wwPDB EM Validation Summary Report

Dec 31, 2024 – 08:44 AM EST

PDB ID	:	8IRU
EMDB ID	:	EMD-35686
Title	:	Dopamine Receptor D4R-Gi-Rotigotine complex
Authors	:	Xu, P.; Huang, S.; Zhuang, Y.; Mao, C.; Zhang, Y.; Wang, Y.; Li, H.; Jiang, Y.; Zhang, Y.; Xu, H.E.
Deposited on	:	2023-03-19
Resolution	:	3.20 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 ⓘ symbol.

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

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

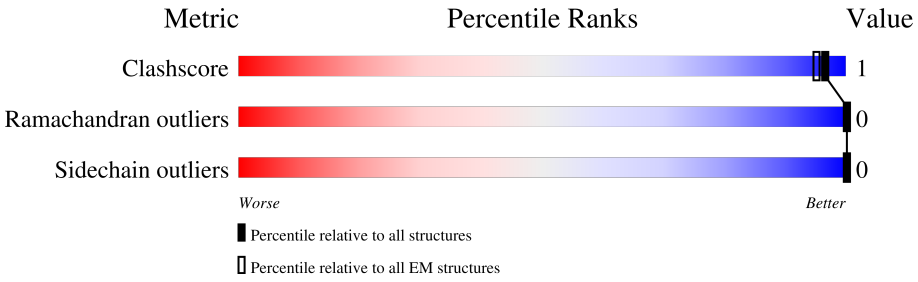
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.20 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	361	62% · 36%
2	B	371	86% · · 9%
3	E	248	89% · 7%
4	G	71	76% · 21%
5	R	785	32% · 66%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18094 atoms, of which 9088 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	H	N	O	S		
1	A	231	3771	1198	1877	336	352	8	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	337	5094	1599	2503	466	505	21	0	0

There are 32 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
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	THR	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TYR	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	GLU	-	expression tag	UNP P62873
B	364	GLU	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	LEU	-	expression tag	UNP P62873

- Molecule 3 is a protein called ScFv16.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	231	Total	C	H	N	O	S	0	0
			3492	1128	1715	294	345	10		

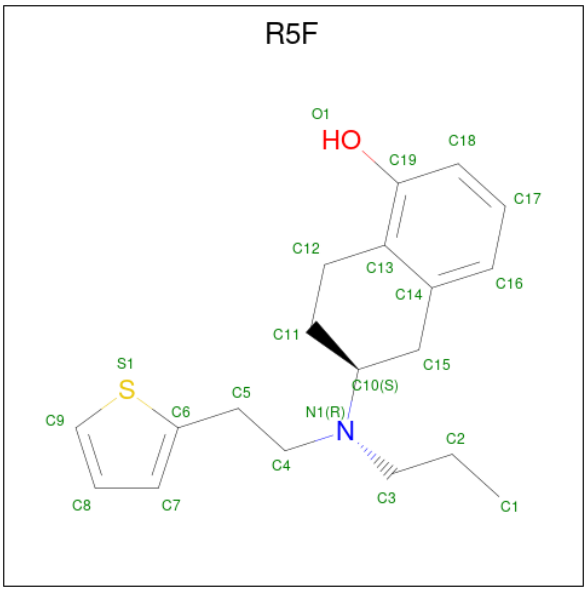
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	56	Total	C	H	N	O	S	0	0
			887	274	451	77	82	3		

- Molecule 5 is a protein called D(4) dopamine receptor.

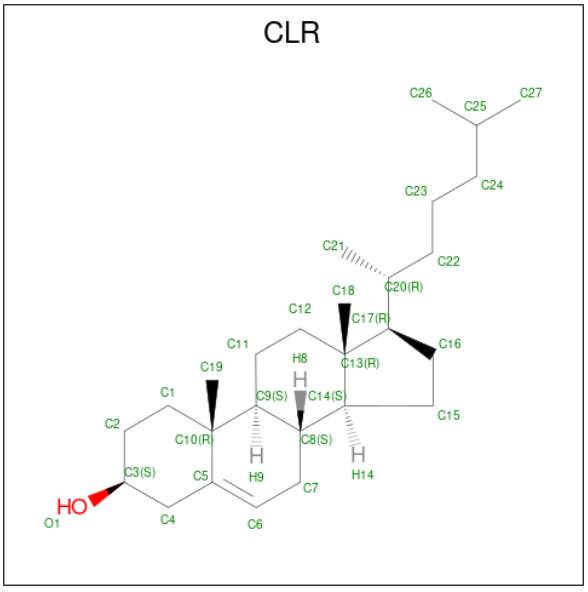
Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	268	Total	C	H	N	O	S	0	0
			4137	1327	2103	348	343	16		

- Molecule 6 is Rotigotine (three-letter code: R5F) (formula: $C_{19}H_{25}NOS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	R	1	Total	C	H	N	O	S	0
			47	19	25	1	1	1	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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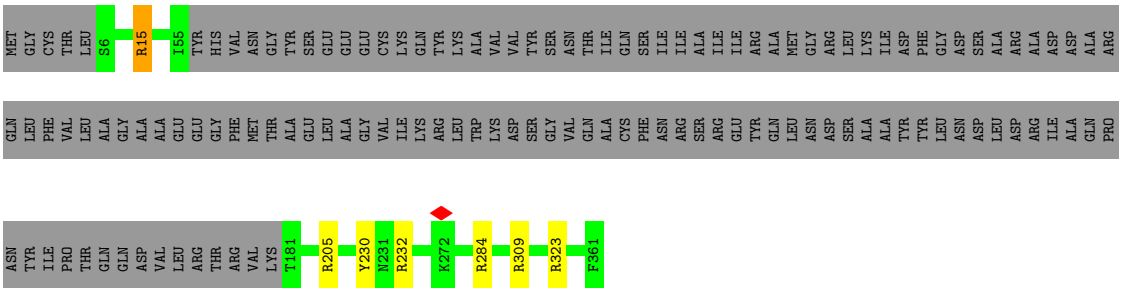
Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	H	O	0
			74	27	46	1	
7	R	1	Total	C	H	O	0
			74	27	46	1	
7	R	1	Total	C	H	O	0
			74	27	46	1	
7	R	1	Total	C	H	O	0
			74	27	46	1	
7	R	1	Total	C	H	O	0
			74	27	46	1	
7	R	1	Total	C	H	O	0
			74	27	46	1	

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.

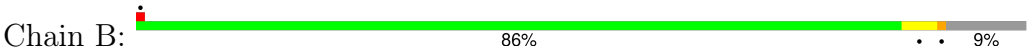
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

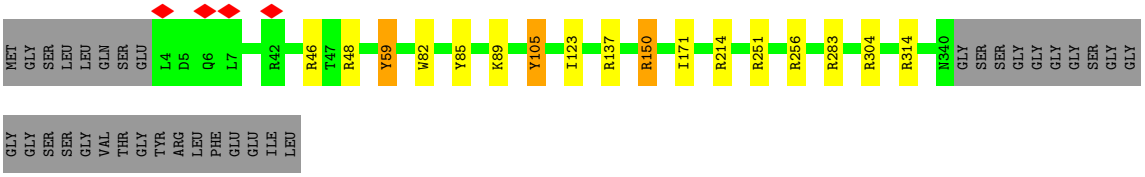
Chain A:



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

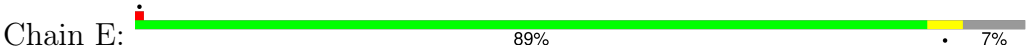
Chain B:

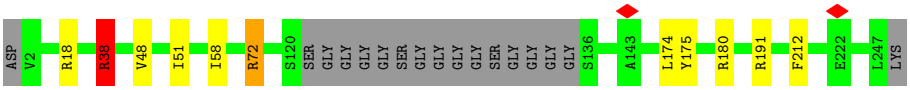




• Molecule 3: ScFv16

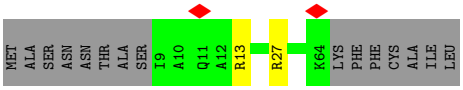
Chain E:





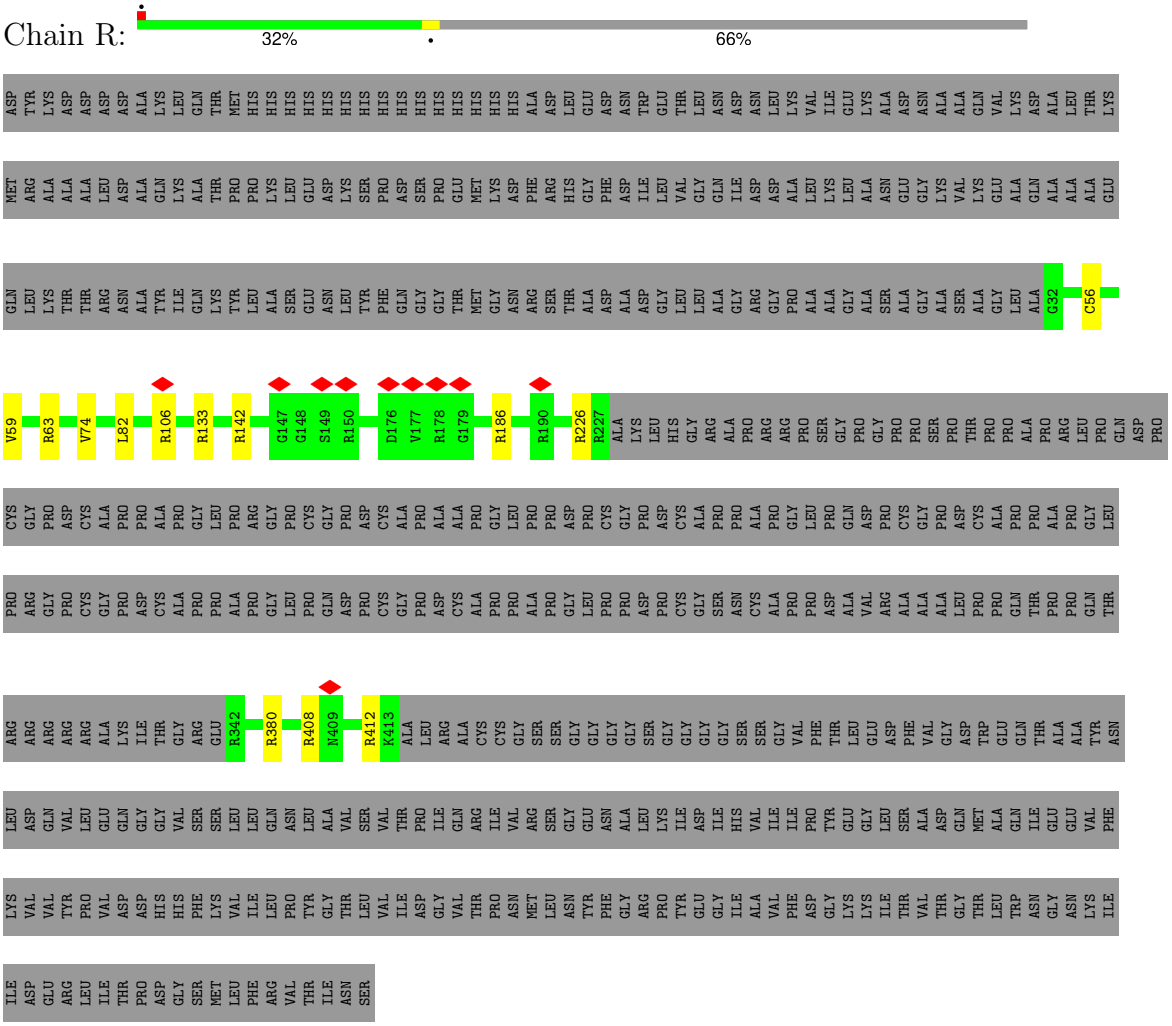
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



• Molecule 5: D(4) dopamine receptor

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	471638	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 ($e^-/Å^2$)	64	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	0.111	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R5F, 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	0.66	0/1930	1.04	8/2599 (0.3%)
2	B	0.61	0/2638	1.08	14/3577 (0.4%)
3	E	0.65	0/1821	1.02	7/2469 (0.3%)
4	G	0.58	0/442	0.99	2/595 (0.3%)
5	R	0.63	0/2079	1.01	8/2844 (0.3%)
All	All	0.63	0/8910	1.04	39/12084 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
3	E	0	3
5	R	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	105	TYR	CB-CG-CD1	-9.90	115.06	121.00
4	G	27	ARG	NE-CZ-NH2	9.39	125.00	120.30
1	A	309	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	205	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	B	59	TYR	CB-CG-CD1	-7.81	116.31	121.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
2	B	105	TYR	Sidechain
2	B	150	ARG	Sidechain
2	B	59	TYR	Sidechain
3	E	38	ARG	Sidechain

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	1894	1877	1873	0	0
2	B	2591	2503	2499	2	0
3	E	1777	1715	1712	3	0
4	G	436	451	450	0	0
5	R	2034	2103	2101	5	0
6	R	22	25	0	0	0
7	R	252	414	414	8	0
All	All	9006	9088	9049	13	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.

The worst 5 of 13 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)
7:R:607:CLR:H183	7:R:607:CLR:H212	1.53	0.89
5:R:56:CYS:SG	7:R:607:CLR:H213	2.35	0.66
3:E:38:ARG:HD3	3:E:48:VAL:CG1	2.42	0.49
7:R:606:CLR:H71	7:R:607:CLR:H14	1.95	0.48
7:R:607:CLR:H212	7:R:607:CLR:C18	2.34	0.46

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	227/361 (63%)	215 (95%)	12 (5%)	0	100	100
2	B	335/371 (90%)	324 (97%)	11 (3%)	0	100	100
3	E	227/248 (92%)	222 (98%)	5 (2%)	0	100	100
4	G	54/71 (76%)	54 (100%)	0	0	100	100
5	R	264/785 (34%)	254 (96%)	10 (4%)	0	100	100
All	All	1107/1836 (60%)	1069 (97%)	38 (3%)	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	206/314 (66%)	206 (100%)	0	100	100
2	B	280/302 (93%)	280 (100%)	0	100	100
3	E	196/201 (98%)	196 (100%)	0	100	100
4	G	46/58 (79%)	46 (100%)	0	100	100
5	R	217/622 (35%)	217 (100%)	0	100	100
All	All	945/1497 (63%)	945 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	88	ASN

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)

10 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	CLR	R	609	-	31,31,31	1.17	1 (3%)	48,48,48	0.58	0
7	CLR	R	607	-	31,31,31	0.35	0	48,48,48	0.82	1 (2%)
7	CLR	R	610	-	31,31,31	1.18	2 (6%)	48,48,48	0.46	0
7	CLR	R	606	-	31,31,31	1.08	2 (6%)	48,48,48	0.60	0
7	CLR	R	608	-	31,31,31	1.19	2 (6%)	48,48,48	0.65	0
7	CLR	R	605	-	31,31,31	1.16	2 (6%)	48,48,48	0.86	2 (4%)
7	CLR	R	604	-	31,31,31	1.16	2 (6%)	48,48,48	0.64	0
7	CLR	R	603	-	31,31,31	1.17	2 (6%)	48,48,48	0.50	0
7	CLR	R	602	-	31,31,31	1.14	1 (3%)	48,48,48	0.68	1 (2%)
6	R5F	R	601	-	24,24,24	1.21	3 (12%)	25,32,32	1.29	3 (12%)

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	CLR	R	609	-	-	2/10/68/68	0/4/4/4
7	CLR	R	607	-	-	9/10/68/68	0/4/4/4
7	CLR	R	610	-	-	3/10/68/68	0/4/4/4
7	CLR	R	606	-	-	0/10/68/68	0/4/4/4
7	CLR	R	608	-	-	1/10/68/68	0/4/4/4
7	CLR	R	605	-	-	2/10/68/68	0/4/4/4
7	CLR	R	604	-	-	3/10/68/68	0/4/4/4
7	CLR	R	603	-	-	2/10/68/68	0/4/4/4
7	CLR	R	602	-	-	0/10/68/68	0/4/4/4
6	R5F	R	601	-	-	2/11/21/21	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	R5F	C4-N1	4.05	1.53	1.47
6	R	601	R5F	C3-N1	2.72	1.51	1.47
7	R	605	CLR	C11-C9	2.65	1.58	1.53
7	R	609	CLR	C11-C9	2.65	1.58	1.53
7	R	604	CLR	C11-C9	2.59	1.58	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	601	R5F	C3-N1-C10	-3.87	105.77	113.23
7	R	607	CLR	C7-C8-C9	2.76	112.91	109.72
6	R	601	R5F	C8-C9-S1	2.65	115.13	112.98
6	R	601	R5F	C3-N1-C4	-2.54	108.06	112.22
7	R	605	CLR	C11-C9-C8	2.44	115.18	111.78

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	R5F	N1-C4-C5-C6
7	R	607	CLR	C13-C17-C20-C21
7	R	607	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
7	R	610	CLR	C17-C20-C22-C23
7	R	603	CLR	C17-C20-C22-C23

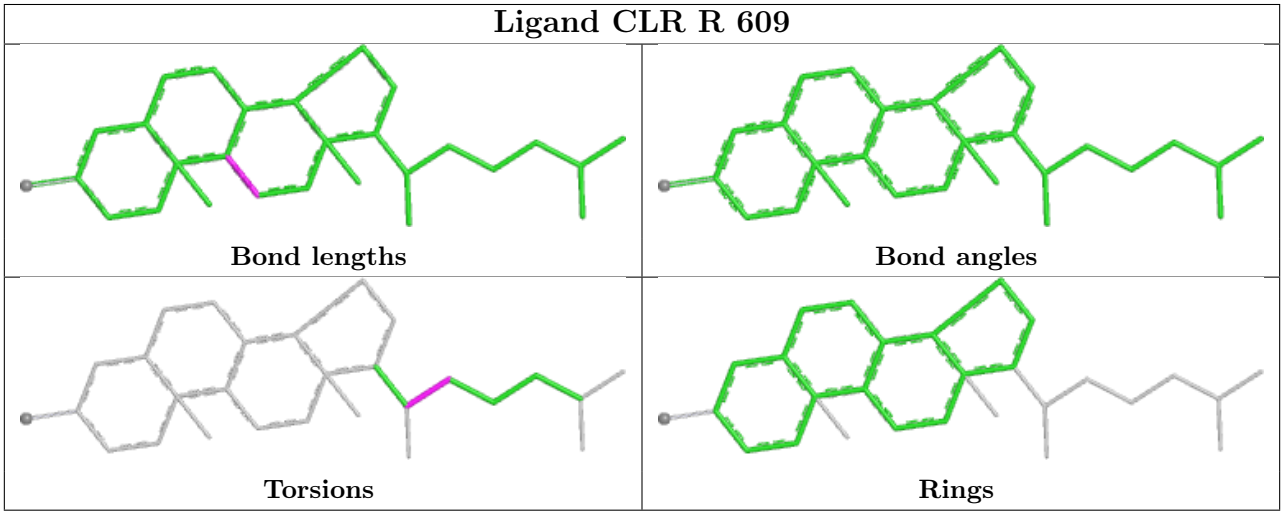
There are no ring outliers.

