Full wwPDB EM Validation Report (i)

Oct 1, 2024 – 02:51 PM JST

PDB ID	:	7XW6
EMDB ID	:	EMD-33492
Title	:	TSHR-Gs-M22 antibody-ML109 complex
Authors	:	Duan, J.; Xu, P.; Luan, X.; Ji, Y.; Yuan, Q.; He, X.; Ye, J.; Cheng, X.; Jiang, H.; Zhang, S.; Jiang, Y.; Xu, H.E.
Deposited on	:	2022-05-26
Resolution	:	2.78 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 (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 (1)) were used in the production of this report:

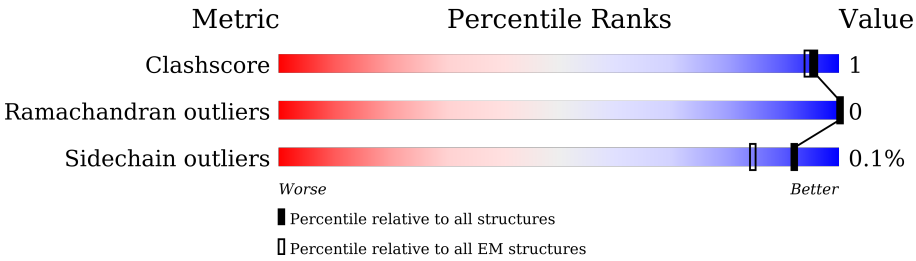
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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 <=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	249	89% 5% 6%
2	B	350	92% 5%
3	G	71	7% 76% 20%
4	L	112	8% 97%
5	N	134	90% 5%
6	R	702	78% 20%
7	Y	120	14% 96%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26020 atoms, of which 13139 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	233	3879	1228	1932	356	356	7	0	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	338	5107	1604	2506	467	509	21	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	G	57	885	273	449	77	83	3	0	0

- Molecule 4 is a protein called M22 antibody light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	L	112	1648	518	807	147	174	2	0	0

- Molecule 5 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	N	128	1911	605	938	170	192	6	0	0

- Molecule 6 is a protein called Thyrotropin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	R	562	9053	2940	4575	715	791	32	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	281	ILE	SER	variant	UNP P16473
R	?	-	ALA	deletion	UNP P16473
R	?	-	LEU	deletion	UNP P16473
R	?	-	ASN	deletion	UNP P16473
R	?	-	SER	deletion	UNP P16473
R	?	-	PRO	deletion	UNP P16473
R	?	-	LEU	deletion	UNP P16473
R	?	-	HIS	deletion	UNP P16473
R	?	-	GLN	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	TYR	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	ASN	deletion	UNP P16473
R	?	-	LEU	deletion	UNP P16473
R	?	-	GLY	deletion	UNP P16473
R	?	-	ASP	deletion	UNP P16473
R	?	-	SER	deletion	UNP P16473
R	?	-	ILE	deletion	UNP P16473
R	?	-	VAL	deletion	UNP P16473
R	?	-	GLY	deletion	UNP P16473
R	?	-	TYR	deletion	UNP P16473
R	?	-	LYS	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	LYS	deletion	UNP P16473

Continued on next page...

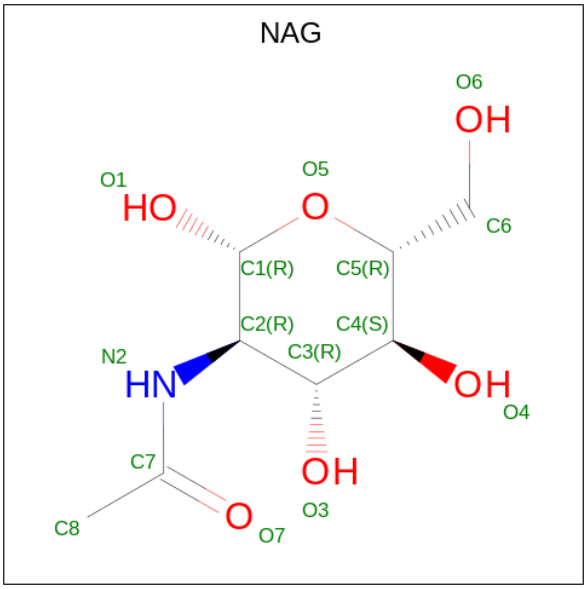
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	SER	deletion	UNP P16473
R	?	-	LYS	deletion	UNP P16473
R	?	-	PHE	deletion	UNP P16473
R	?	-	GLN	deletion	UNP P16473
R	?	-	ASP	deletion	UNP P16473
R	?	-	THR	deletion	UNP P16473
R	?	-	HIS	deletion	UNP P16473
R	?	-	ASN	deletion	UNP P16473
R	?	-	ASN	deletion	UNP P16473
R	?	-	ALA	deletion	UNP P16473
R	?	-	HIS	deletion	UNP P16473
R	?	-	TYR	deletion	UNP P16473
R	?	-	TYR	deletion	UNP P16473
R	?	-	VAL	deletion	UNP P16473
R	?	-	PHE	deletion	UNP P16473
R	?	-	PHE	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	GLN	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	ASP	deletion	UNP P16473
R	?	-	GLU	deletion	UNP P16473
R	?	-	ILE	deletion	UNP P16473
R	?	-	ILE	deletion	UNP P16473
R	?	-	GLY	deletion	UNP P16473
R	?	-	PHE	deletion	UNP P16473
R	367	ASN	GLY	conflict	UNP P16473
R	368	LYS	GLN	conflict	UNP P16473
R	369	THR	GLU	conflict	UNP P16473
R	765	HIS	-	expression tag	UNP P16473
R	766	HIS	-	expression tag	UNP P16473
R	767	HIS	-	expression tag	UNP P16473
R	768	HIS	-	expression tag	UNP P16473
R	769	HIS	-	expression tag	UNP P16473
R	770	HIS	-	expression tag	UNP P16473
R	771	HIS	-	expression tag	UNP P16473
R	772	HIS	-	expression tag	UNP P16473

- Molecule 7 is a protein called M22 antibody heavy chain.

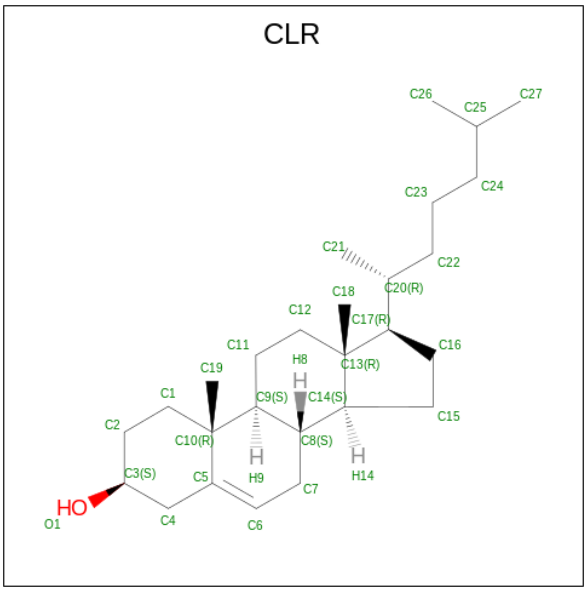
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	Y	120	1854	600	910	160	180	4	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
8	R	1	28	8	14	1	5	0
			Total	C	H	N	O	
8	R	1	28	8	14	1	5	0
			Total	C	H	N	O	
8	R	1	28	8	14	1	5	0
			Total	C	H	N	O	
8	R	1	28	8	14	1	5	0

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



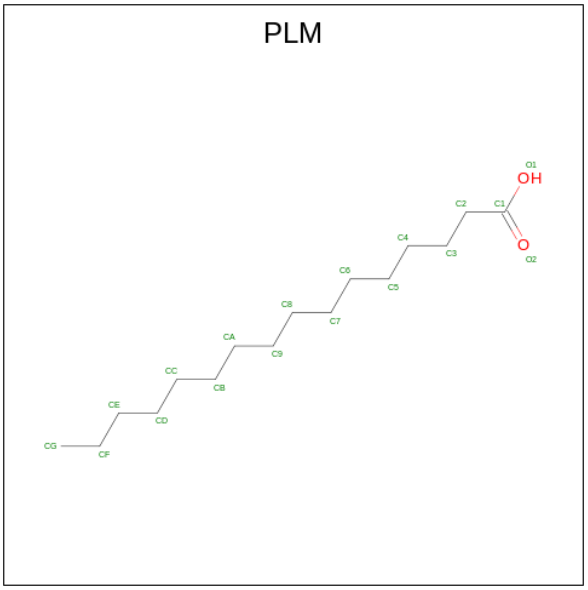
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0
			Total	C	H	O	
9	R	1	74	27	46	1	0

Continued on next page...

Continued from previous page...

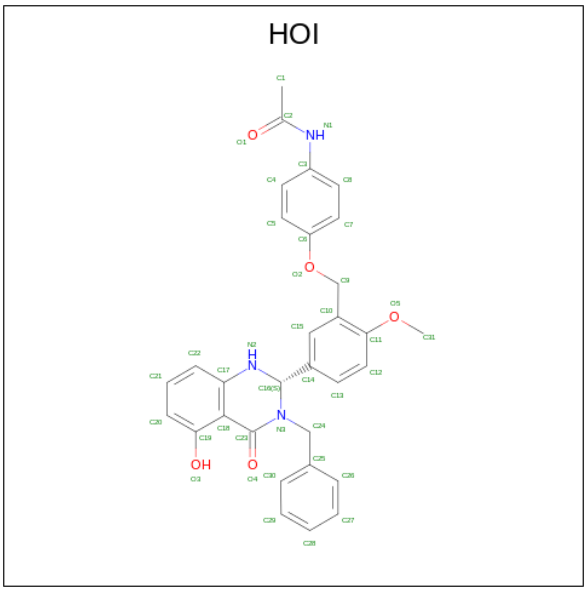
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0

- Molecule 10 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
10	R	1	49	16	31	2	0
10	R	1	49	16	31	2	0
10	R	1	49	16	31	2	0
10	R	1	49	16	31	2	0
10	R	1	49	16	31	2	0

- Molecule 11 is {N}-[4-[[2-methoxy-5-[(2 {S})-5-oxidanyl-4-oxidanylidene-3-(phenylmethyl)-1,2-dihydroquinazolin-2-yl]phenyl]methoxy]phenyl]ethanamide (three-letter code: HOI) (formula: $C_{31}H_{29}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



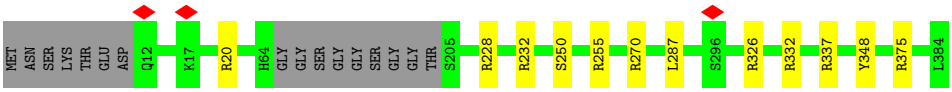
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
11	R	1	68	31	29	3	5	0

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.

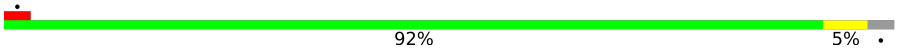
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A:



• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:

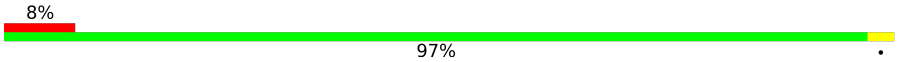


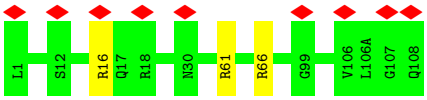
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

• Molecule 4: M22 antibody light chain

Chain L:



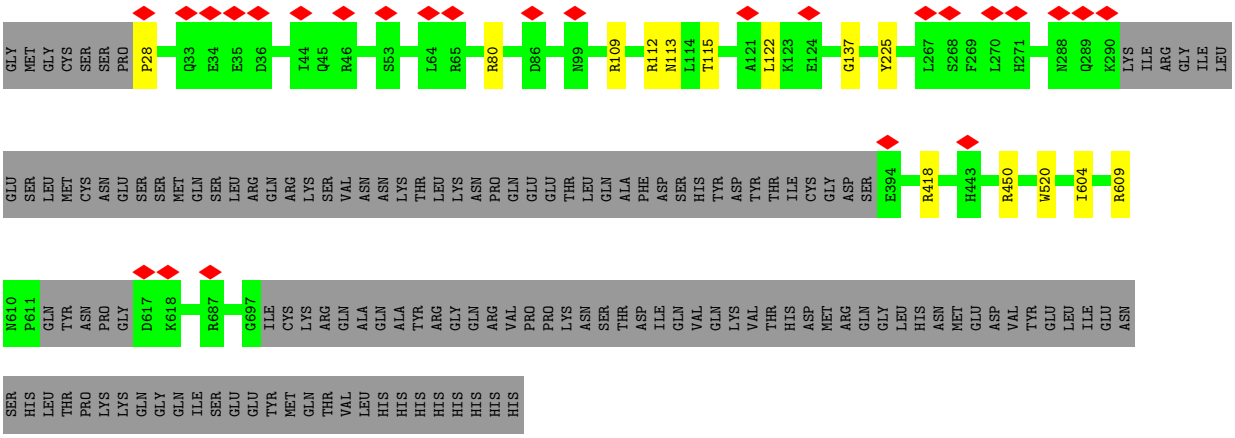


• Molecule 5: Nanobody35

Chain N:

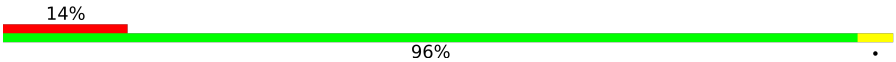
• Molecule 6: Thyrotropin receptor

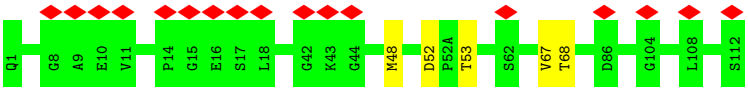
Chain R:



• Molecule 7: M22 antibody heavy chain

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	455661	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.846	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	247.2, 247.2, 247.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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: PLM, NAG, CLR, HOI

