wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 03:49 AM JST

PDB ID	:	7E2X
EMDB ID	:	EMD-30971
Title	:	Apo serotonin 1A (5-HT1A) receptor-Gi protein complex
Authors	:	Xu, P.; Huang, S.; Zhang, H.; Mao, C.; Zhou, X.E.; Shen, D.D.; Jiang, Y.; Zhang, Y.; Xu, H.E.
Deposited on	:	2021-02-07
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

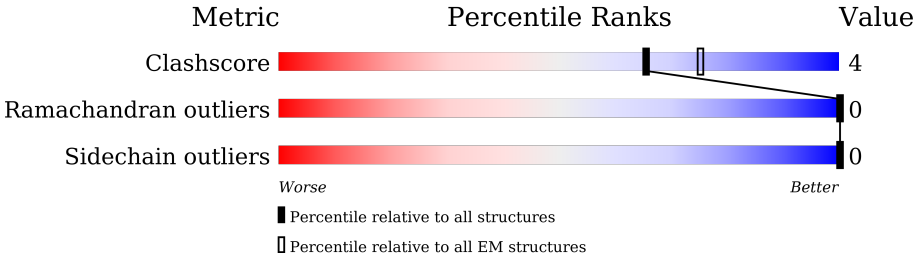
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	354	6% 55% 7% 38%
2	B	345	9% 86% 9% 5%
3	G	71	17% 61% • 37%
4	R	543	• 47% • 49%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7226 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	219	1766	1126	295	333	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- 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	N	O	S		
2	B	328	2516	1554	452	489	21	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	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	N	O	S		
3	G	45	347	218	60	66	3	0	0

- Molecule 4 is a protein called Soluble cytochrome b562,5-hydroxytryptamine receptor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	278	2197	1453	362	365	17	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-120	ASP	-	expression tag	UNP P0ABE7
R	-119	TYR	-	expression tag	UNP P0ABE7
R	-118	LYS	-	expression tag	UNP P0ABE7
R	-117	ASP	-	expression tag	UNP P0ABE7
R	-116	ASP	-	expression tag	UNP P0ABE7
R	-115	ASP	-	expression tag	UNP P0ABE7
R	-114	ASP	-	expression tag	UNP P0ABE7
R	-113	ALA	-	expression tag	UNP P0ABE7
R	-112	LYS	-	expression tag	UNP P0ABE7
R	-111	LEU	-	expression tag	UNP P0ABE7
R	-110	GLN	-	expression tag	UNP P0ABE7
R	-109	THR	-	expression tag	UNP P0ABE7
R	-108	MET	-	expression tag	UNP P0ABE7
R	-107	HIS	-	expression tag	UNP P0ABE7
R	-106	HIS	-	expression tag	UNP P0ABE7
R	-105	HIS	-	expression tag	UNP P0ABE7
R	-104	HIS	-	expression tag	UNP P0ABE7
R	-103	HIS	-	expression tag	UNP P0ABE7
R	-102	HIS	-	expression tag	UNP P0ABE7
R	-101	HIS	-	expression tag	UNP P0ABE7
R	-100	HIS	-	expression tag	UNP P0ABE7
R	-99	HIS	-	expression tag	UNP P0ABE7
R	-98	HIS	-	expression tag	UNP P0ABE7
R	-97	HIS	-	expression tag	UNP P0ABE7
R	-96	HIS	-	expression tag	UNP P0ABE7
R	-95	HIS	-	expression tag	UNP P0ABE7
R	-94	HIS	-	expression tag	UNP P0ABE7
R	-93	HIS	-	expression tag	UNP P0ABE7
R	-86	TRP	MET	engineered mutation	UNP P0ABE7
R	9	ILE	HIS	engineered mutation	UNP P0ABE7
R	13	LEU	ARG	engineered mutation	UNP P0ABE7

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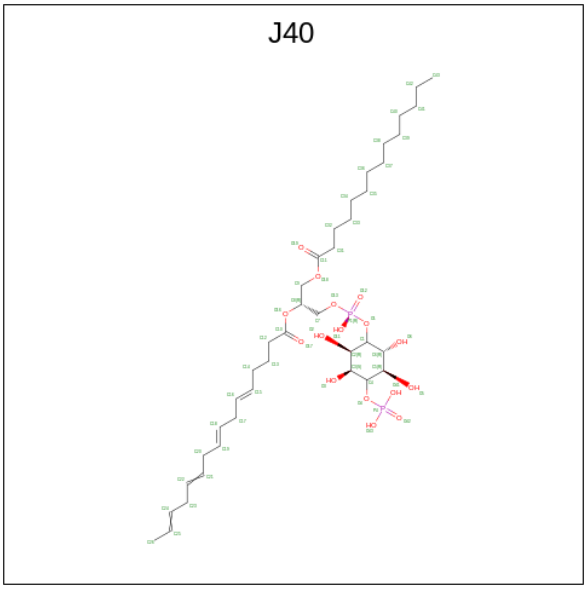
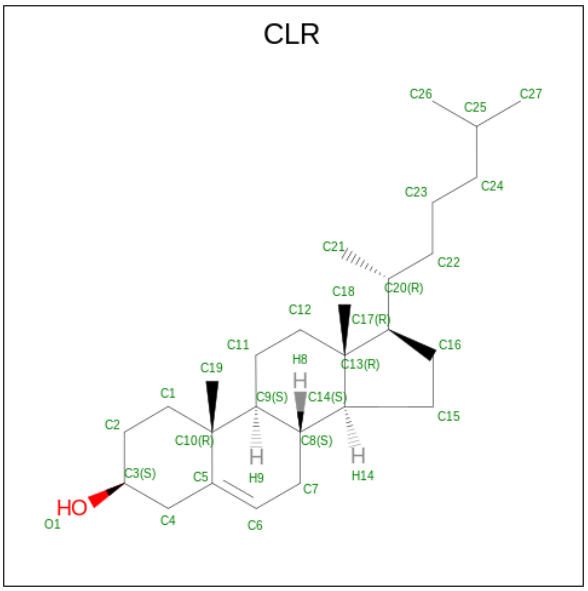
Chain	Residue	Modelled	Actual	Comment	Reference
R	14	ALA	-	linker	UNP P0ABE7
R	15	SER	-	linker	UNP P0ABE7
R	16	GLU	-	linker	UNP P0ABE7
R	17	ASN	-	linker	UNP P0ABE7
R	18	LEU	-	linker	UNP P0ABE7
R	19	TYR	-	linker	UNP P0ABE7
R	20	PHE	-	linker	UNP P0ABE7
R	21	GLN	-	linker	UNP P0ABE7
R	22	GLY	-	linker	UNP P0ABE7
R	23	GLY	-	linker	UNP P0ABE7
R	24	THR	-	linker	UNP P0ABE7
R	125	TRP	LEU	engineered mutation	UNP P08908

- Molecule 5 is [(2R)-1-[oxidanyl-[(2R,3R,5S,6R)-2,3,5,6-tetrakis(oxidanyl)-4-phosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-3-tetradecanoyloxy-propan-2-yl] (5E,8E)-hexadeca-5,8,11,14-tetraenoate (three-letter code: J40) (formula: $C_{39}H_{68}O_{16}P_2$) (labeled as "Ligand of Interest" by depositor).



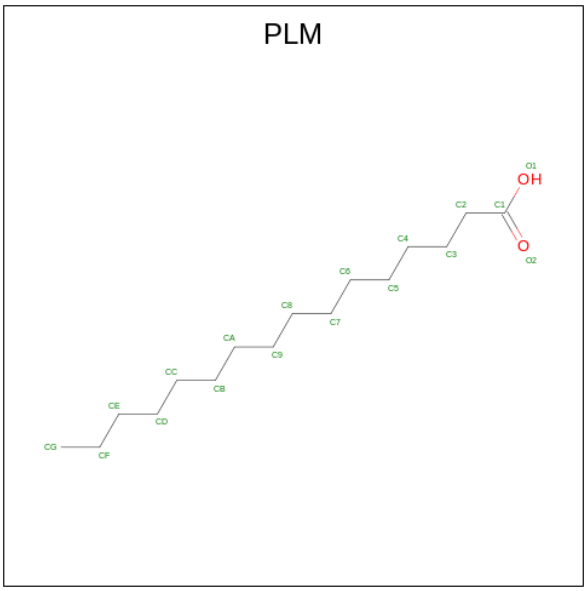
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
5	R	1	57	39	16	2	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0
			Total	C	O	
6	R	1	280	270	10	0

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	R	1	54	48	6	0
			Total	C	O	
7	R	1	54	48	6	0
			Total	C	O	
7	R	1	54	48	6	0

- Molecule 8 is water.