2 monomers are involved in 8 short contacts:

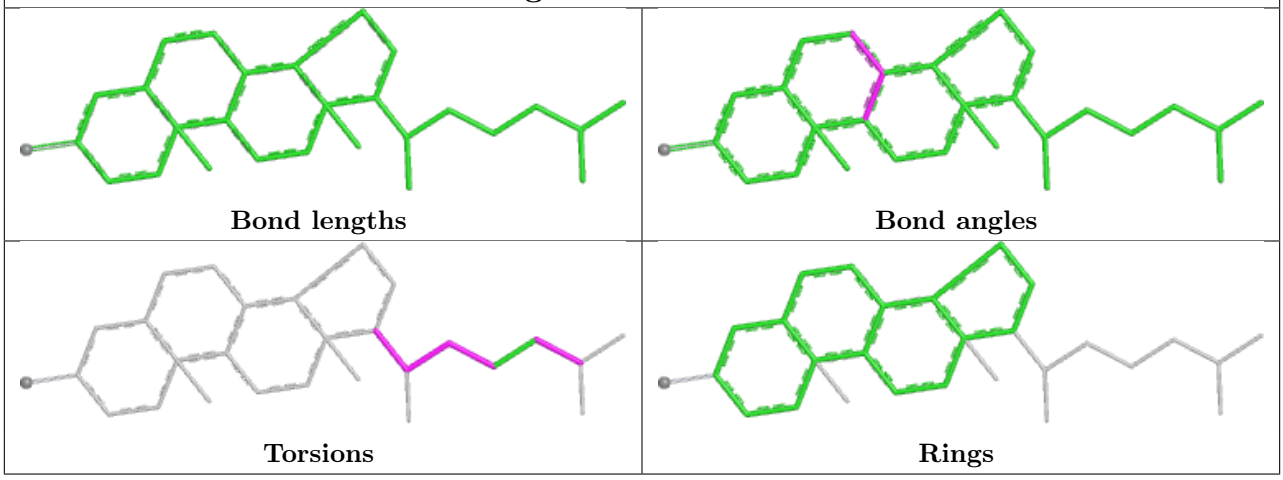
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	607	CLR	8	0
7	R	606	CLR	1	0

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.

