



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 04:01 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

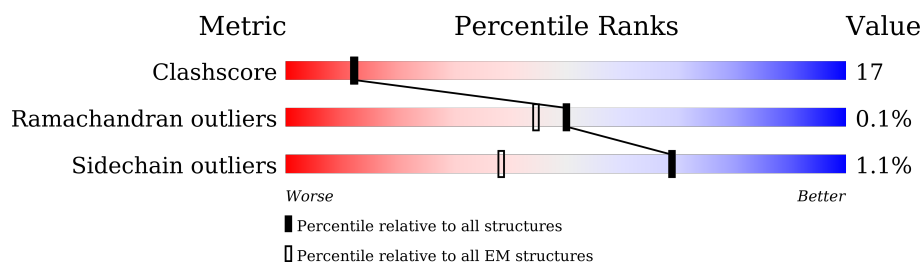
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1838	<div> <div>7%</div> <div>41%</div> <div>20%</div> <div>•</div> <div>39%</div> </div>

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:

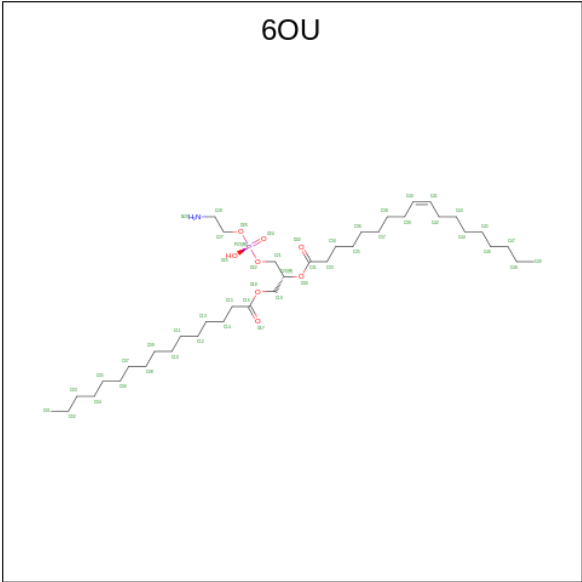
Chain	Residue	Modelled	Actual	Comment	Reference
A	1487	GLN	ILE	engineered mutation	UNP P15389
A	1488	GLN	PHE	engineered mutation	UNP P15389
A	1489	GLN	MET	engineered mutation	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389
A	1902	PHE	-	linker	UNP 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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).



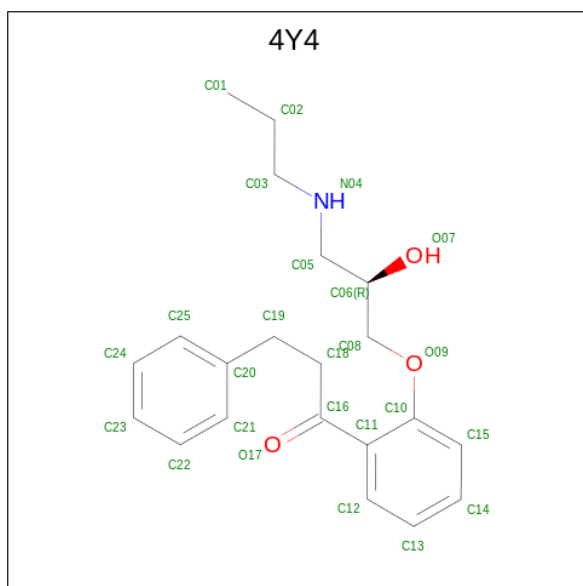
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0

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



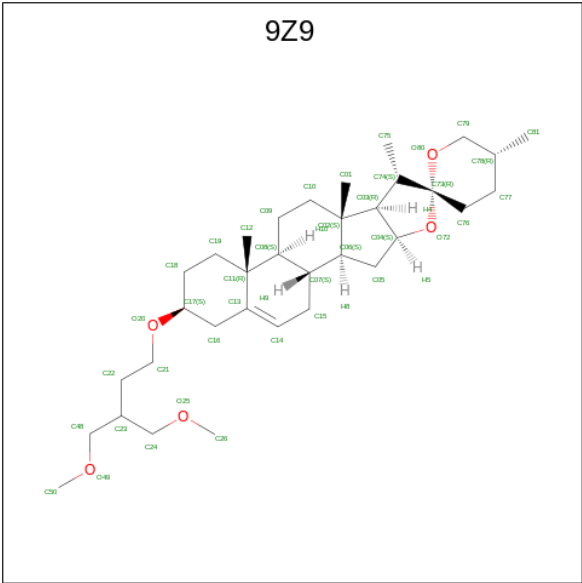
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
3	A	1	Total	C	O			0
			15	12	3			
3	A	1	Total	C	O			0
			26	21	5			
3	A	1	Total	C	O			0
			29	25	4			
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	A	1	Total	C	O			0
			27	23	4			
3	A	1	Total	C	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 (three-letter code: 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 (three-letter code: 9Z9) (formula: C₃₄H₅₆O₅).

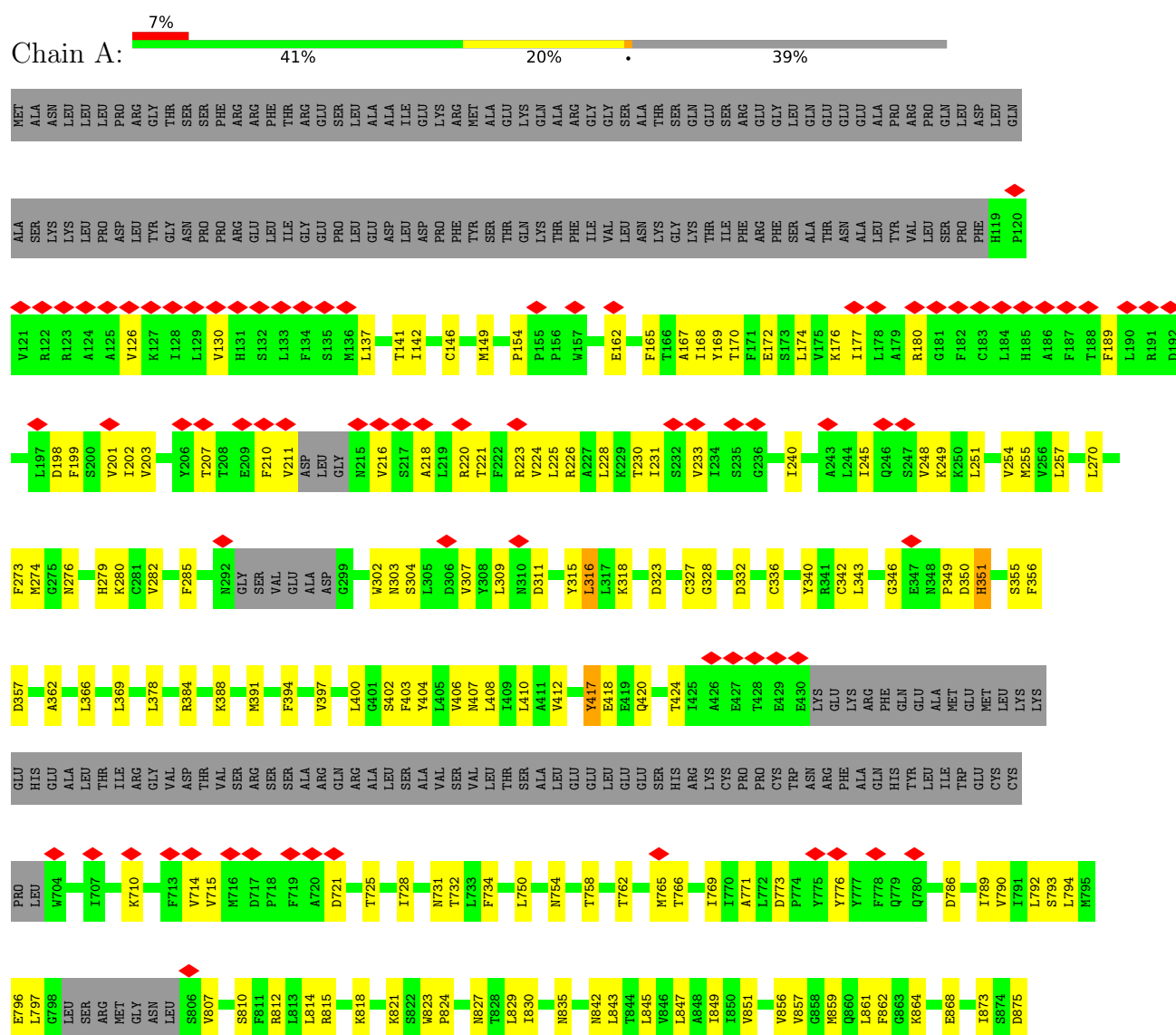


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			34	31	3	
5	A	1	Total	C	O	0
			30	27	3	

