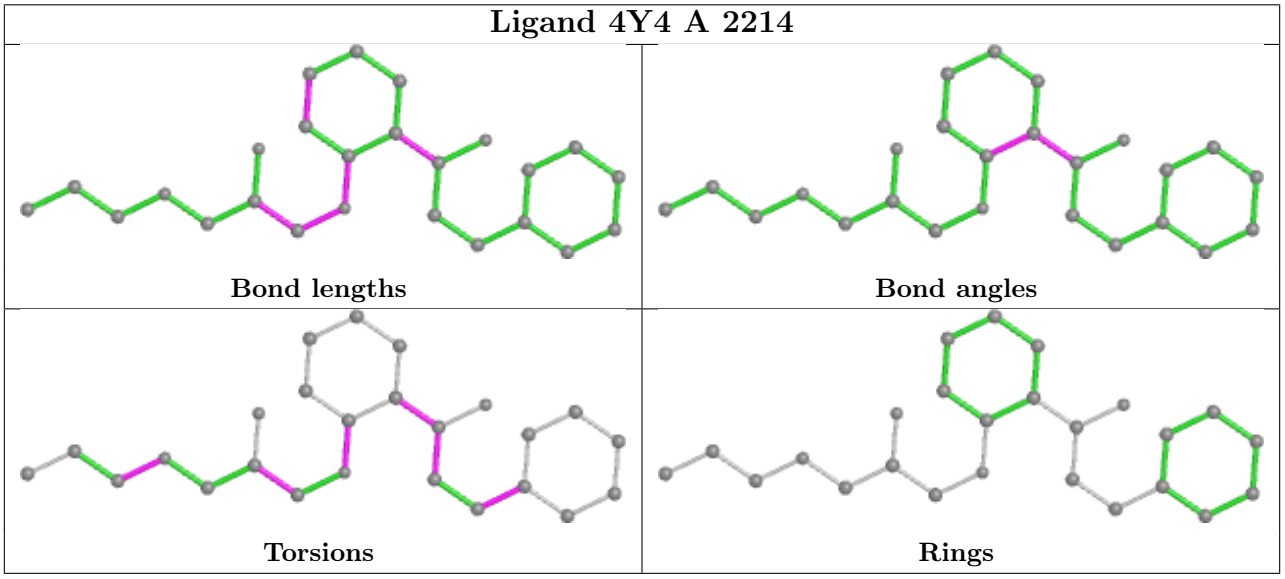
Ligand 6OU A 2212



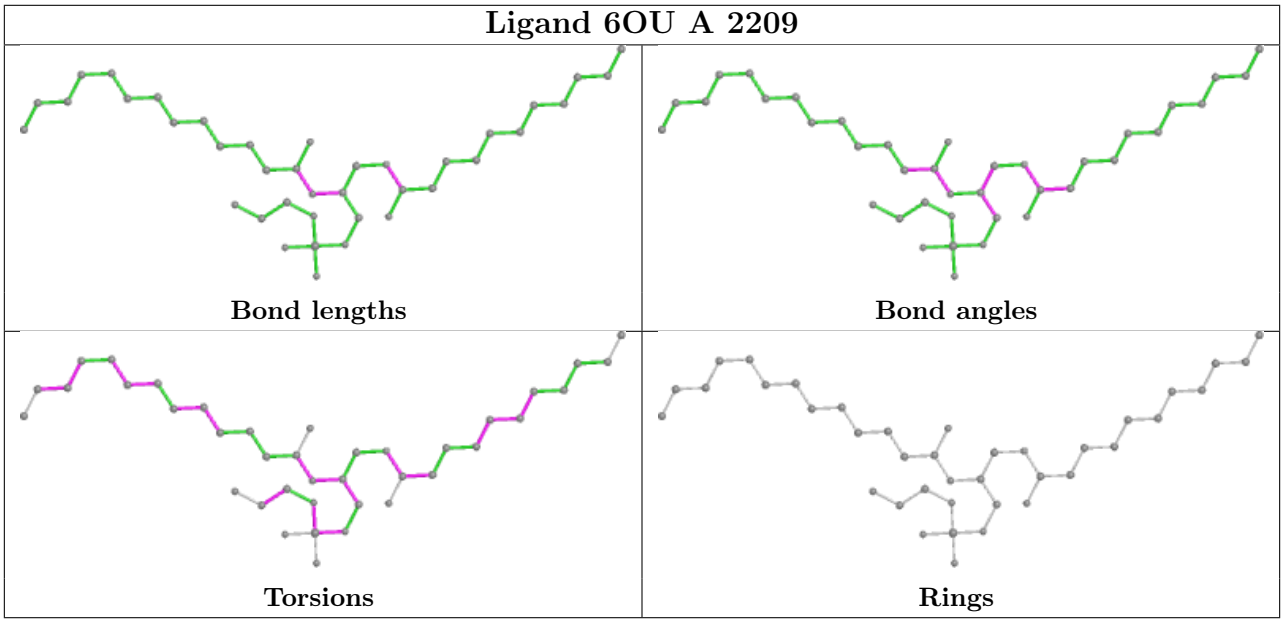
Ligand 6OU A 2210



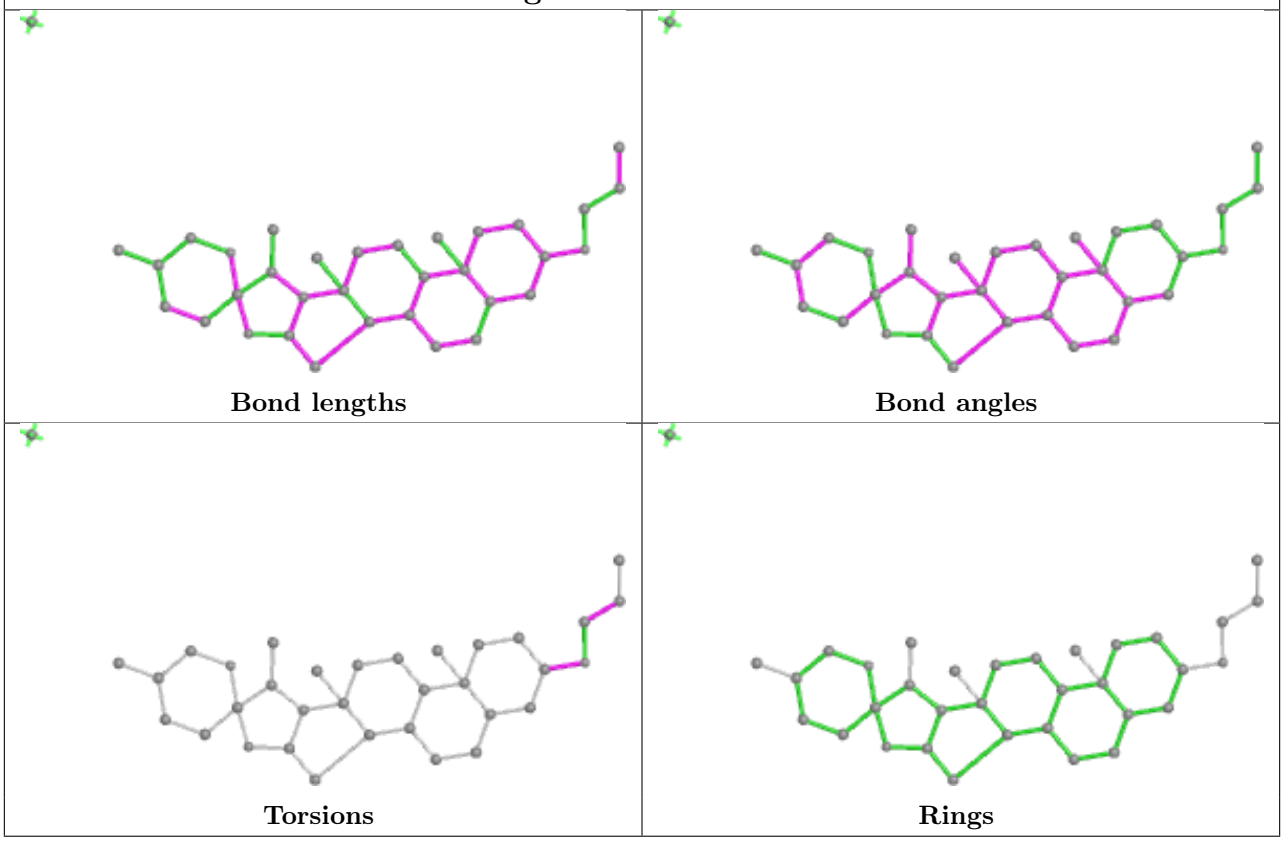
Ligand 4Y4 A 2214