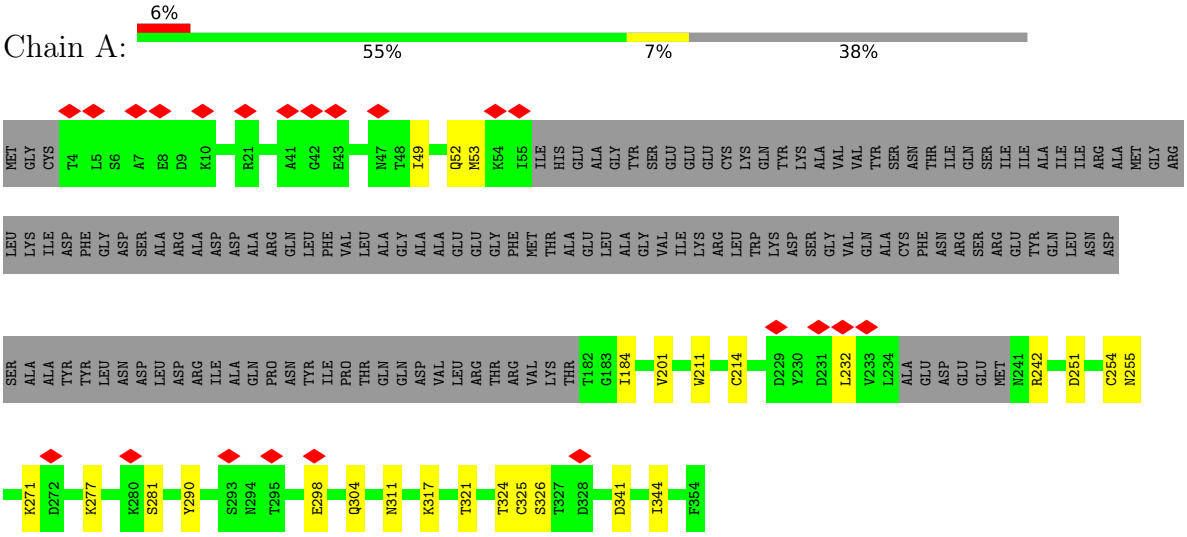
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	R	9	9	9	0

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.

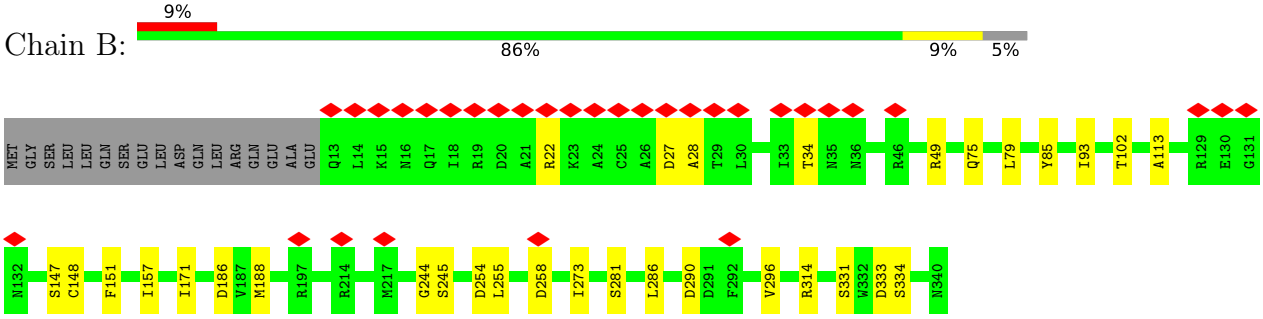
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



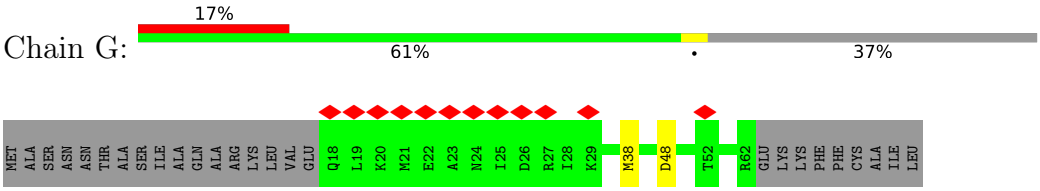
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



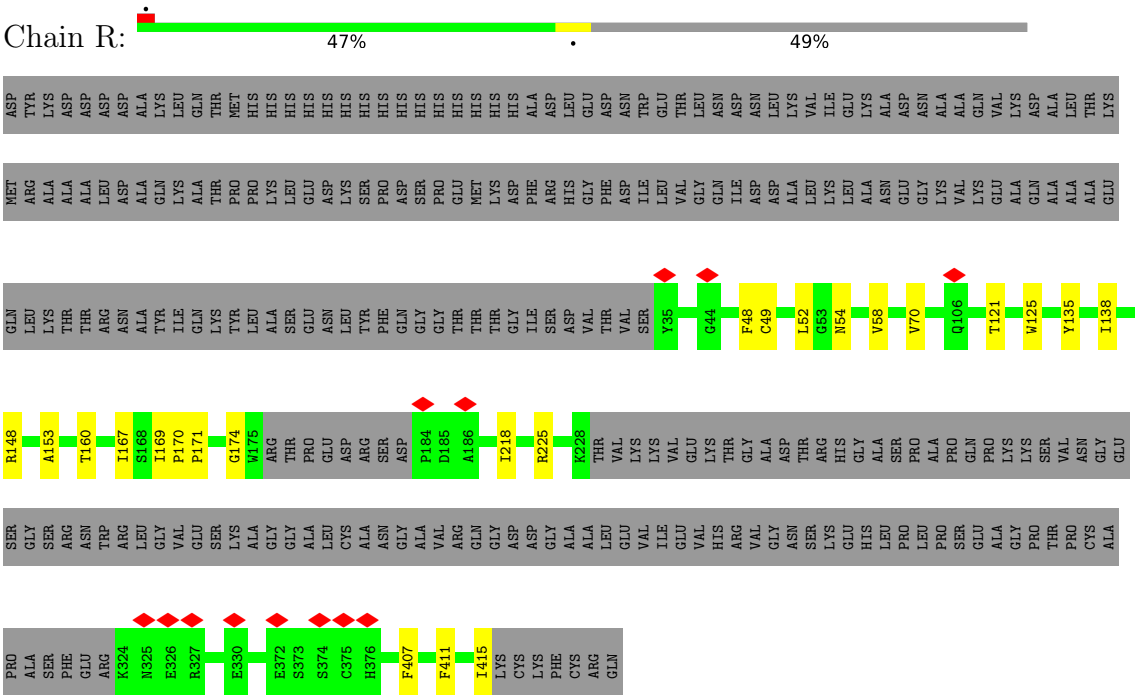
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



• Molecule 4: Soluble cytochrome b562,5-hydroxytryptamine receptor 1A

Chain R:


47%
49%
ASP TYR LYS ASP ASP ASP ASP ALA LYS LEU GLN THR MET HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS ALA ASP LEU GLU ASP ASN TRP GLU THR LEU ASN ASP ASN LEU LYS VAL ILE GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA LEU THR LYS
MET ARG ALA ALA ALA LEU ASP ALA GLN LYS LEU ALA THR PRO PRO LYS LEU GLU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ASP ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA GLU
GLN LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU ALA SER GLU ASN LEU TYR PHE GLN GLY GLY THR THR THR GLY ILE SER ASP VAL THR VAL SER Y35 G44 F48 C49 L52 G53 N54 V58 V70 Q106 T121 W125 Y135 I138
R148 A153 T160 I167 S168 I169 P170 P171 G174 W175 ARG THR PRO GLU ASP ARG SER ASP P184 D185 A186 I218 R225 K228 THR VAL LYS LYS VAL GLU LYS THR GLY ALA ASP THR ARG HIS GLY ALA SER PRO ALA PRO GLN PRO LYS LYS SER VAL ASN GLY GLU
SER GLY SER ARG ASN TRP ARG LEU GLY VAL GLU GLU SER LYS ALA GLY GLY ALA LEU CYS ALA ASN GLY ALA VAL ARG GLN GLY ASP ASP GLY ALA ALA LEU GLU VAL ILE GLU VAL HIS ARG VAL GLY ASN SER LYS GLU HIS LEU PRO LEU PRO SER GLU ALA GLY PRO THR PRO CYS ALA
PRO ALA SER PHE GLU ARG K324 N325 E326 R327 E330 E372 S373 S374 C375 H376 F407 F411 I415 LYS CYS LYS PHE CYS ARG GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	245886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	49310	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.183	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	194.68802, 194.68802, 194.68802	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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, J40, CLR

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	0.25	0/1795	0.38	0/2407
2	B	0.24	0/2563	0.44	0/3475
3	G	0.25	0/353	0.36	0/477
4	R	0.24	0/2248	0.37	0/3058
All	All	0.24	0/6959	0.40	0/9417

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	1766	0	1768	20	0
2	B	2516	0	2425	24	0
3	G	347	0	350	2	0
4	R	2197	0	2298	16	0
5	R	57	0	0	1	0
6	R	280	0	450	4	0
7	R	54	0	93	0	0
8	R	9	0	0	0	0
All	All	7226	0	7384	60	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 4.