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



TYR	TYR	TYR	THR	SER	ILE	GLU	W1686	V1601	P1513	Y1436	N1338	T1211	ARG	LEU	ALA	ARG	S876
GLN	GLN	GLU	THR	GLY	HIS	ASP		I1602	R1514	E1437	V1339	I1214	LYS	ALA	ALA	THR	G877
ASN	ASN	LEU	THR	LYS	CYS	ASP	D1692	I1603	P1515	E1438	L1340		GLU	ARG	ILE	ARG	L878
ASP	ASP	LEU	THR	GLU	MET	THR	M1693	S1604	L1516	Q1439	L1341	L1219	THR	GLN	ILE	ARG	L879
ASP	ASP	GLY	THR	LEU	ASP	MET	F1694	I1605	M1517		V1342	S1220	PHE	ARG	ARG	PHE	P880
ILE	ILE	ILE	VAL	PHE	LEU	PHE	N1695	G1607	K1518	W1442	C1343	S1221	GLU	GLY	GLY	GLY	R881
GLY	GLY	ASP	GLN	THR	THR	TYR	F1696	T1608	Y1519	E1443	L1344	L1224	LEU	LEU	LEU	F888	
ASP	ASP	PHE	CYS	GLY	ALA	GLU	Q1697	V1609	Q1520	N1445	I1345		ARG	ARG	ARG	H889	
GLY	GLY	VAL	PHE	VAL	PHE	ILE	T1698	L1610	G1521	N1446	F1346	L1224	PHE	PHE	PHE	A890	
VAL	VAL	ARG	THR	VAL	THR	TRP	F1699	S1611	F1522	Y1447	W1347	L1231	ASP	ASP	ASP	I894	
LEU	LEU	ILE	TYR	ILE	ARG	GLU	A1700	D1612	I1523	M1448	S1351	E1232	PRO	LYS	LYS	F895	
LEU	LEU	VAL	PHE	LEU	VAL	PHE	N1701	I1613	I1526	Y1449	V1355	E1233	GLY	GLY	GLY	R896	
PRO	PRO	VAL	ASP	VAL	LEU	ASP	L1704	I1614	I1529	I1450	F1358	R1234	PRO	VAL	VAL	THR	I897
ASN	ASN	GLY	GLY	GLY	GLY	GLU	I1709	Q1615	Q1530		K1361		GLN	ARG	ARG	THR	L898
THR	THR	GLY	GLY	GLY	GLY	THR	L1718	K1616	A1531	V1454	F1362	I1237	PRO	ASP	ASP	PHE	E901
LEU	LEU	ASP	GLU	ASP	GLU	GLN		Y1617		I1456	G1363	V1253	SER	CYS	CYS	GLY	D908
SER	SER	VAL	VAL	VAL	MET	PHE	I1722	F1618	V1534	I1457	C1364	L1257	GLU	VAL	VAL	THR	Q915
THR	THR	GLY	PHE	ASN	ASP	ILE	L1723	F1619	T1535	G1458	C1365		PRO	VAL	VAL	GLY	S916
GLN	GLN	ASP	THR	GLY	ALA	GLU	N1724	S1620	I1536	G1459			VAL	CYS	ARG	ARG	L917
SER	SER	HIS	PHE	GLY	LYS	TYR	I1725		M1537	F1461	Q1368	Y1263	VAL	GLY	GLY	VAL	C918
ALA	ALA	LYS	LYS	LYS	LYS	LEU	G1726	F1624	I1540	F1462	D1372		PRO	ARG	ARG	ARG	L919
LEU	LEU	ASN	ALA	PHE	ILE	ALA	P1727		C1541	T1463	L1373	W1273	VAL	ILE	ILE	PRO	L920
SER	SER	SER	ALA	SER	GLN	LEU	P1728	I1627	L1542	L1464	P1374		ALA	LYS	LYS	LYS	V921
LYS	LYS	ASN	VAL	VAL	MET	SER	Y1729	R1628	L1543		N1376	L1276	VAL	VAL	VAL	VAL	F922
ASP	ASP	VAL	GLU	SER	GLU	ASP	C1730		M1544				ALA	ALA	ALA	ALA	L931
PRO	PRO	VAL	TYR	GLY	GLU	PHE		R1631	M1544			V1281	GLU	GLU	GLU	GLU	N935
ASN	ASN	ILE	TYR	GLY	LYS	ASP	L1734	I1632	V1545		I1379	D1285	SER	ALA	ALA	ALA	L936
GLU	GLU	GLY	VAL	GLY	GLY	ASP	P1735	G1633	V1549			V1286	THR	LEU	LEU	LEU	F937
LYS	LYS	ALA	GLU	GLY	ALA	LEU	N1736	R1634				L1287	GLU	ALA	ALA	ALA	L942
ARG	ARG	LYS	GLU	GLY	ASN	SER	I1751	L1638	D1553				ASP	THR	THR	HIS	L943
THR	THR	GLN	THR	ALA	ASN	GLU	L1752	R1639	I1561				GLN	GLU	GLN	SER	S943
ILE	ILE	LYS	ILE	THR	PRO	PRO	F1753	I1639	I1565				GLY	GLU	GLY	GLN	S944
VAL	VAL	ASN	PHE	TYR	LYS	LEU	F1754	R1640	L1568				ASP	PRO	PRO	PRO	F945
LEU	LEU	ILE	GLY	GLY	LYS	ARG	T1755	G1641	I1565				GLY	ASP	ASP	ASP	
LEU	LEU	ILE	LEU	LYS	ILE	ILE	T1756		L1568				GLU	SER	SER	SER	
PHE	PHE	VAL	ASP	LEU	THR	LYS	M1768	R1646	F1569				ASN	CYS	CYS	ALA	ALA
GLU	GLU	VAL	GLY	LEU	GLU	PRO	Y1769	T1647	V1570				GLU	ILE	ILE	ALA	ASP
VAL	VAL	ASN	ASN	LYS	PRO	ASN		L1648	K1494				GLU	THR	THR	ASN	ASN
THR	THR	PHE	TYR	ILE	ILE	GLN	I1772	L1652	I1572					ALA	ALA	ALA	LEU
ALA	ALA	ARG	THR	CYS	THR	ILE	I1773		C1577					PRO	PRO	PRO	PRO
ALA	ALA	HIS	ALA	THR	THR	LEU	F1777	S1655	M1581					ALA	ALA	ALA	ALA
GLY	GLY	THR	GLU	GLY	GLU	ILE	SER	L1656	L1498					THR	THR	THR	THR
LEU	LEU	ILE	VAL	GLY	VAL	ASN	VAL	P1657	A1499					ARG	ARG	ARG	ARG
VAL	VAL	LYS	VAL	LYS	VAL	MET	ALA	A1658	M1500					SER	SER	SER	SER
ASP	ASP	GLY	PHE	LEU	LEU	ASP	THR	L1659	K1501					GLY	GLY	GLY	GLY
GLU	GLU	GLY	GLU	PRO	GLN	LEU	GLU		K1502					VAL	VAL	VAL	VAL
LEU	LEU	VAL	GLY	PRO	GLY	MET	GLU	I1662	L1503					GLY	GLY	GLY	GLY
THR	THR	ASP	GLY	VAL	THR	SER	SER		G1504					LYS	LYS	LYS	LYS
LYS	LYS	PRO	GLY	TRP	PRO	VAL	THR	M1670	S1506					VAL	VAL	VAL	VAL
GLY	GLY	LEU	THR	PRO	GLY	SER	GLU	S1674	I1594					GLY	GLY	GLY	GLY
VAL	VAL	ALA	LEU	THR	GLY	ASP	LEU	I1675	F1596					ALA	ALA	ALA	ALA
ASN	ASN	ASP	VAL	LEU	MET	ASP	LEU	F1676	D1597					PRO	PRO	PRO	PRO
		HIS	ASN	SER	VAL	ARG	SER		F1598					ALA	ALA	ALA	ALA
								N1680	V1599					ALA	ALA	ALA	ALA
								F1681									

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: 6OU, 9Z9, NAG, 4Y4

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 [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	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.

All (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
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: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: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:1670:MET:O	1:A:1674:SER:OG	2.04	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: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:146:CYS:HA	1:A:149:MET:HE2	1.73	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:309:LEU:HD23	1:A:309:LEU:C	2.17	0.65
1:A:316:LEU:HD23	1:A:316:LEU:C	2.16	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1344:LEU:O	1:A:1411:TYR:OH	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1751:ILE:O	1:A:1755:THR:OG1	2.18	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1526:ILE:HA	1:A:1529:LYS:HZ1	1.75	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:1537:MET:CE	1:A:1641:GLY:HA3	2.42	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
1:A:336:CYS:SG	1:A:342:CYS:HB3	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:793:SER:HA	1:A:796:GLU:CD	2.35	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1293:LEU:O	1:A:1293:LEU:HG	2.17	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:1495:LYS:HE2	1:A:1495:LYS:HB3	1.86	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:309:LEU:C	1:A:309:LEU:CD2	2.85	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:ASP:OD1	1:A:776:TYR:HB2	2.20	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:1537:MET:HE2	1:A:1641:GLY:HA3	2.02	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: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 ⓘ

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%)	70	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	351	HIS
1	A	391	MET
1	A	417	TYR
1	A	1358	PHE
1	A	1372	ASP
1	A	1373	LEU
1	A	1379	ILE
1	A	1423	TRP
1	A	1730	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	276	ASN
1	A	407	ASN
1	A	422	GLN
1	A	731	ASN
1	A	754	ASN
1	A	783	ASN
1	A	871	HIS
1	A	1327	ASN
1	A	1356	ASN
1	A	1376	ASN
1	A	1439	GLN
1	A	1517	ASN
1	A	1520	GLN
1	A	1543	ASN

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Mol	Chain	Res	Type
1	A	1566	ASN
1	A	1701	ASN
1	A	1736	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	2207	-	25,25,48	1.07	3 (12%)	27,27,53	1.33	2 (7%)
3	6OU	A	2208	-	28,28,48	1.16	3 (10%)	30,30,53	1.40	3 (10%)
3	6OU	A	2204	-	31,31,48	1.08	4 (12%)	34,36,53	1.29	2 (5%)
3	6OU	A	2212	-	16,16,48	1.26	3 (18%)	16,16,53	1.12	1 (6%)
4	4Y4	A	2214	-	26,26,26	1.61	5 (19%)	30,32,32	1.01	1 (3%)
3	6OU	A	2213	-	14,14,48	1.34	3 (21%)	14,14,53	0.99	0
3	6OU	A	2209	-	38,38,48	0.97	3 (7%)	41,43,53	1.17	3 (7%)
2	NAG	A	2203	-	14,14,15	0.43	0	17,19,21	0.39	0
3	6OU	A	2211	-	24,24,48	1.26	4 (16%)	28,29,53	1.28	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6OU	A	2215	-	33,33,48	1.04	3 (9%)	35,38,53	1.22	2 (5%)
5	9Z9	A	2217	-	35,35,44	8.14	23 (65%)	58,58,68	2.15	23 (39%)
3	6OU	A	2210	-	26,26,48	0.95	2 (7%)	27,27,53	1.27	2 (7%)
5	9Z9	A	2216	-	38,38,44	8.22	23 (60%)	60,61,68	2.28	25 (41%)
3	6OU	A	2206	-	14,14,48	0.94	1 (7%)	14,14,53	1.32	1 (7%)
2	NAG	A	2201	-	14,14,15	0.38	0	17,19,21	0.42	0
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

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	2208	-	-	15/29/29/52	-
3	6OU	A	2204	-	-	17/35/35/52	-
3	6OU	A	2212	-	-	4/15/15/52	-
4	4Y4	A	2214	-	-	11/19/19/19	0/2/2/2
3	6OU	A	2213	-	-	5/13/13/52	-
3	6OU	A	2209	-	-	24/42/42/52	-
2	NAG	A	2203	-	-	4/6/23/26	0/1/1/1
3	6OU	A	2211	-	-	13/26/26/52	-
3	6OU	A	2215	-	-	17/37/37/52	-
5	9Z9	A	2217	-	-	-	0/6/6/6
3	6OU	A	2210	-	-	18/26/26/52	-
5	9Z9	A	2216	-	-	2/4/92/100	0/6/6/6
3	6OU	A	2206	-	-	5/13/13/52	-
2	NAG	A	2201	-	-	2/6/23/26	0/1/1/1
3	6OU	A	2205	-	-	23/38/38/52	-
2	NAG	A	2202	-	-	2/6/23/26	0/1/1/1

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
5	A	2216	9Z9	C11-C13	-18.39	1.16	1.52
5	A	2216	9Z9	C10-C02	-17.33	1.23	1.54
5	A	2217	9Z9	C10-C02	-17.16	1.23	1.54
5	A	2216	9Z9	C23-C22	16.82	2.88	1.49
5	A	2217	9Z9	C05-C04	11.11	1.77	1.52
5	A	2216	9Z9	C10-C09	-11.11	1.29	1.53
5	A	2216	9Z9	C05-C04	11.08	1.77	1.52
5	A	2217	9Z9	C10-C09	-10.97	1.30	1.53
5	A	2217	9Z9	C11-C08	10.73	1.74	1.56
5	A	2217	9Z9	C07-C08	-10.34	1.33	1.53
5	A	2216	9Z9	C11-C08	10.23	1.73	1.56
5	A	2216	9Z9	C07-C08	-10.14	1.34	1.53
5	A	2217	9Z9	C18-C17	-8.78	1.30	1.51
5	A	2217	9Z9	C19-C11	8.68	1.70	1.54
5	A	2216	9Z9	C19-C11	8.25	1.69	1.54
5	A	2216	9Z9	C18-C17	-7.56	1.30	1.51
5	A	2217	9Z9	C02-C03	5.65	1.67	1.56
5	A	2216	9Z9	C15-C14	5.64	1.62	1.50
5	A	2217	9Z9	C15-C14	5.63	1.62	1.50
5	A	2216	9Z9	C02-C03	5.41	1.67	1.56
5	A	2216	9Z9	C03-C04	-5.27	1.43	1.54
5	A	2217	9Z9	C03-C04	-5.13	1.44	1.54
5	A	2216	9Z9	C03-C74	-4.51	1.39	1.54
5	A	2217	9Z9	O72-C73	-4.44	1.32	1.42
5	A	2216	9Z9	O72-C73	-4.34	1.33	1.42
5	A	2217	9Z9	C03-C74	-4.26	1.40	1.54
5	A	2217	9Z9	C16-C13	4.10	1.60	1.51
5	A	2217	9Z9	C16-C17	4.06	1.59	1.52
5	A	2216	9Z9	C16-C13	3.92	1.60	1.51
3	A	2208	6OU	O30-C20	-3.87	1.40	1.47
4	A	2214	4Y4	O09-C08	-3.71	1.32	1.44
3	A	2212	6OU	C08-C07	-3.50	1.31	1.51
3	A	2213	6OU	C08-C07	-3.49	1.32	1.51
5	A	2216	9Z9	C76-C77	-3.00	1.47	1.53
5	A	2217	9Z9	C76-C77	-2.96	1.47	1.53
4	A	2214	4Y4	C14-C15	2.94	1.45	1.38
4	A	2214	4Y4	C11-C16	2.81	1.54	1.48
5	A	2217	9Z9	O20-C17	2.80	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2216	9Z9	C16-C17	2.77	1.58	1.52
4	A	2214	4Y4	C08-C06	2.73	1.60	1.51
4	A	2214	4Y4	O09-C10	2.72	1.43	1.37
3	A	2211	6OU	P23-O26	2.68	1.65	1.54
3	A	2207	6OU	O30-C20	-2.67	1.39	1.46
5	A	2217	9Z9	O80-C73	2.65	1.46	1.42
5	A	2216	9Z9	O80-C73	2.63	1.46	1.42
3	A	2215	6OU	O30-C20	-2.62	1.40	1.46
3	A	2205	6OU	O30-C20	-2.61	1.40	1.46
3	A	2211	6OU	O30-C20	-2.55	1.40	1.46
3	A	2205	6OU	O18-C16	2.53	1.40	1.33
3	A	2215	6OU	O18-C19	-2.53	1.39	1.45
3	A	2204	6OU	O30-C20	-2.52	1.40	1.46
3	A	2208	6OU	O18-C16	2.49	1.40	1.33
3	A	2210	6OU	O18-C16	2.48	1.40	1.33
3	A	2209	6OU	O18-C16	2.46	1.40	1.33
5	A	2216	9Z9	O20-C17	2.46	1.50	1.43
3	A	2204	6OU	O18-C16	2.38	1.40	1.33
3	A	2207	6OU	O18-C19	-2.38	1.39	1.45
5	A	2217	9Z9	C05-C06	2.35	1.59	1.54
5	A	2217	9Z9	C19-C18	-2.34	1.48	1.53
3	A	2209	6OU	O30-C20	-2.33	1.40	1.46
3	A	2210	6OU	O30-C31	2.31	1.40	1.33
3	A	2212	6OU	O18-C16	2.27	1.40	1.33
3	A	2213	6OU	O18-C16	2.26	1.40	1.33
5	A	2216	9Z9	C19-C18	-2.25	1.48	1.53
5	A	2216	9Z9	C05-C06	2.24	1.59	1.54
3	A	2212	6OU	O18-C19	-2.21	1.40	1.45
3	A	2211	6OU	O18-C19	-2.20	1.40	1.45
5	A	2217	9Z9	C76-C73	2.19	1.55	1.52
3	A	2213	6OU	O18-C19	-2.18	1.40	1.45
3	A	2207	6OU	O18-C16	2.16	1.39	1.33
3	A	2206	6OU	O30-C31	2.14	1.39	1.33
3	A	2211	6OU	O18-C16	2.12	1.39	1.33
3	A	2209	6OU	O30-C31	2.10	1.40	1.34
3	A	2204	6OU	O30-C31	2.09	1.40	1.34
3	A	2215	6OU	O18-C16	2.09	1.39	1.33
3	A	2208	6OU	O30-C31	2.08	1.40	1.34
3	A	2204	6OU	O18-C19	-2.08	1.40	1.45