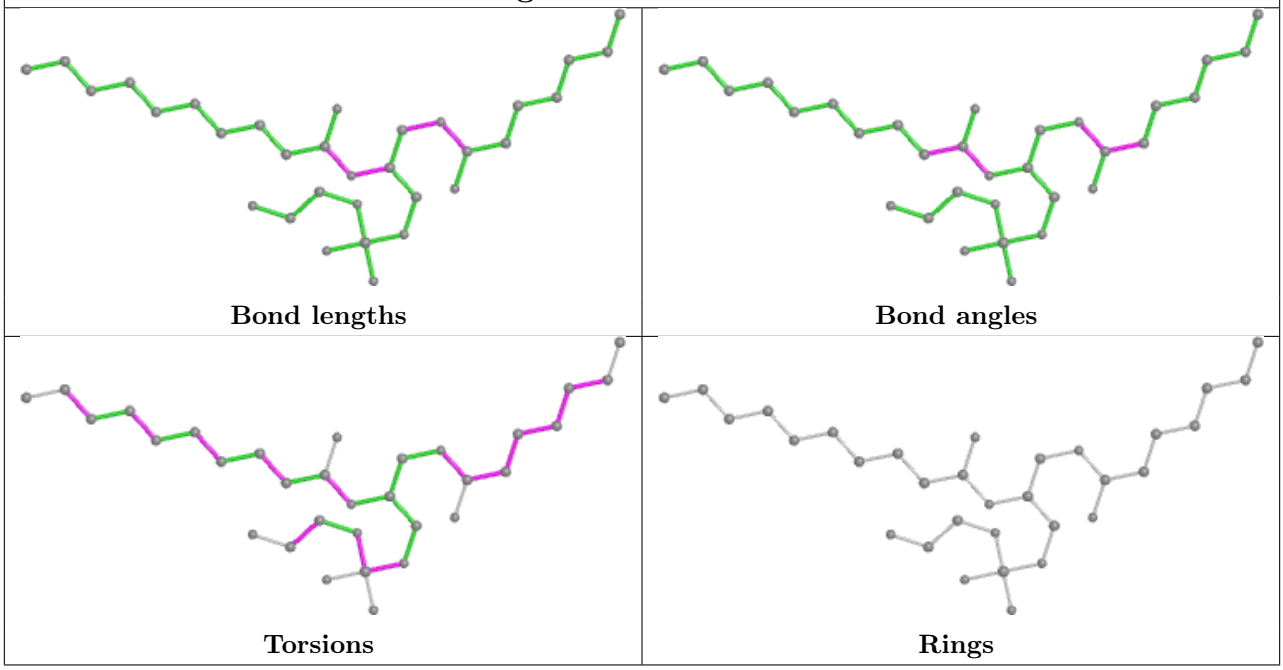
Ligand 6OU A 2209

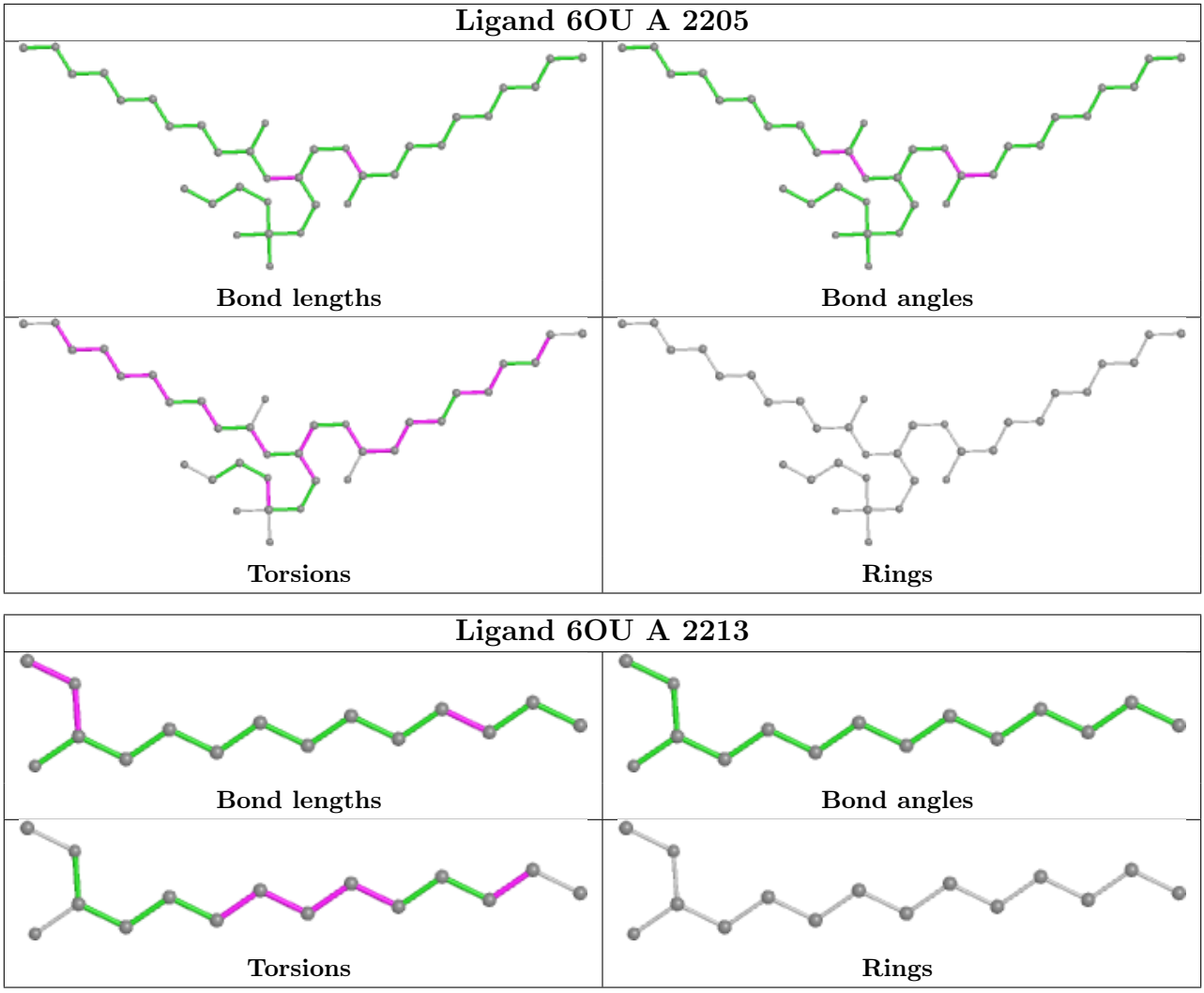


Ligand 9Z9 A 2216



Ligand 6OU A 2204





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

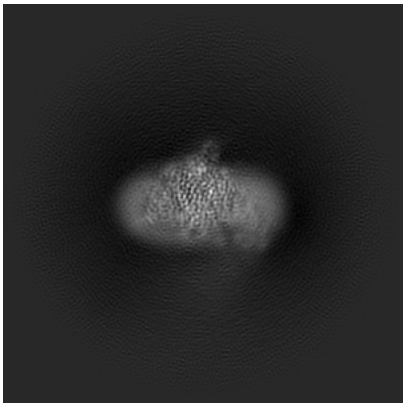
6 Map visualisation

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

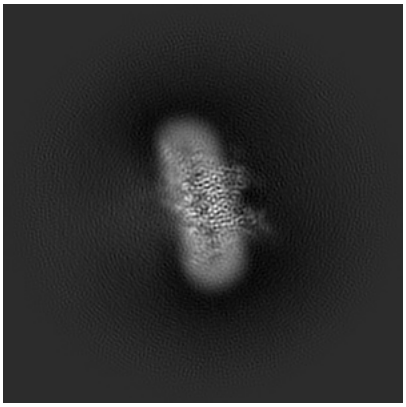
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