The worst 5 of 60 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)
4:R:135:TYR:HA	4:R:218:ILE:HD11	1.64	0.80
2:B:314:ARG:O	2:B:331:SER:OG	2.01	0.79
2:B:147:SER:OG	2:B:188:MET:O	2.02	0.77
1:A:271:LYS:NZ	1:A:324:THR:O	2.20	0.75
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.21	0.73

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	213/354 (60%)	211 (99%)	2 (1%)	0	100	100
2	B	326/345 (94%)	317 (97%)	9 (3%)	0	100	100
3	G	43/71 (61%)	43 (100%)	0	0	100	100
4	R	272/543 (50%)	270 (99%)	2 (1%)	0	100	100
All	All	854/1313 (65%)	841 (98%)	13 (2%)	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	195/305 (64%)	195 (100%)	0	100	100
2	B	272/287 (95%)	272 (100%)	0	100	100
3	G	37/58 (64%)	37 (100%)	0	100	100
4	R	237/453 (52%)	237 (100%)	0	100	100
All	All	741/1103 (67%)	741 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	304	GLN
2	B	75	GLN
4	R	126	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
7	PLM	R	606	-	17,17,17	0.58	0	17,17,17	1.11	0
6	CLR	R	610	-	31,31,31	1.82	5 (16%)	48,48,48	1.36	7 (14%)
6	CLR	R	605	-	31,31,31	1.84	6 (19%)	48,48,48	1.40	8 (16%)
7	PLM	R	614	-	17,17,17	0.58	0	17,17,17	1.12	0
6	CLR	R	603	-	31,31,31	1.78	5 (16%)	48,48,48	1.33	6 (12%)
6	CLR	R	608	-	31,31,31	1.79	5 (16%)	48,48,48	1.37	7 (14%)
6	CLR	R	607	-	31,31,31	1.83	5 (16%)	48,48,48	1.35	9 (18%)
6	CLR	R	611	-	31,31,31	1.80	5 (16%)	48,48,48	1.40	9 (18%)
6	CLR	R	612	-	31,31,31	1.79	5 (16%)	48,48,48	1.38	6 (12%)
6	CLR	R	609	-	31,31,31	1.80	5 (16%)	48,48,48	1.35	7 (14%)
7	PLM	R	613	-	17,17,17	0.58	0	17,17,17	1.12	1 (5%)
6	CLR	R	604	-	31,31,31	1.80	5 (16%)	48,48,48	1.39	7 (14%)
6	CLR	R	602	-	31,31,31	1.83	6 (19%)	48,48,48	1.38	8 (16%)
5	J40	R	601	-	57,57,57	1.45	11 (19%)	69,72,72	1.17	3 (4%)

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
7	PLM	R	606	-	-	6/15/15/15	-
6	CLR	R	610	-	-	2/10/68/68	0/4/4/4
6	CLR	R	605	-	-	5/10/68/68	0/4/4/4
7	PLM	R	614	-	-	2/15/15/15	-
6	CLR	R	603	-	-	0/10/68/68	0/4/4/4
6	CLR	R	608	-	-	0/10/68/68	0/4/4/4
6	CLR	R	607	-	-	1/10/68/68	0/4/4/4
6	CLR	R	611	-	-	0/10/68/68	0/4/4/4
6	CLR	R	612	-	-	0/10/68/68	0/4/4/4
6	CLR	R	609	-	-	0/10/68/68	0/4/4/4
7	PLM	R	613	-	-	6/15/15/15	-
6	CLR	R	604	-	-	4/10/68/68	0/4/4/4
6	CLR	R	602	-	-	6/10/68/68	0/4/4/4
5	J40	R	601	-	-	24/53/77/77	0/1/1/1

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	605	CLR	C6-C5	6.52	1.47	1.33
6	R	610	CLR	C6-C5	6.50	1.47	1.33
6	R	602	CLR	C6-C5	6.50	1.47	1.33
6	R	608	CLR	C6-C5	6.45	1.47	1.33
6	R	612	CLR	C6-C5	6.44	1.47	1.33

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	601	J40	O16-C10-C12	4.19	120.53	111.50
6	R	604	CLR	C12-C11-C9	3.41	119.03	113.11
6	R	612	CLR	C4-C5-C10	3.37	120.90	116.42
6	R	608	CLR	C4-C5-C10	3.33	120.85	116.42
6	R	609	CLR	C4-C5-C10	3.32	120.83	116.42

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	601	J40	O16-C8-C9-O18
5	R	601	J40	C19-C20-C21-C22
5	R	601	J40	C23-C24-C25-C26
6	R	602	CLR	C13-C17-C20-C21
6	R	602	CLR	C13-C17-C20-C22

There are no ring outliers.

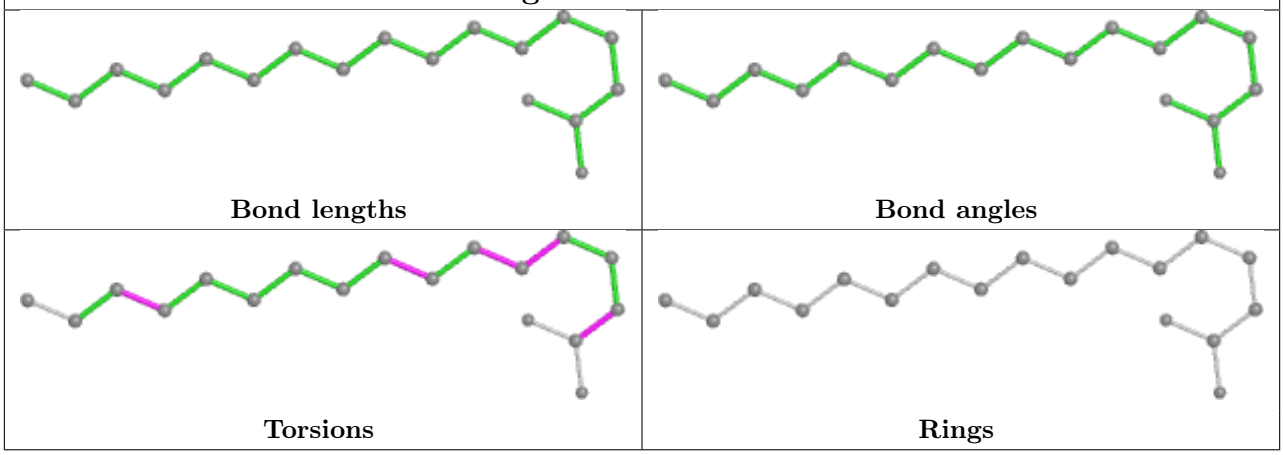
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	603	CLR	1	0
6	R	608	CLR	1	0
6	R	612	CLR	2	0
5	R	601	J40	1	0

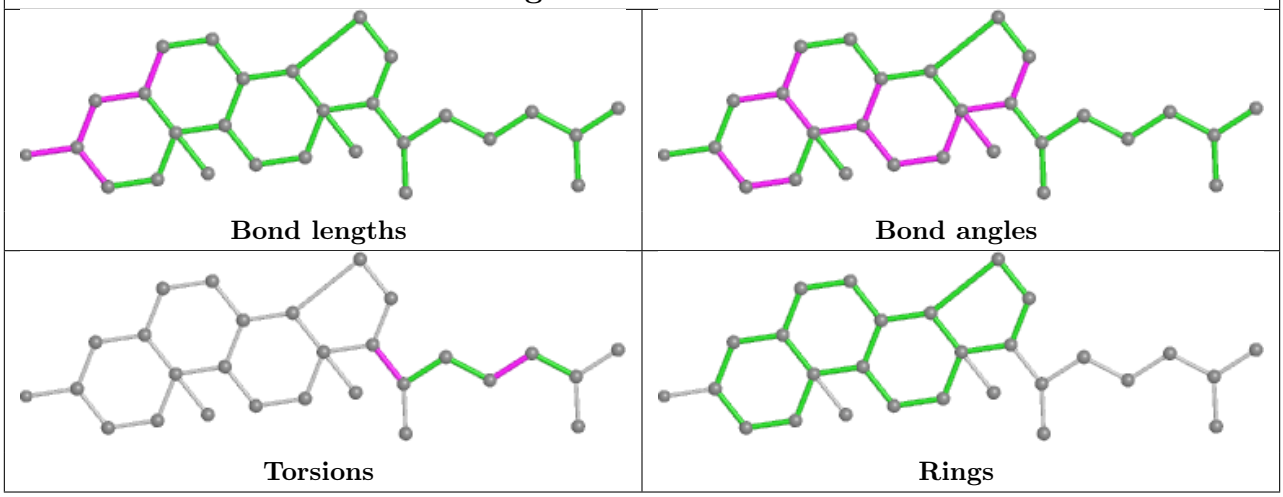
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

