Full wwPDB EM Validation Report ⓘ

May 8, 2024 – 08:13 PM JST

PDB ID	:	8J7M
EMDB ID	:	EMD-36042
Title	:	ion channel
Authors	:	Chen, H.W.; Chen, H.W.
Deposited on	:	2023-04-27
Resolution	:	3.10 Å(reported)

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

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

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

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

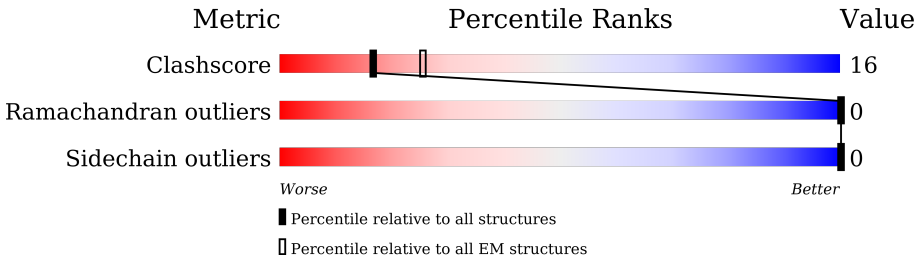
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	803	25% 7% 68%
1	B	803	25% 7% 68%
1	C	803	24% 8% 68%
1	D	803	24% 8% 68%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8806 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 ion channel,Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	257	Total	C	N	O	S	0	0
			2096	1411	329	345	11		
1	D	257	Total	C	N	O	S	0	0
			2096	1411	329	345	11		
1	B	257	Total	C	N	O	S	0	0
			2096	1411	329	345	11		
1	C	257	Total	C	N	O	S	0	0
			2096	1411	329	345	11		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	ALA	-	linker	UNP R1FVI4
A	544	ALA	-	linker	UNP R1FVI4
A	545	ALA	-	linker	UNP R1FVI4
A	546	LEU	-	linker	UNP R1FVI4
A	547	GLU	-	linker	UNP R1FVI4
A	548	VAL	-	linker	UNP R1FVI4
A	549	LEU	-	linker	UNP R1FVI4
A	550	PHE	-	linker	UNP R1FVI4
A	551	GLN	-	linker	UNP R1FVI4
A	552	GLY	-	linker	UNP R1FVI4
A	553	PRO	-	linker	UNP R1FVI4
A	554	SER	-	linker	UNP R1FVI4
A	582	ARG	SER	conflict	UNP A0A059PIQ0
A	624	SER	ALA	conflict	UNP A0A059PIQ0
A	632	ARG	GLN	conflict	UNP A0A059PIQ0
A	758	VAL	ALA	conflict	UNP A0A059PIQ0
A	788	TRP	-	expression tag	UNP A0A059PIQ0
A	789	SER	-	expression tag	UNP A0A059PIQ0
A	790	HIS	-	expression tag	UNP A0A059PIQ0
A	791	PRO	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	792	GLN	-	expression tag	UNP A0A059PIQ0
A	793	PHE	-	expression tag	UNP A0A059PIQ0
A	794	GLU	-	expression tag	UNP A0A059PIQ0
A	795	LYS	-	expression tag	UNP A0A059PIQ0
A	796	GLY	-	expression tag	UNP A0A059PIQ0
A	797	GLY	-	expression tag	UNP A0A059PIQ0
A	798	GLY	-	expression tag	UNP A0A059PIQ0
A	799	SER	-	expression tag	UNP A0A059PIQ0
A	800	GLY	-	expression tag	UNP A0A059PIQ0
A	801	GLY	-	expression tag	UNP A0A059PIQ0
A	802	GLY	-	expression tag	UNP A0A059PIQ0