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	0.66	0/1985	1.05	9/2668 (0.3%)
2	B	0.60	0/2648	1.04	8/3589 (0.2%)
3	G	0.60	0/442	1.00	3/597 (0.5%)
4	L	0.65	0/857	1.04	4/1166 (0.3%)
5	N	0.67	0/993	1.07	9/1345 (0.7%)
6	R	0.64	0/4587	0.96	8/6241 (0.1%)
7	Y	0.70	0/971	0.99	0/1320
All	All	0.64	0/12483	1.01	41/16926 (0.2%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	80	ARG	NE-CZ-NH2	10.88	125.74	120.30
1	A	228	ARG	NE-CZ-NH2	9.74	125.17	120.30
5	N	98	ARG	NE-CZ-NH2	8.77	124.68	120.30
1	A	255	ARG	NE-CZ-NH2	7.91	124.26	120.30
6	R	450	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	B	96	ARG	NE-CZ-NH2	7.46	124.03	120.30
6	R	418	ARG	NE-CZ-NH2	6.74	123.67	120.30
2	B	219	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	326	ARG	NE-CZ-NH2	6.47	123.53	120.30
4	L	66	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	B	304	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	B	85	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	20	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	G	62	ARG	NE-CZ-NH2	6.09	123.35	120.30
3	G	27	ARG	NE-CZ-NH2	6.06	123.33	120.30
5	N	67	ARG	NE-CZ-NH2	6.02	123.31	120.30
5	N	38	ARG	NE-CZ-NH2	5.96	123.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ARG	NE-CZ-NH2	5.91	123.25	120.30
5	N	72	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	337	ARG	NE-CZ-NH2	5.83	123.21	120.30
6	R	28	PRO	CA-N-CD	-5.82	103.35	111.50
1	A	332	ARG	NE-CZ-NH2	5.75	123.18	120.30
6	R	225	TYR	CB-CG-CD2	-5.65	117.61	121.00
6	R	609	ARG	NE-CZ-NH2	5.44	123.02	120.30
5	N	98	ARG	NE-CZ-NH1	-5.43	117.58	120.30
2	B	68	ARG	NE-CZ-NH2	5.41	123.01	120.30
5	N	118	ARG	NE-CZ-NH2	5.41	123.00	120.30
2	B	283	ARG	NE-CZ-NH2	5.39	123.00	120.30
4	L	61	ARG	NE-CZ-NH2	5.36	122.98	120.30
5	N	38	ARG	NE-CZ-NH1	-5.31	117.64	120.30
2	B	256	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	332	ARG	NE-CZ-NH1	-5.26	117.67	120.30
3	G	13	ARG	NE-CZ-NH2	5.24	122.92	120.30
4	L	16	ARG	NE-CZ-NH2	5.12	122.86	120.30
5	N	68	PHE	CB-CG-CD2	-5.12	117.22	120.80
4	L	66	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	232	ARG	NE-CZ-NH2	5.09	122.84	120.30
6	R	109	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	B	49	ARG	NE-CZ-NH2	5.03	122.81	120.30
5	N	19	ARG	NE-CZ-NH2	5.01	122.80	120.30
6	R	112	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	1947	1932	1930	3	0
2	B	2601	2506	2505	5	0
3	G	436	449	448	0	0
4	L	841	807	807	0	0
5	N	973	938	938	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	4478	4575	4573	4	0
7	Y	944	910	910	4	0
8	R	56	56	52	0	0
9	R	476	782	782	7	0
10	R	90	155	155	0	0
11	R	39	29	0	0	0
All	All	12881	13139	13100	23	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 1.

All (23) 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)
9:R:812:CLR:H213	9:R:812:CLR:H183	1.59	0.82
9:R:812:CLR:H213	9:R:812:CLR:C18	2.20	0.71
2:B:315:VAL:HG13	2:B:329:THR:HG23	1.74	0.69
9:R:812:CLR:H222	9:R:812:CLR:H121	1.76	0.67
2:B:315:VAL:HG13	2:B:329:THR:CG2	2.25	0.67
1:A:348:TYR:CZ	1:A:375:ARG:NH1	2.70	0.60
1:A:250:SER:OG	1:A:287:LEU:HD22	2.04	0.58
6:R:113:ASN:O	6:R:115:THR:HG23	2.06	0.55
9:R:812:CLR:C18	9:R:812:CLR:C21	2.85	0.55
6:R:115:THR:HG22	6:R:137:GLY:O	2.07	0.54
7:Y:48:MET:HE2	7:Y:67:VAL:HG21	1.90	0.52
7:Y:67:VAL:HG12	7:Y:68:THR:N	2.27	0.49
7:Y:52:ASP:OD1	7:Y:53:THR:HG22	2.14	0.47
6:R:122:LEU:HD12	6:R:122:LEU:O	2.16	0.46
2:B:315:VAL:CG1	2:B:329:THR:HG23	2.45	0.45
9:R:817:CLR:H212	9:R:817:CLR:H121	1.99	0.44
1:A:375:ARG:HD2	1:A:375:ARG:HA	1.80	0.44
2:B:79:LEU:HG	2:B:95:LEU:HD11	2.00	0.43
9:R:812:CLR:H232	9:R:812:CLR:H17	1.85	0.43
6:R:520:TRP:HA	6:R:604:ILE:HD11	2.00	0.43
2:B:128:THR:HG21	2:B:132:ASN:O	2.20	0.41
7:Y:67:VAL:CG1	7:Y:68:THR:N	2.83	0.41
9:R:808:CLR:H121	9:R:808:CLR:H212	2.02	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	229/249 (92%)	220 (96%)	9 (4%)	0	100	100
2	B	336/350 (96%)	319 (95%)	17 (5%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	L	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
5	N	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
6	R	556/702 (79%)	526 (95%)	30 (5%)	0	100	100
7	Y	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
All	All	1530/1738 (88%)	1461 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/221 (96%)	211 (100%)	0	100	100
2	B	281/292 (96%)	279 (99%)	2 (1%)	81	93
3	G	46/58 (79%)	46 (100%)	0	100	100
4	L	94/94 (100%)	94 (100%)	0	100	100
5	N	106/112 (95%)	106 (100%)	0	100	100
6	R	508/637 (80%)	508 (100%)	0	100	100
7	Y	103/103 (100%)	103 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1349/1517 (89%)	1347 (100%)	2 (0%)	92 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	105	TYR
2	B	340	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
8	NAG	R	803	6	14,14,15	1.37	2 (14%)	17,19,21	0.79	0
9	CLR	R	809	-	31,31,31	1.19	2 (6%)	48,48,48	0.62	0
9	CLR	R	821	-	31,31,31	1.22	2 (6%)	48,48,48	0.48	0
9	CLR	R	808	-	31,31,31	1.22	2 (6%)	48,48,48	0.54	0
10	PLM	R	823	-	17,17,17	0.97	1 (5%)	17,17,17	0.57	0
9	CLR	R	819	-	31,31,31	1.17	1 (3%)	48,48,48	0.50	0
10	PLM	R	824	-	17,17,17	0.93	1 (5%)	17,17,17	0.58	0
9	CLR	R	818	-	31,31,31	1.22	2 (6%)	48,48,48	0.56	0
8	NAG	R	804	6	14,14,15	1.29	2 (14%)	17,19,21	0.99	0
9	CLR	R	814	-	31,31,31	1.21	2 (6%)	48,48,48	0.50	0
10	PLM	R	825	-	17,17,17	0.96	1 (5%)	17,17,17	0.51	0
9	CLR	R	806	-	31,31,31	1.27	2 (6%)	48,48,48	0.62	1 (2%)
9	CLR	R	815	-	31,31,31	1.22	2 (6%)	48,48,48	0.80	1 (2%)
9	CLR	R	817	-	31,31,31	1.19	1 (3%)	48,48,48	0.56	0
8	NAG	R	801	6	14,14,15	1.26	1 (7%)	17,19,21	0.88	1 (5%)
10	PLM	R	826	-	17,17,17	0.94	1 (5%)	17,17,17	0.59	0
8	NAG	R	802	6	14,14,15	1.34	3 (21%)	17,19,21	0.84	1 (5%)
9	CLR	R	820	-	31,31,31	1.22	2 (6%)	48,48,48	0.50	0
9	CLR	R	807	-	31,31,31	1.13	2 (6%)	48,48,48	0.62	0
9	CLR	R	811	-	31,31,31	1.20	3 (9%)	48,48,48	0.68	2 (4%)
10	PLM	R	822	-	17,17,17	0.90	1 (5%)	17,17,17	0.63	0
9	CLR	R	810	-	31,31,31	1.23	2 (6%)	48,48,48	0.75	1 (2%)
9	CLR	R	805	-	31,31,31	1.22	2 (6%)	48,48,48	0.56	0
9	CLR	R	813	-	31,31,31	1.19	2 (6%)	48,48,48	0.67	0
11	HOI	R	827	-	42,43,43	0.96	0	53,60,60	1.14	7 (13%)
9	CLR	R	812	-	31,31,31	0.90	2 (6%)	48,48,48	1.47	9 (18%)
9	CLR	R	816	-	31,31,31	1.37	7 (22%)	48,48,48	0.87	1 (2%)

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
8	NAG	R	803	6	-	0/6/23/26	0/1/1/1
9	CLR	R	809	-	-	3/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLR	R	821	-	-	0/10/68/68	0/4/4/4
9	CLR	R	808	-	-	0/10/68/68	0/4/4/4
10	PLM	R	823	-	-	3/15/15/15	-
9	CLR	R	819	-	-	3/10/68/68	0/4/4/4
10	PLM	R	824	-	-	3/15/15/15	-
9	CLR	R	818	-	-	0/10/68/68	0/4/4/4
8	NAG	R	804	6	-	0/6/23/26	0/1/1/1
9	CLR	R	814	-	-	0/10/68/68	0/4/4/4
10	PLM	R	825	-	-	4/15/15/15	-
9	CLR	R	806	-	-	3/10/68/68	0/4/4/4
9	CLR	R	815	-	-	2/10/68/68	0/4/4/4
9	CLR	R	817	-	-	2/10/68/68	0/4/4/4
8	NAG	R	801	6	-	0/6/23/26	0/1/1/1
10	PLM	R	826	-	-	3/15/15/15	-
8	NAG	R	802	6	-	0/6/23/26	0/1/1/1
9	CLR	R	820	-	-	1/10/68/68	0/4/4/4
9	CLR	R	807	-	-	2/10/68/68	0/4/4/4
9	CLR	R	811	-	-	4/10/68/68	0/4/4/4
10	PLM	R	822	-	-	4/15/15/15	-
9	CLR	R	810	-	-	0/10/68/68	0/4/4/4
9	CLR	R	805	-	-	0/10/68/68	0/4/4/4
9	CLR	R	813	-	-	0/10/68/68	0/4/4/4
11	HOI	R	827	-	-	6/19/35/35	0/5/5/5
9	CLR	R	812	-	-	7/10/68/68	0/4/4/4
9	CLR	R	816	-	-	2/10/68/68	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	803	NAG	O5-C1	3.05	1.48	1.43
8	R	804	NAG	O5-C5	2.81	1.49	1.43
9	R	818	CLR	C11-C9	2.81	1.58	1.53
9	R	816	CLR	C11-C9	2.79	1.58	1.53
8	R	802	NAG	O5-C5	2.72	1.49	1.43
9	R	806	CLR	C20-C17	2.68	1.59	1.54
8	R	801	NAG	O5-C5	2.62	1.48	1.43
9	R	805	CLR	C11-C9	2.60	1.58	1.53
9	R	809	CLR	C20-C17	2.58	1.58	1.54
10	R	823	PLM	O1-C1	-2.55	1.22	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	803	NAG	O5-C5	2.54	1.48	1.43
9	R	819	CLR	C11-C9	2.54	1.58	1.53
10	R	826	PLM	O1-C1	-2.54	1.22	1.30
10	R	822	PLM	O1-C1	-2.52	1.22	1.30
10	R	825	PLM	O1-C1	-2.49	1.22	1.30
9	R	806	CLR	C11-C9	2.49	1.57	1.53
9	R	813	CLR	C20-C17	2.48	1.58	1.54
9	R	815	CLR	C11-C9	2.48	1.57	1.53
10	R	824	PLM	O1-C1	-2.47	1.22	1.30
9	R	821	CLR	C11-C9	2.45	1.57	1.53
9	R	810	CLR	C11-C9	2.43	1.57	1.53
9	R	808	CLR	C11-C9	2.42	1.57	1.53
9	R	813	CLR	C11-C9	2.42	1.57	1.53
9	R	810	CLR	C20-C17	2.42	1.58	1.54
9	R	820	CLR	C11-C9	2.39	1.57	1.53
9	R	807	CLR	C11-C9	2.39	1.57	1.53
9	R	816	CLR	C20-C17	2.39	1.58	1.54
9	R	814	CLR	C20-C17	2.32	1.58	1.54
8	R	802	NAG	C1-C2	2.30	1.55	1.52
9	R	814	CLR	C11-C9	2.28	1.57	1.53
9	R	808	CLR	C20-C17	2.23	1.58	1.54
9	R	809	CLR	C11-C9	2.23	1.57	1.53
9	R	811	CLR	C11-C9	2.23	1.57	1.53
9	R	817	CLR	C11-C9	2.21	1.57	1.53
9	R	807	CLR	C20-C17	2.19	1.58	1.54
9	R	816	CLR	C8-C9	2.18	1.57	1.53
9	R	820	CLR	C20-C17	2.16	1.58	1.54
9	R	805	CLR	C20-C17	2.15	1.58	1.54
8	R	802	NAG	O5-C1	2.15	1.47	1.43
9	R	812	CLR	C12-C13	-2.14	1.50	1.54
9	R	812	CLR	C13-C14	-2.12	1.51	1.55
9	R	816	CLR	C1-C10	2.11	1.58	1.54
9	R	818	CLR	C20-C17	2.10	1.58	1.54
9	R	811	CLR	C20-C17	2.08	1.58	1.54
9	R	816	CLR	C4-C3	2.08	1.55	1.52
8	R	804	NAG	C1-C2	2.06	1.55	1.52
9	R	811	CLR	C18-C13	2.06	1.57	1.54
9	R	816	CLR	C18-C13	2.06	1.57	1.54
9	R	821	CLR	C20-C17	2.05	1.58	1.54
9	R	816	CLR	C10-C9	2.02	1.59	1.56
9	R	815	CLR	C20-C17	2.01	1.57	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	812	CLR	C4-C5-C10	3.91	121.61	116.42
9	R	812	CLR	C10-C9-C8	-3.30	107.78	112.73
9	R	812	CLR	C11-C12-C13	-3.25	107.20	112.78
11	R	827	HOI	C14-C16-N3	2.97	116.20	112.92
9	R	811	CLR	C16-C17-C20	2.86	116.57	112.15
9	R	812	CLR	C4-C5-C6	-2.82	116.55	120.61
11	R	827	HOI	O5-C11-C12	-2.80	119.56	124.37
11	R	827	HOI	O5-C11-C10	2.76	119.82	115.97
9	R	812	CLR	C7-C8-C9	-2.70	106.44	109.71
9	R	812	CLR	C14-C8-C9	2.60	112.57	109.09
11	R	827	HOI	C25-C24-N3	2.58	118.27	113.54
11	R	827	HOI	C14-C16-N2	-2.57	107.76	112.59
9	R	812	CLR	C23-C22-C20	-2.57	107.66	115.03
11	R	827	HOI	O4-C23-C18	-2.57	119.46	124.25
8	R	802	NAG	C1-O5-C5	2.56	115.66	112.19
9	R	806	CLR	C21-C20-C22	-2.35	106.68	110.36
9	R	812	CLR	C1-C10-C9	2.35	112.01	108.73
9	R	812	CLR	C13-C14-C8	-2.34	110.92	114.38
8	R	801	NAG	C1-O5-C5	2.27	115.27	112.19
9	R	816	CLR	C1-C10-C9	2.21	111.81	108.73
9	R	815	CLR	C7-C8-C9	2.18	112.35	109.71
9	R	811	CLR	C21-C20-C17	-2.04	109.79	112.92
9	R	810	CLR	C11-C9-C8	2.03	114.68	111.75
11	R	827	HOI	C3-N1-C2	2.02	131.66	127.99