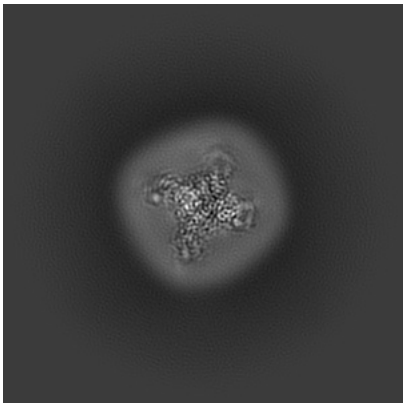
6.1.1 Primary map



X



Y

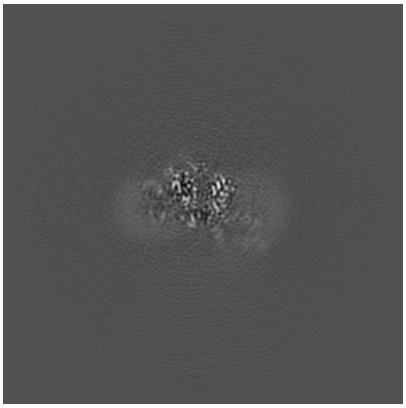


Z

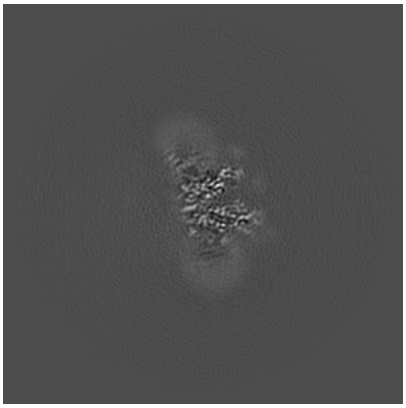
The images above show the map projected in three orthogonal directions.

6.2 Central slices

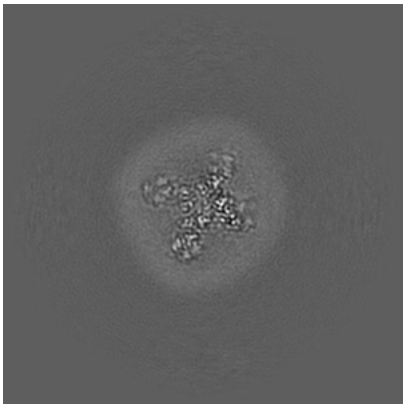
6.2.1 Primary map



X Index: 160



Y Index: 160

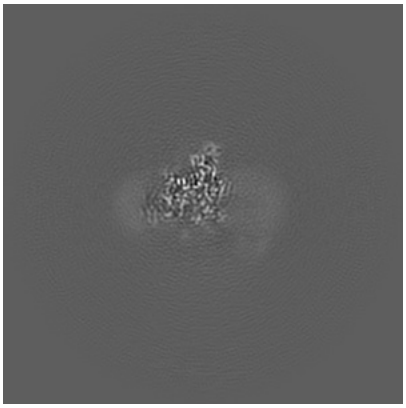


Z Index: 160

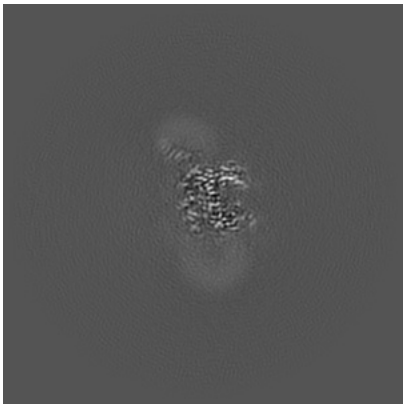
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

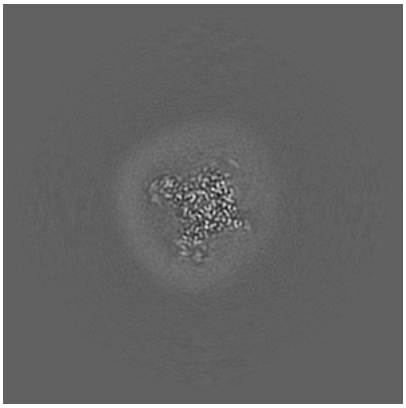
6.3.1 Primary map



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 surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