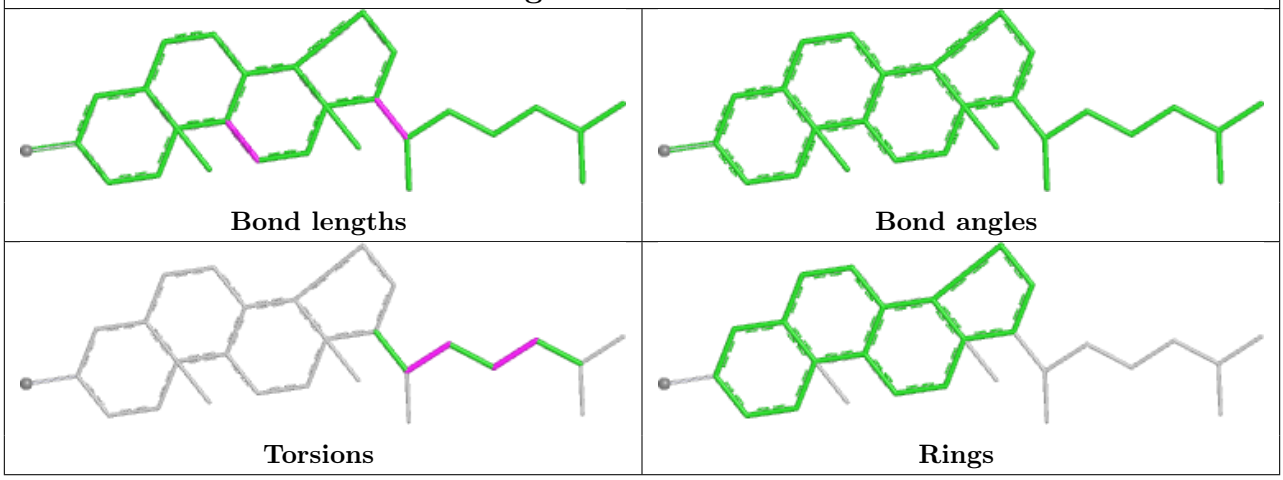
Ligand CLR R 609



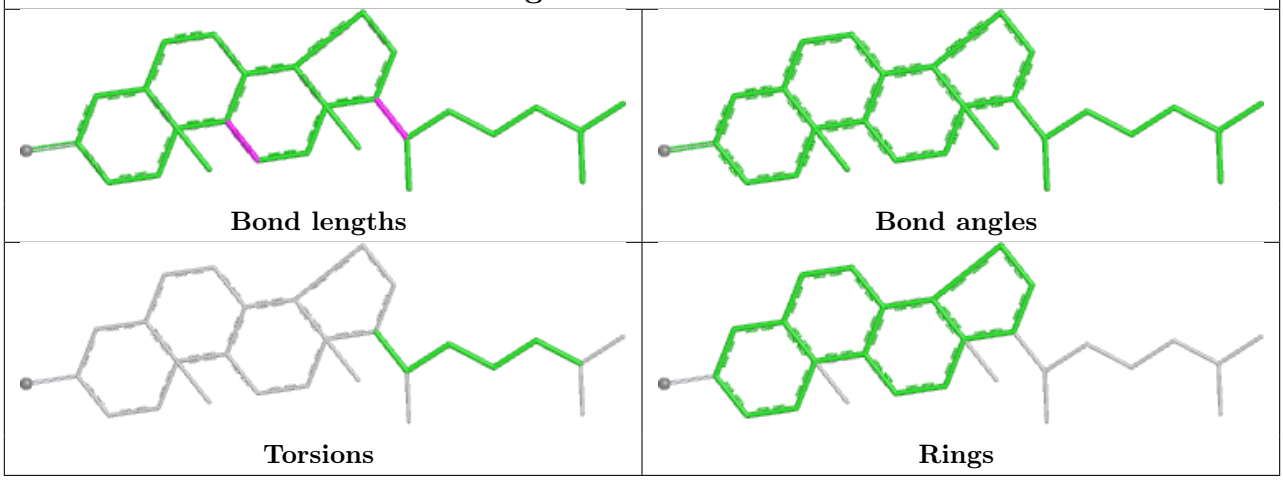
Ligand CLR R 607



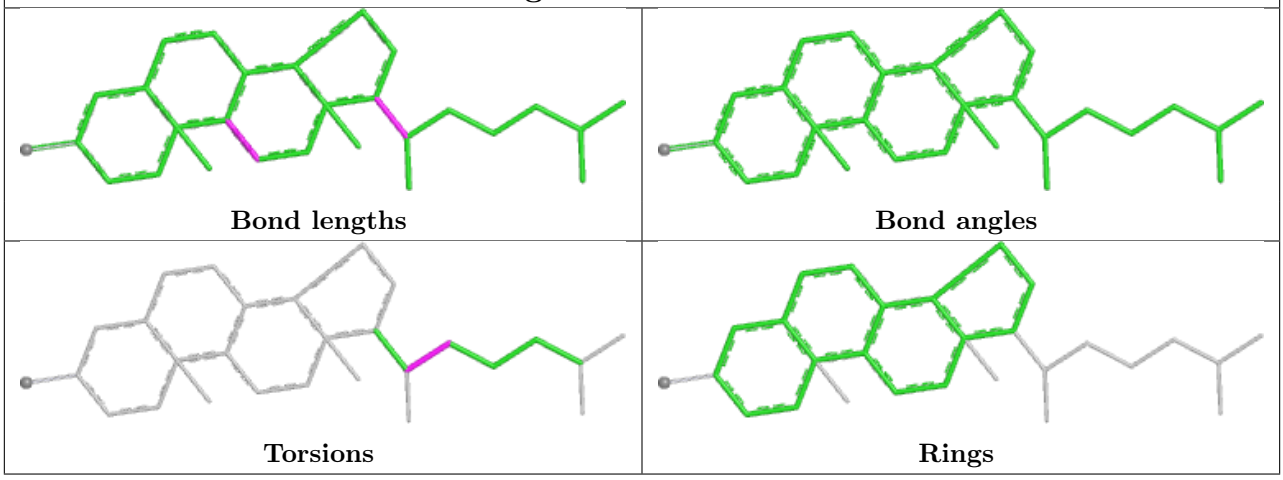
Ligand CLR R 610



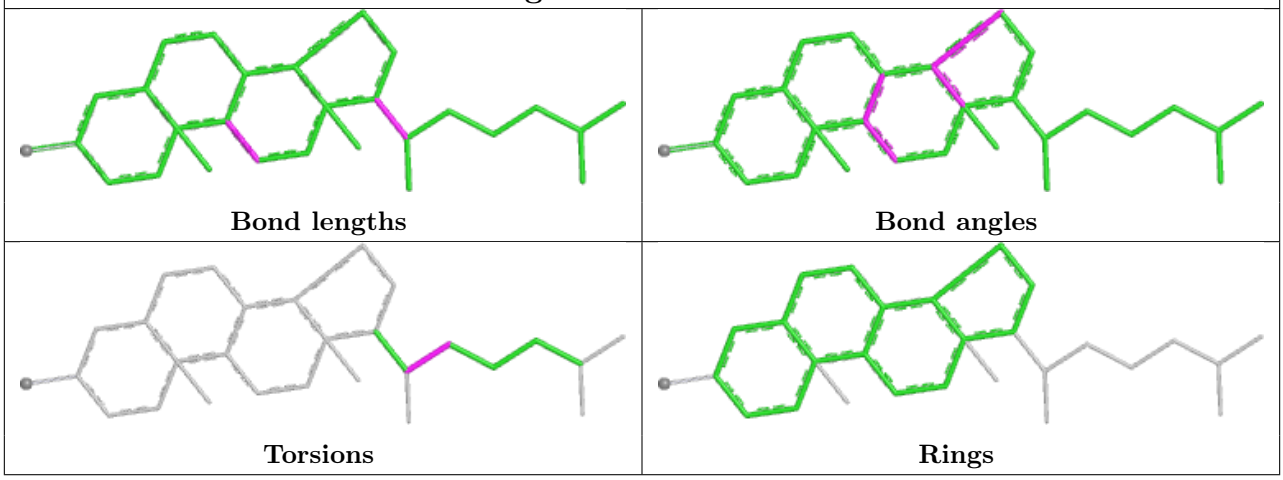
Ligand CLR R 606



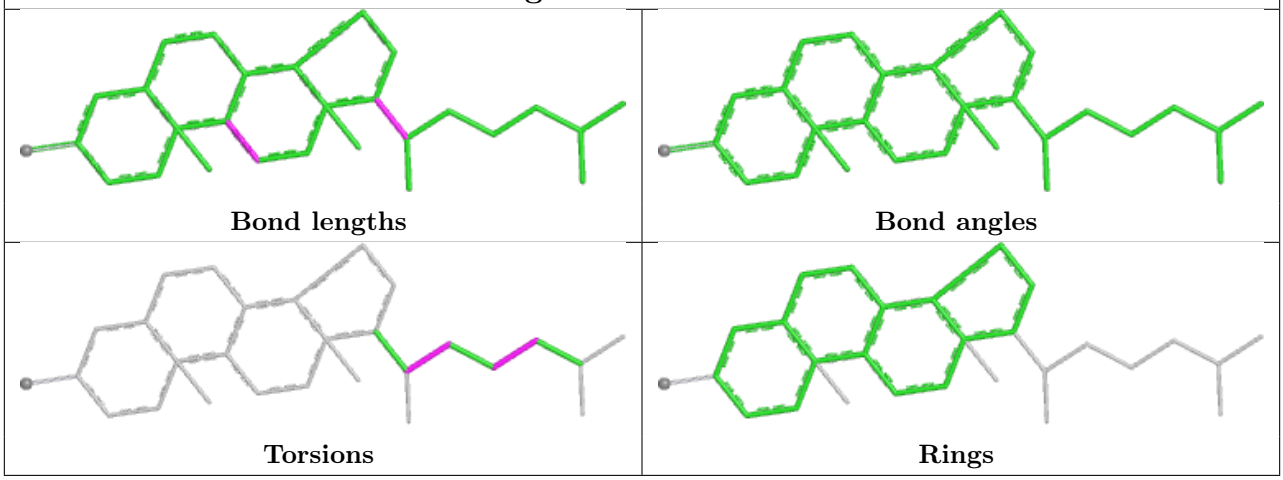
Ligand CLR R 608



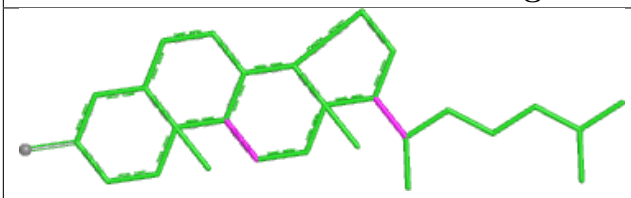
Ligand CLR R 605



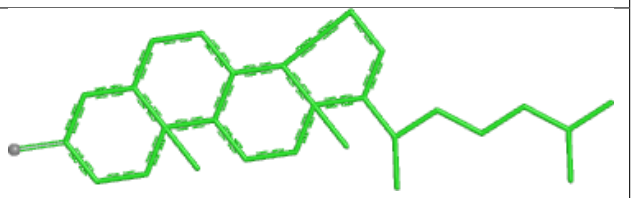
Ligand CLR R 604



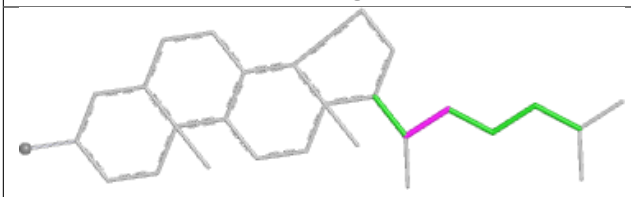
Ligand CLR R 603



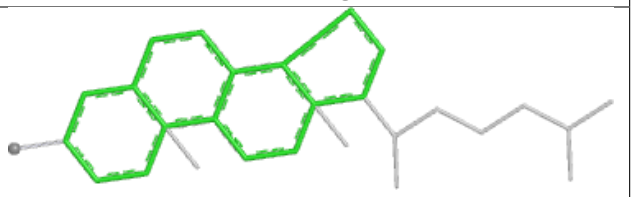
Bond lengths



Bond angles

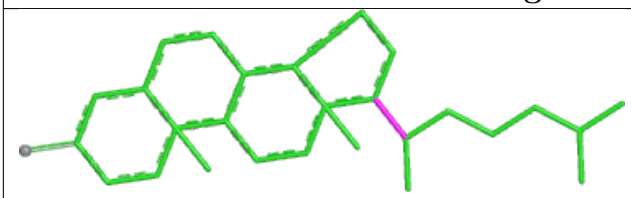


Torsions

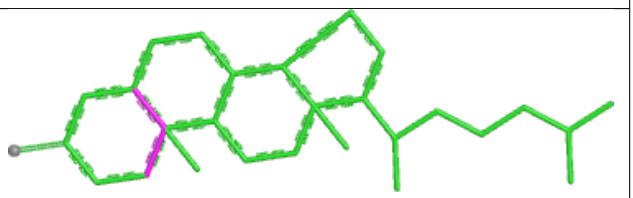


Rings

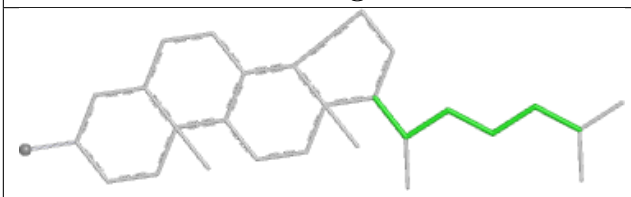
Ligand CLR R 602



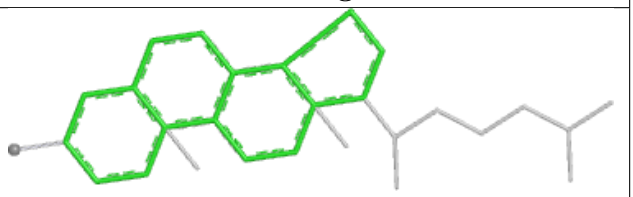
Bond lengths



Bond angles

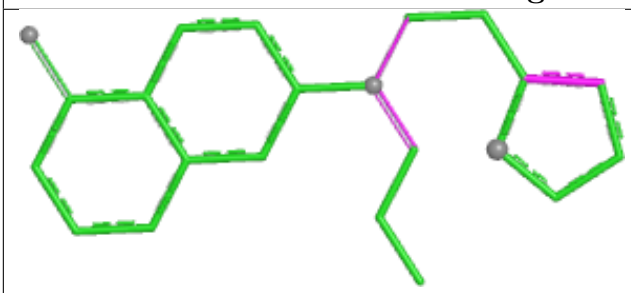


Torsions

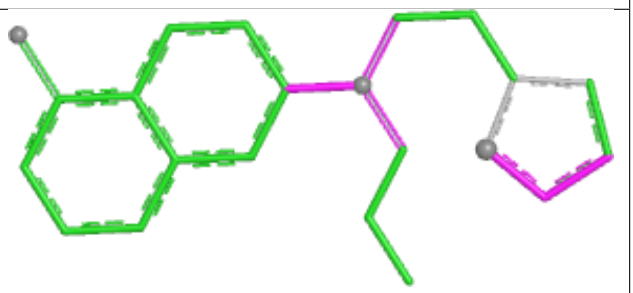


Rings

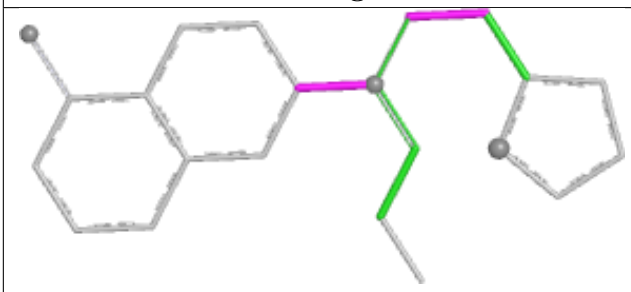
Ligand R5F R 601



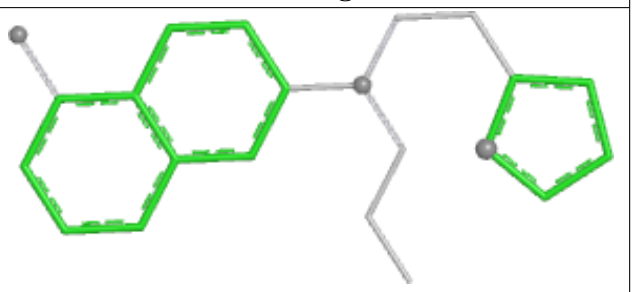
Bond lengths



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.