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	827	HOI	C12-C11-O5-C31
9	R	807	CLR	C17-C20-C22-C23
9	R	820	CLR	C22-C23-C24-C25
9	R	812	CLR	C13-C17-C20-C22
9	R	806	CLR	C20-C22-C23-C24
9	R	807	CLR	C21-C20-C22-C23
11	R	827	HOI	C10-C11-O5-C31
9	R	812	CLR	C22-C23-C24-C25
9	R	812	CLR	C16-C17-C20-C22
9	R	809	CLR	C20-C22-C23-C24
9	R	812	CLR	C16-C17-C20-C21
9	R	809	CLR	C21-C20-C22-C23
9	R	809	CLR	C17-C20-C22-C23
9	R	812	CLR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	R	816	CLR	C20-C22-C23-C24
11	R	827	HOI	C7-C6-O2-C9
9	R	819	CLR	C17-C20-C22-C23
9	R	812	CLR	C21-C20-C22-C23
9	R	806	CLR	C21-C20-C22-C23
10	R	823	PLM	C8-C9-CA-CB
11	R	827	HOI	C5-C6-O2-C9
9	R	806	CLR	C17-C20-C22-C23
9	R	812	CLR	C23-C24-C25-C27
9	R	811	CLR	C16-C17-C20-C21
9	R	811	CLR	C16-C17-C20-C22
9	R	811	CLR	C13-C17-C20-C22
9	R	819	CLR	C21-C20-C22-C23
9	R	811	CLR	C13-C17-C20-C21
9	R	817	CLR	C23-C24-C25-C27
11	R	827	HOI	C10-C9-O2-C6
9	R	816	CLR	C22-C23-C24-C25
9	R	817	CLR	C23-C24-C25-C26
10	R	824	PLM	C8-C9-CA-CB
10	R	822	PLM	CA-CB-CC-CD
10	R	822	PLM	C4-C5-C6-C7
9	R	819	CLR	C20-C22-C23-C24
10	R	823	PLM	O2-C1-C2-C3
10	R	825	PLM	O2-C1-C2-C3
10	R	825	PLM	O1-C1-C2-C3
10	R	826	PLM	C4-C5-C6-C7
10	R	823	PLM	O1-C1-C2-C3
9	R	815	CLR	C13-C17-C20-C21
10	R	826	PLM	O2-C1-C2-C3
10	R	824	PLM	O2-C1-C2-C3
10	R	824	PLM	O1-C1-C2-C3
9	R	815	CLR	C16-C17-C20-C22
10	R	825	PLM	CC-CD-CE-CF
10	R	822	PLM	O1-C1-C2-C3
10	R	826	PLM	O1-C1-C2-C3
10	R	822	PLM	O2-C1-C2-C3
11	R	827	HOI	C13-C14-C16-N2
10	R	825	PLM	C3-C4-C5-C6

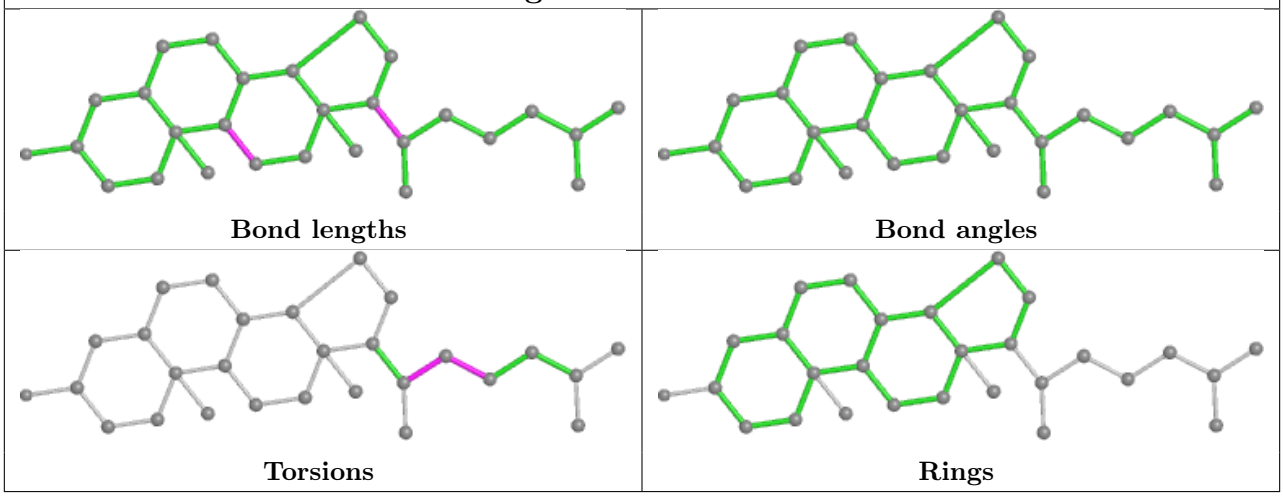
There are no ring outliers.

3 monomers are involved in 7 short contacts:

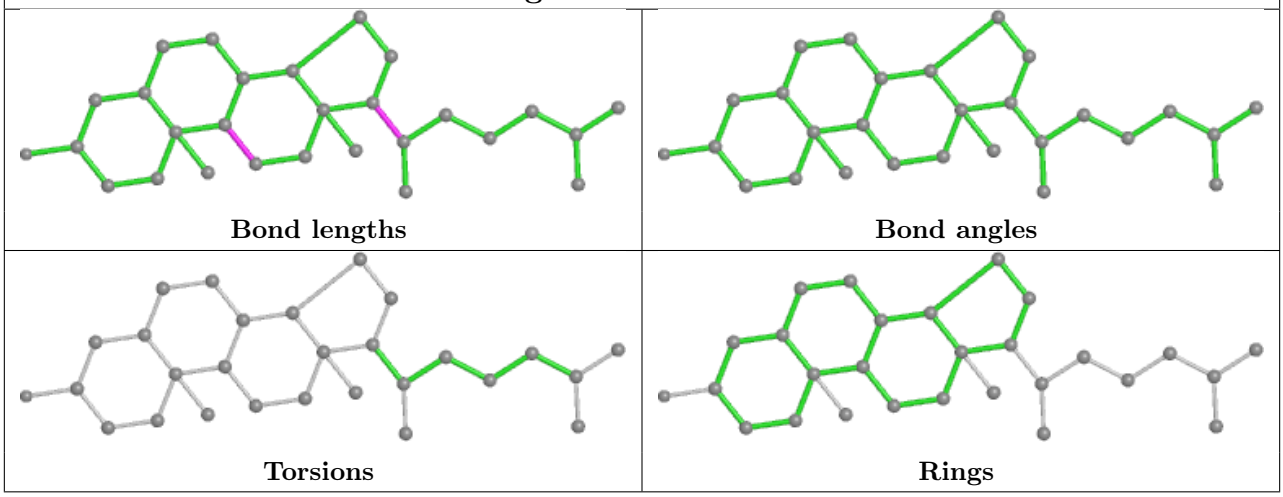
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	808	CLR	1	0
9	R	817	CLR	1	0
9	R	812	CLR	5	0