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	A	2211	6OU	O30-C31-C33	4.37	120.93	111.50
5	A	2217	9Z9	C10-C02-C03	4.27	122.29	115.46
3	A	2208	6OU	O30-C31-C33	4.26	120.67	111.50
5	A	2216	9Z9	C01-C02-C06	-4.21	103.86	111.71
3	A	2209	6OU	O30-C31-C33	4.17	120.48	111.50
5	A	2216	9Z9	C10-C02-C06	4.16	113.73	107.27
3	A	2215	6OU	O30-C31-C33	4.16	120.46	111.50
3	A	2205	6OU	O30-C31-C33	4.08	120.29	111.50
5	A	2216	9Z9	C05-C06-C02	-4.05	98.51	103.91
5	A	2216	9Z9	C16-C13-C11	-4.00	111.10	116.42
5	A	2216	9Z9	C10-C02-C03	3.95	121.78	115.46
4	A	2214	4Y4	C10-C11-C16	-3.89	119.71	125.34
5	A	2217	9Z9	C10-C02-C06	3.79	113.16	107.27
5	A	2217	9Z9	C01-C02-C10	-3.79	104.60	110.59
3	A	2207	6OU	O30-C31-C33	3.77	119.62	111.50
5	A	2217	9Z9	C15-C14-C13	-3.75	118.14	125.06
5	A	2216	9Z9	C12-C11-C08	-3.54	107.45	111.68
5	A	2217	9Z9	C01-C02-C06	-3.52	105.16	111.71
5	A	2216	9Z9	C03-C02-C06	3.43	105.27	100.23
5	A	2216	9Z9	C01-C02-C10	-3.37	105.27	110.59
5	A	2217	9Z9	C03-C02-C06	3.34	105.15	100.23
5	A	2216	9Z9	C15-C07-C08	3.32	113.74	109.71
5	A	2216	9Z9	C08-C07-C06	3.20	113.37	109.09
5	A	2217	9Z9	C08-C11-C13	3.16	114.61	109.65
5	A	2217	9Z9	C75-C74-C73	-3.10	109.26	114.92
5	A	2216	9Z9	C09-C08-C11	-3.01	109.12	113.08
5	A	2216	9Z9	C09-C10-C02	2.99	117.91	112.78
3	A	2210	6OU	O30-C31-C33	2.96	121.19	111.91
5	A	2216	9Z9	C02-C03-C74	-2.94	110.56	120.56
5	A	2217	9Z9	C02-C03-C74	-2.92	110.62	120.56
5	A	2217	9Z9	C77-C78-C79	2.91	112.61	108.56
3	A	2210	6OU	O18-C16-C15	2.91	121.05	111.91
5	A	2217	9Z9	C08-C07-C06	2.89	112.96	109.09
3	A	2206	6OU	O30-C31-C33	2.88	120.94	111.91
5	A	2216	9Z9	C75-C74-C73	-2.82	109.76	114.92
3	A	2209	6OU	O18-C16-C15	2.80	120.68	111.91
5	A	2217	9Z9	C01-C02-C03	-2.72	105.00	111.63
3	A	2204	6OU	O18-C16-C15	2.70	120.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2217	9Z9	C05-C06-C02	-2.64	100.39	103.91
5	A	2217	9Z9	C75-C74-C03	-2.64	108.64	114.50
5	A	2216	9Z9	C08-C11-C13	2.63	113.77	109.65
5	A	2216	9Z9	C01-C02-C03	-2.62	105.25	111.63
5	A	2216	9Z9	C02-C03-C04	2.58	107.25	104.13
3	A	2207	6OU	O18-C16-C15	2.54	119.87	111.91
3	A	2208	6OU	O18-C16-C15	2.54	119.86	111.91
3	A	2205	6OU	O18-C16-C15	2.47	119.65	111.91
5	A	2216	9Z9	C05-C06-C07	2.40	124.62	119.48
5	A	2217	9Z9	C15-C07-C08	2.40	112.62	109.71
3	A	2215	6OU	O18-C16-C15	2.38	119.36	111.91
5	A	2217	9Z9	C02-C03-C04	2.35	106.98	104.13
5	A	2217	9Z9	C12-C11-C08	-2.35	108.88	111.68
5	A	2217	9Z9	C05-C06-C07	2.34	124.48	119.48
5	A	2216	9Z9	C11-C08-C07	-2.26	109.34	112.73
3	A	2211	6OU	O18-C16-C15	2.24	118.94	111.91
3	A	2208	6OU	C20-O30-C31	-2.22	115.02	117.88
5	A	2216	9Z9	C77-C78-C79	2.21	111.63	108.56
5	A	2217	9Z9	C79-O80-C73	-2.17	109.60	113.72
5	A	2217	9Z9	C09-C10-C02	2.17	116.50	112.78
5	A	2216	9Z9	C73-C74-C03	-2.15	99.87	103.37
3	A	2209	6OU	C21-C20-C19	-2.13	106.74	111.79
5	A	2216	9Z9	C75-C74-C03	-2.08	109.87	114.50
5	A	2216	9Z9	C76-C73-C74	-2.05	111.48	115.69
5	A	2217	9Z9	C76-C77-C78	2.04	116.11	111.81
3	A	2212	6OU	O18-C16-C15	2.02	120.19	112.23

There are no chirality outliers.

All (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
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

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Mol	Chain	Res	Type	Atoms
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	2212	6OU	C06-C07-C08-C09
3	A	2208	6OU	C15-C16-O18-C19
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	2205	6OU	C34-C35-C36-C37
3	A	2207	6OU	C15-C16-O18-C19
3	A	2205	6OU	C33-C31-O30-C20
3	A	2212	6OU	C04-C05-C06-C07
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
3	A	2215	6OU	C31-C33-C34-C35
2	A	2201	NAG	C4-C5-C6-O6
3	A	2204	6OU	C13-C14-C15-C16
3	A	2205	6OU	C13-C14-C15-C16
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	2215	6OU	C13-C14-C15-C16
4	A	2214	4Y4	C05-C06-C08-O09
3	A	2205	6OU	O32-C31-O30-C20
4	A	2214	4Y4	O07-C06-C08-O09
3	A	2209	6OU	C27-O26-P23-O22

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Mol	Chain	Res	Type	Atoms
5	A	2216	9Z9	O20-C21-C22-C23
3	A	2204	6OU	O32-C31-O30-C20
3	A	2206	6OU	O30-C20-C21-O22
3	A	2204	6OU	C33-C31-O30-C20
3	A	2209	6OU	C33-C31-O30-C20
3	A	2208	6OU	C06-C07-C08-C09
3	A	2209	6OU	O32-C31-O30-C20
2	A	2201	NAG	O5-C5-C6-O6
3	A	2211	6OU	C34-C35-C36-C37
3	A	2205	6OU	C10-C11-C12-C13
3	A	2207	6OU	C33-C34-C35-C36
3	A	2209	6OU	C35-C36-C37-C38
3	A	2209	6OU	C34-C35-C36-C37
3	A	2210	6OU	C35-C36-C37-C38
3	A	2205	6OU	C12-C13-C14-C15
3	A	2210	6OU	O18-C19-C20-O30
3	A	2204	6OU	C12-C13-C14-C15
3	A	2207	6OU	C35-C36-C37-C38
3	A	2210	6OU	C41-C42-C43-C44
3	A	2210	6OU	C31-C33-C34-C35
3	A	2204	6OU	C34-C35-C36-C37
3	A	2215	6OU	C10-C11-C12-C13
3	A	2210	6OU	C37-C38-C39-C40
3	A	2204	6OU	C31-C33-C34-C35
3	A	2210	6OU	C33-C31-O30-C20
3	A	2210	6OU	C38-C39-C40-C41
3	A	2213	6OU	C11-C12-C13-C14
3	A	2208	6OU	C33-C34-C35-C36
3	A	2215	6OU	C11-C12-C13-C14
3	A	2210	6OU	C11-C12-C13-C14
3	A	2213	6OU	C08-C09-C10-C11
3	A	2206	6OU	C31-C33-C34-C35
3	A	2208	6OU	C31-C33-C34-C35
3	A	2212	6OU	C13-C14-C15-C16
4	A	2214	4Y4	C11-C16-C18-C19
3	A	2207	6OU	O18-C19-C20-C21
3	A	2215	6OU	C34-C35-C36-C37
3	A	2209	6OU	C10-C11-C12-C13
3	A	2206	6OU	C35-C36-C37-C38
3	A	2206	6OU	C34-C35-C36-C37
3	A	2210	6OU	C42-C43-C44-C45
3	A	2205	6OU	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	A	2205	6OU	C07-C08-C09-C10
3	A	2204	6OU	C10-C11-C12-C13
3	A	2211	6OU	C21-O22-P23-O24
3	A	2205	6OU	C38-C39-C40-C41
3	A	2210	6OU	O32-C31-O30-C20
4	A	2214	4Y4	C15-C10-O09-C08
3	A	2209	6OU	C09-C10-C11-C12
3	A	2205	6OU	C15-C16-O18-C19
3	A	2205	6OU	O18-C19-C20-C21
4	A	2214	4Y4	C11-C10-O09-C08
3	A	2205	6OU	O18-C19-C20-O30
3	A	2215	6OU	C20-C21-O22-P23
3	A	2210	6OU	C36-C37-C38-C39
3	A	2215	6OU	C40-C41-C42-C43
3	A	2208	6OU	C34-C35-C36-C37
3	A	2210	6OU	C33-C34-C35-C36
3	A	2207	6OU	C12-C13-C14-C15
4	A	2214	4Y4	O17-C16-C18-C19
3	A	2212	6OU	C08-C09-C10-C11
3	A	2209	6OU	C11-C12-C13-C14
3	A	2205	6OU	O30-C20-C21-O22
3	A	2205	6OU	C35-C36-C37-C38
3	A	2207	6OU	O18-C19-C20-O30
3	A	2211	6OU	O18-C19-C20-O30
3	A	2205	6OU	O17-C16-O18-C19
3	A	2215	6OU	C33-C34-C35-C36
3	A	2215	6OU	C15-C16-O18-C19
3	A	2205	6OU	C09-C10-C11-C12
3	A	2204	6OU	C36-C37-C38-C39
3	A	2209	6OU	C21-O22-P23-O24
3	A	2215	6OU	C27-O26-P23-O24
3	A	2205	6OU	C19-C20-C21-O22
3	A	2209	6OU	C37-C38-C39-C40
3	A	2215	6OU	O17-C16-O18-C19
3	A	2209	6OU	C19-C20-O30-C31
3	A	2208	6OU	C36-C37-C38-C39
3	A	2204	6OU	C27-O26-P23-O22
3	A	2209	6OU	C21-O22-P23-O26
3	A	2213	6OU	C05-C06-C07-C08
3	A	2211	6OU	C20-C21-O22-P23
3	A	2208	6OU	C07-C08-C09-C10
3	A	2208	6OU	C37-C38-C39-C40