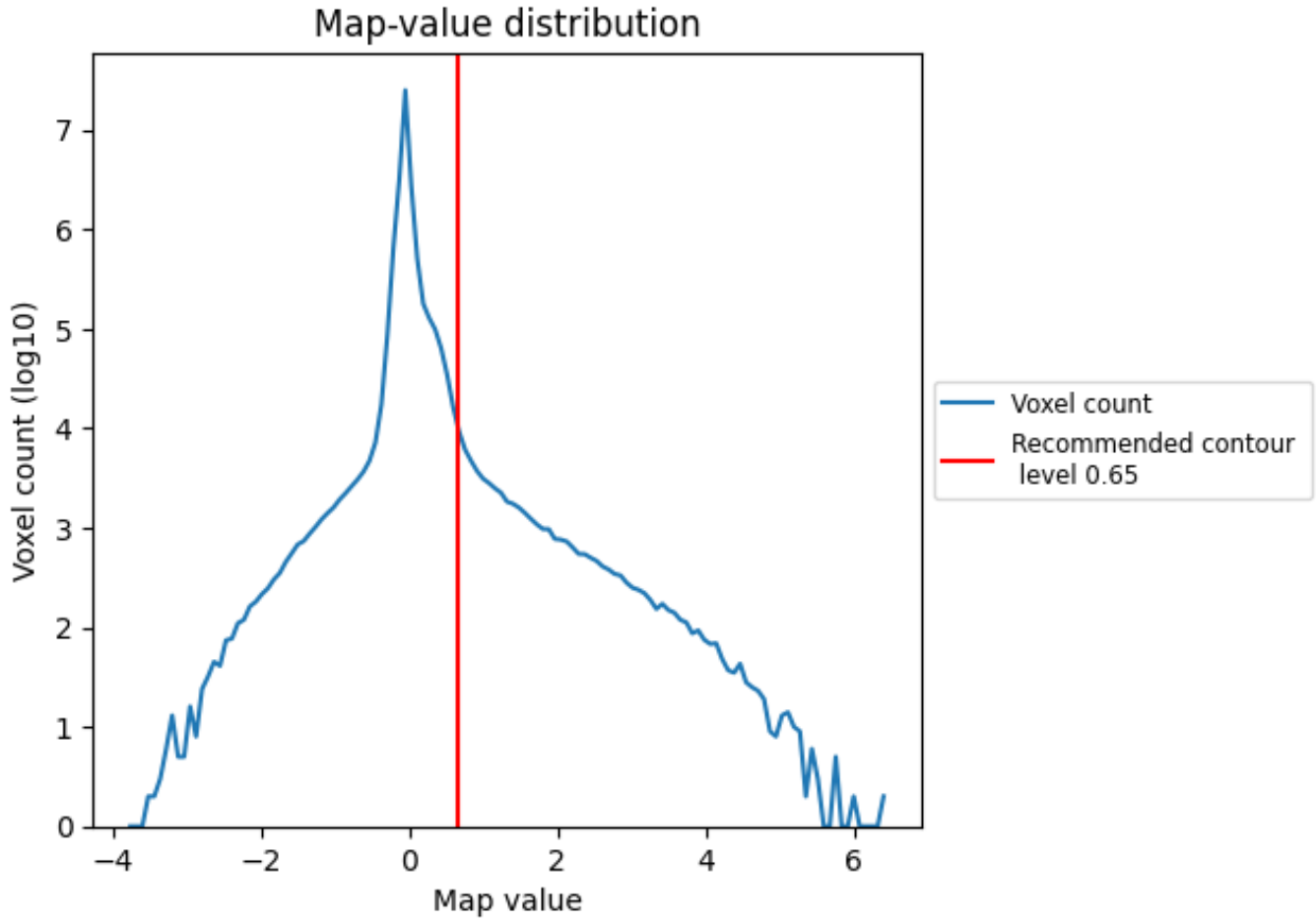
6.5 Mask visualisation (i)

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

7 Map analysis

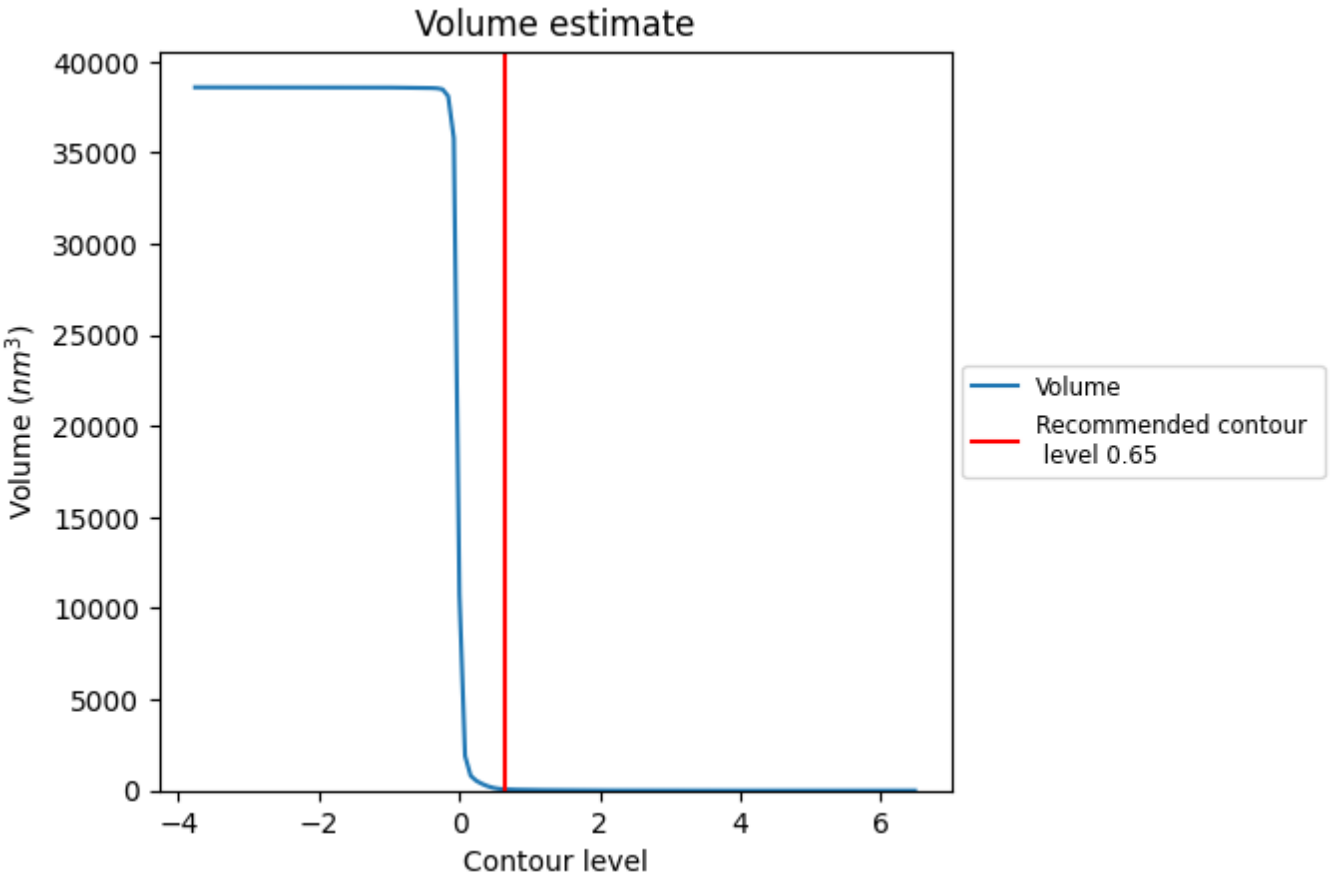
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