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

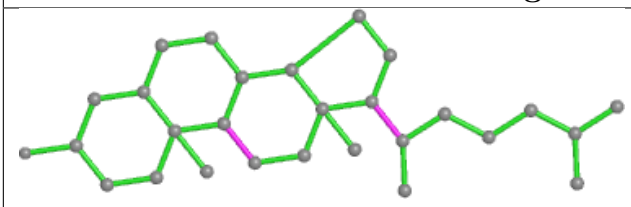
Ligand CLR R 809



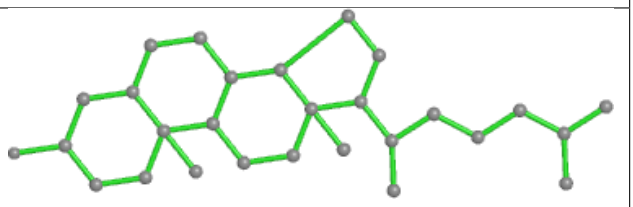
Ligand CLR R 821



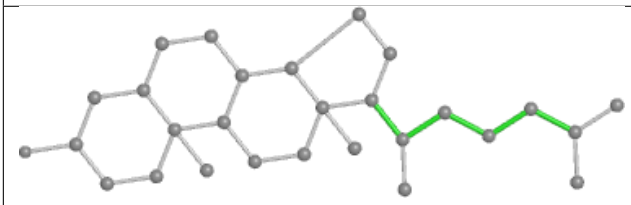
Ligand CLR R 808



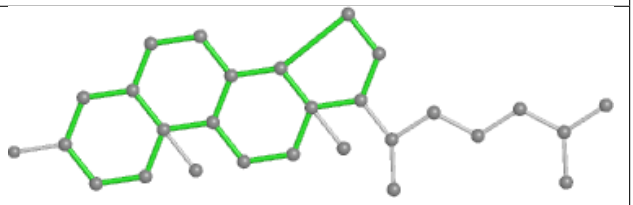
Bond lengths



Bond angles

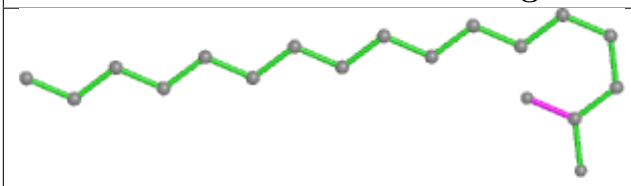


Torsions

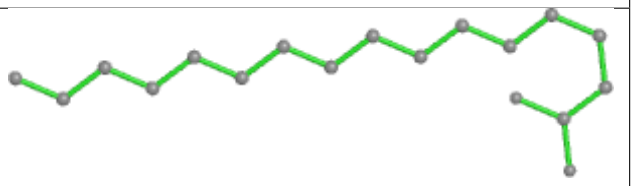


Rings

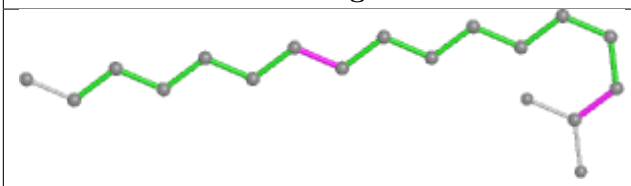
Ligand PLM R 823



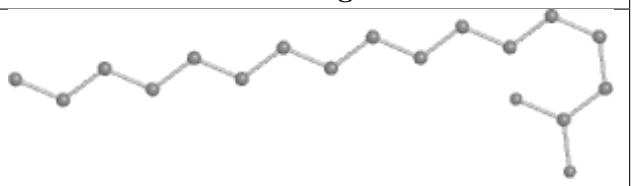
Bond lengths



Bond angles

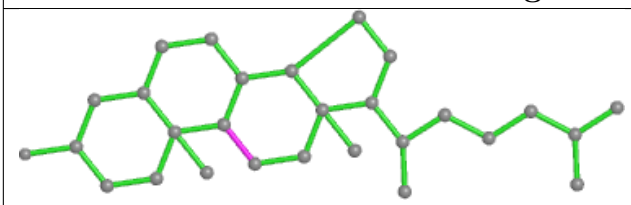


Torsions

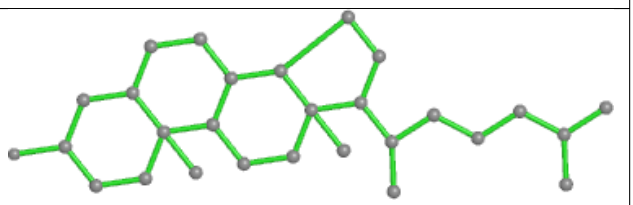


Rings

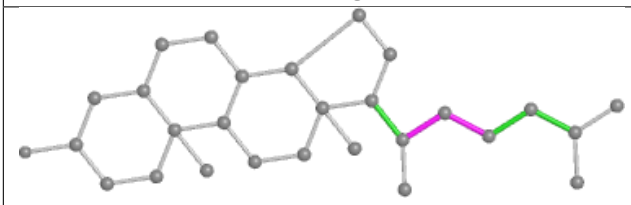
Ligand CLR R 819



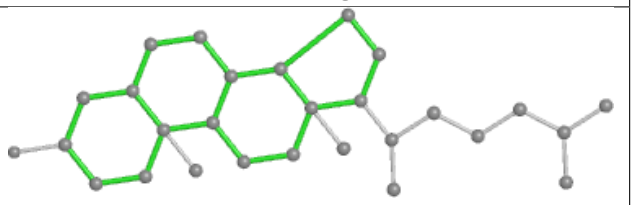
Bond lengths



Bond angles

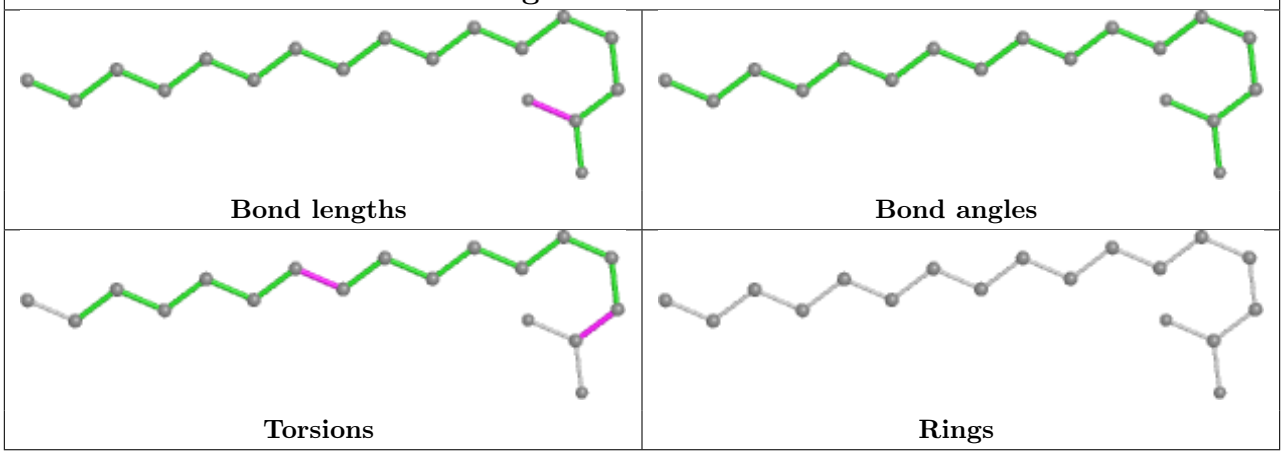


Torsions

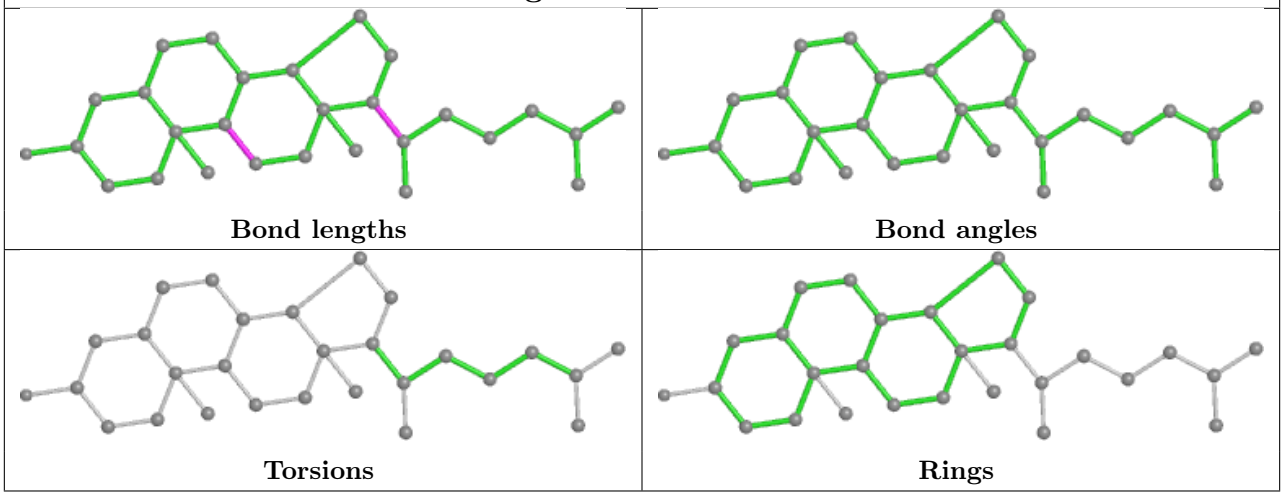


Rings

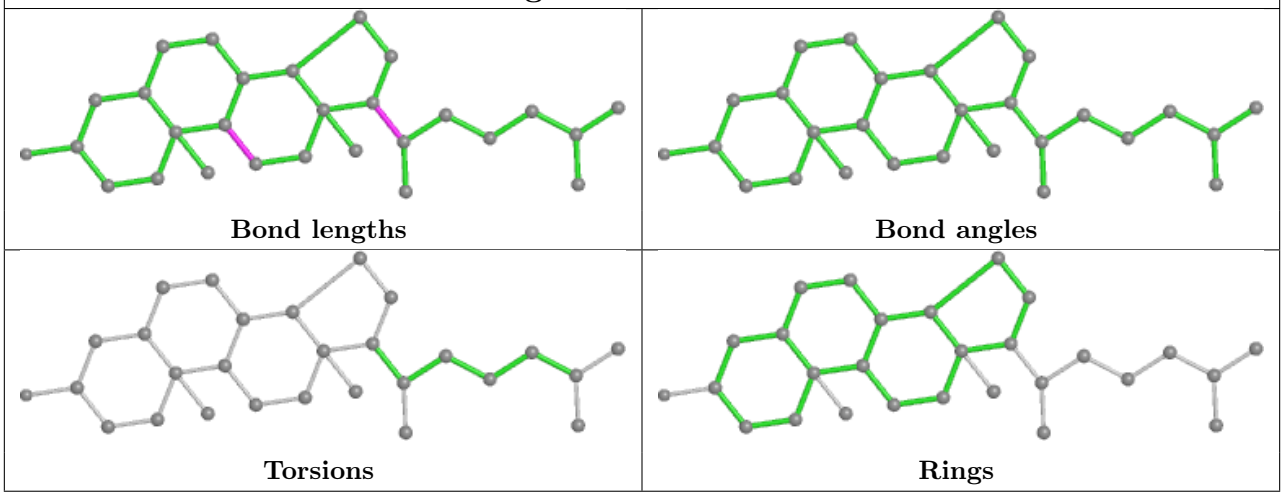
Ligand PLM R 824



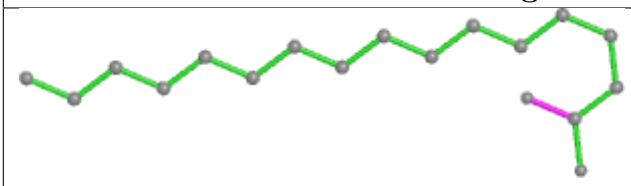
Ligand CLR R 818



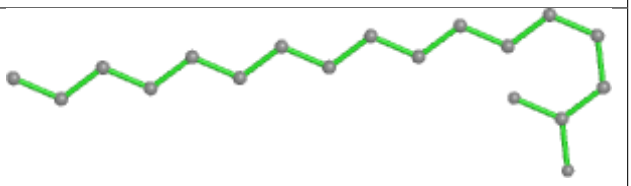
Ligand CLR R 814



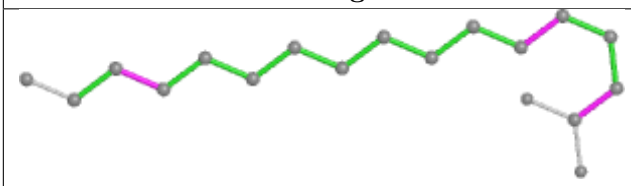
Ligand PLM R 825



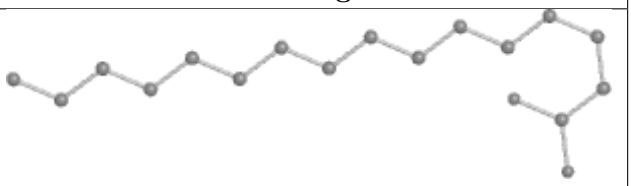
Bond lengths



Bond angles

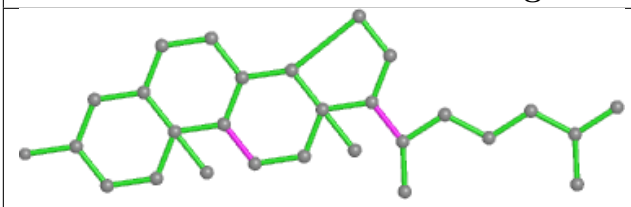


Torsions

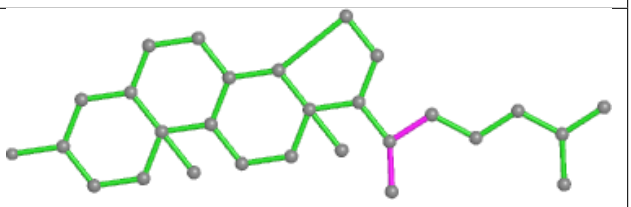


Rings

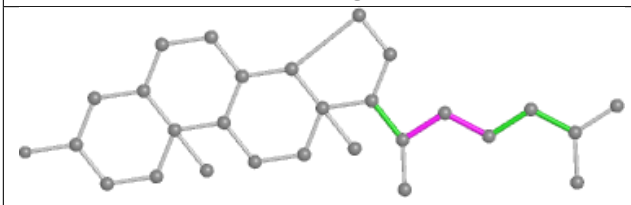
Ligand CLR R 806



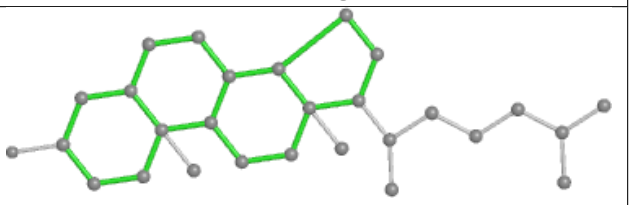
Bond lengths



Bond angles

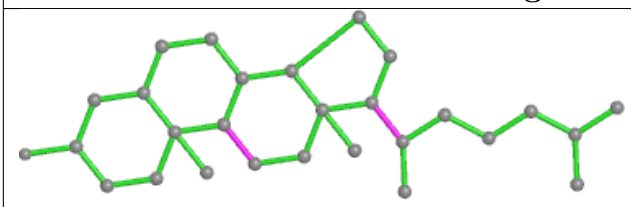


Torsions

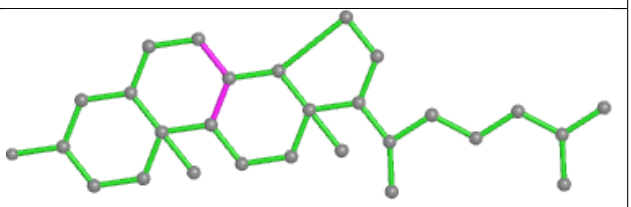


Rings

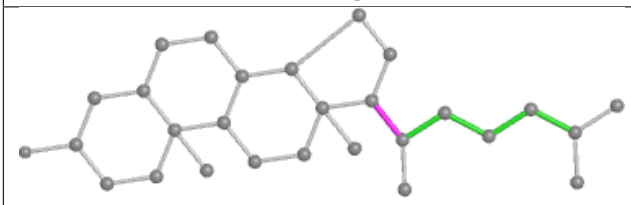
Ligand CLR R 815



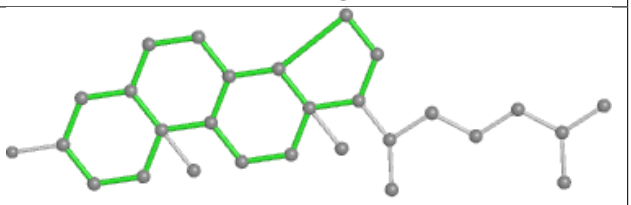
Bond lengths



Bond angles

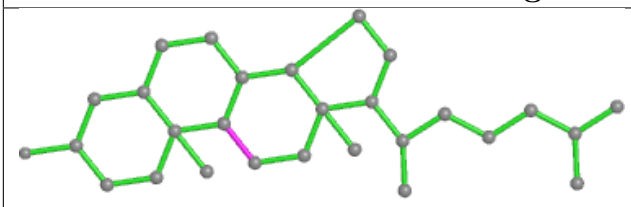


Torsions

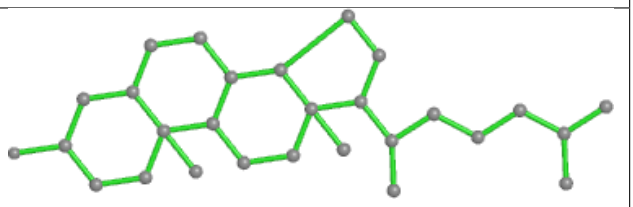