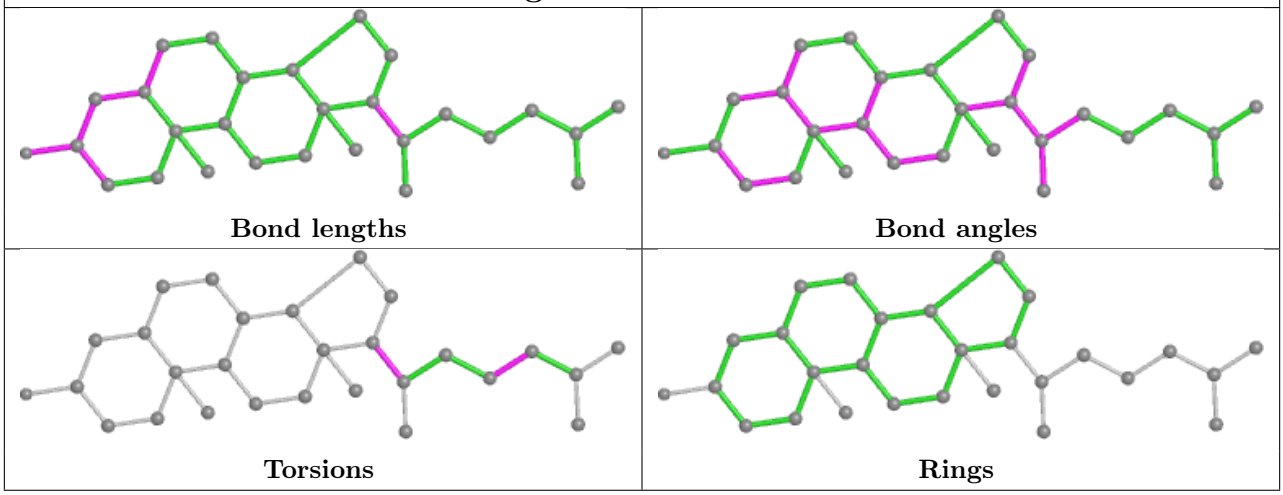
Ligand PLM R 606



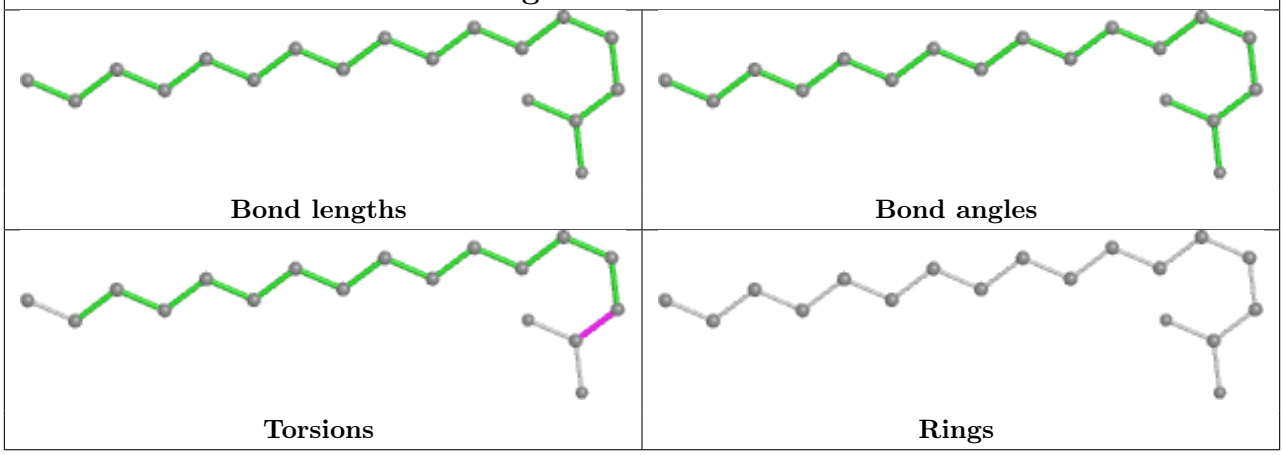
Ligand CLR R 610



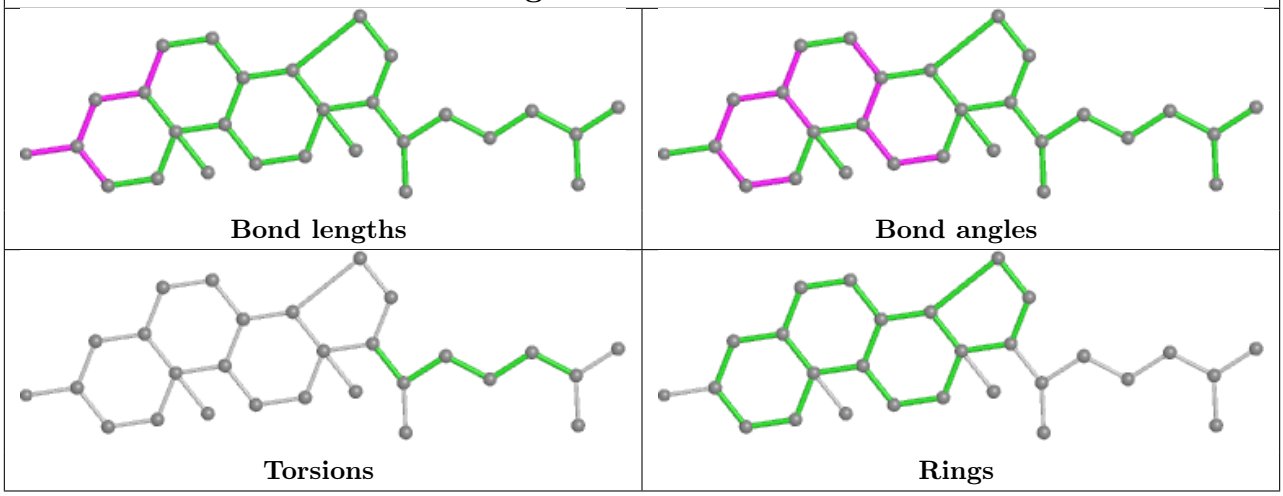
Ligand CLR R 605



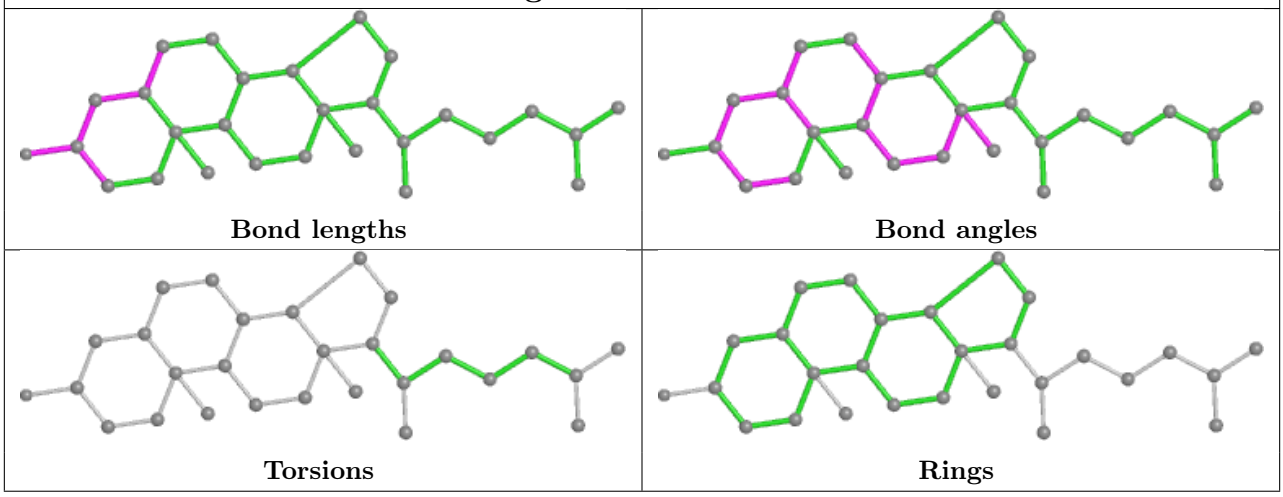
Ligand PLM R 614



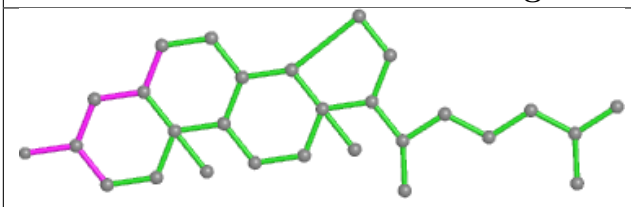
Ligand CLR R 603



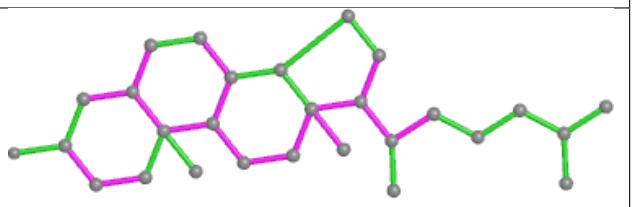
Ligand CLR R 608



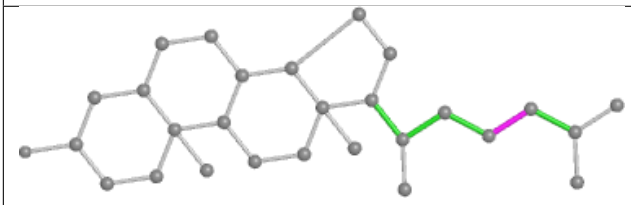
Ligand CLR R 607



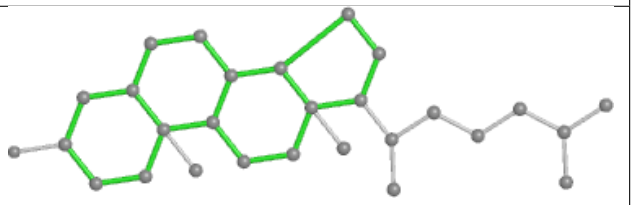
Bond lengths



Bond angles

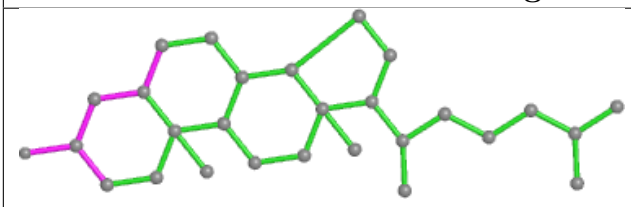


Torsions

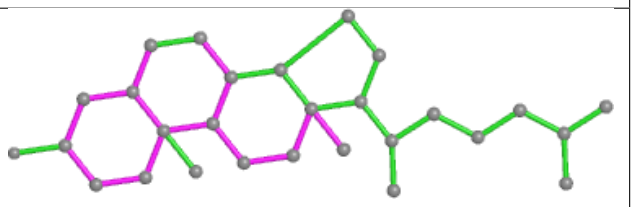


Rings

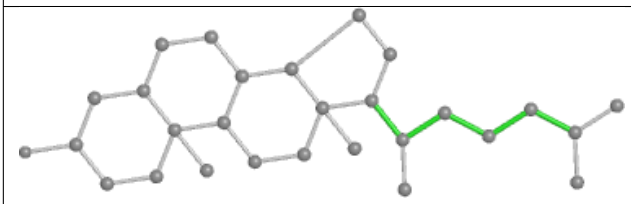
Ligand CLR R 611



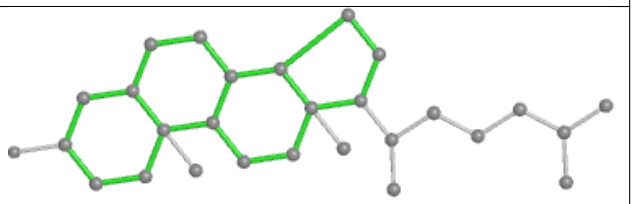
Bond lengths



Bond angles

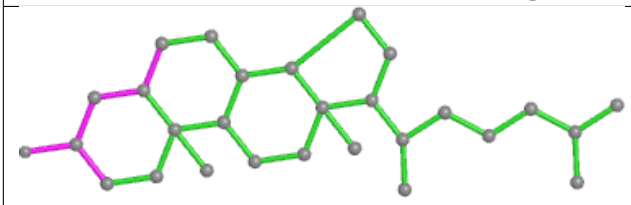


Torsions

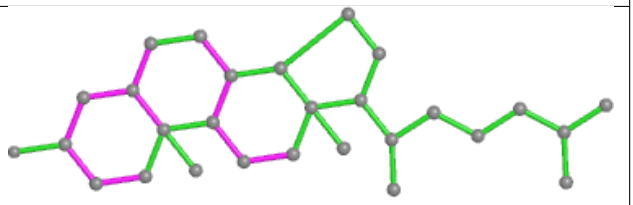


Rings