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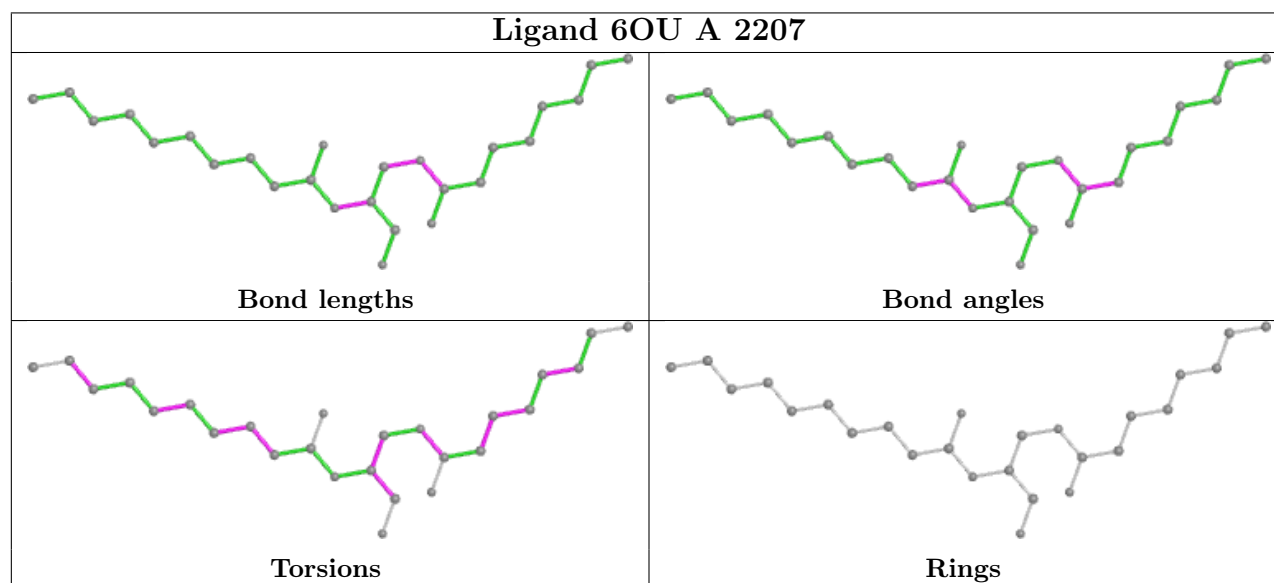
Mol	Chain	Res	Type	Atoms
3	A	2209	6OU	C41-C42-C43-C44
3	A	2213	6OU	C10-C11-C12-C13
3	A	2211	6OU	O18-C19-C20-C21
3	A	2210	6OU	C10-C11-C12-C13
3	A	2208	6OU	O32-C31-O30-C20
3	A	2204	6OU	C11-C12-C13-C14
3	A	2207	6OU	C38-C39-C40-C41
3	A	2207	6OU	C13-C14-C15-C16
3	A	2207	6OU	O30-C20-C21-O22
3	A	2213	6OU	C09-C10-C11-C12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

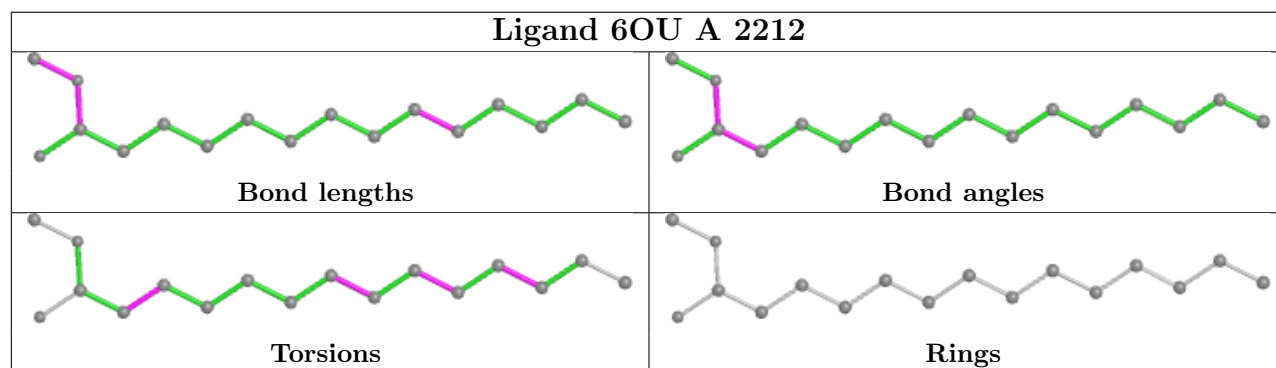
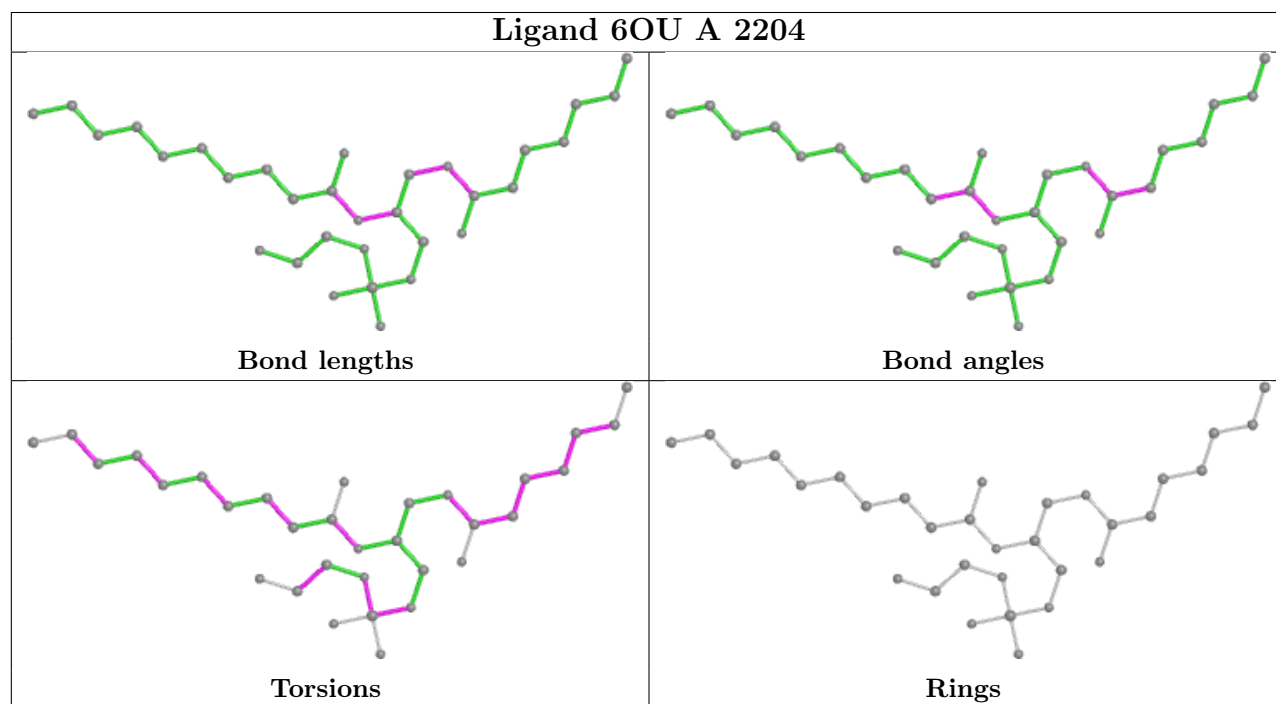
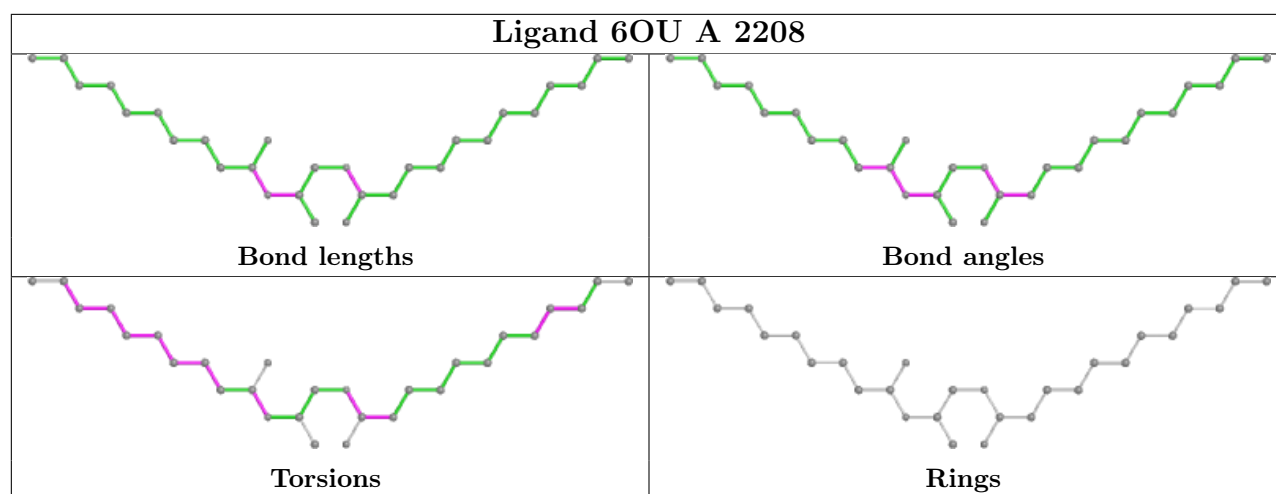
There are no ring outliers.

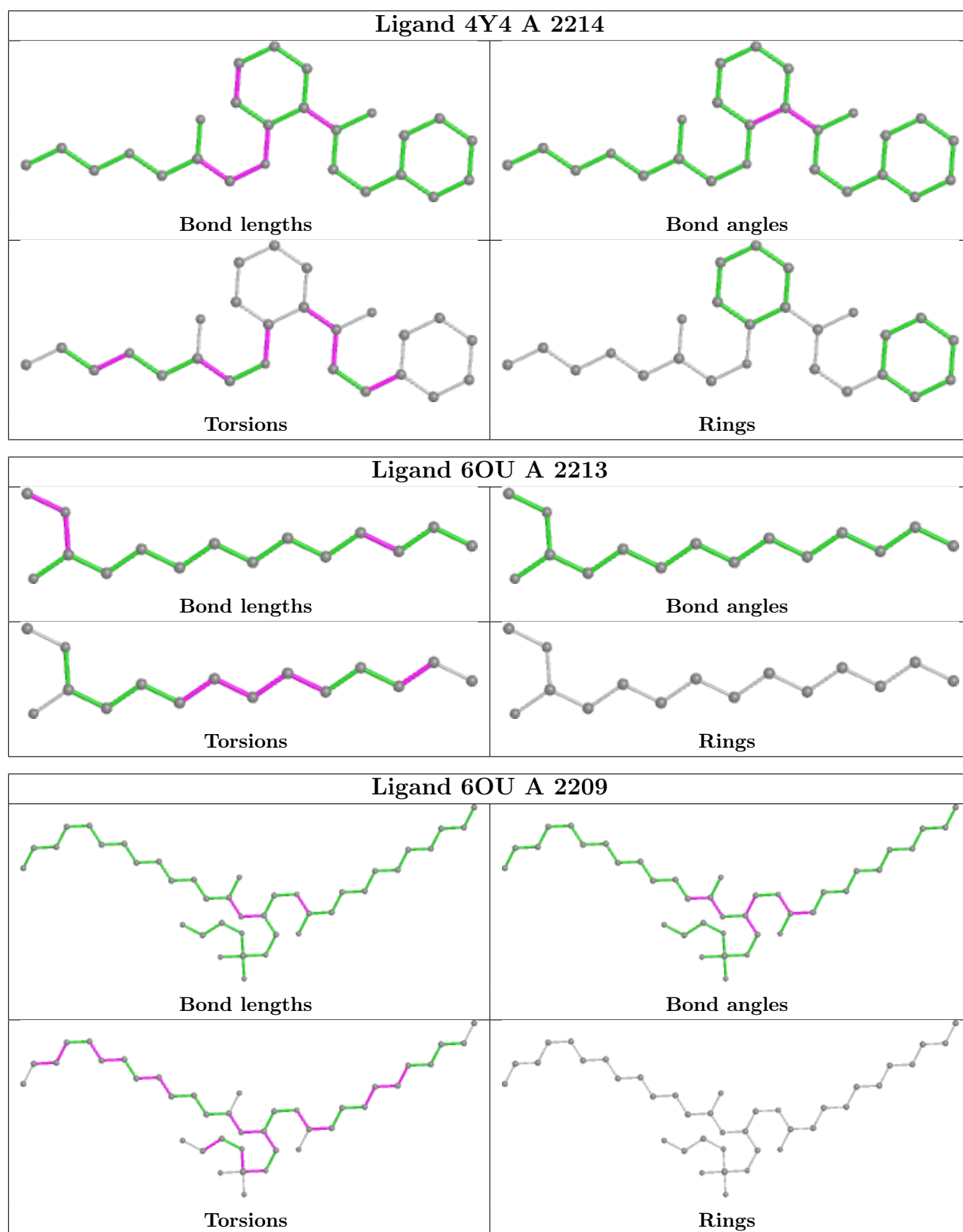
4 monomers are involved in 21 short contacts:

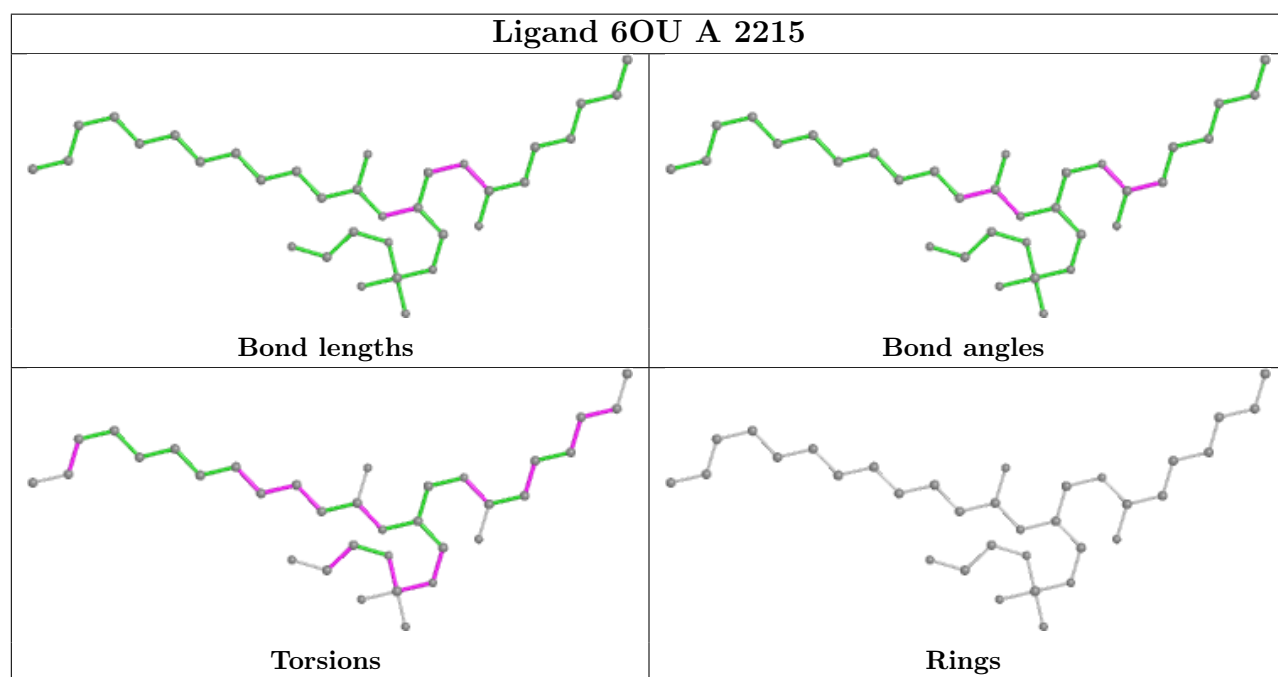
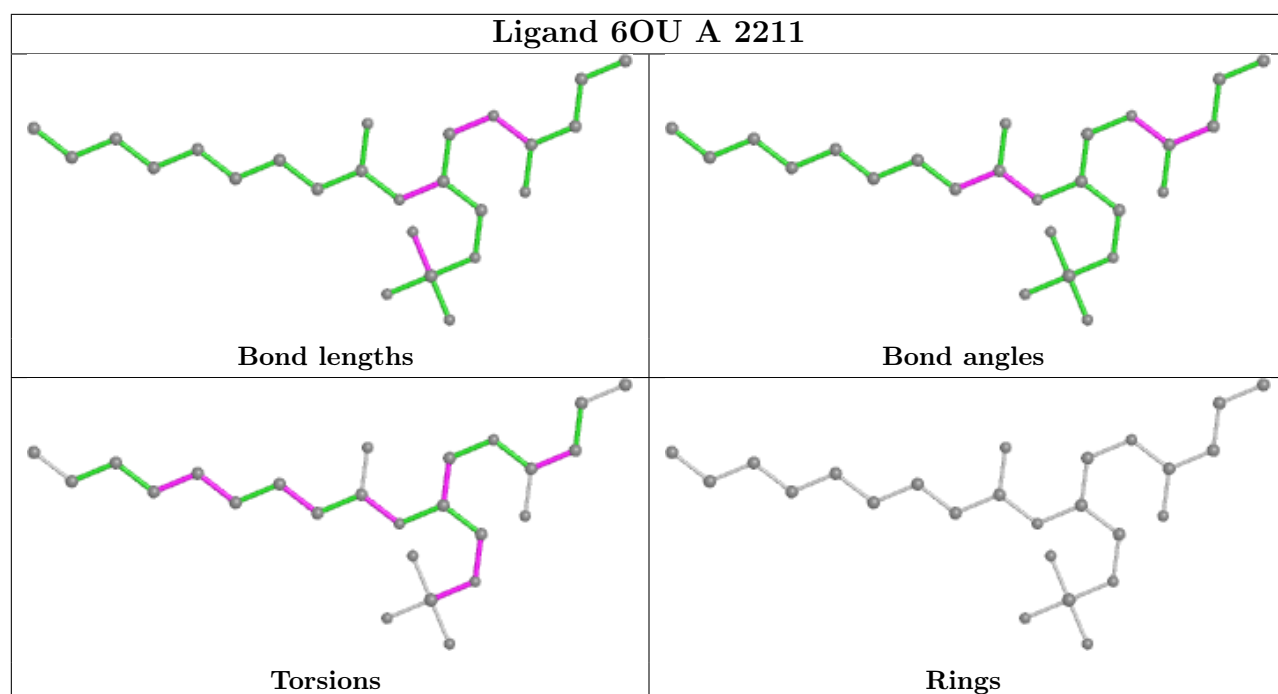
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2217	9Z9	5	0
5	A	2216	9Z9	8	0
2	A	2201	NAG	5	0
2	A	2202	NAG	4	0

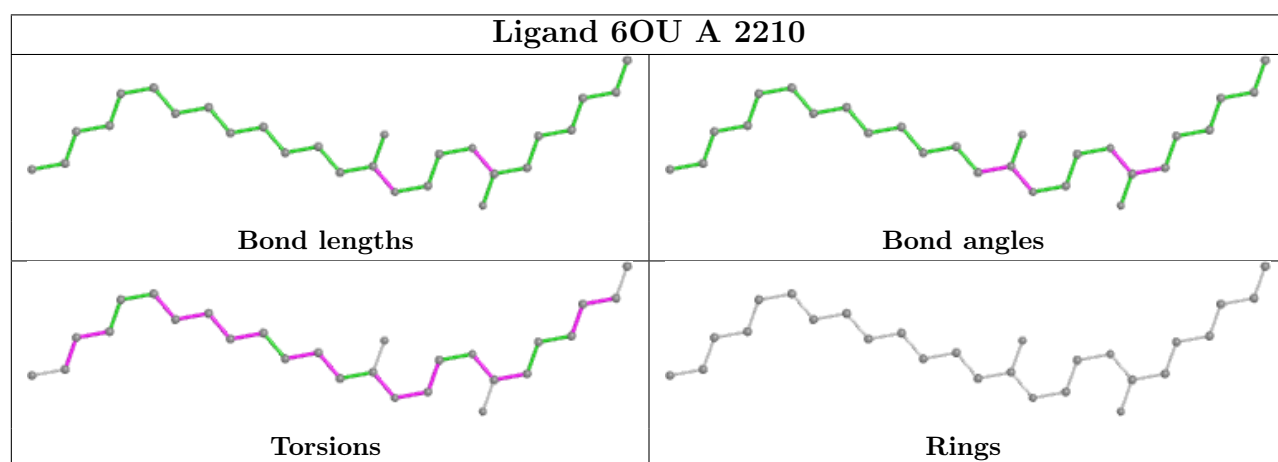
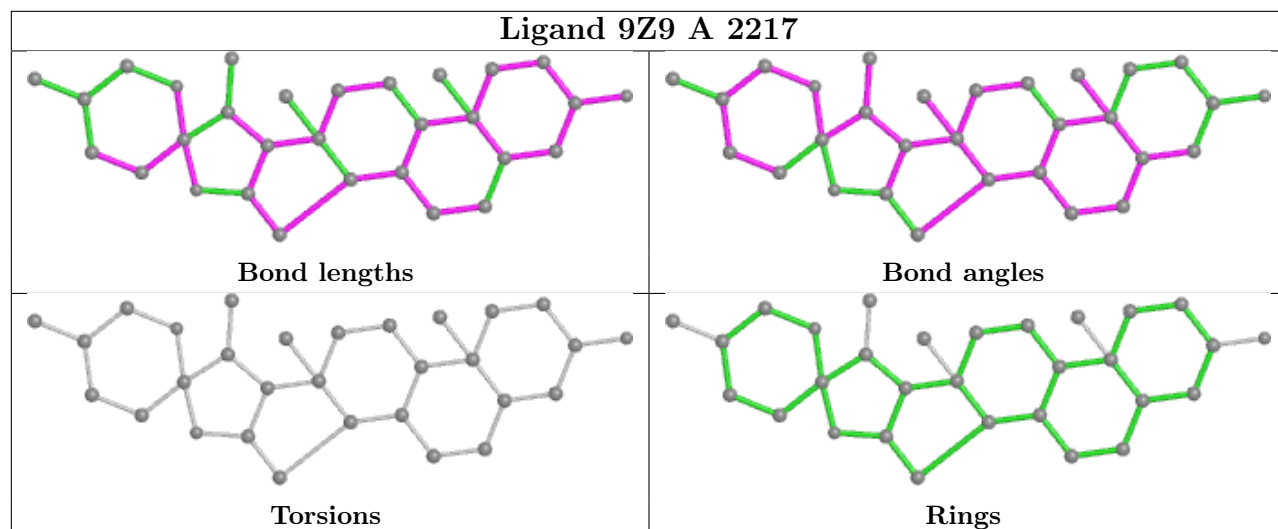
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