Rings

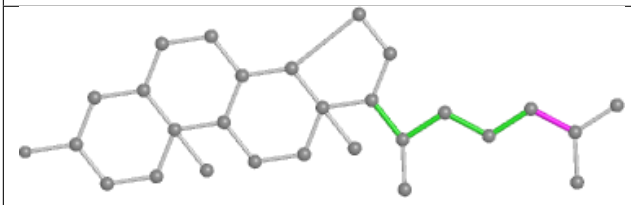
Ligand CLR R 817



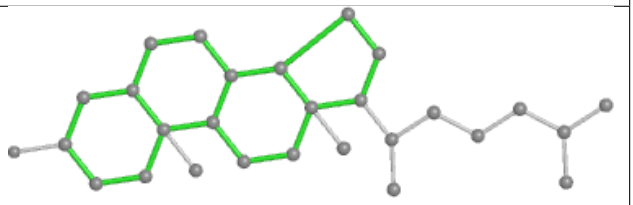
Bond lengths



Bond angles

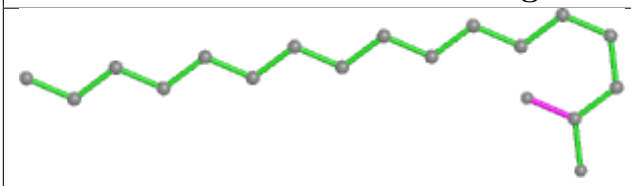


Torsions

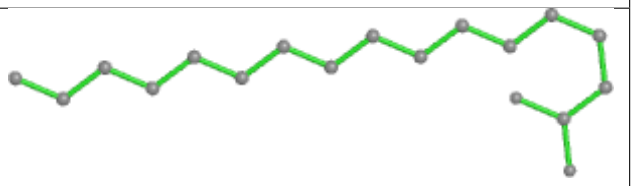


Rings

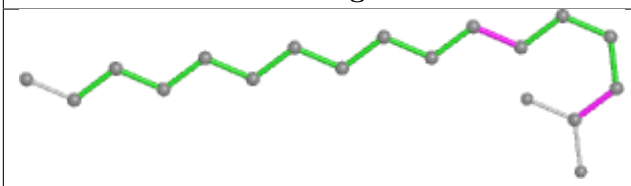
Ligand PLM R 826



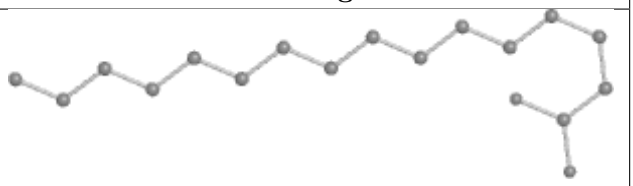
Bond lengths



Bond angles

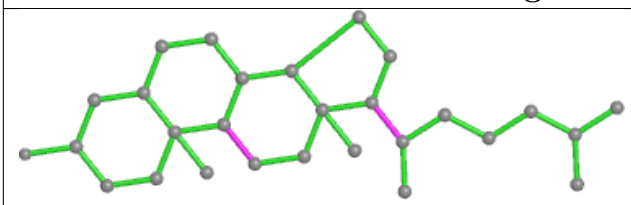


Torsions

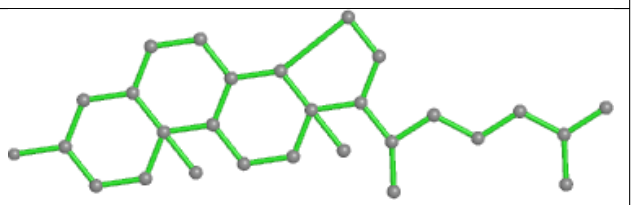


Rings

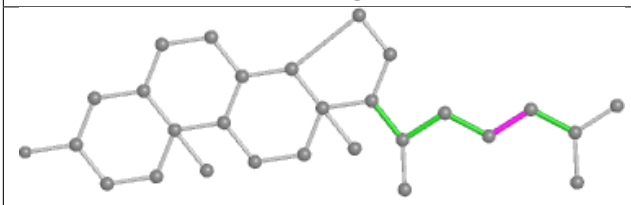
Ligand CLR R 820



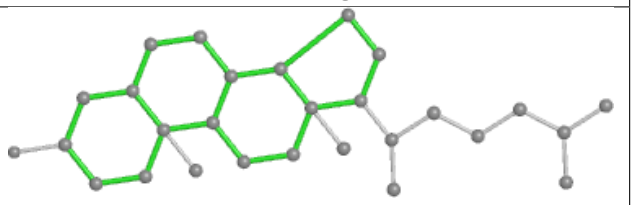
Bond lengths



Bond angles

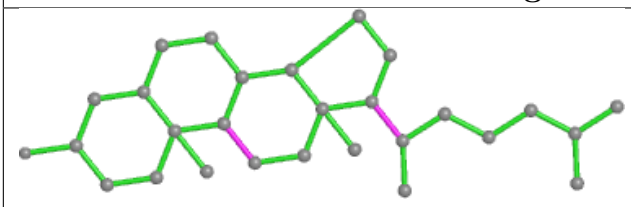


Torsions

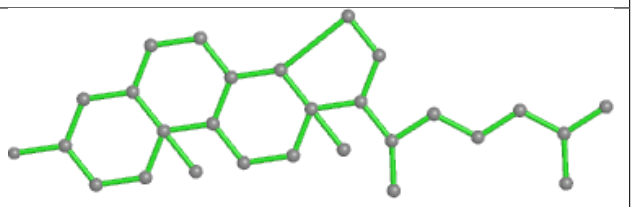


Rings

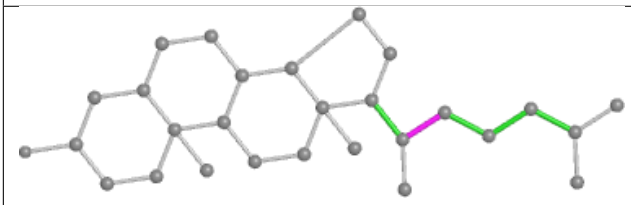
Ligand CLR R 807



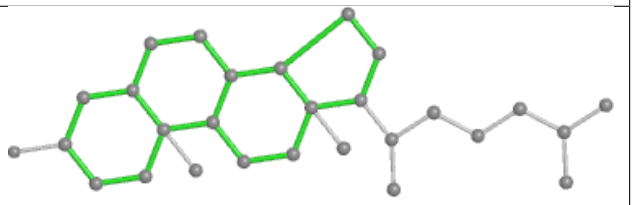
Bond lengths



Bond angles

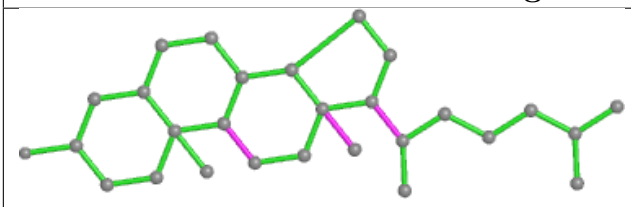


Torsions

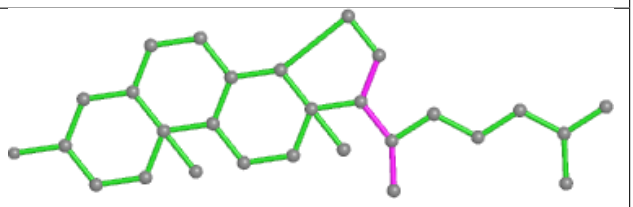


Rings

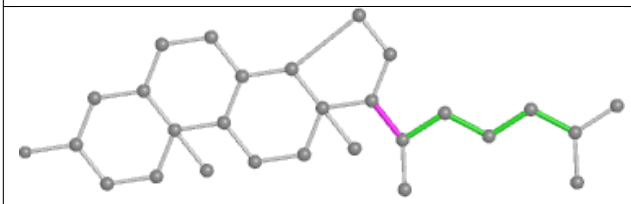
Ligand CLR R 811



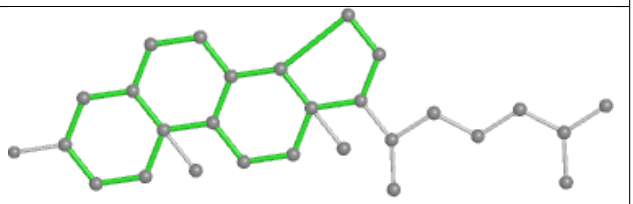
Bond lengths



Bond angles

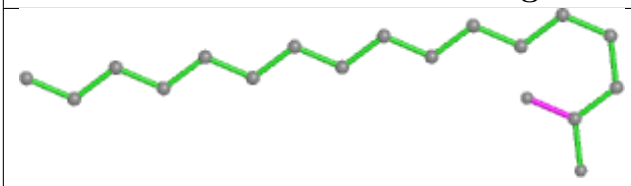


Torsions

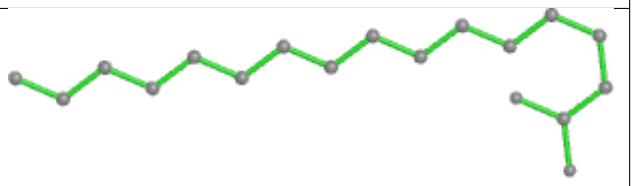


Rings

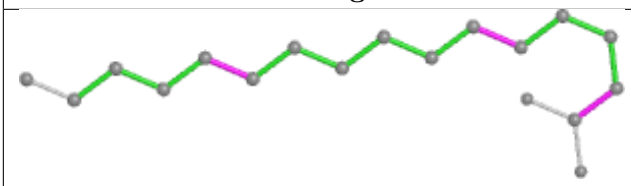
Ligand PLM R 822



Bond lengths



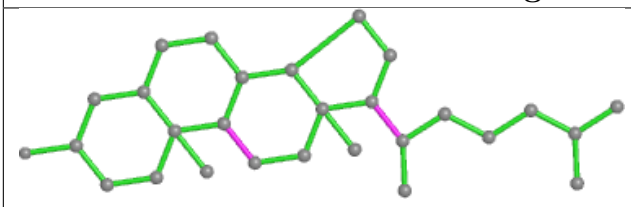
Bond angles



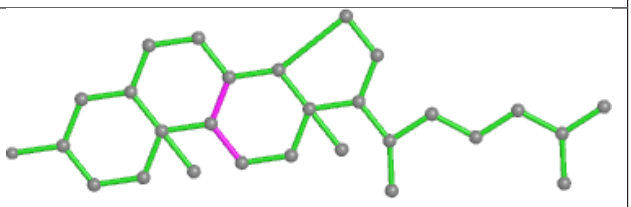
Torsions

Rings

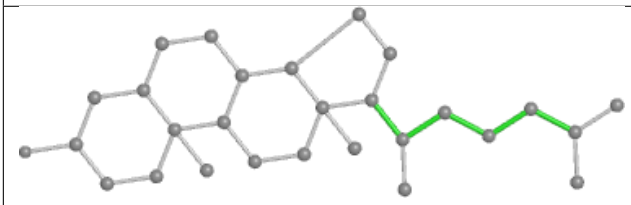
Ligand CLR R 810



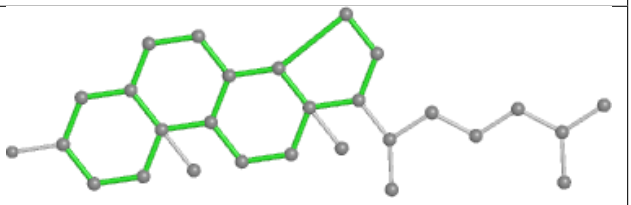
Bond lengths



Bond angles

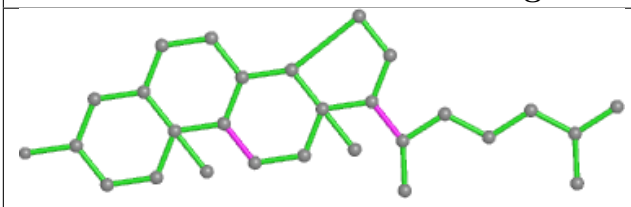


Torsions

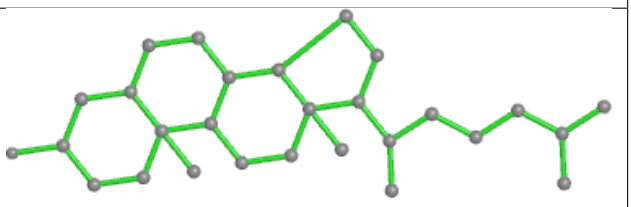


Rings

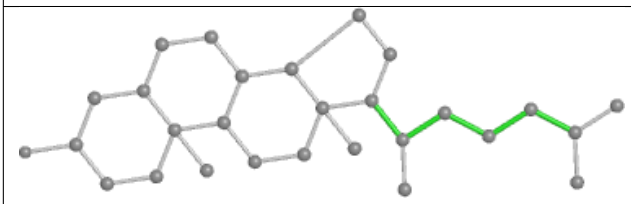
Ligand CLR R 805



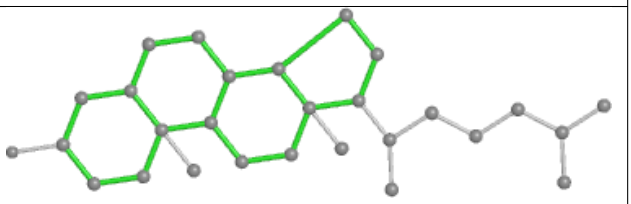
Bond lengths



Bond angles