A	803	SER	-	expression tag	UNP A0A059PIQ0
A	804	GLY	-	expression tag	UNP A0A059PIQ0
A	805	GLY	-	expression tag	UNP A0A059PIQ0
A	806	SER	-	expression tag	UNP A0A059PIQ0
A	807	ALA	-	expression tag	UNP A0A059PIQ0
A	808	TRP	-	expression tag	UNP A0A059PIQ0
A	809	SER	-	expression tag	UNP A0A059PIQ0
A	810	HIS	-	expression tag	UNP A0A059PIQ0
A	811	PRO	-	expression tag	UNP A0A059PIQ0
A	812	GLN	-	expression tag	UNP A0A059PIQ0
A	813	PHE	-	expression tag	UNP A0A059PIQ0
A	814	GLU	-	expression tag	UNP A0A059PIQ0
A	815	LYS	-	expression tag	UNP A0A059PIQ0
D	543	ALA	-	linker	UNP R1FVI4
D	544	ALA	-	linker	UNP R1FVI4
D	545	ALA	-	linker	UNP R1FVI4
D	546	LEU	-	linker	UNP R1FVI4
D	547	GLU	-	linker	UNP R1FVI4
D	548	VAL	-	linker	UNP R1FVI4
D	549	LEU	-	linker	UNP R1FVI4
D	550	PHE	-	linker	UNP R1FVI4
D	551	GLN	-	linker	UNP R1FVI4
D	552	GLY	-	linker	UNP R1FVI4
D	553	PRO	-	linker	UNP R1FVI4
D	554	SER	-	linker	UNP R1FVI4
D	582	ARG	SER	conflict	UNP A0A059PIQ0
D	624	SER	ALA	conflict	UNP A0A059PIQ0
D	632	ARG	GLN	conflict	UNP A0A059PIQ0
D	758	VAL	ALA	conflict	UNP A0A059PIQ0
D	788	TRP	-	expression tag	UNP A0A059PIQ0
D	789	SER	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	790	HIS	-	expression tag	UNP A0A059PIQ0
D	791	PRO	-	expression tag	UNP A0A059PIQ0
D	792	GLN	-	expression tag	UNP A0A059PIQ0
D	793	PHE	-	expression tag	UNP A0A059PIQ0
D	794	GLU	-	expression tag	UNP A0A059PIQ0
D	795	LYS	-	expression tag	UNP A0A059PIQ0
D	796	GLY	-	expression tag	UNP A0A059PIQ0
D	797	GLY	-	expression tag	UNP A0A059PIQ0
D	798	GLY	-	expression tag	UNP A0A059PIQ0
D	799	SER	-	expression tag	UNP A0A059PIQ0
D	800	GLY	-	expression tag	UNP A0A059PIQ0
D	801	GLY	-	expression tag	UNP A0A059PIQ0
D	802	GLY	-	expression tag	UNP A0A059PIQ0
D	803	SER	-	expression tag	UNP A0A059PIQ0
D	804	GLY	-	expression tag	UNP A0A059PIQ0
D	805	GLY	-	expression tag	UNP A0A059PIQ0
D	806	SER	-	expression tag	UNP A0A059PIQ0
D	807	ALA	-	expression tag	UNP A0A059PIQ0
D	808	TRP	-	expression tag	UNP A0A059PIQ0
D	809	SER	-	expression tag	UNP A0A059PIQ0
D	810	HIS	-	expression tag	UNP A0A059PIQ0
D	811	PRO	-	expression tag	UNP A0A059PIQ0
D	812	GLN	-	expression tag	UNP A0A059PIQ0
D	813	PHE	-	expression tag	UNP A0A059PIQ0
D	814	GLU	-	expression tag	UNP A0A059PIQ0