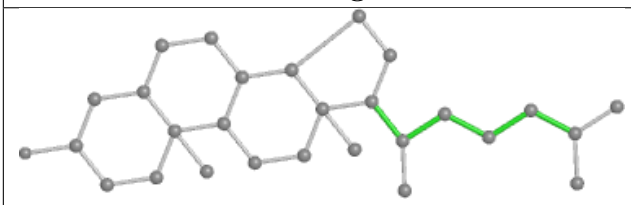
Ligand CLR R 612



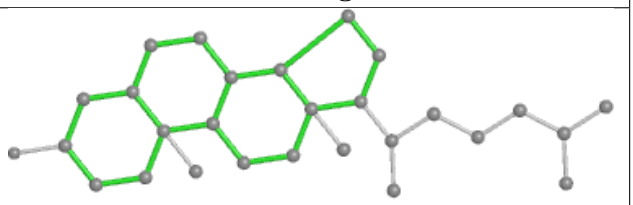
Bond lengths



Bond angles

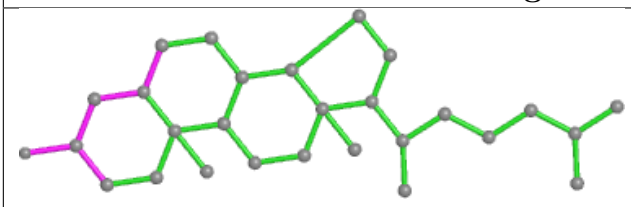


Torsions

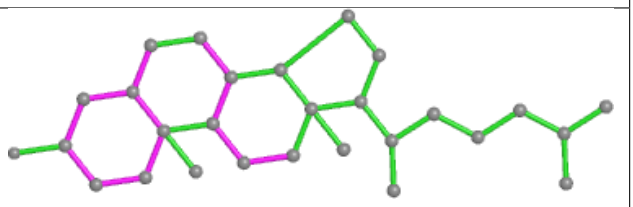


Rings

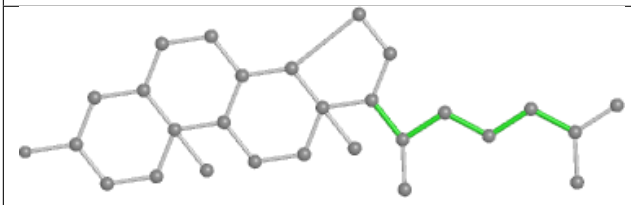
Ligand CLR R 609



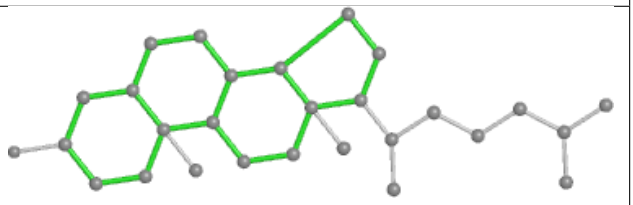
Bond lengths



Bond angles

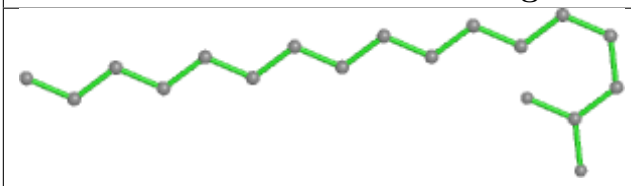


Torsions

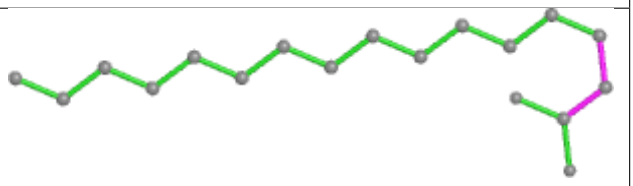


Rings

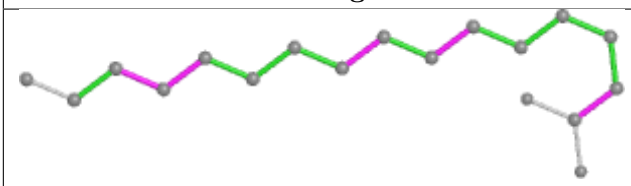
Ligand PLM R 613



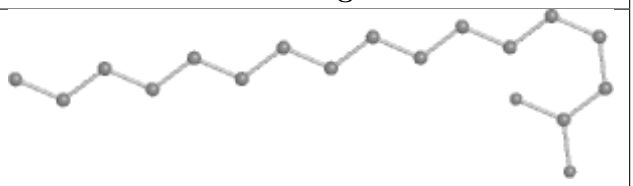
Bond lengths



Bond angles

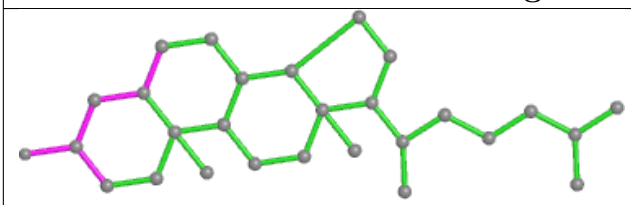


Torsions

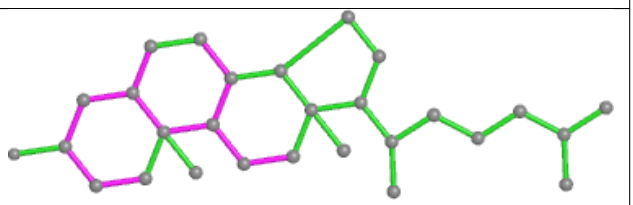


Rings

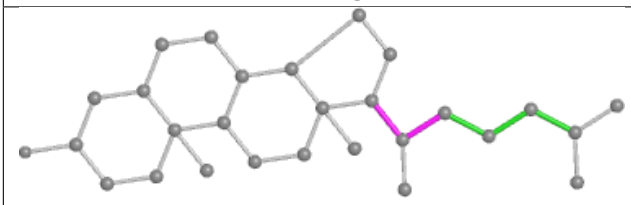
Ligand CLR R 604



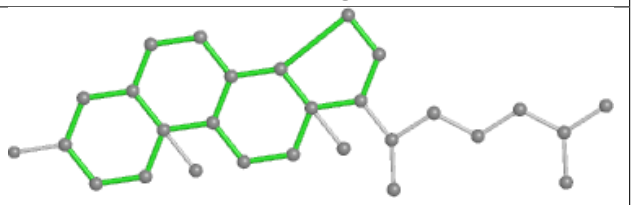
Bond lengths



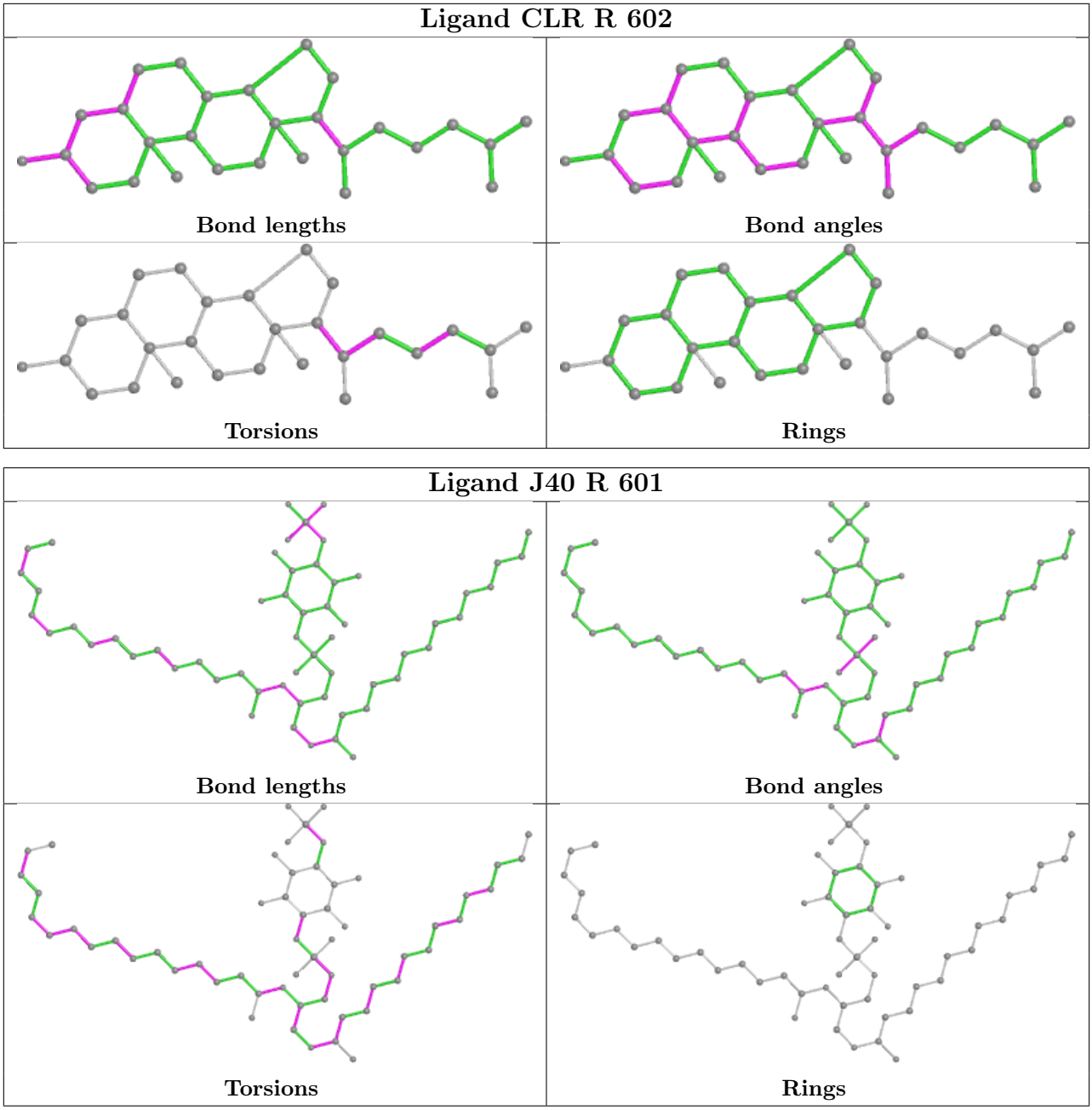