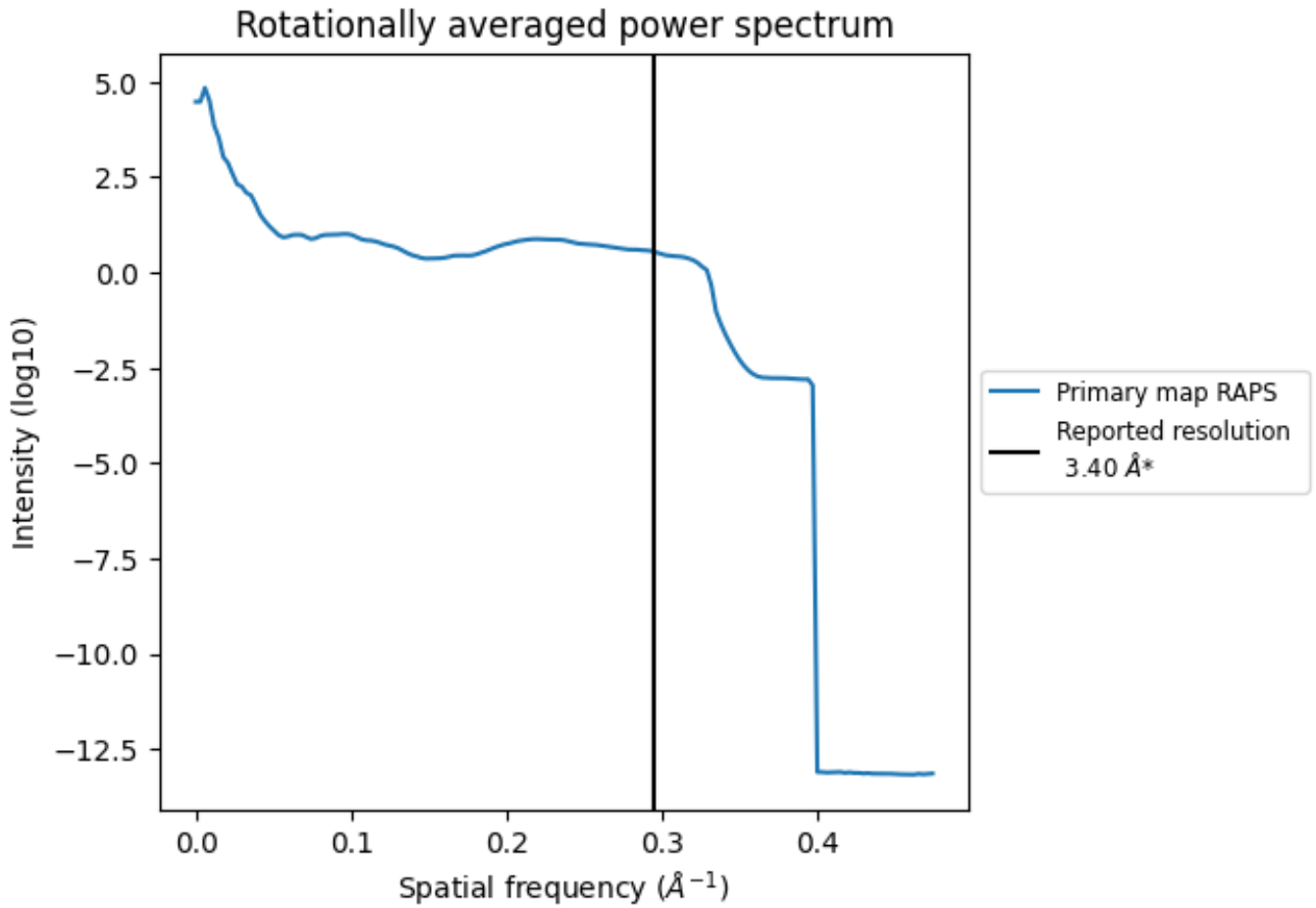
7.2 Volume estimate (i)



The volume at the recommended contour level is 69 nm^3; 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 (i)