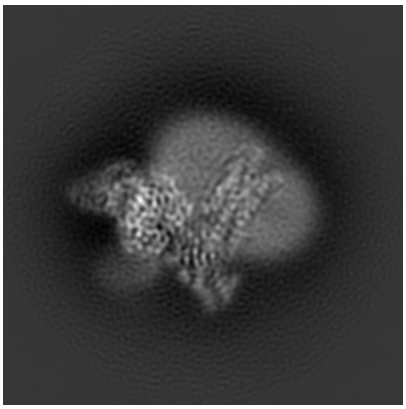
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35686. These allow visual inspection of the internal detail of the map and identification of artifacts.

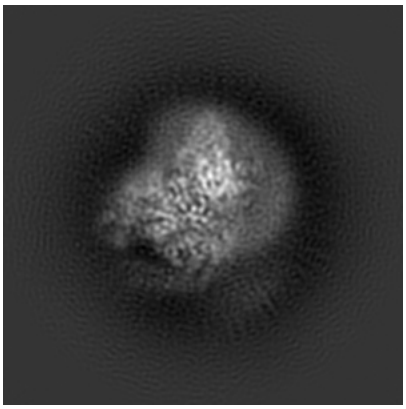
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

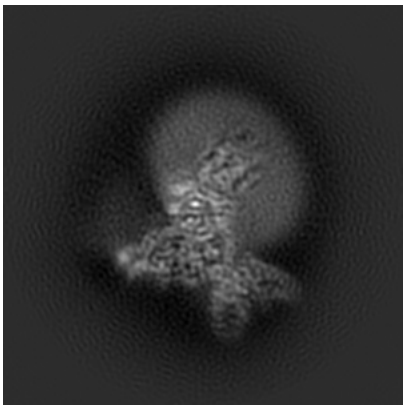
6.1.1 Primary map



X

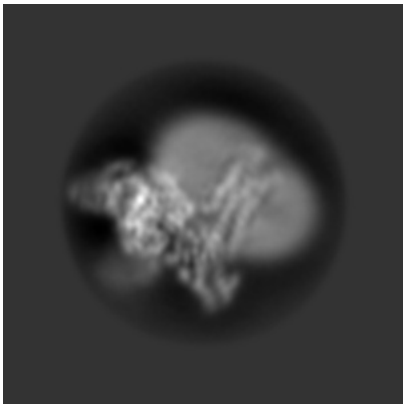


Y

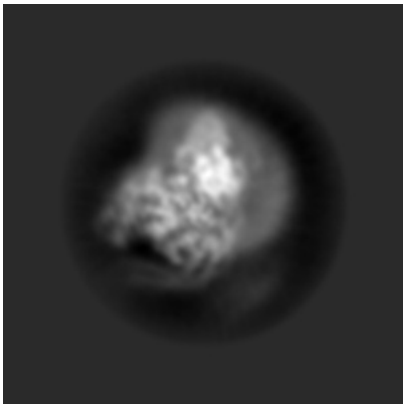


Z

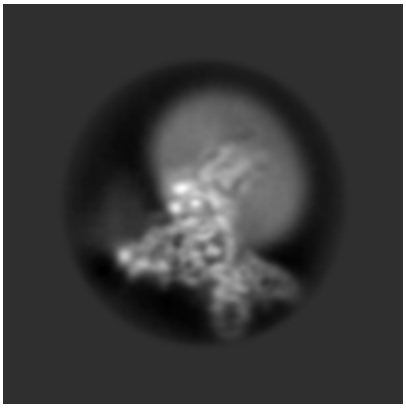
6.1.2 Raw map



X



Y

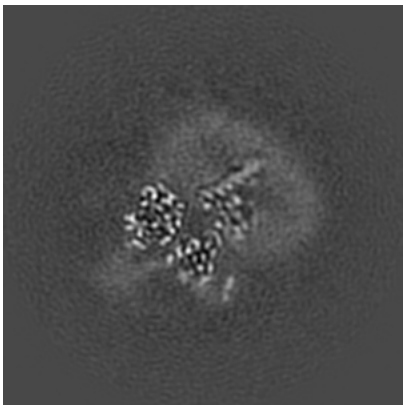


Z

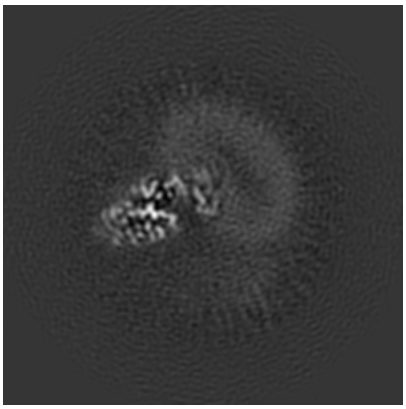
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

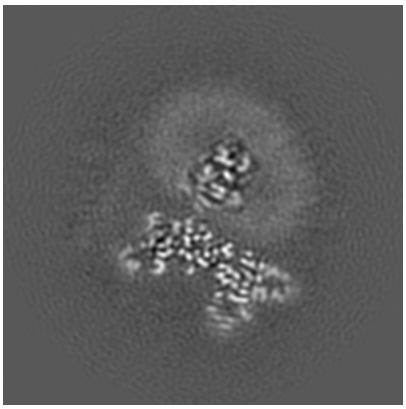
6.2.1 Primary map



X Index: 100

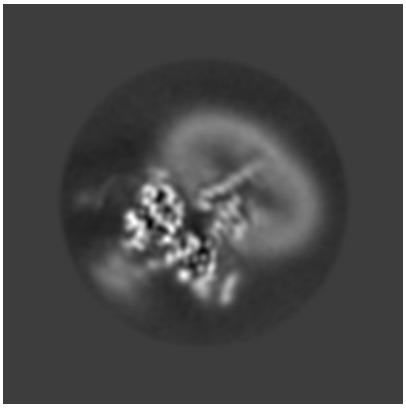


Y Index: 100

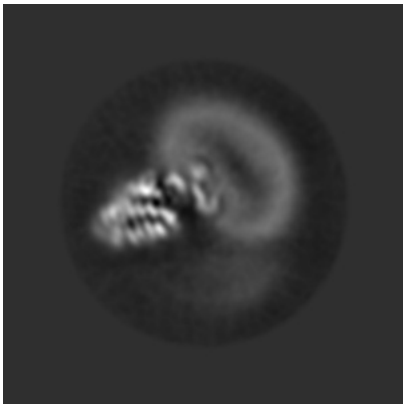


Z Index: 100

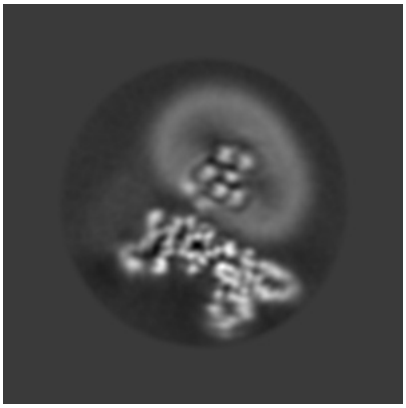
6.2.2 Raw map



X Index: 100



Y Index: 100

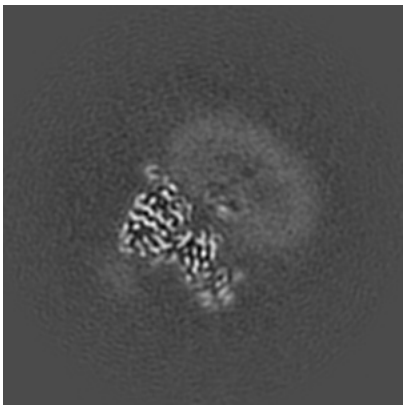


Z Index: 100

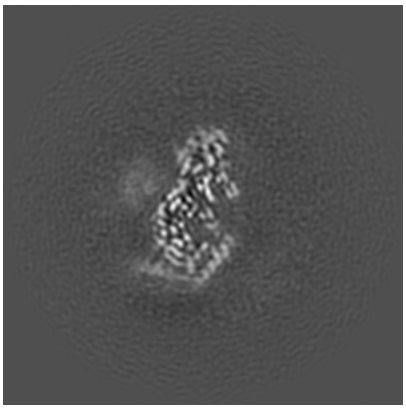
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