Bond angles



Torsions



Rings



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.

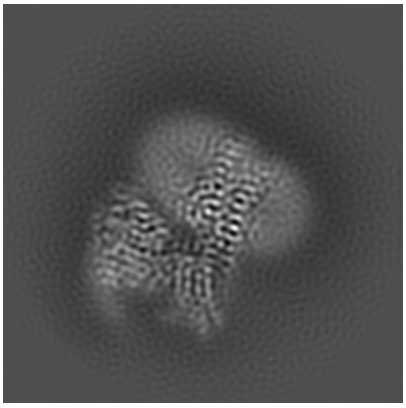
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30971. These allow visual inspection of the internal detail of the map and identification of artifacts.

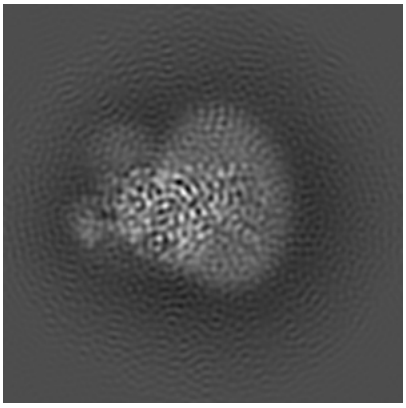
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

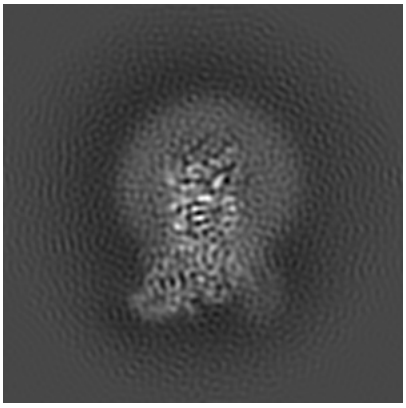
6.1.1 Primary map



X



Y

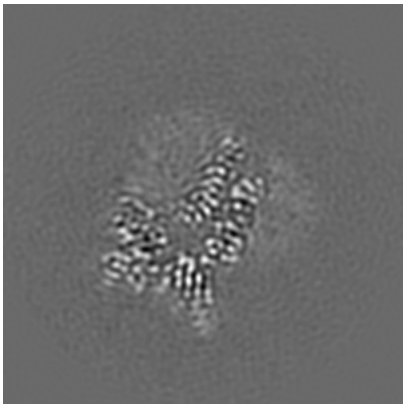


Z

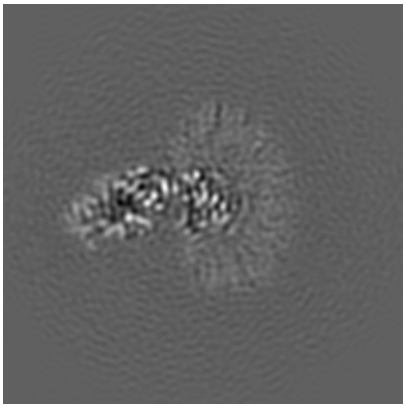
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

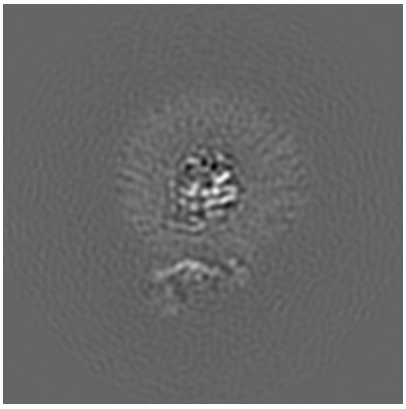
6.2.1 Primary map



X Index: 96



Y Index: 96

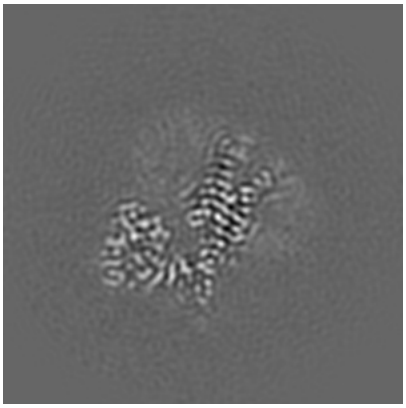


Z Index: 96

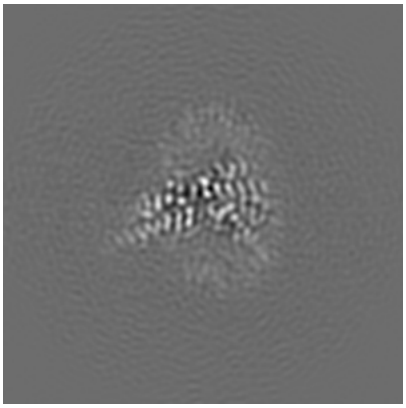
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