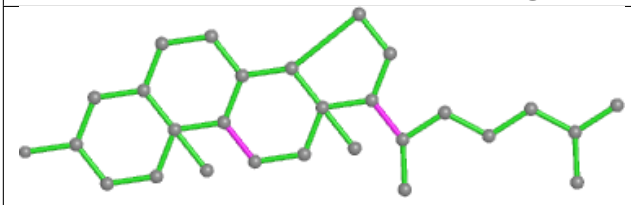


Torsions

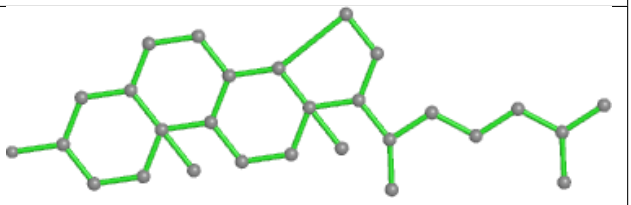


Rings

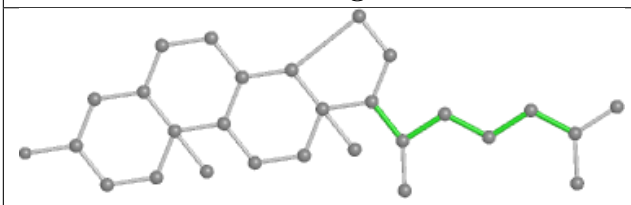
Ligand CLR R 813



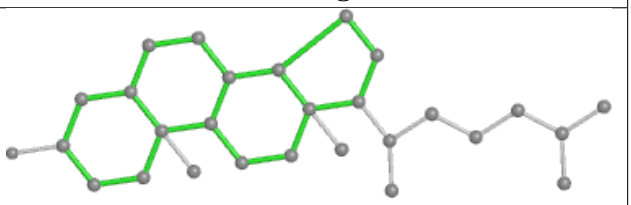
Bond lengths



Bond angles

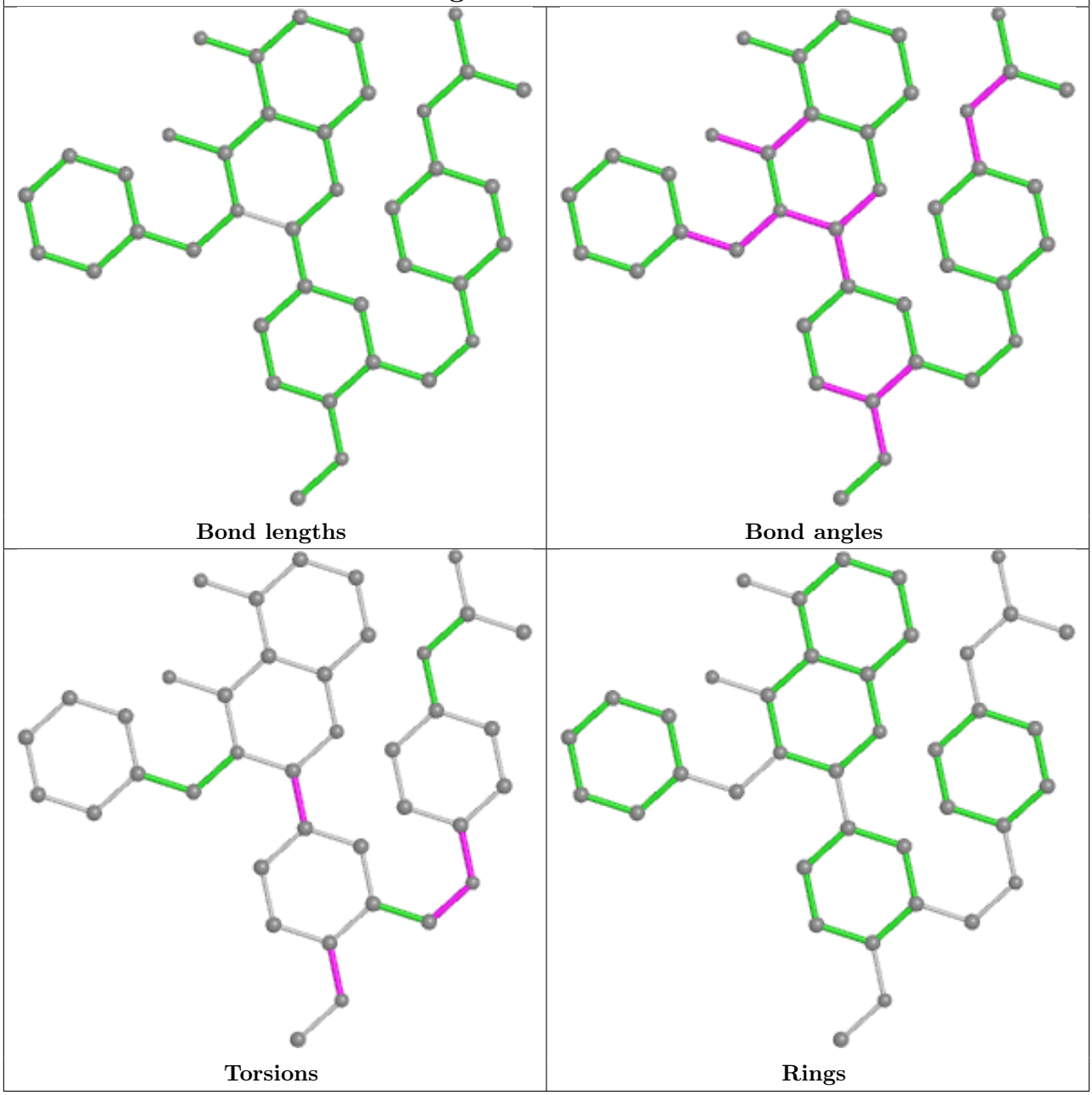


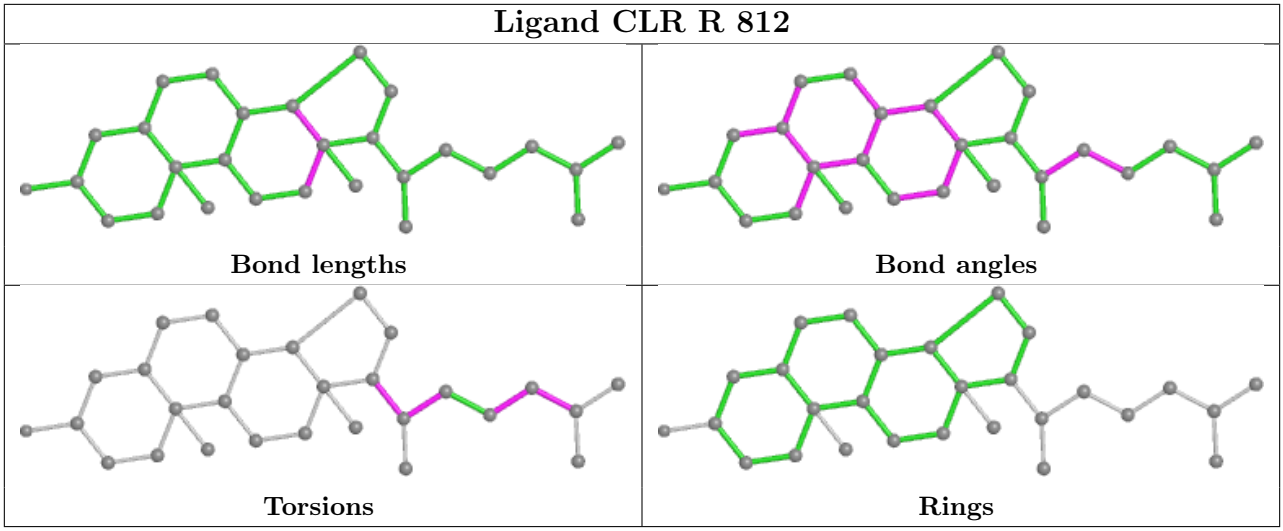
Torsions

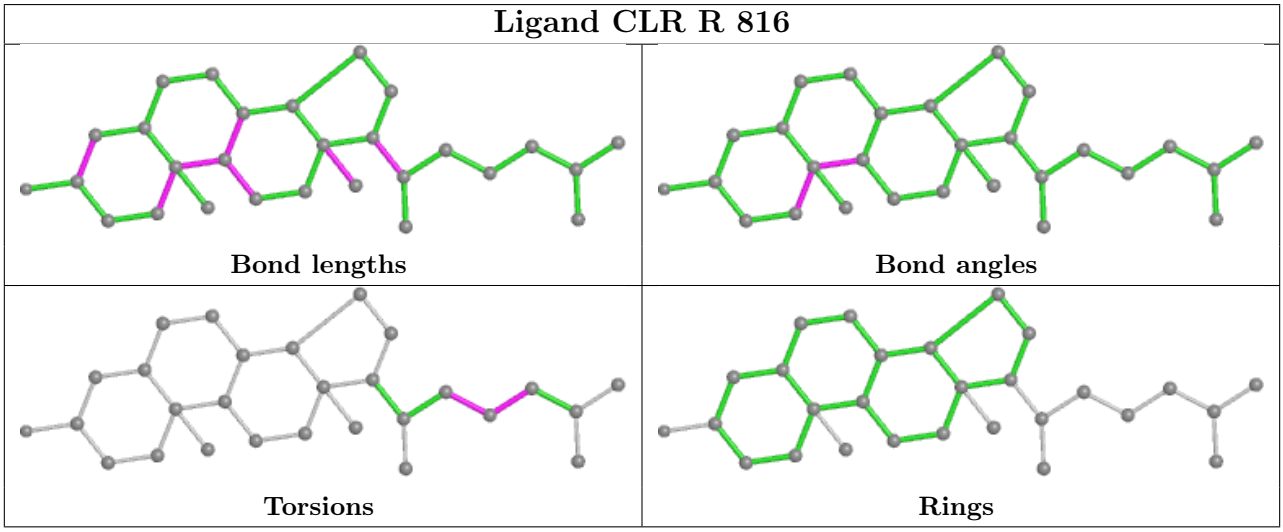


Rings

Ligand HOI R 827







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.

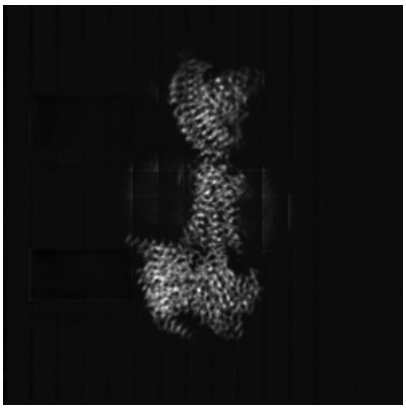
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33492. These allow visual inspection of the internal detail of the map and identification of artifacts.

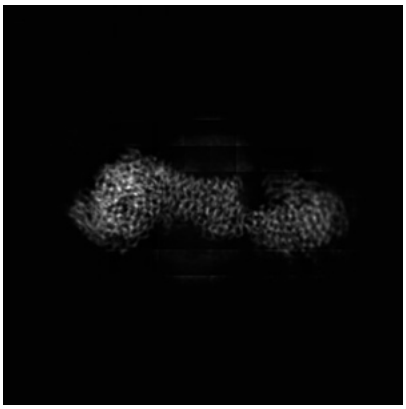
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

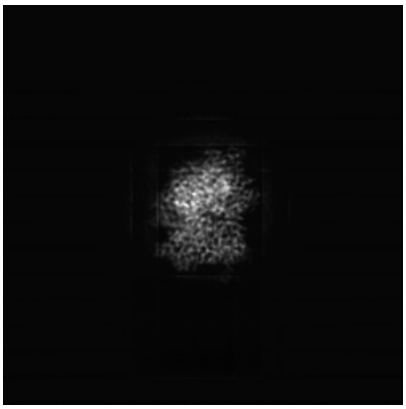
6.1.1 Primary map



X

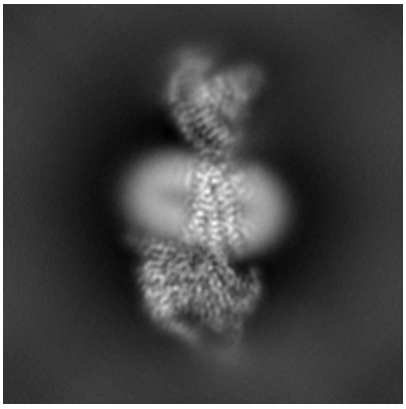


Y

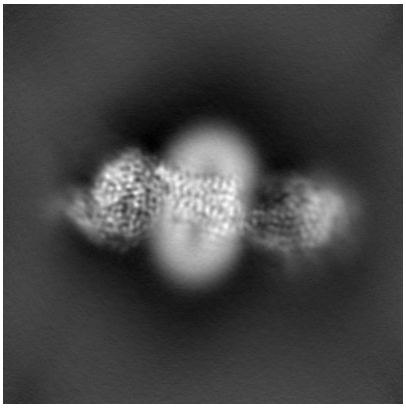


Z

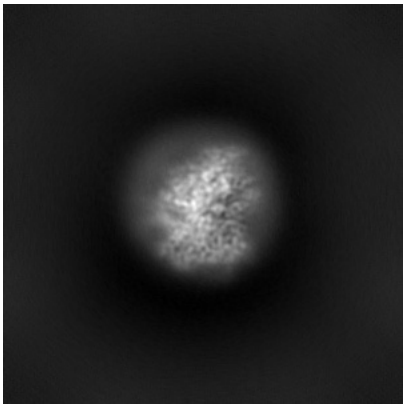
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

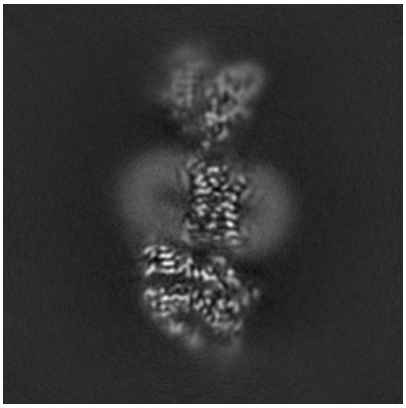
6.2.1 Primary map

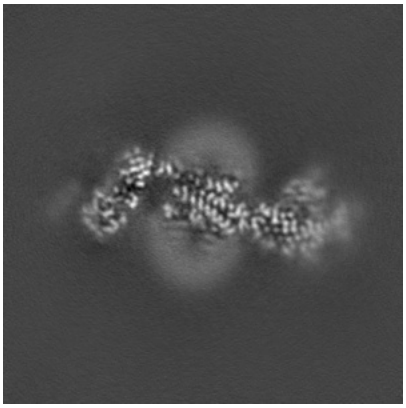
X Index: 150

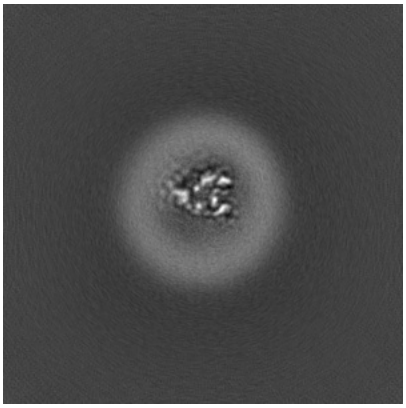
Y Index: 150

Z Index: 150

6.2.2 Raw map


X Index: 150


Y Index: 150

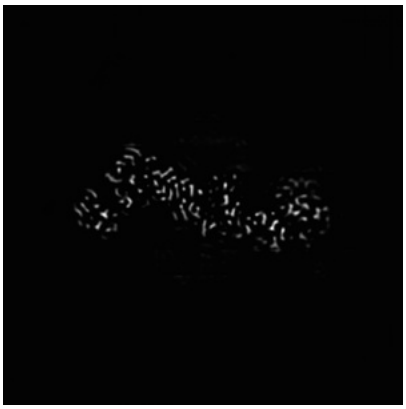

Z Index: 150

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

6.3 Largest variance slices (i)

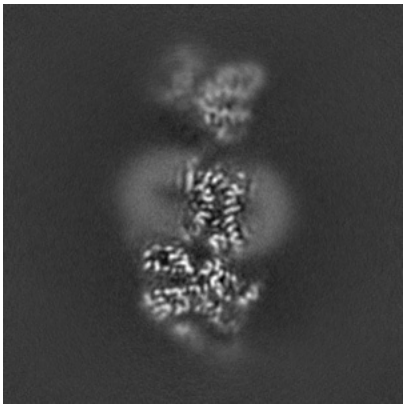
6.3.1 Primary map

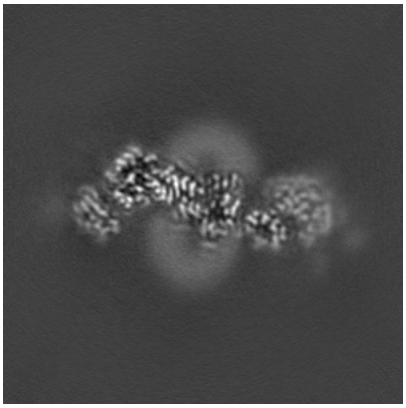
X Index: 142

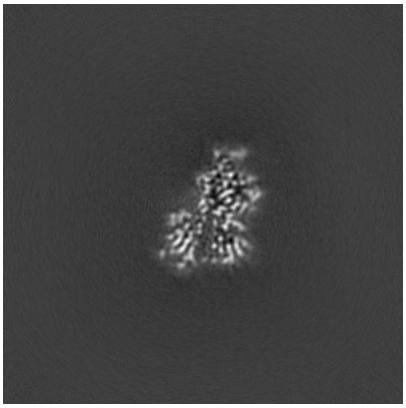

Y Index: 158

Z Index: 96

6.3.2 Raw map


X Index: 154

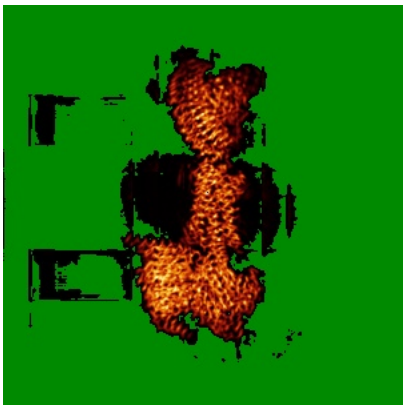

Y Index: 159


Z Index: 96

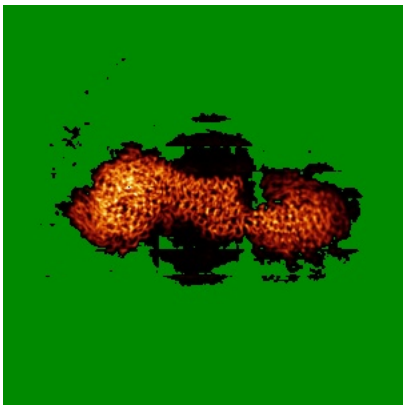
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