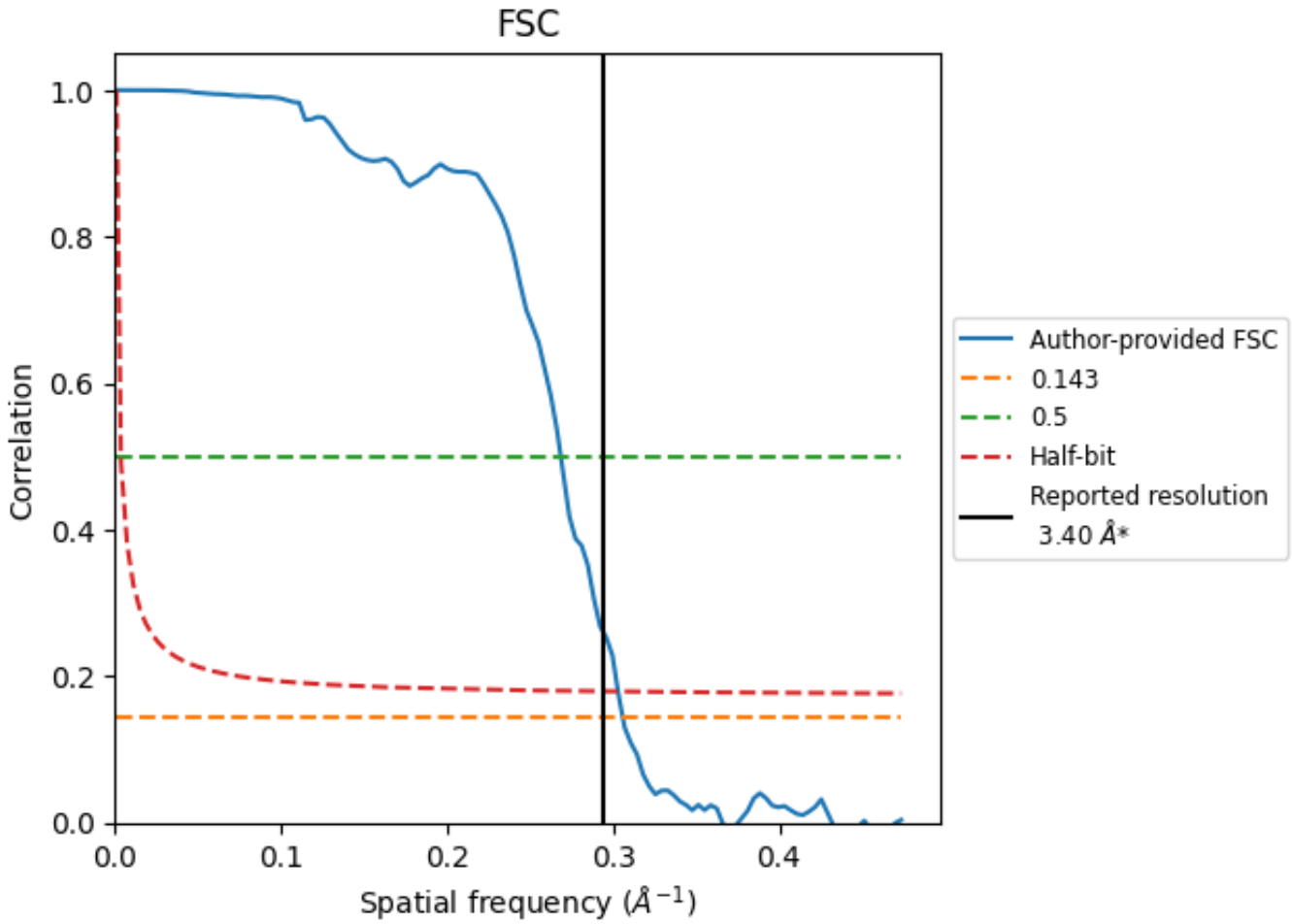


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

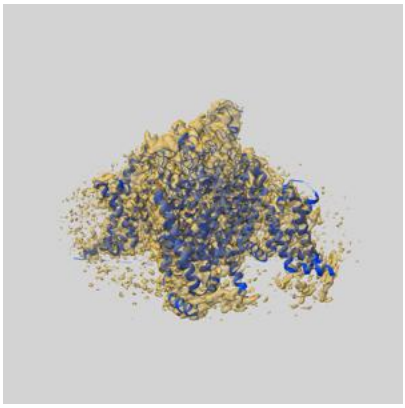
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.27	3.72	3.30
Unmasked-calculated*	-	-	-

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

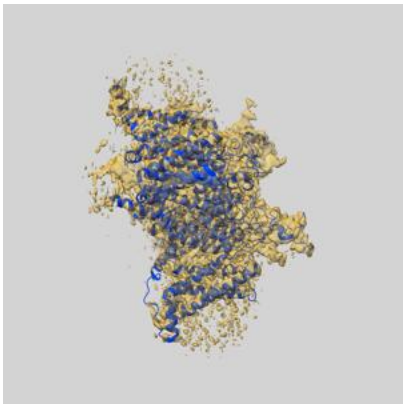
9 Map-model fit

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.

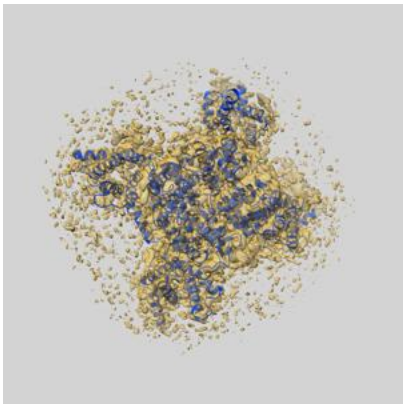
9.1 Map-model overlay



X



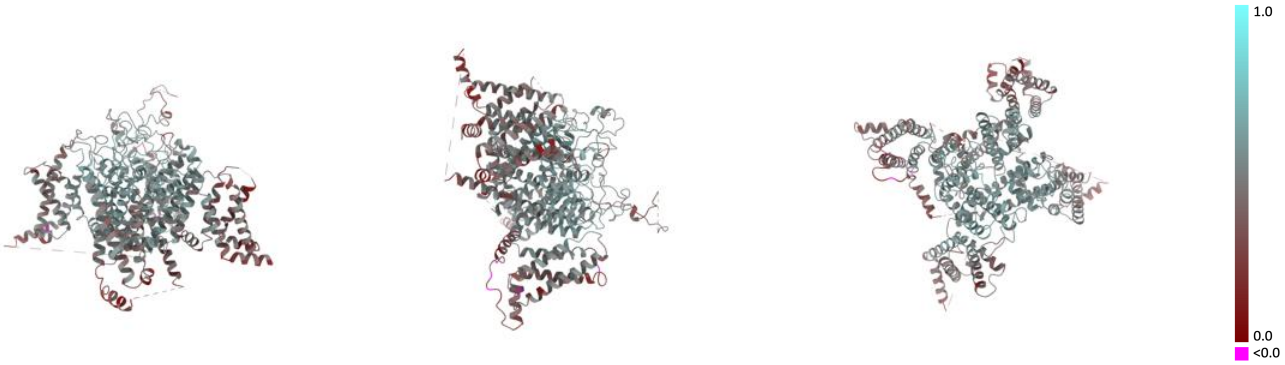
Y



Z

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.