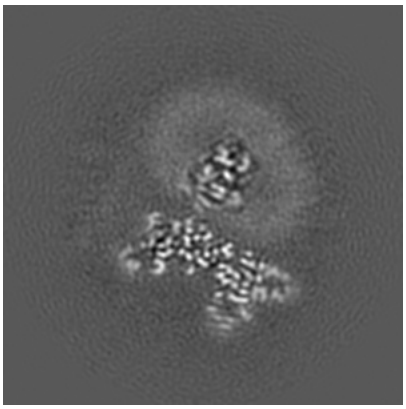
6.3.1 Primary map



X Index: 94

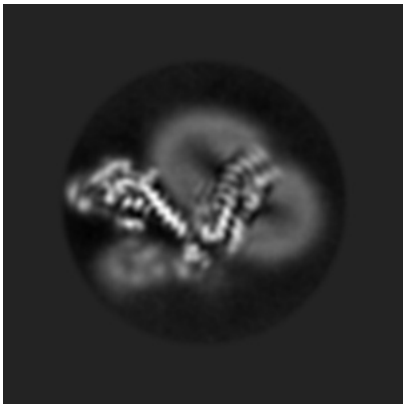


Y Index: 68

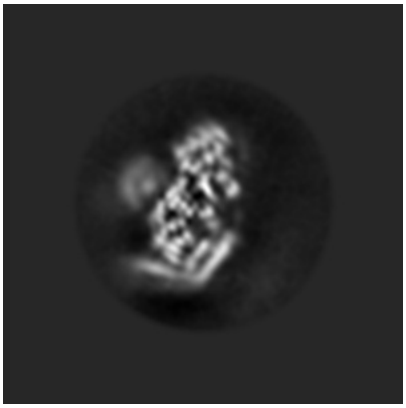


Z Index: 100

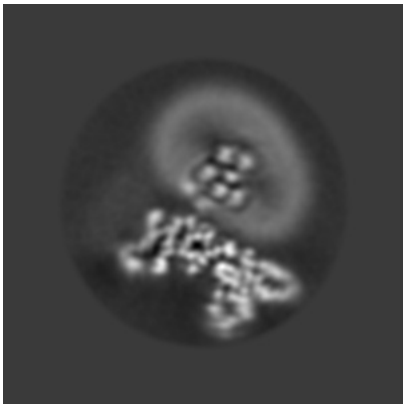
6.3.2 Raw map



X Index: 112



Y Index: 68

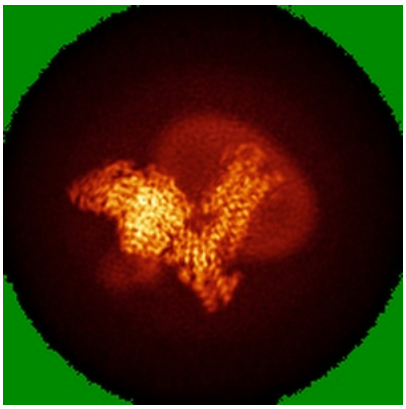


Z Index: 100

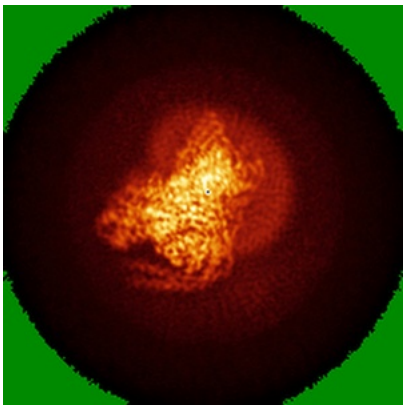
The images above show the largest variance slices of the map in three orthogonal directions.

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

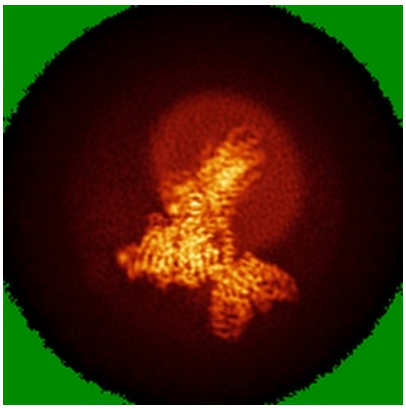
6.4.1 Primary map



X

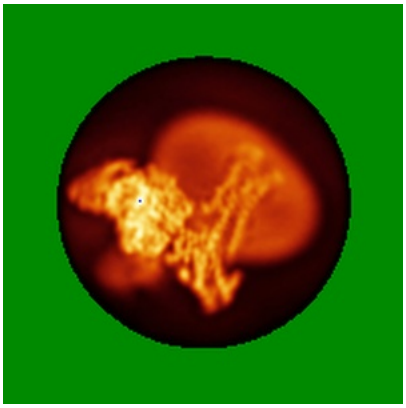


Y

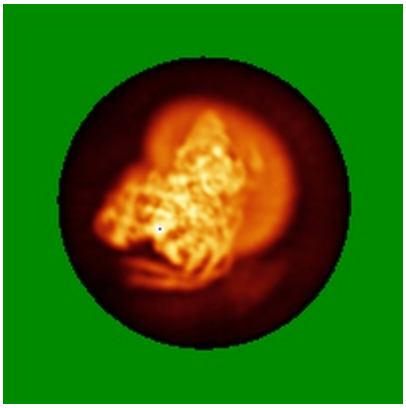


Z

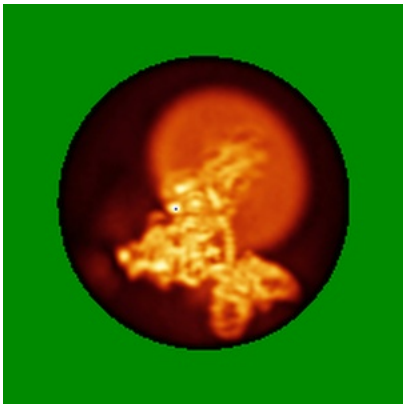
6.4.2 Raw map



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 0.016. 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.

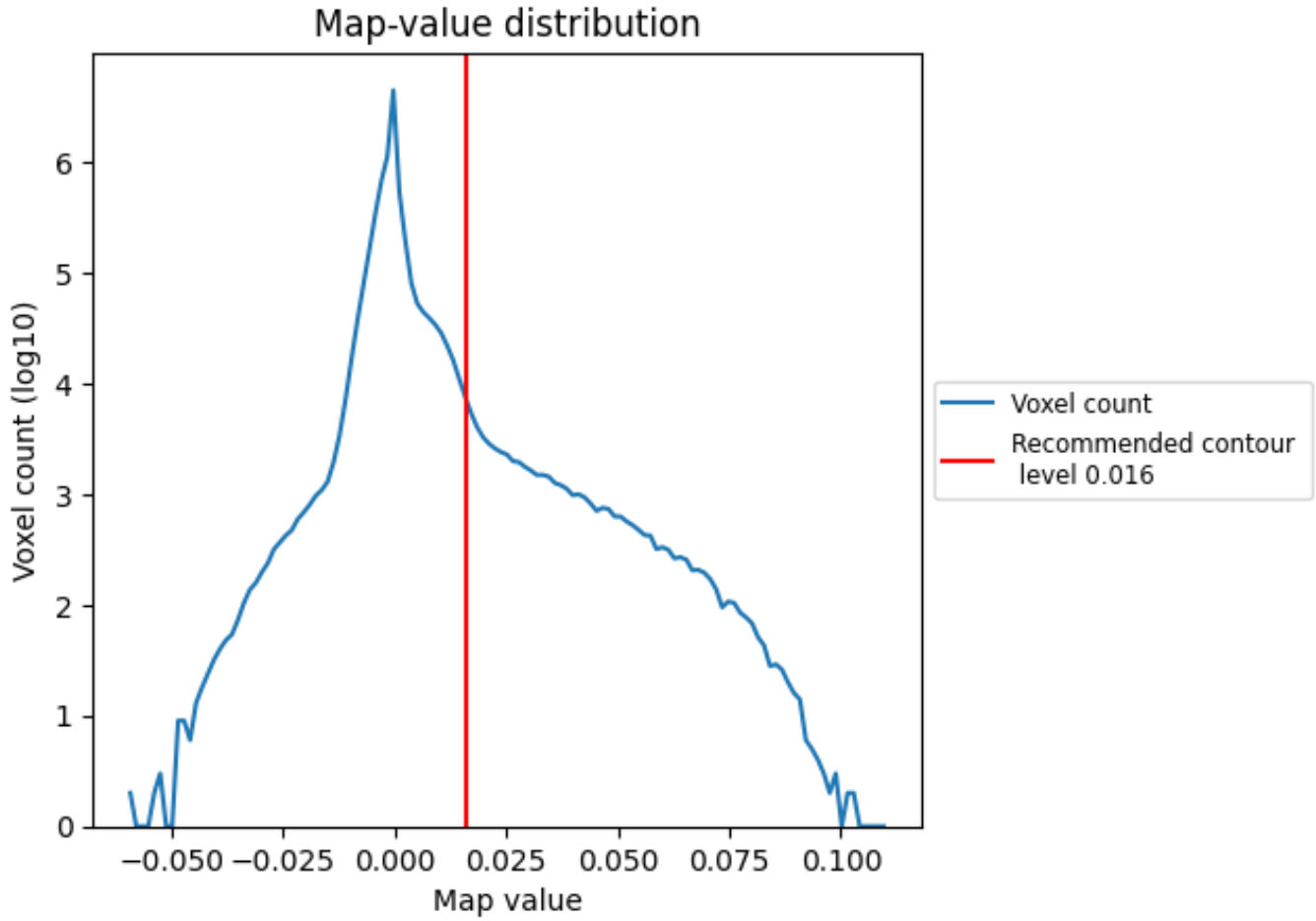
6.6 Mask visualisation (i)