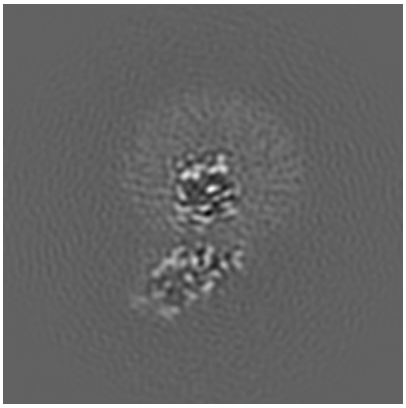
6.3.1 Primary map



X Index: 100



Y Index: 109



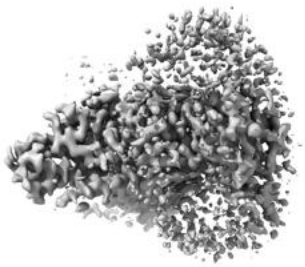
Z Index: 89

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

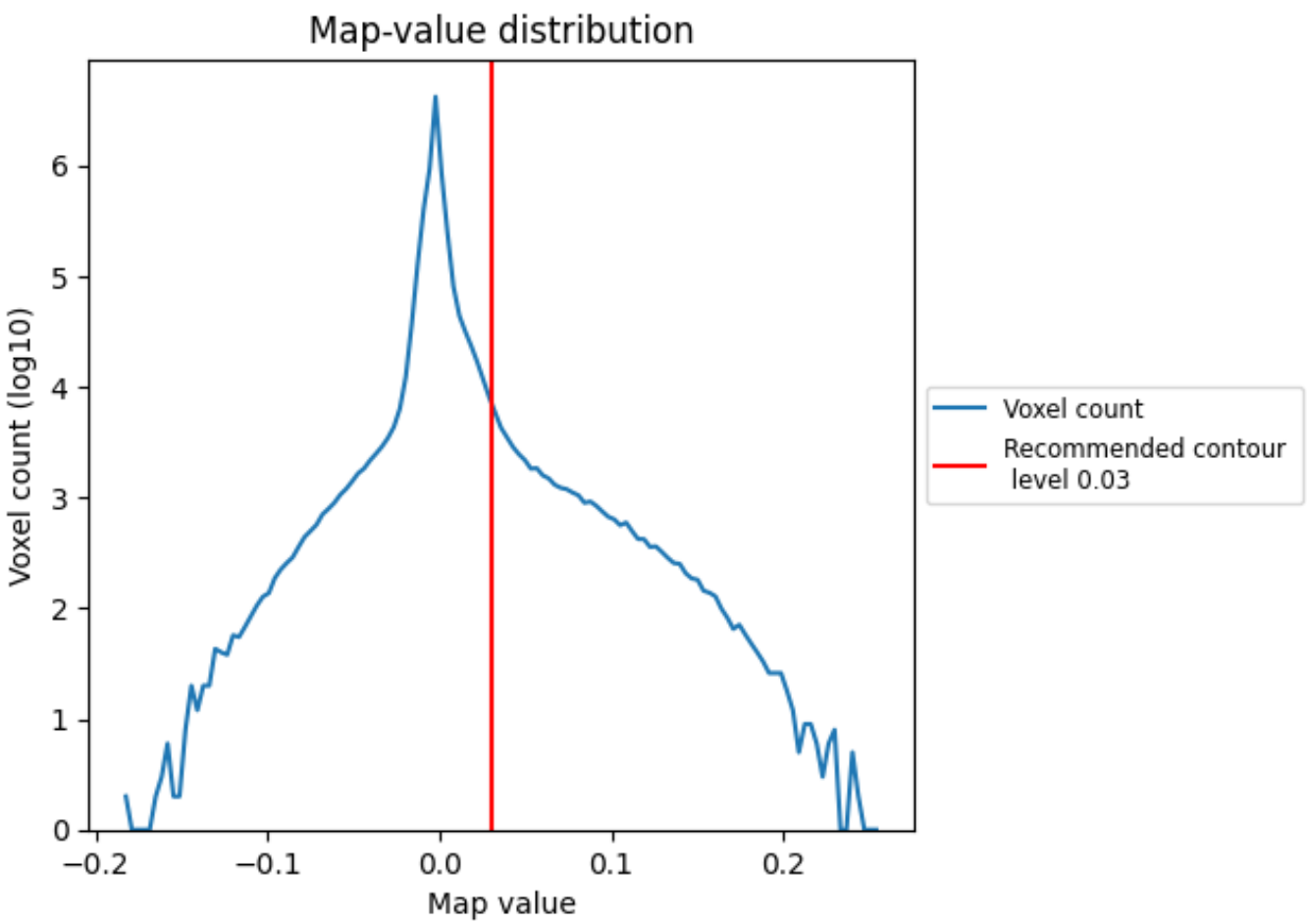
6.5 Mask visualisation (i)

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

7 Map analysis (i)

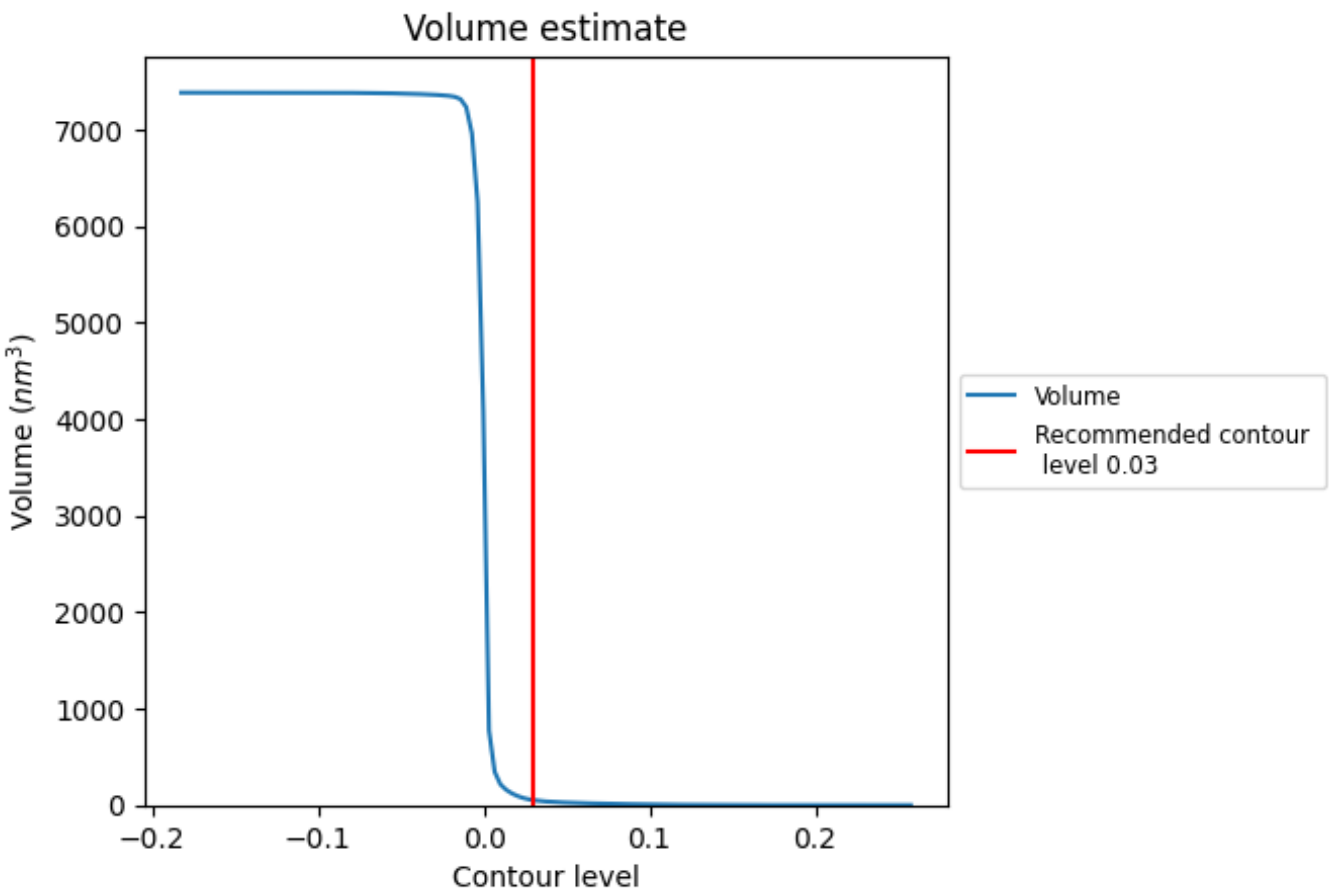
This section contains the results of statistical analysis of the map.

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.

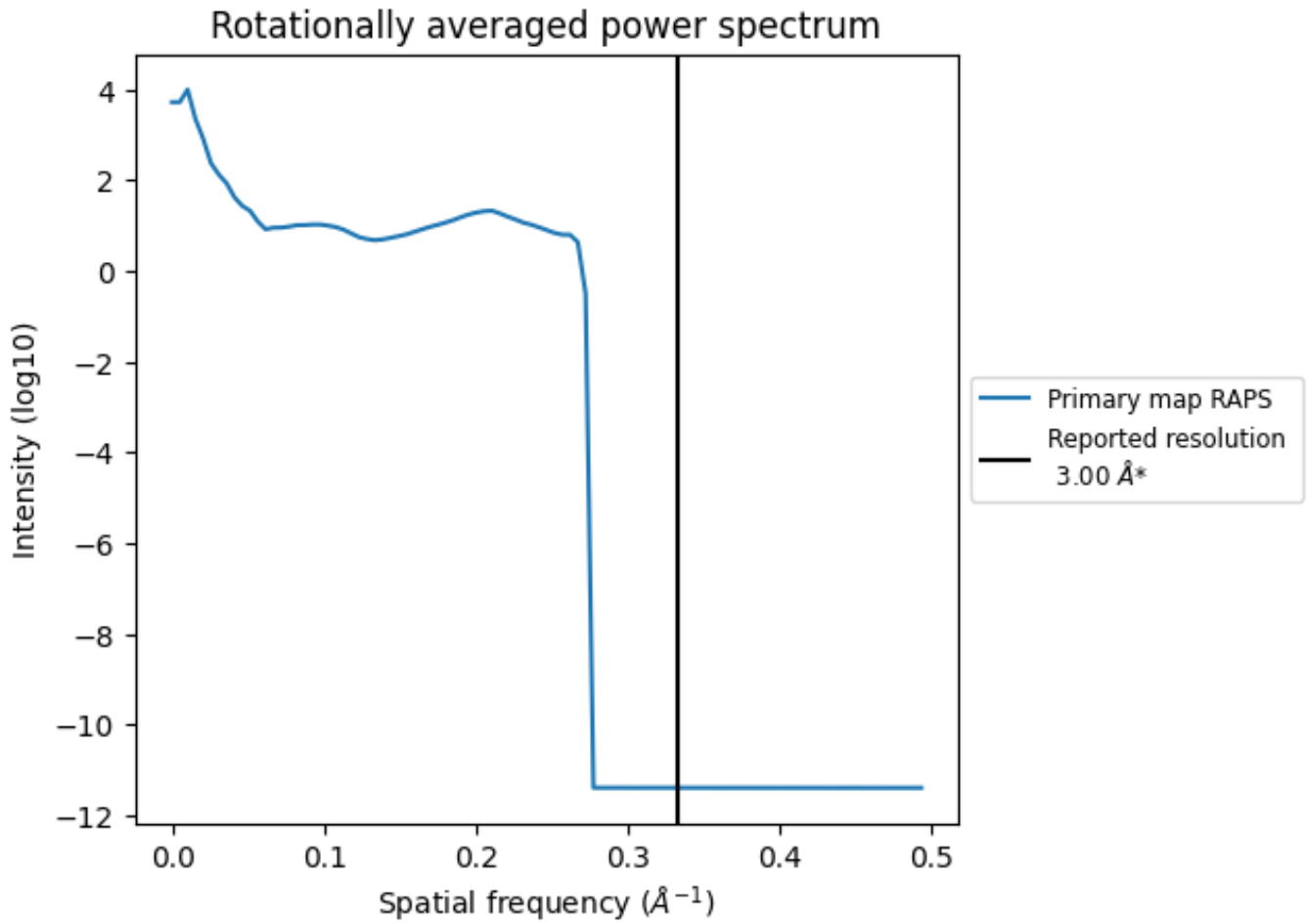
7.2 Volume estimate (i)