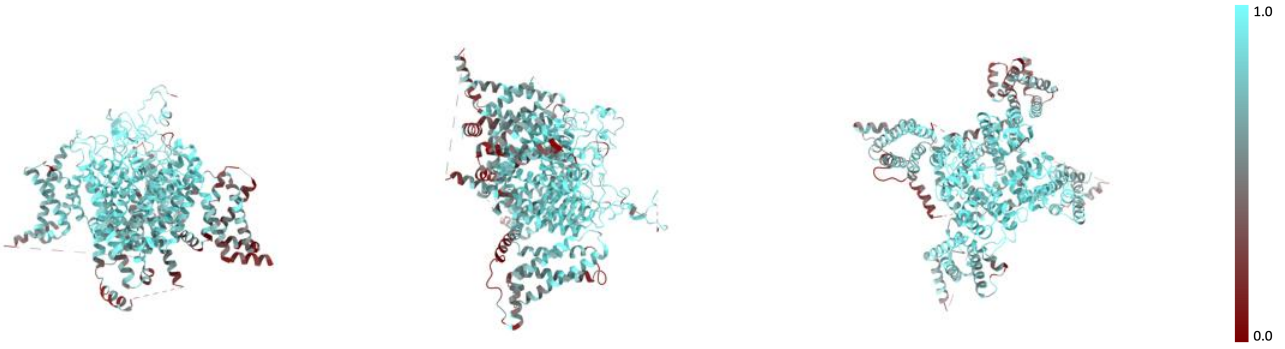
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

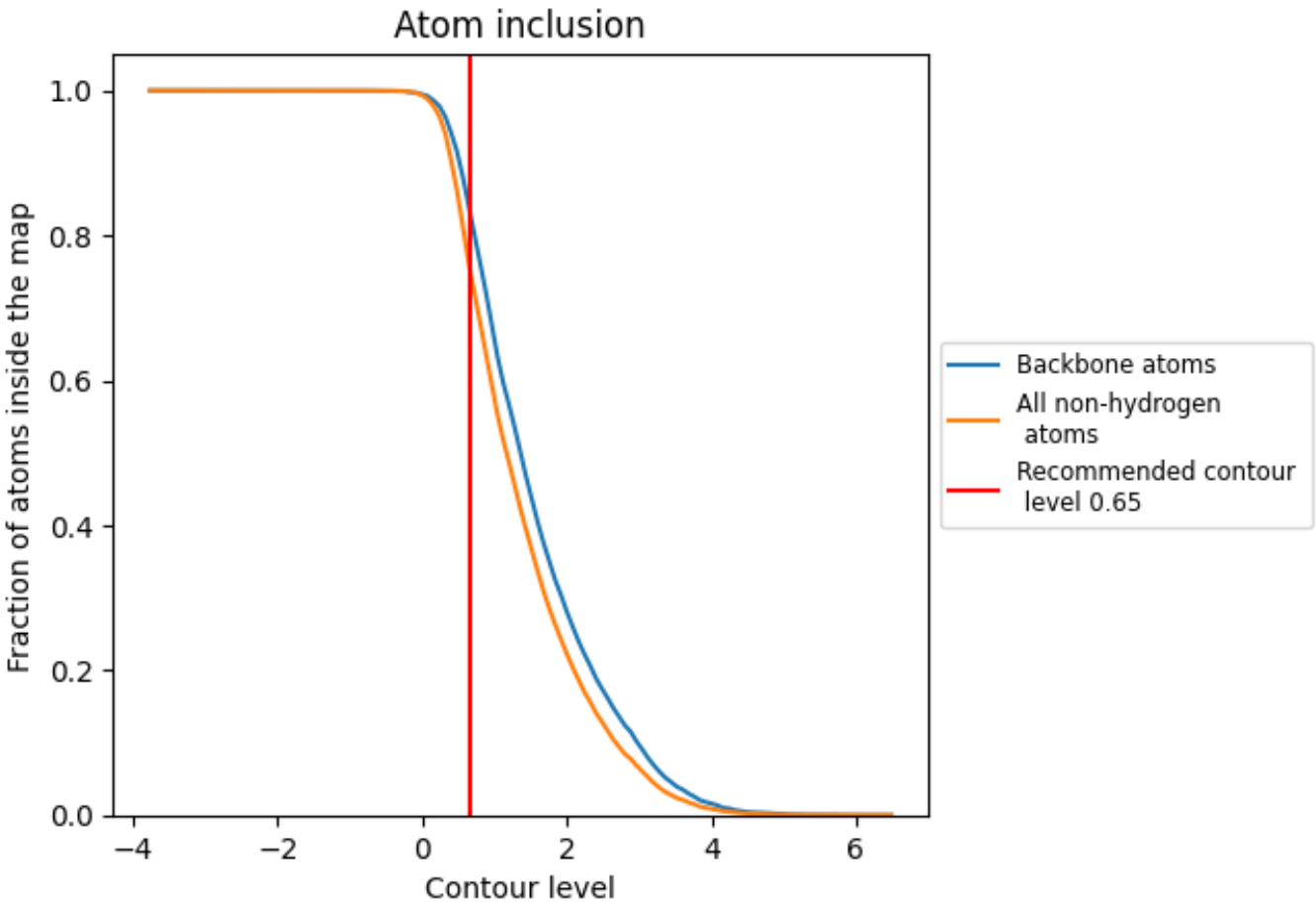
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).

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	0.7579	0.4770
A	0.7579	0.4770