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

7 Map analysis

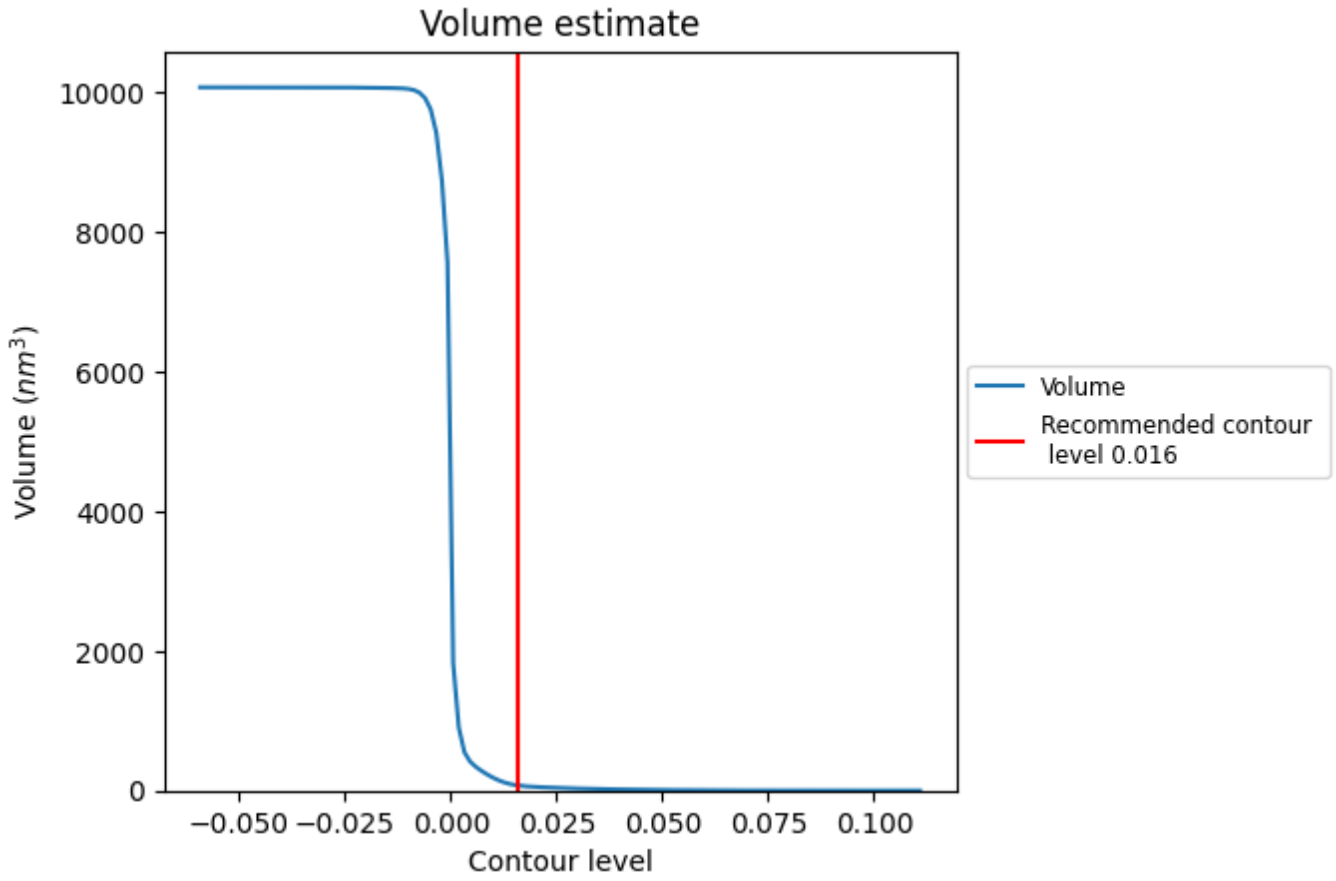
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

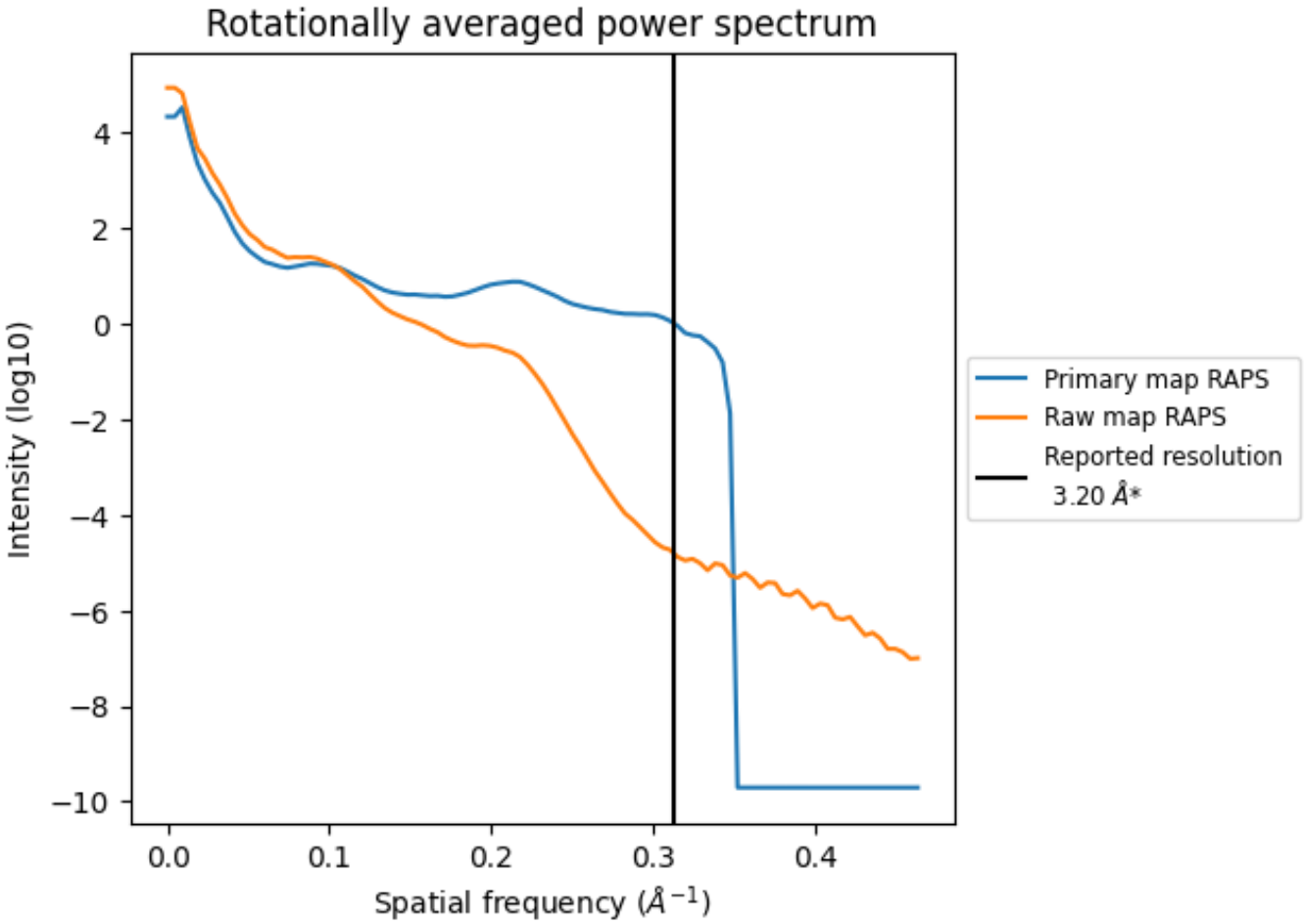
7.2 Volume estimate (i)



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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)

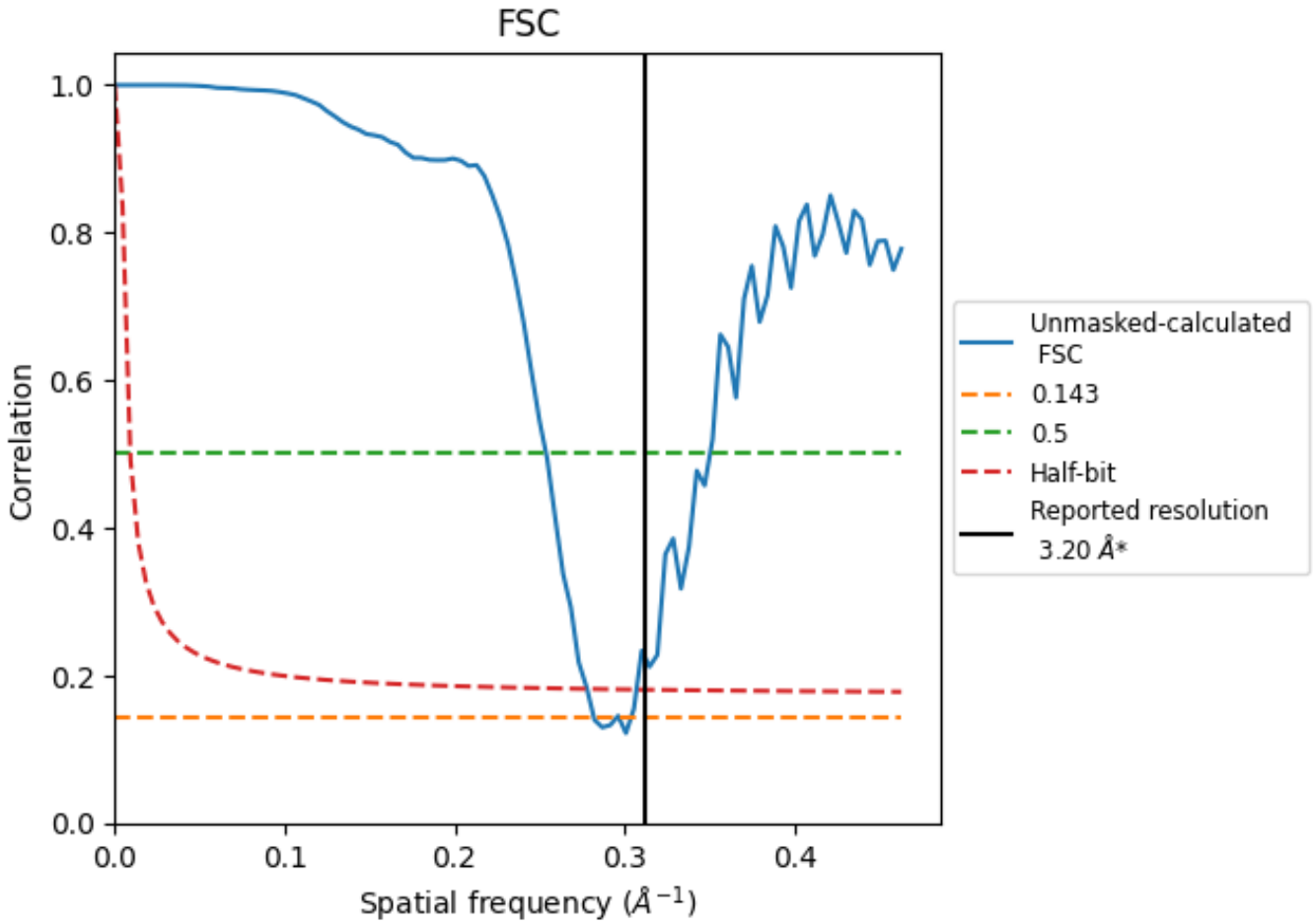


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

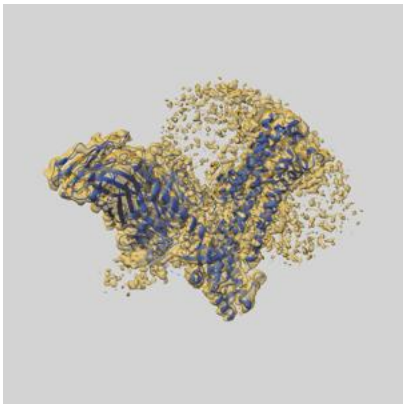
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	3.94	3.60