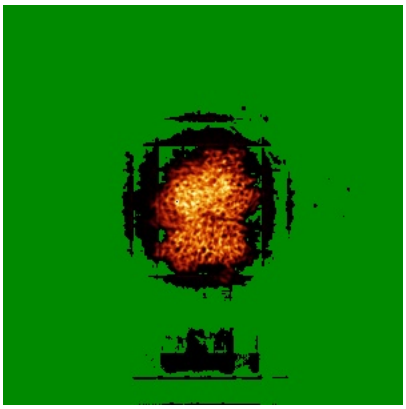
6.4.1 Primary map



X

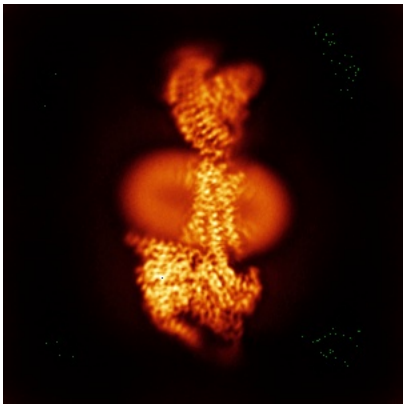


Y

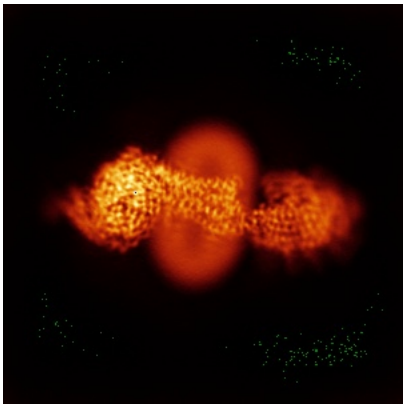


Z

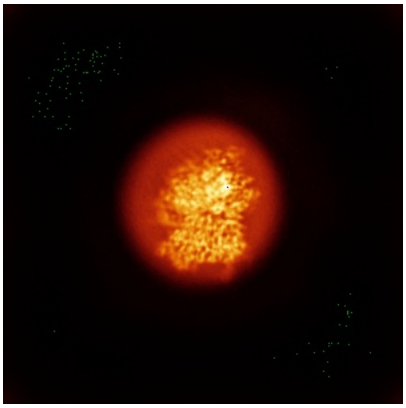
6.4.2 Raw map



X



Y

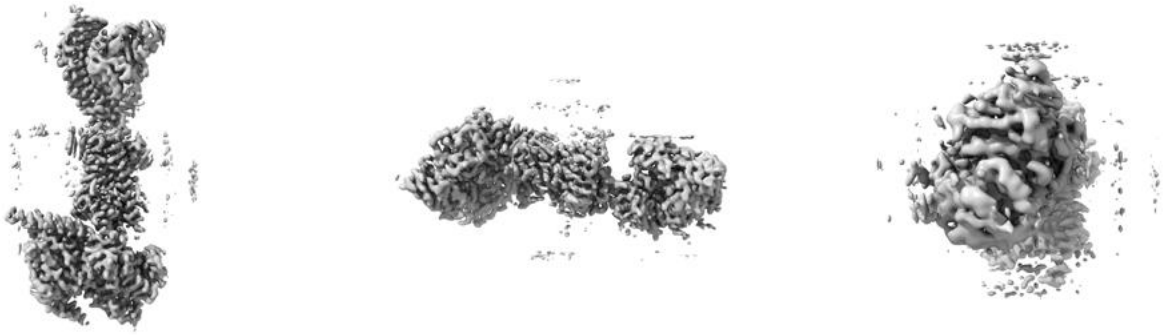


Z

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)

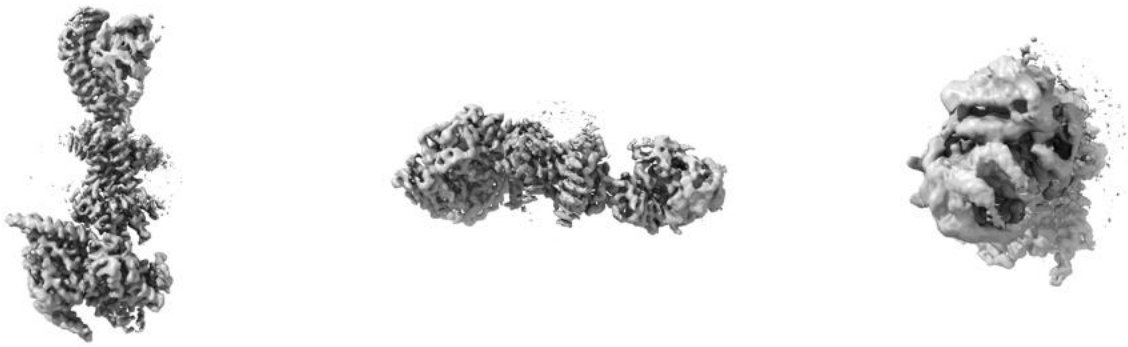
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

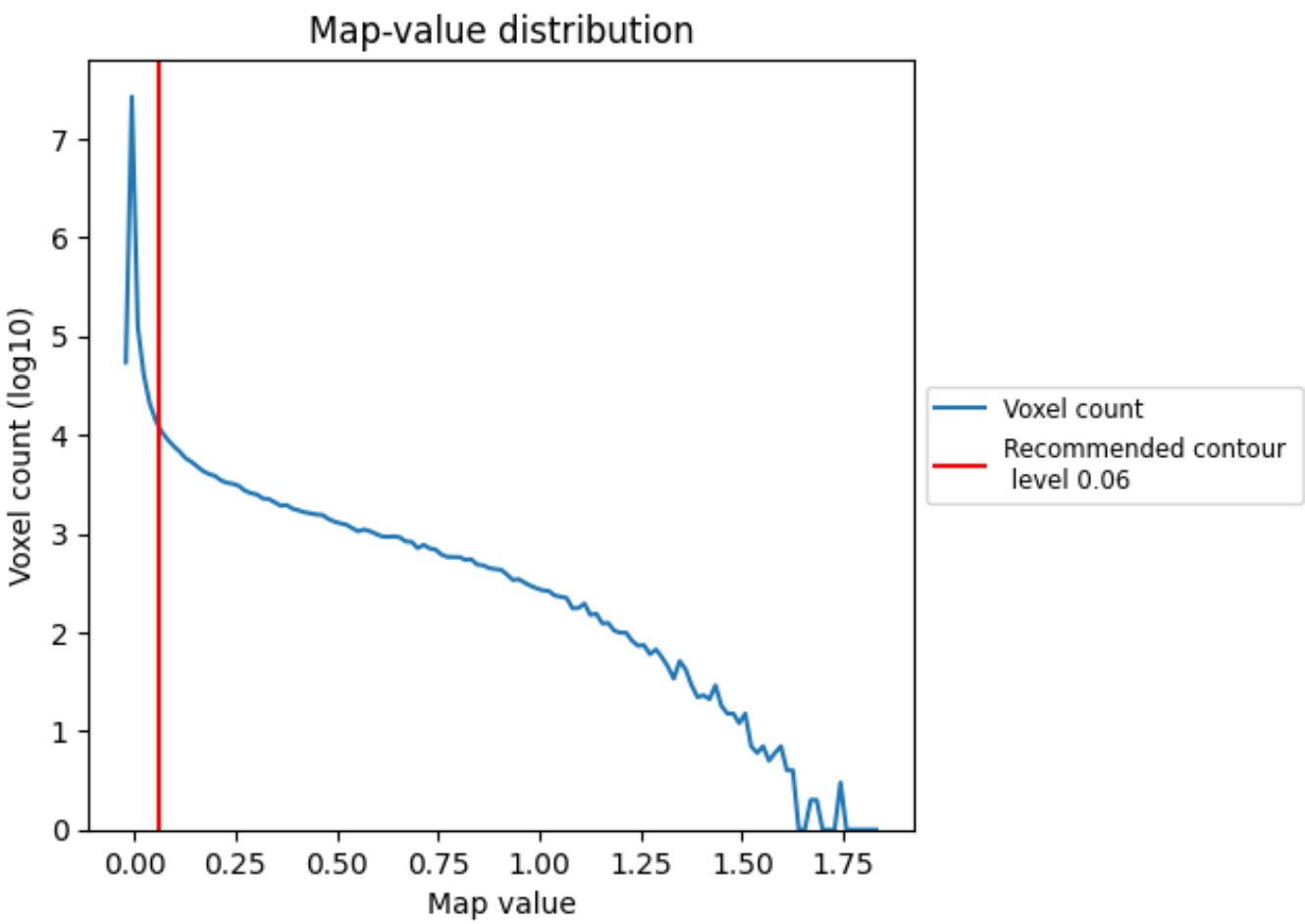
6.6 Mask visualisation (i)

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

7 Map analysis (i)

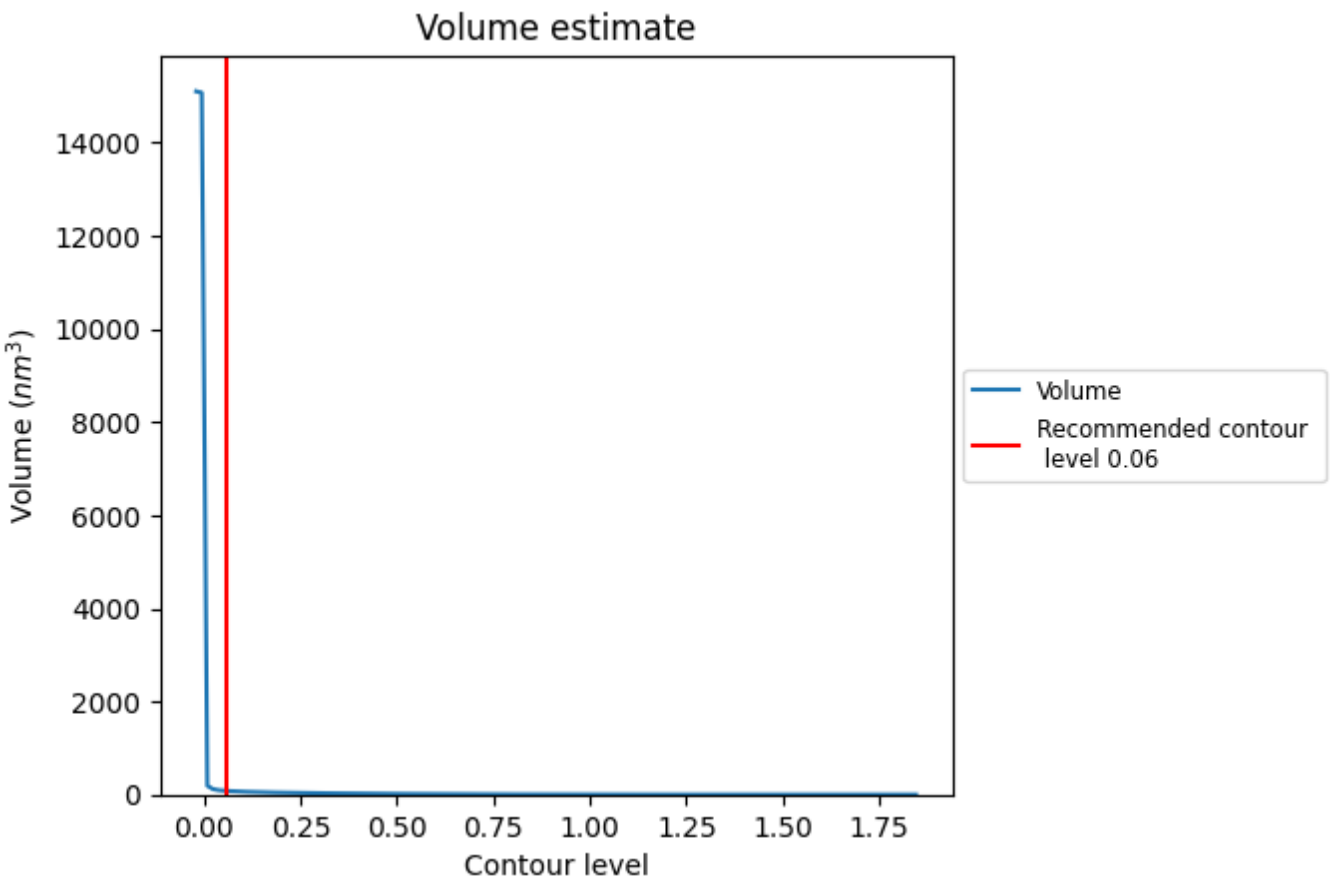
This section contains the results of statistical analysis of the map.

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.