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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 0.333 Å^{-1}

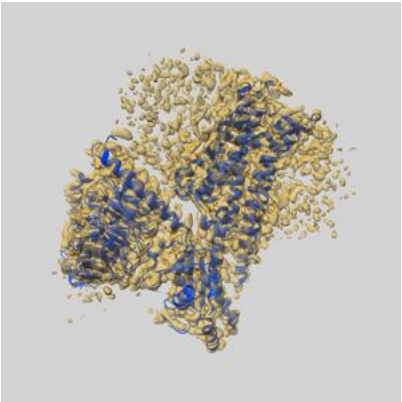
8 Fourier-Shell correlation (i)

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

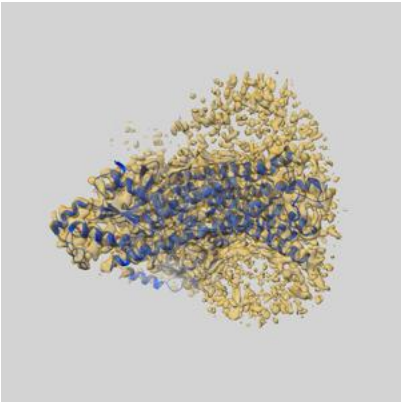
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30971 and PDB model 7E2X. Per-residue inclusion information can be found in section 3 on page 8.

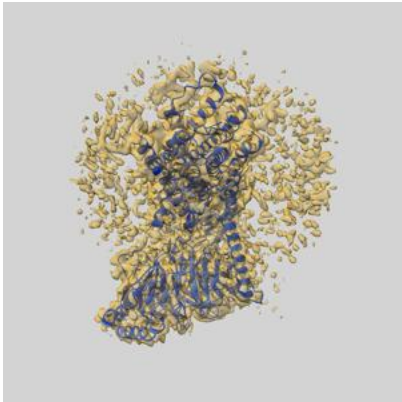
9.1 Map-model overlay (i)



X



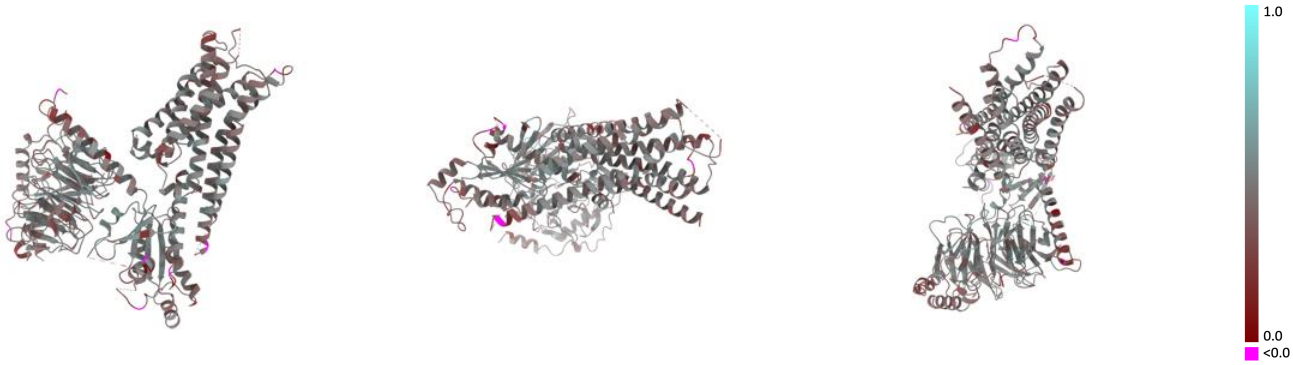
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

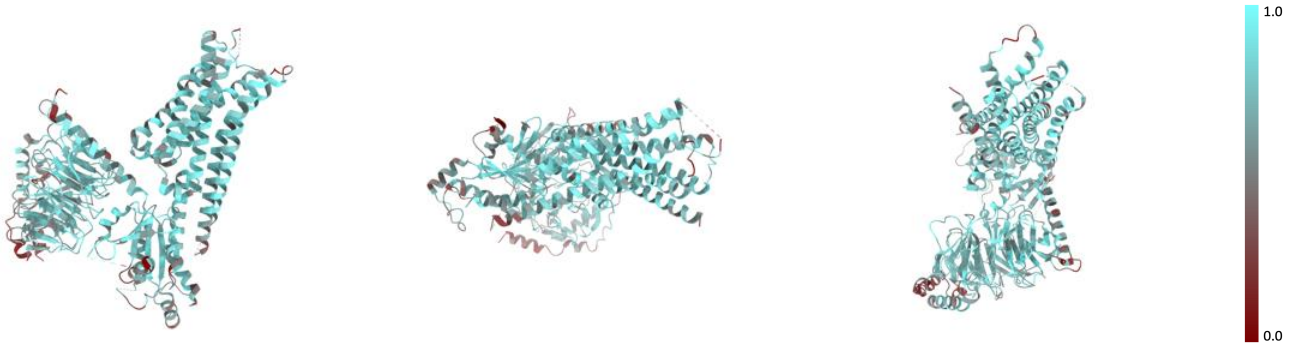
9.2 Q-score mapped to coordinate model (i)



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.

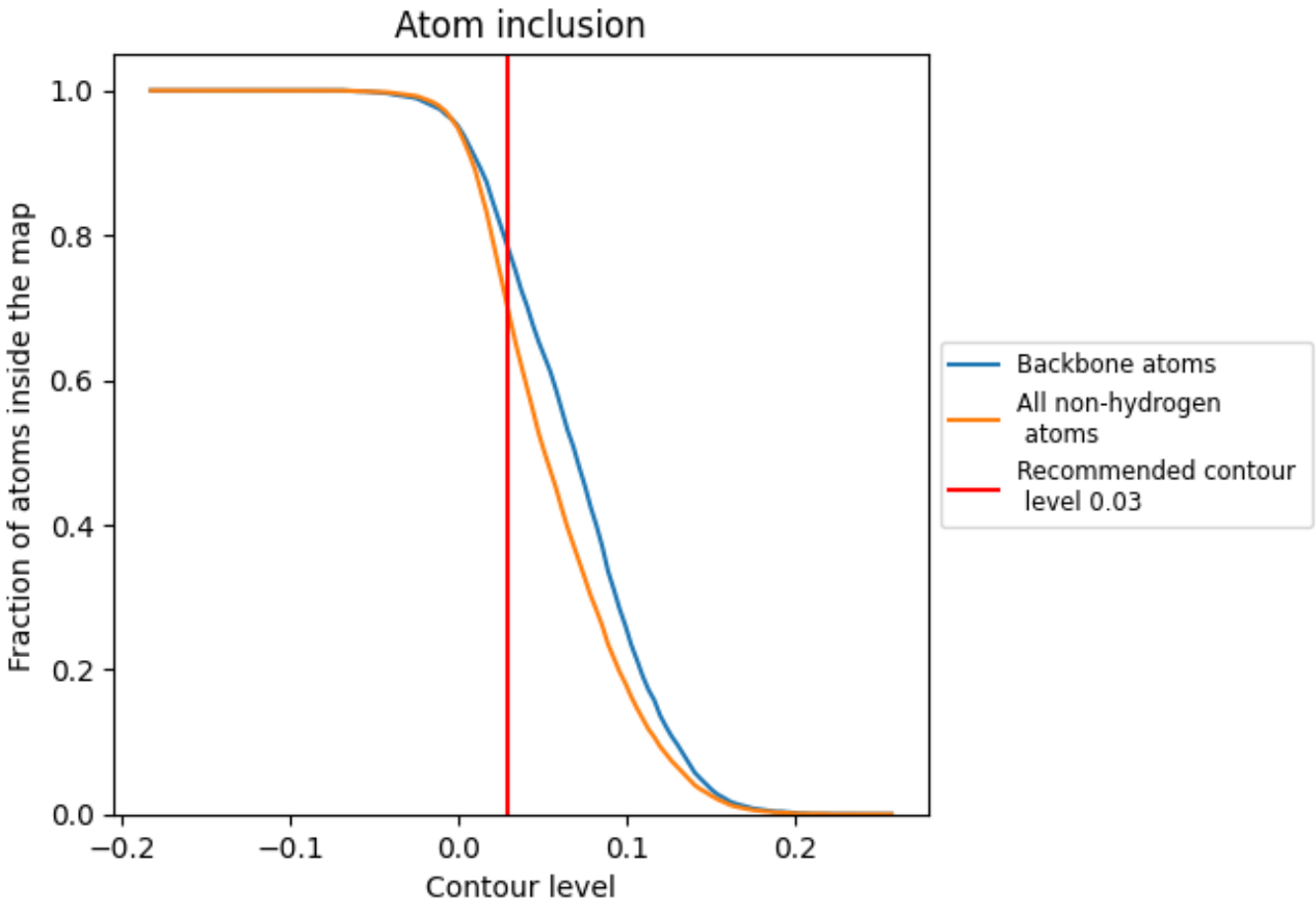
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6934	0.4240
A	0.6831	0.4160
B	0.6961	0.4400
G	0.5000	0.3340
R	0.7237	0.4260