*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 3.55 differs from the reported value 3.2 by more than 10 %

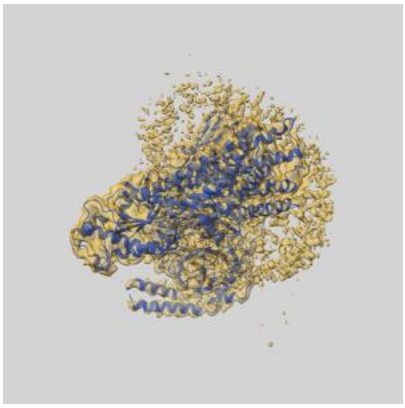
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35686 and PDB model 8IRU. Per-residue inclusion information can be found in section 3 on page 7.

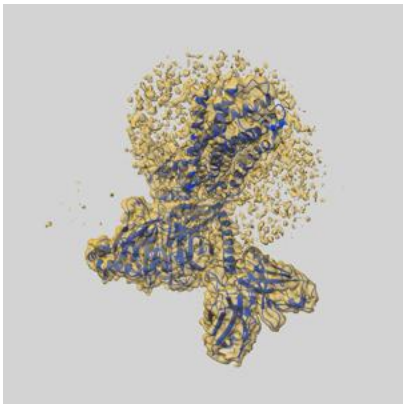
9.1 Map-model overlay



X



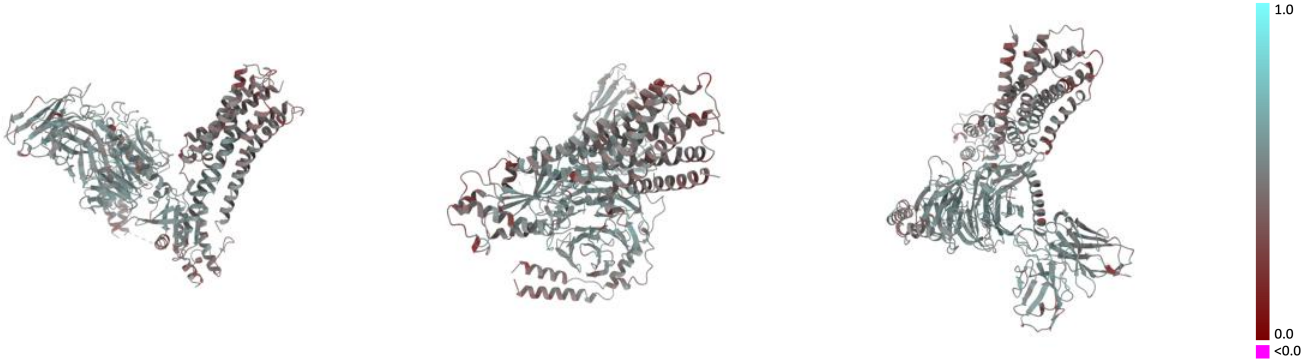
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

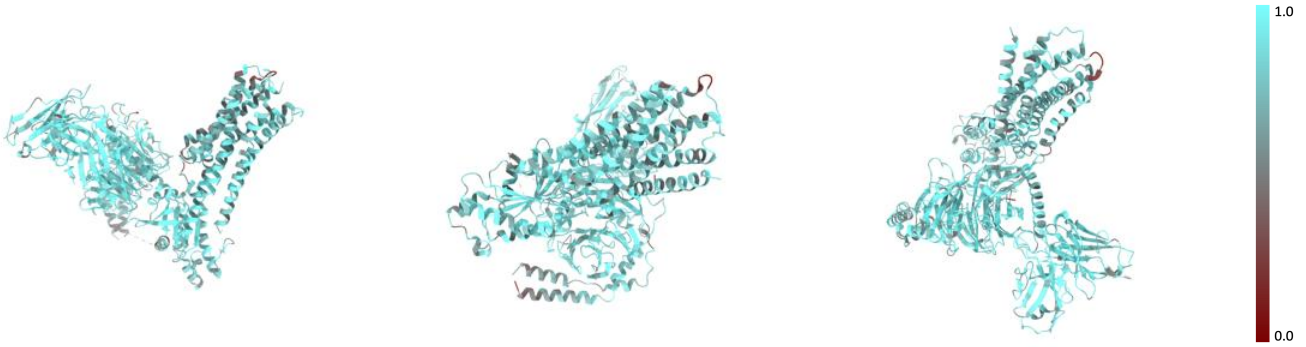
9.2 Q-score mapped to coordinate model (i)



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.

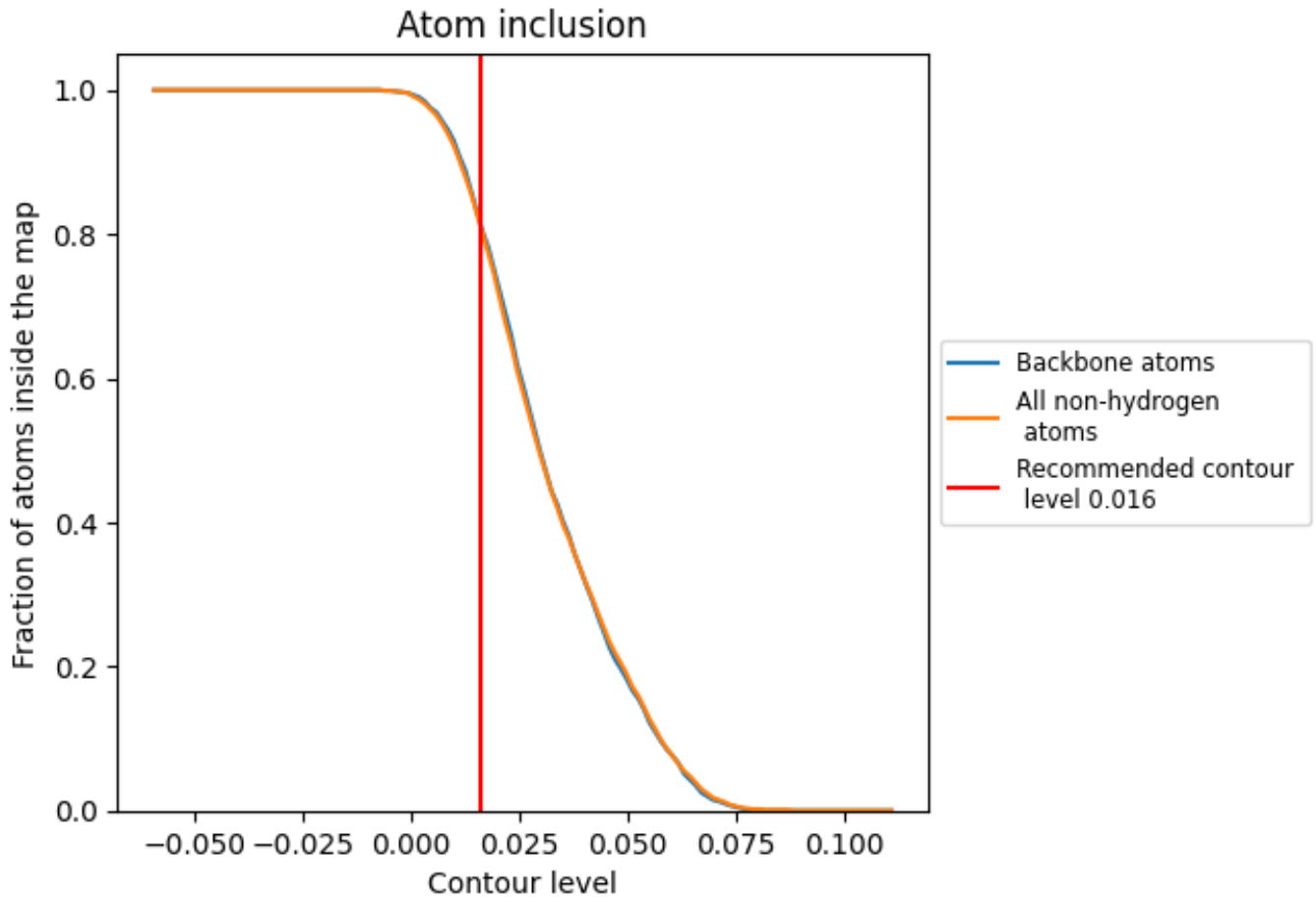
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.4850
A	0.8290	0.4740
B	0.8790	0.5250
E	0.8690	0.5150
G	0.7180	0.4430
R	0.7390	0.4320