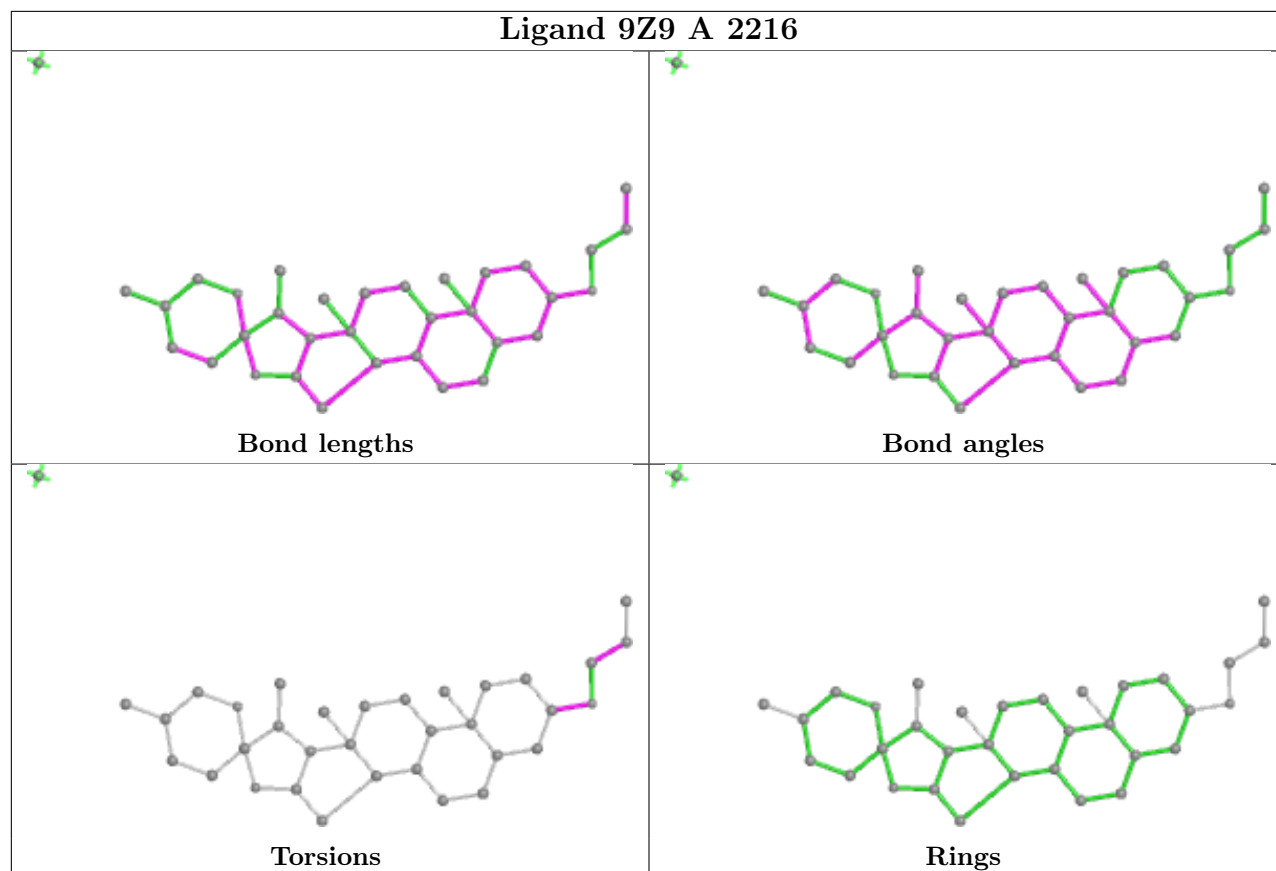




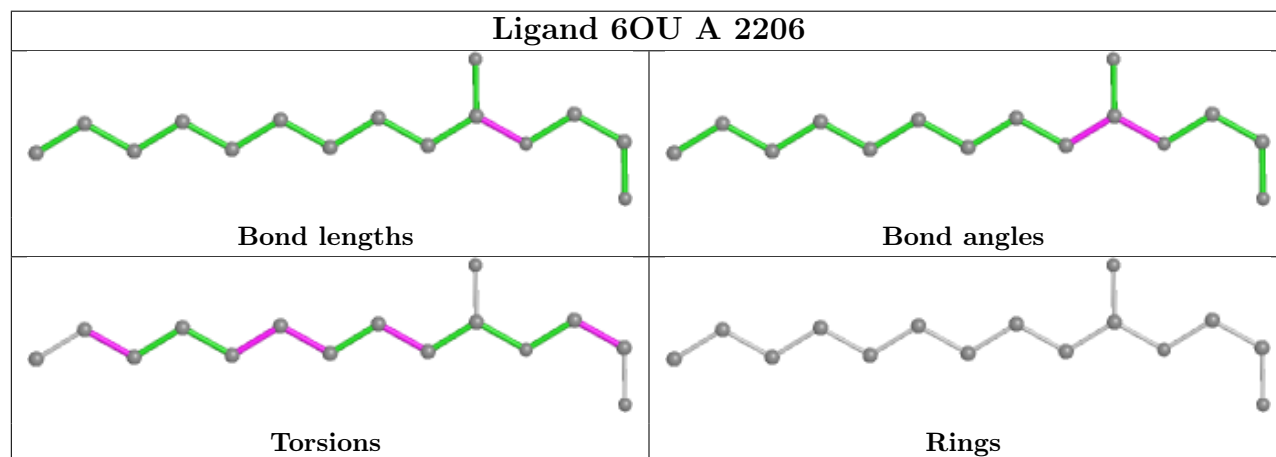


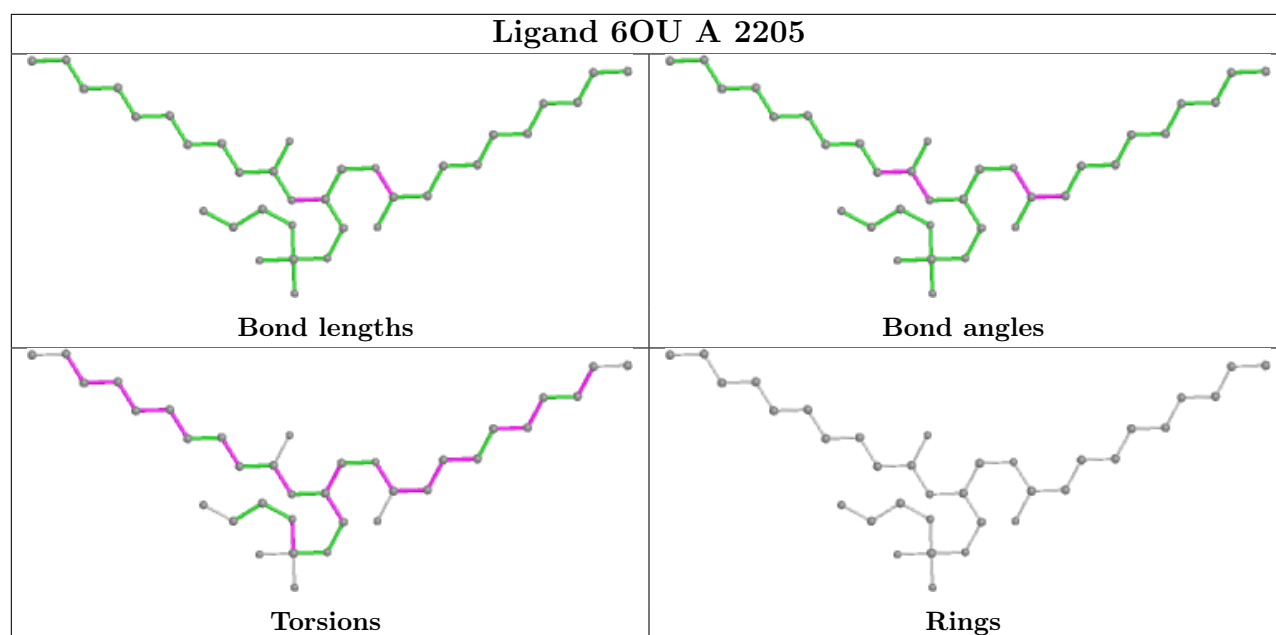


Ligand 9Z9 A 2216



Ligand 6OU A 2206





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.

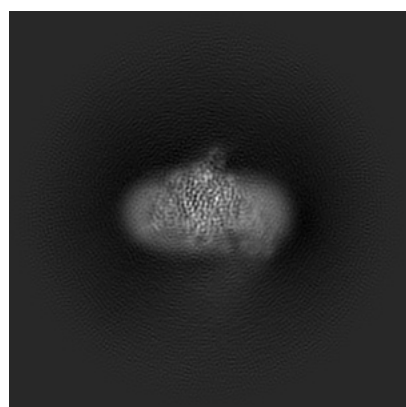
6 Map visualisation [i](#)

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

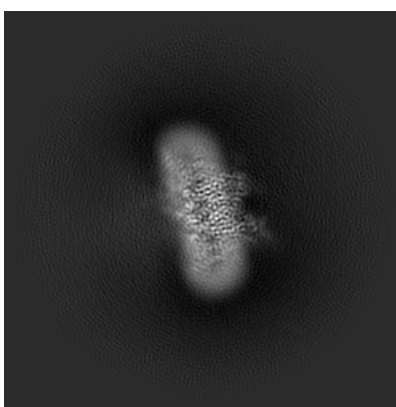
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

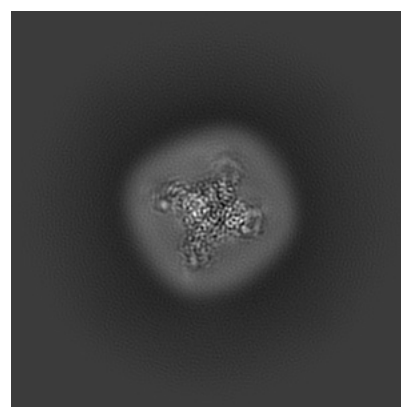
6.1.1 Primary map



X



Y

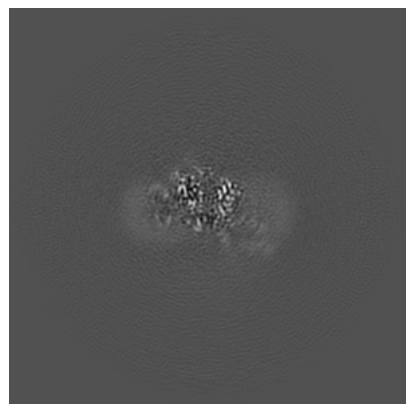


Z

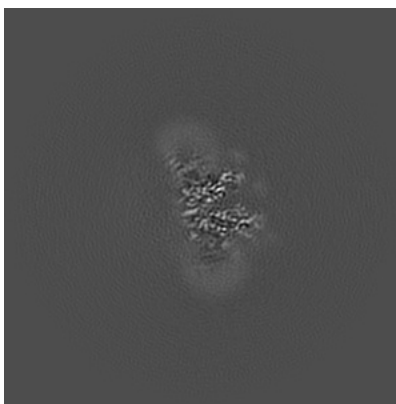
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

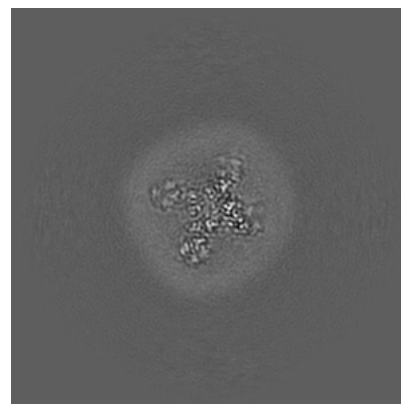
6.2.1 Primary map



X Index: 160



Y Index: 160

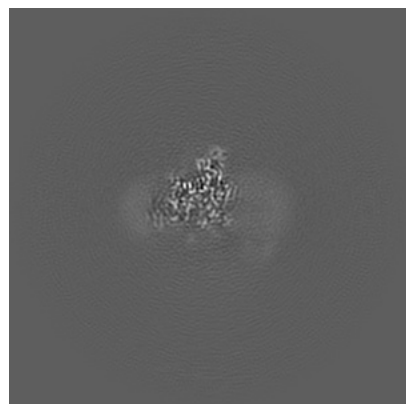


Z Index: 160

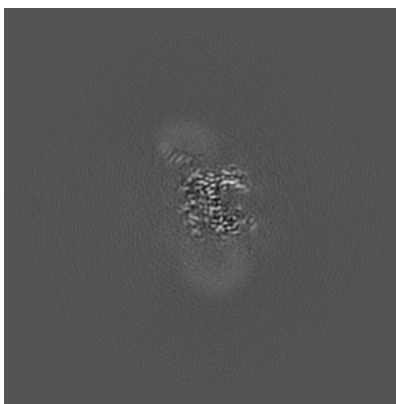
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

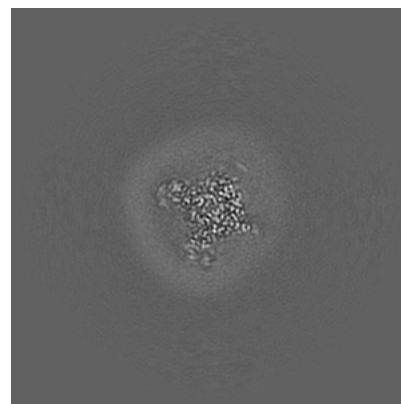
6.3.1 Primary map



X Index: 150



Y Index: 153

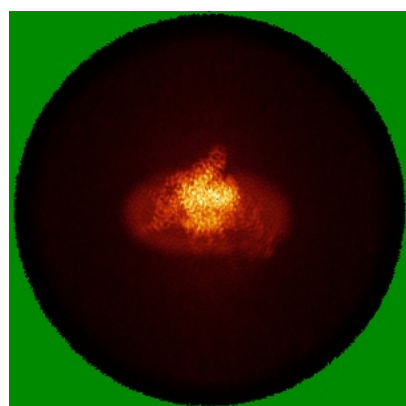


Z Index: 168

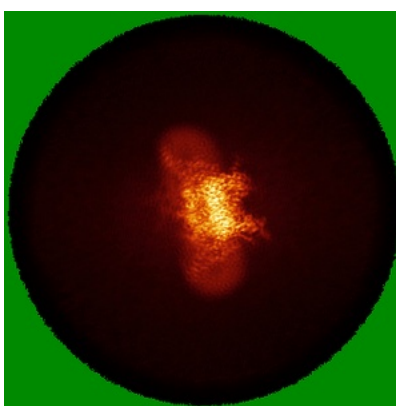
The images above show the largest variance slices of the map in three orthogonal directions.