D	815	LYS	-	expression tag	UNP A0A059PIQ0
B	543	ALA	-	linker	UNP R1FVI4
B	544	ALA	-	linker	UNP R1FVI4
B	545	ALA	-	linker	UNP R1FVI4
B	546	LEU	-	linker	UNP R1FVI4
B	547	GLU	-	linker	UNP R1FVI4
B	548	VAL	-	linker	UNP R1FVI4
B	549	LEU	-	linker	UNP R1FVI4
B	550	PHE	-	linker	UNP R1FVI4
B	551	GLN	-	linker	UNP R1FVI4
B	552	GLY	-	linker	UNP R1FVI4
B	553	PRO	-	linker	UNP R1FVI4
B	554	SER	-	linker	UNP R1FVI4
B	582	ARG	SER	conflict	UNP A0A059PIQ0
B	624	SER	ALA	conflict	UNP A0A059PIQ0
B	632	ARG	GLN	conflict	UNP A0A059PIQ0
B	758	VAL	ALA	conflict	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	788	TRP	-	expression tag	UNP A0A059PIQ0
B	789	SER	-	expression tag	UNP A0A059PIQ0
B	790	HIS	-	expression tag	UNP A0A059PIQ0
B	791	PRO	-	expression tag	UNP A0A059PIQ0
B	792	GLN	-	expression tag	UNP A0A059PIQ0
B	793	PHE	-	expression tag	UNP A0A059PIQ0
B	794	GLU	-	expression tag	UNP A0A059PIQ0
B	795	LYS	-	expression tag	UNP A0A059PIQ0
B	796	GLY	-	expression tag	UNP A0A059PIQ0
B	797	GLY	-	expression tag	UNP A0A059PIQ0
B	798	GLY	-	expression tag	UNP A0A059PIQ0
B	799	SER	-	expression tag	UNP A0A059PIQ0
B	800	GLY	-	expression tag	UNP A0A059PIQ0
B	801	GLY	-	expression tag	UNP A0A059PIQ0
B	802	GLY	-	expression tag	UNP A0A059PIQ0
B	803	SER	-	expression tag	UNP A0A059PIQ0
B	804	GLY	-	expression tag	UNP A0A059PIQ0
B	805	GLY	-	expression tag	UNP A0A059PIQ0
B	806	SER	-	expression tag	UNP A0A059PIQ0
B	807	ALA	-	expression tag	UNP A0A059PIQ0
B	808	TRP	-	expression tag	UNP A0A059PIQ0
B	809	SER	-	expression tag	UNP A0A059PIQ0
B	810	HIS	-	expression tag	UNP A0A059PIQ0
B	811	PRO	-	expression tag	UNP A0A059PIQ0
B	812	GLN	-	expression tag	UNP A0A059PIQ0
B	813	PHE	-	expression tag	UNP A0A059PIQ0
B	814	GLU	-	expression tag	UNP A0A059PIQ0
B	815	LYS	-	expression tag	UNP A0A059PIQ0
C	543	ALA	-	linker	UNP R1FVI4
C	544	ALA	-	linker	UNP R1FVI4
C	545	ALA	-	linker	UNP R1FVI4
C	546	LEU	-	linker	UNP R1FVI4
C	547	GLU	-	linker	UNP R1FVI4
C	548	VAL	-	linker	UNP R1FVI4
C	549	LEU	-	linker	UNP R1FVI4
C	550	PHE	-	linker	UNP R1FVI4
C	551	GLN	-	linker	UNP R1FVI4
C	552	GLY	-	linker	UNP R1FVI4
C	553	PRO	-	linker	UNP R1FVI4
C	554	SER	-	linker	UNP R1FVI4
C	582	ARG	SER	conflict	UNP A0A059PIQ0
C	624	SER	ALA	conflict	UNP A0A059PIQ0