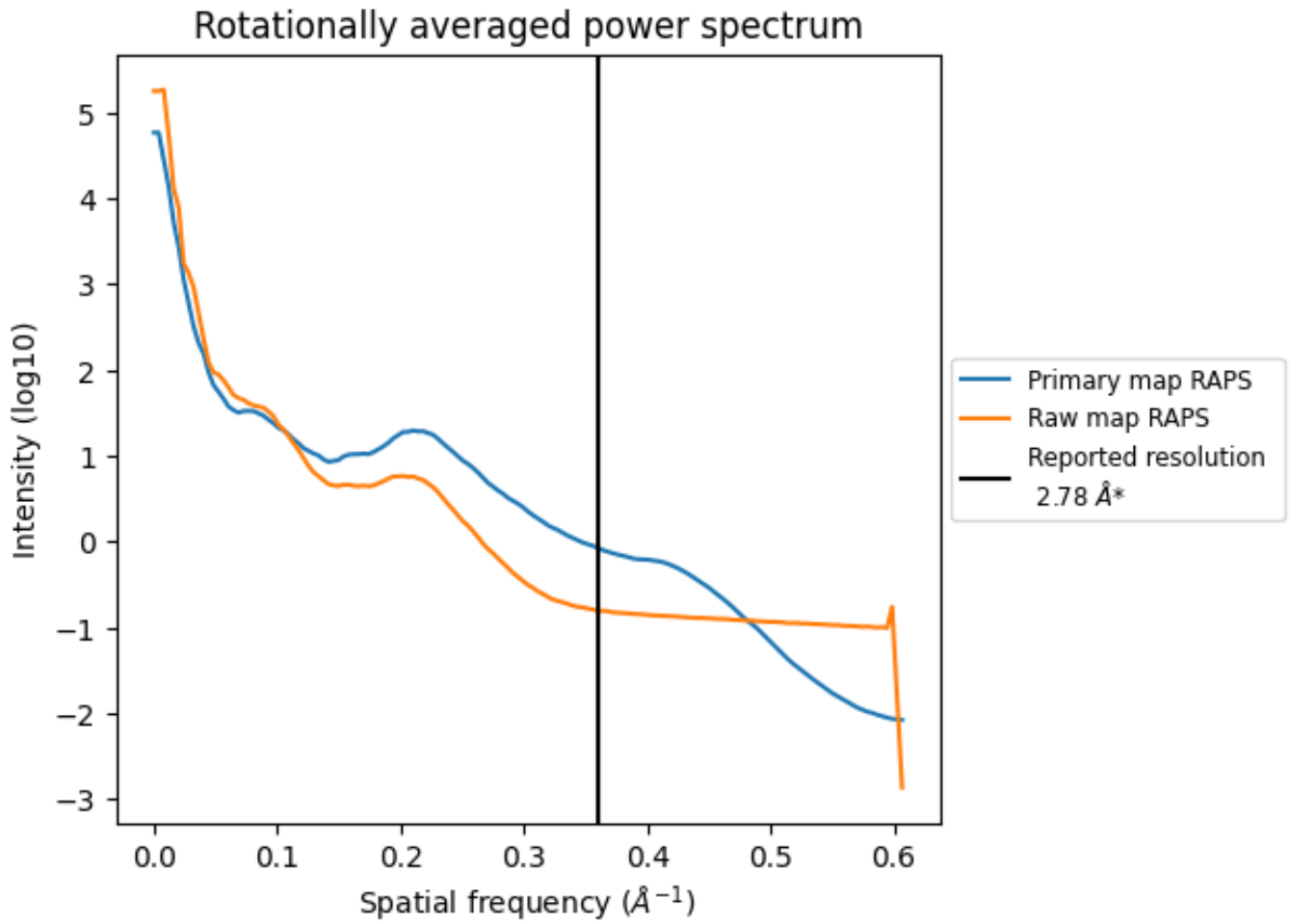
7.2 Volume estimate (i)



The volume at the recommended contour level is 78 nm^3; this corresponds to an approximate mass of 71 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)

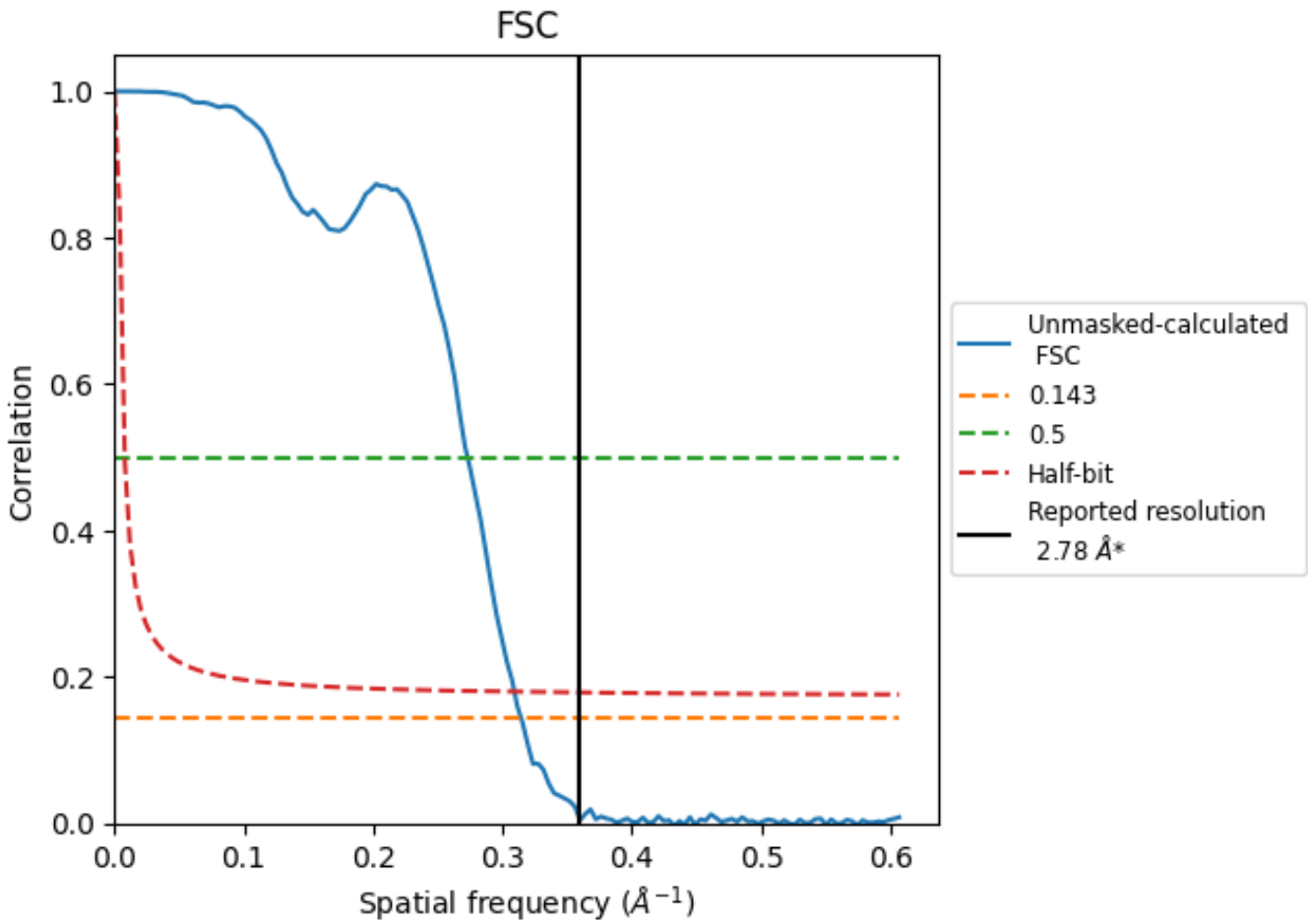


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

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 0.360 Å^{-1}

8.2 Resolution estimates (i)

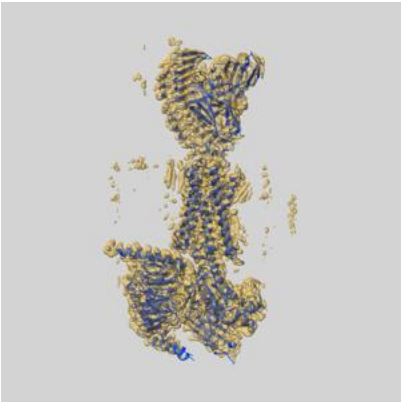
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.66	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.78 by more than 10 %

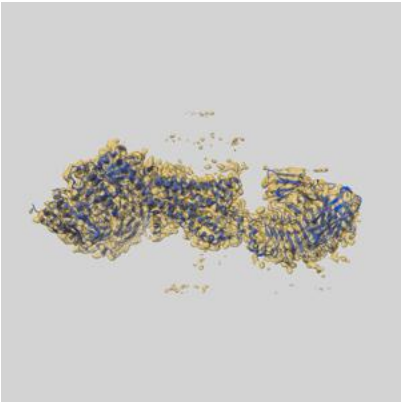
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33492 and PDB model 7XW6. Per-residue inclusion information can be found in section 3 on page 10.

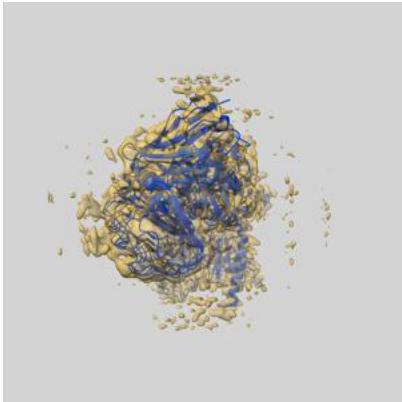
9.1 Map-model overlay (i)



X



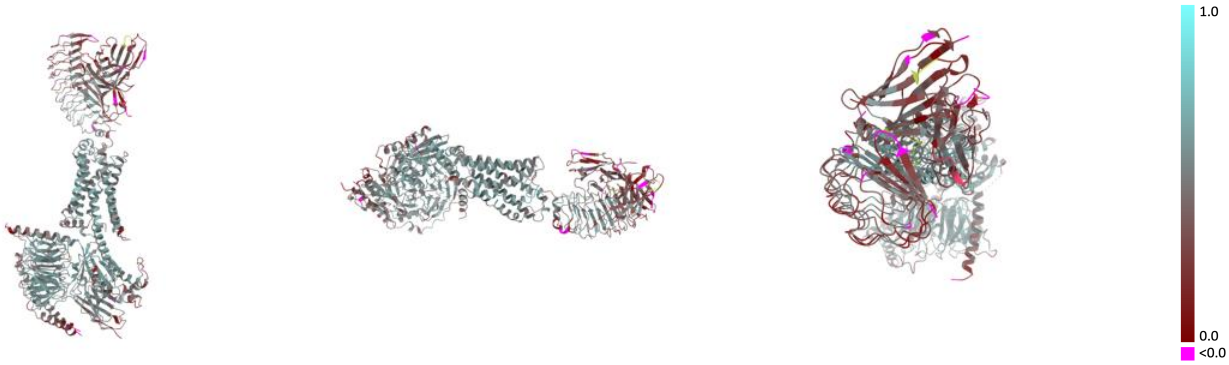
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

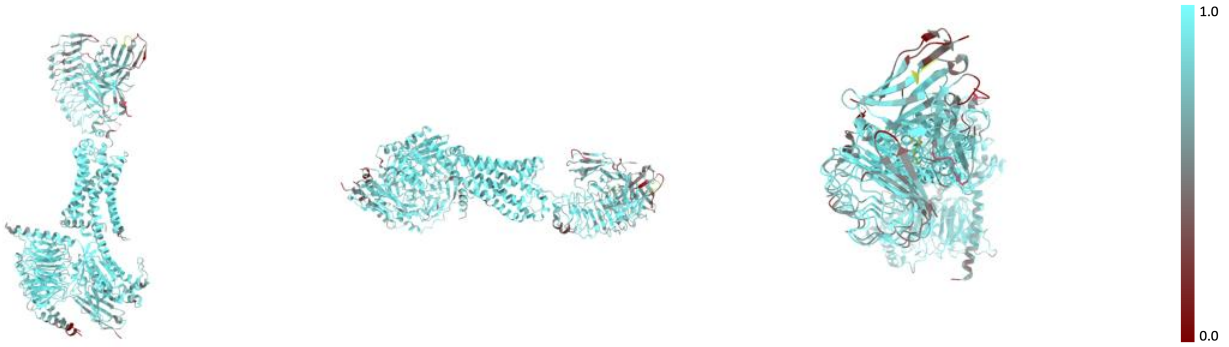
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

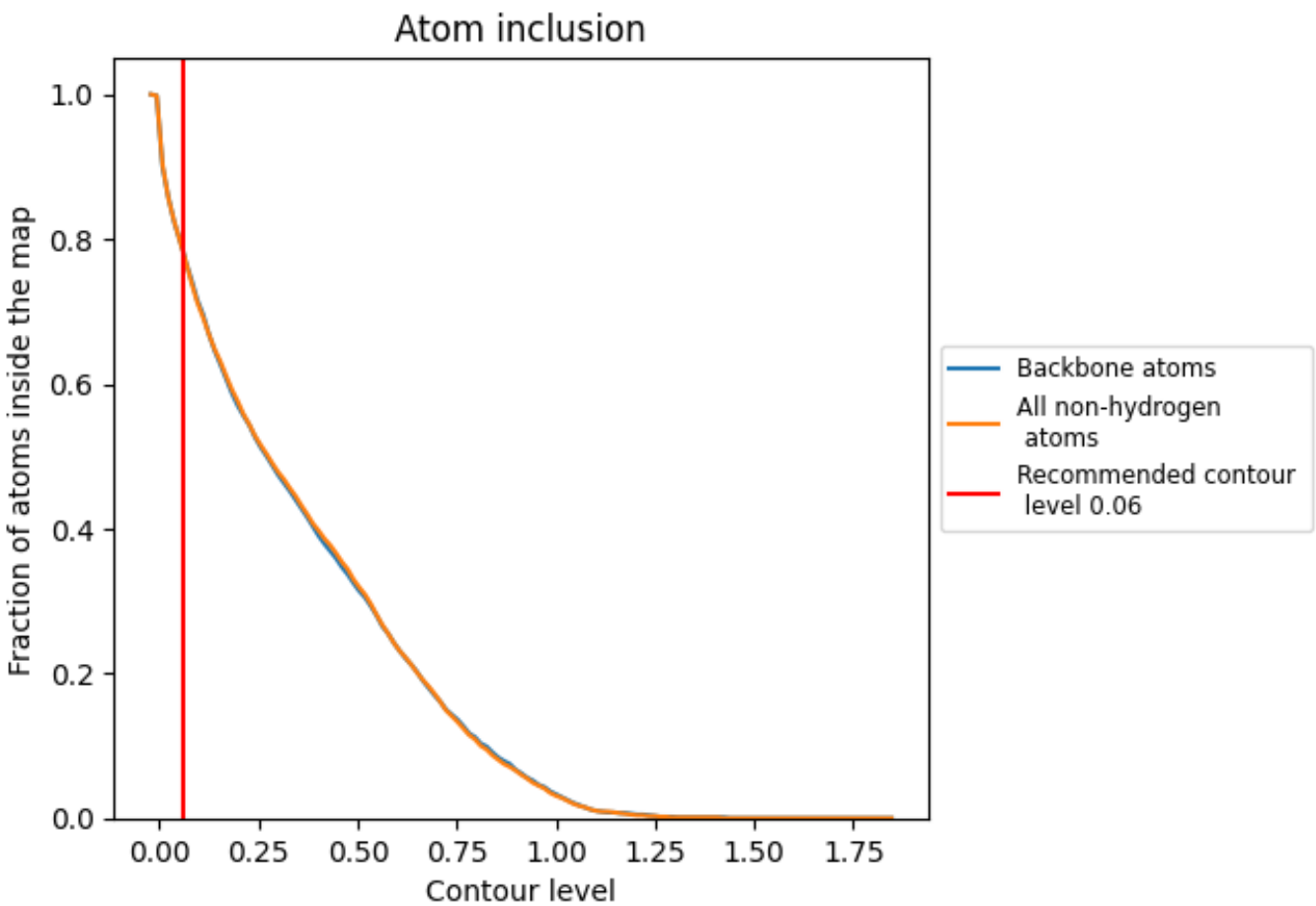
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.4410
A	0.8580	0.4940
B	0.8870	0.5200
G	0.7160	0.4010
L	0.6970	0.3090
N	0.8280	0.4710
R	0.7500	0.4220
Y	0.6880	0.3170