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

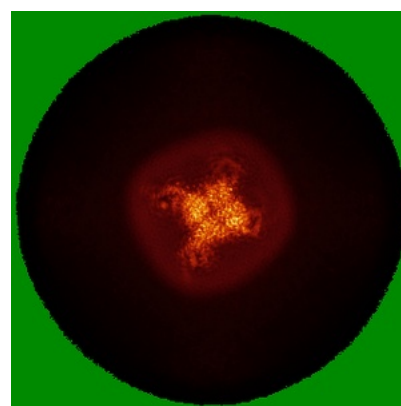
6.4.1 Primary map



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.

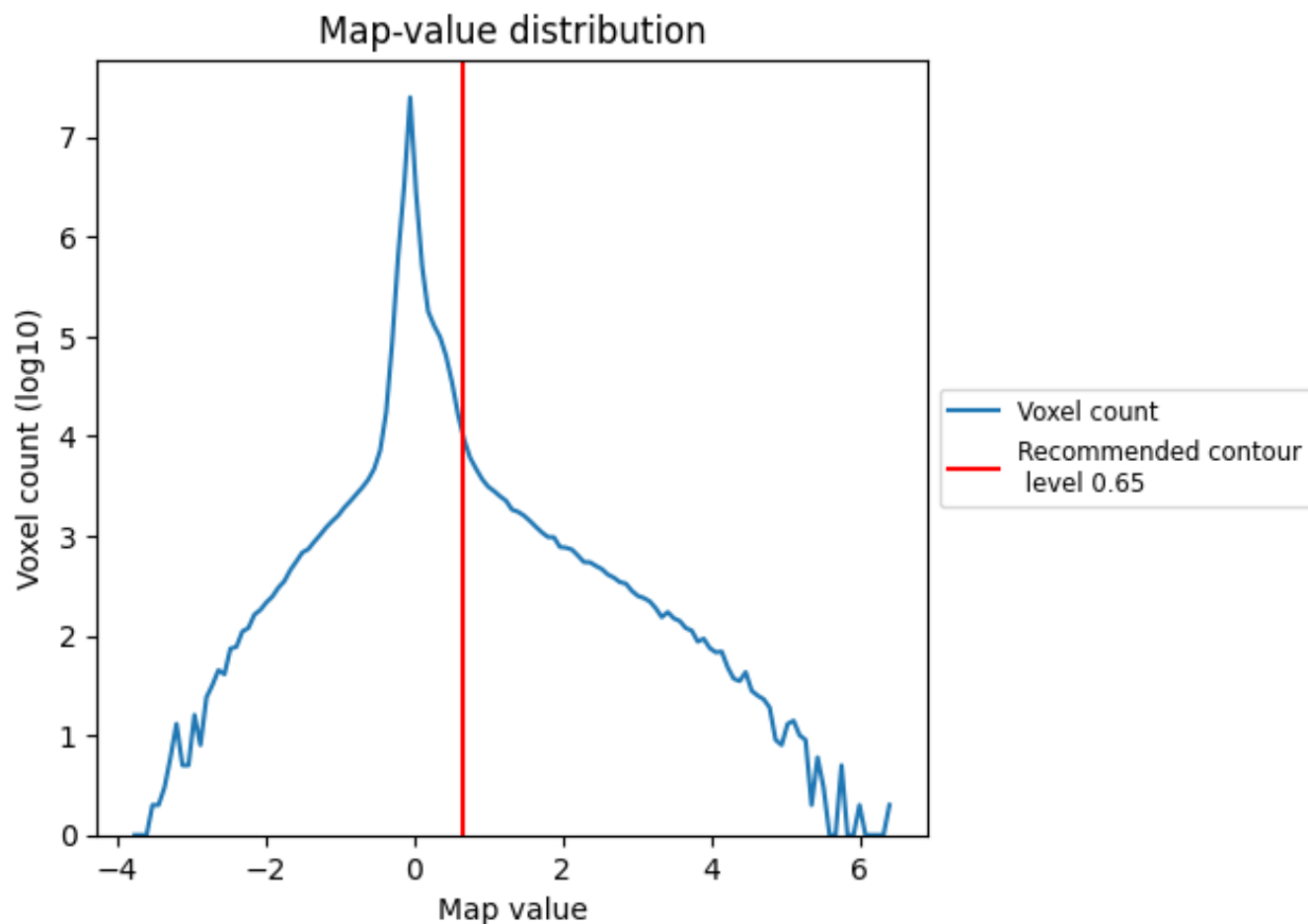
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

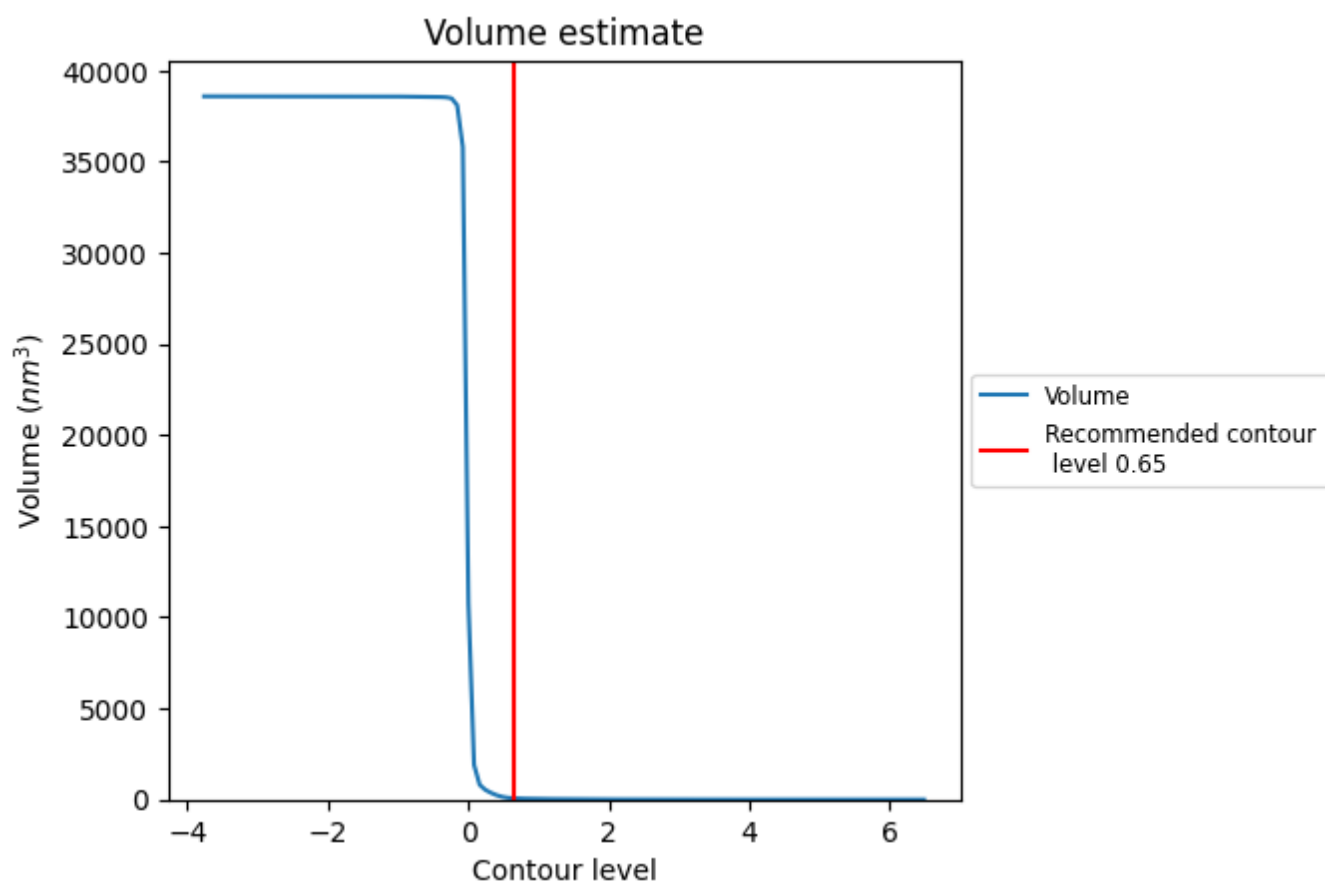
This section contains the results of statistical analysis of the map.

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.

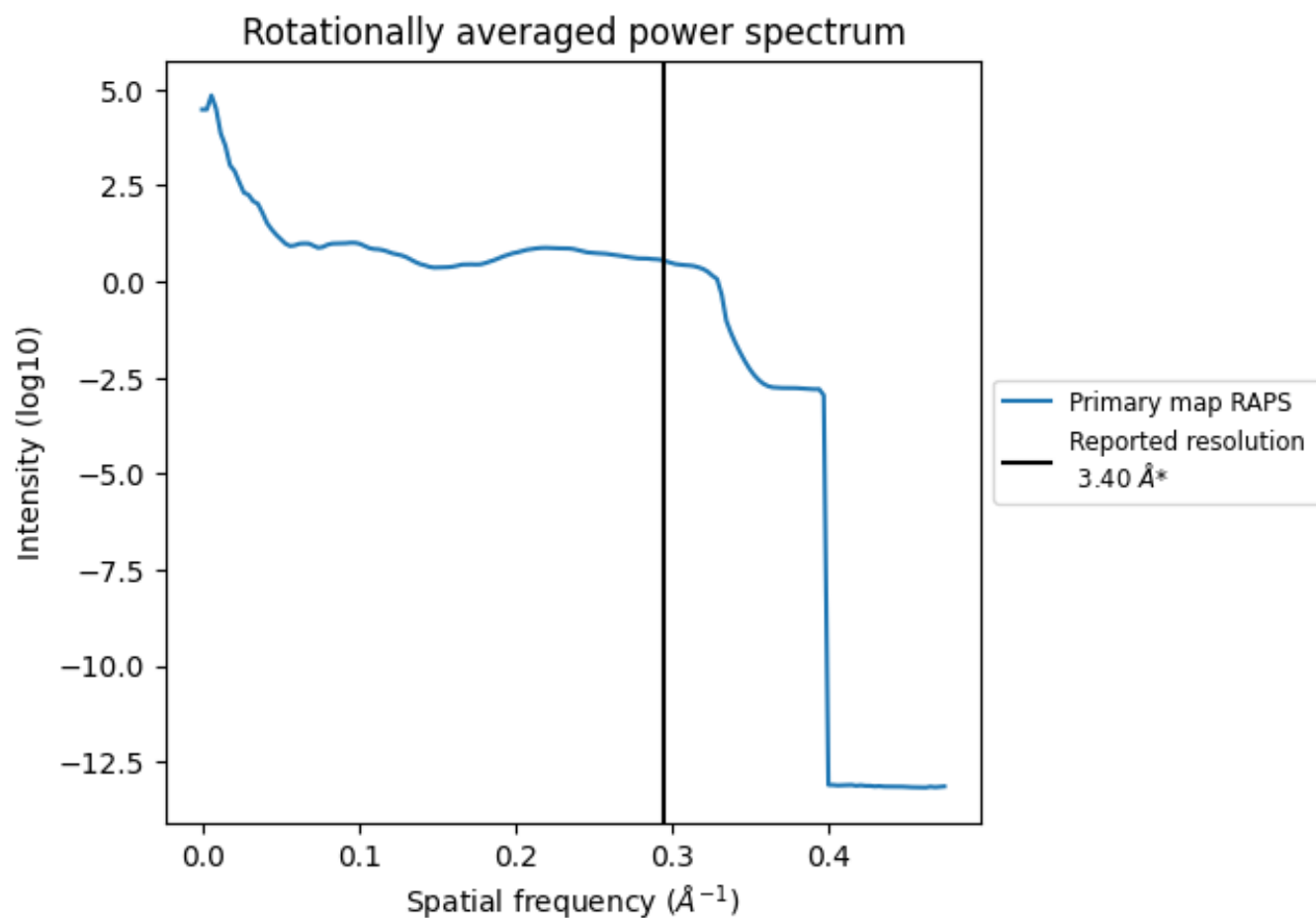
7.2 Volume estimate [i](#)



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 ⓘ

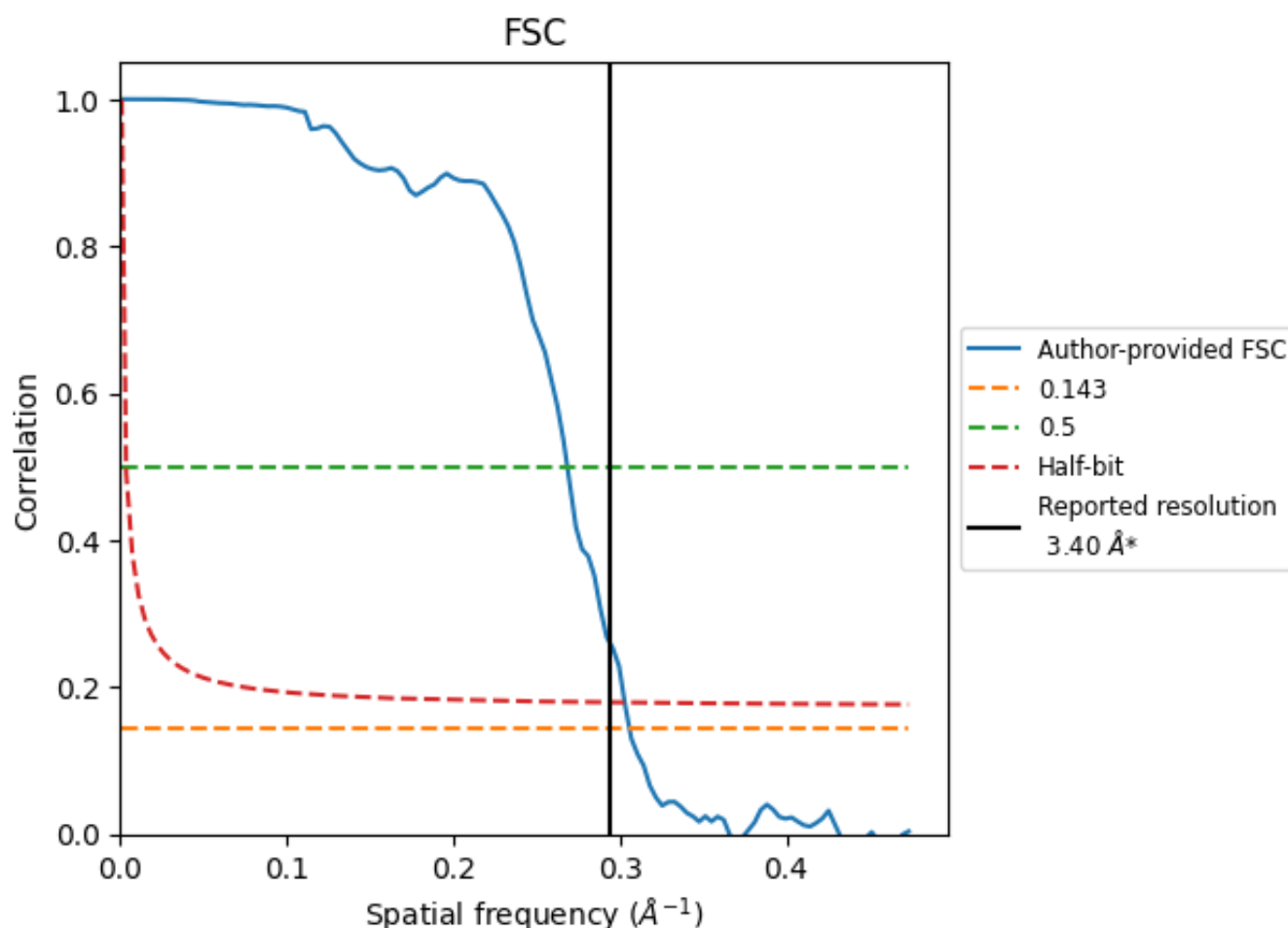


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

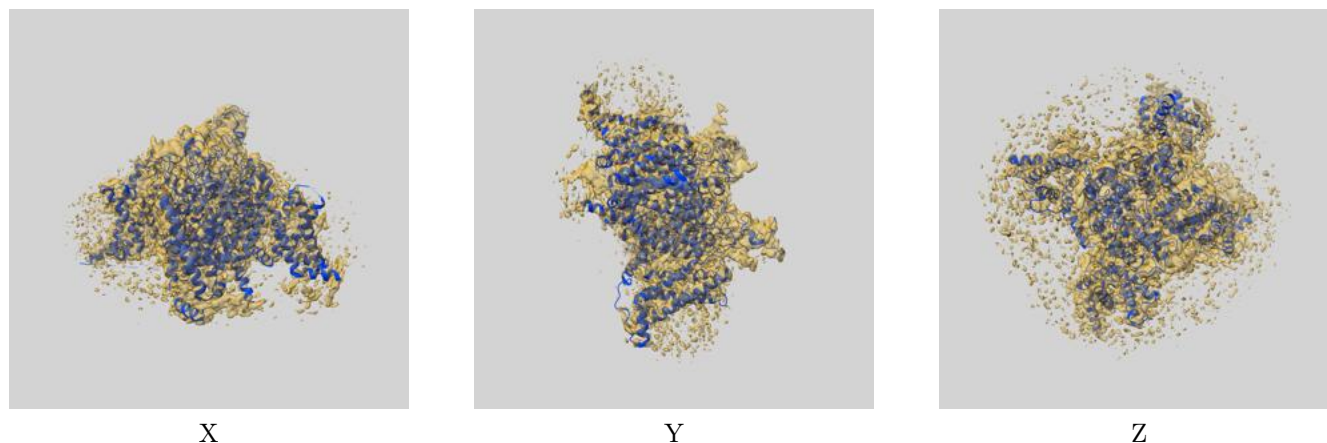
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.27	3.72	3.30
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

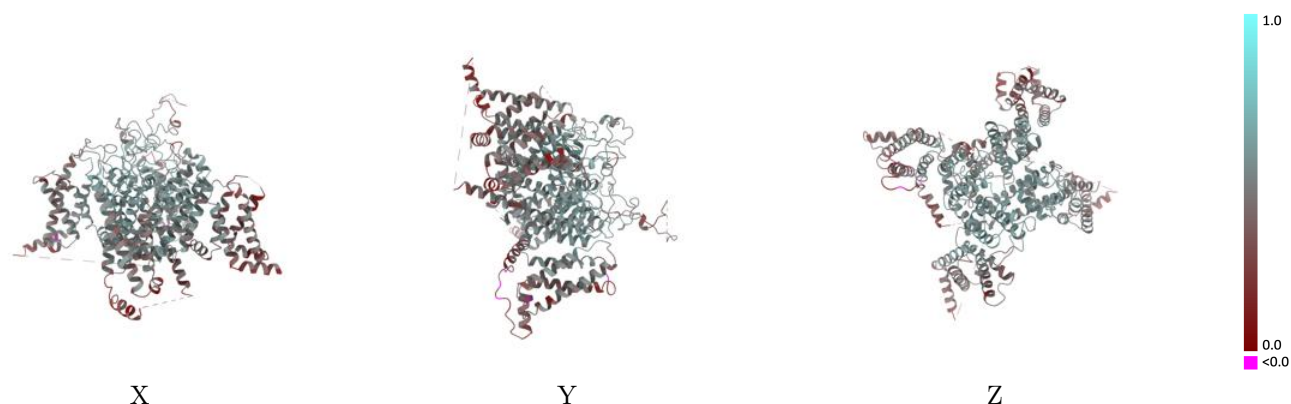
This section contains information regarding the fit between EMDB map EMD-31519 and PDB model 7FBS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



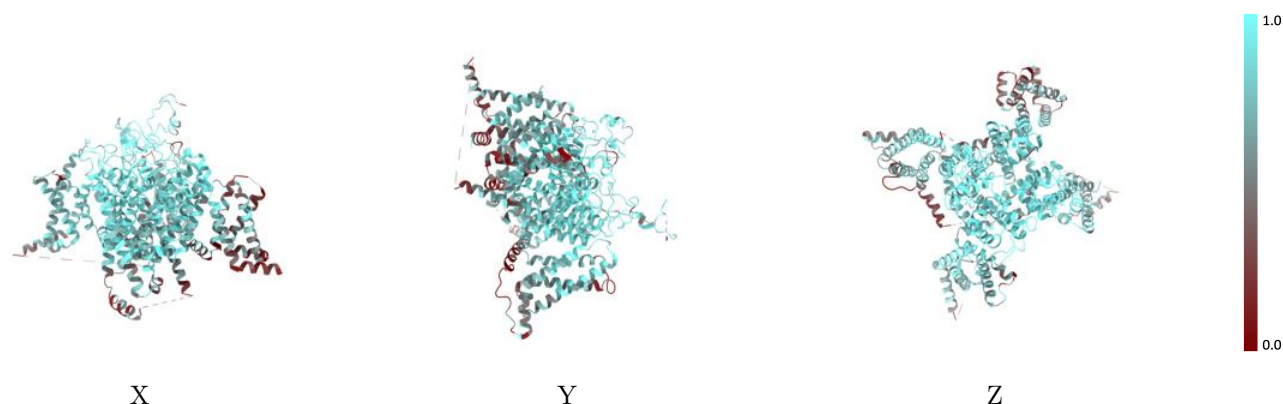
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



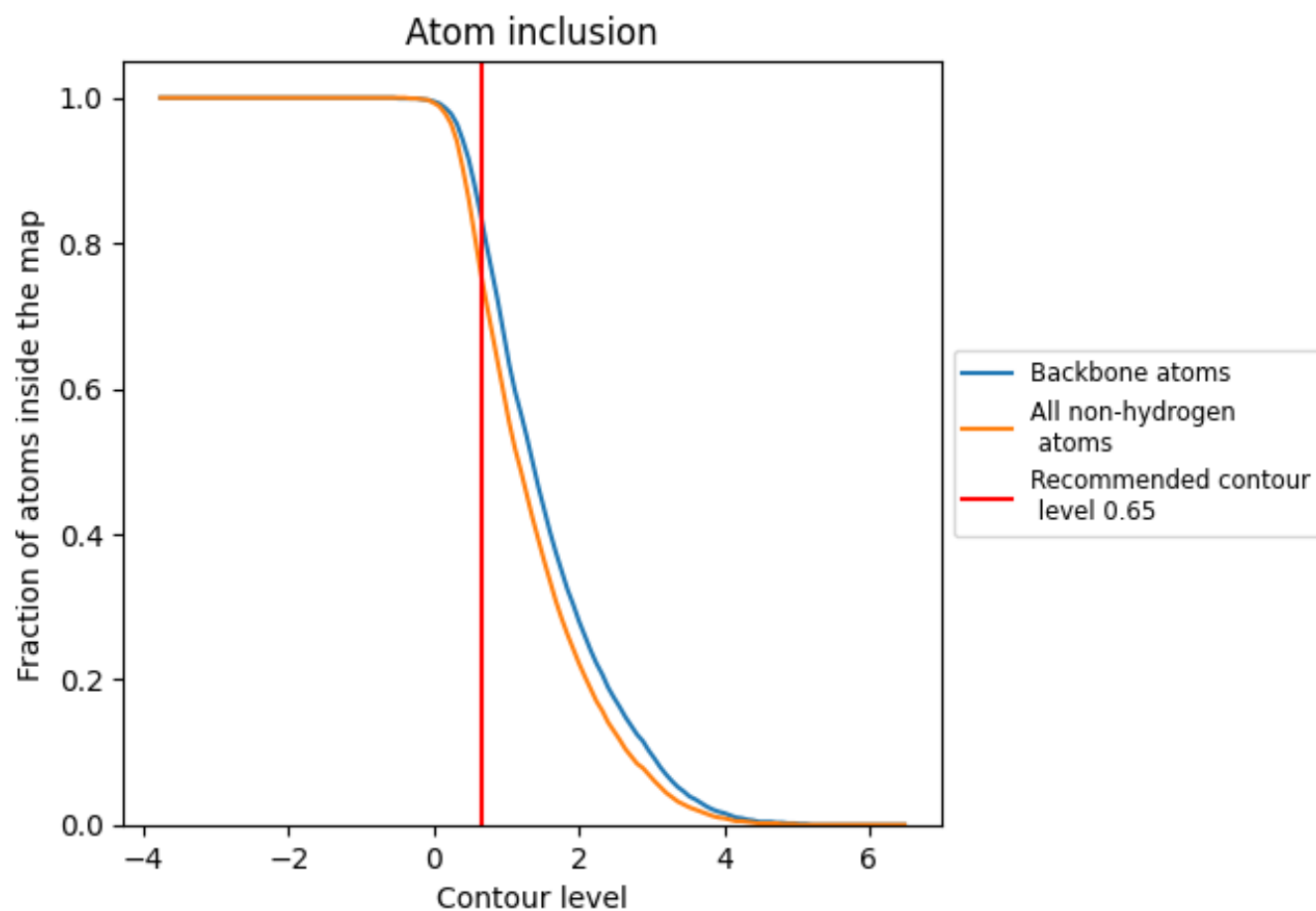
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.7580	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.7580	<div><div></div></div> 0.4770