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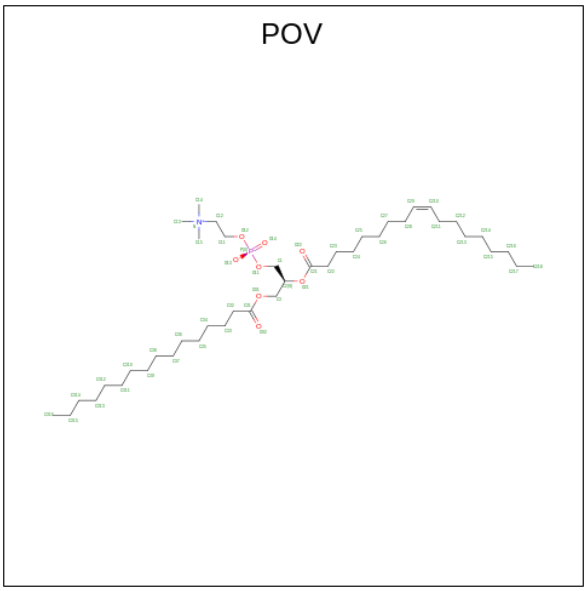
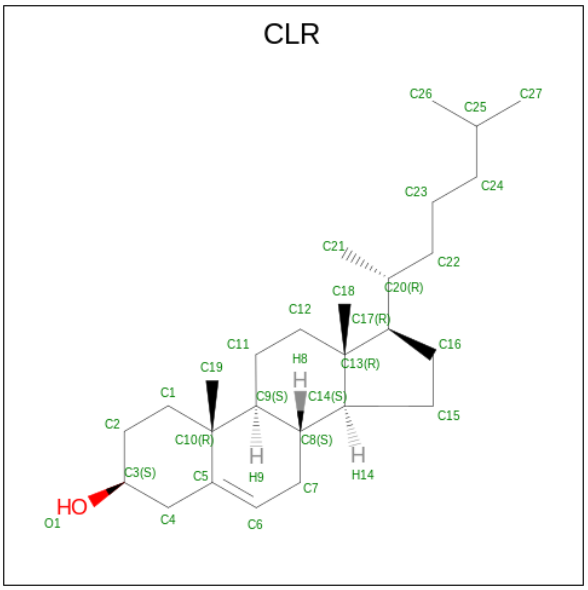
Chain	Residue	Modelled	Actual	Comment	Reference
C	632	ARG	GLN	conflict	UNP A0A059PIQ0
C	758	VAL	ALA	conflict	UNP A0A059PIQ0
C	788	TRP	-	expression tag	UNP A0A059PIQ0
C	789	SER	-	expression tag	UNP A0A059PIQ0
C	790	HIS	-	expression tag	UNP A0A059PIQ0
C	791	PRO	-	expression tag	UNP A0A059PIQ0
C	792	GLN	-	expression tag	UNP A0A059PIQ0
C	793	PHE	-	expression tag	UNP A0A059PIQ0
C	794	GLU	-	expression tag	UNP A0A059PIQ0
C	795	LYS	-	expression tag	UNP A0A059PIQ0
C	796	GLY	-	expression tag	UNP A0A059PIQ0
C	797	GLY	-	expression tag	UNP A0A059PIQ0
C	798	GLY	-	expression tag	UNP A0A059PIQ0
C	799	SER	-	expression tag	UNP A0A059PIQ0
C	800	GLY	-	expression tag	UNP A0A059PIQ0
C	801	GLY	-	expression tag	UNP A0A059PIQ0
C	802	GLY	-	expression tag	UNP A0A059PIQ0
C	803	SER	-	expression tag	UNP A0A059PIQ0
C	804	GLY	-	expression tag	UNP A0A059PIQ0
C	805	GLY	-	expression tag	UNP A0A059PIQ0
C	806	SER	-	expression tag	UNP A0A059PIQ0
C	807	ALA	-	expression tag	UNP A0A059PIQ0
C	808	TRP	-	expression tag	UNP A0A059PIQ0
C	809	SER	-	expression tag	UNP A0A059PIQ0
C	810	HIS	-	expression tag	UNP A0A059PIQ0
C	811	PRO	-	expression tag	UNP A0A059PIQ0
C	812	GLN	-	expression tag	UNP A0A059PIQ0
C	813	PHE	-	expression tag	UNP A0A059PIQ0
C	814	GLU	-	expression tag	UNP A0A059PIQ0
C	815	LYS	-	expression tag	UNP A0A059PIQ0

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	27	8	1	
2	D	1	Total	C	O	P	0
			35	26	8	1	
2	B	1	Total	C	O	P	0
			35	26	8	1	
2	C	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



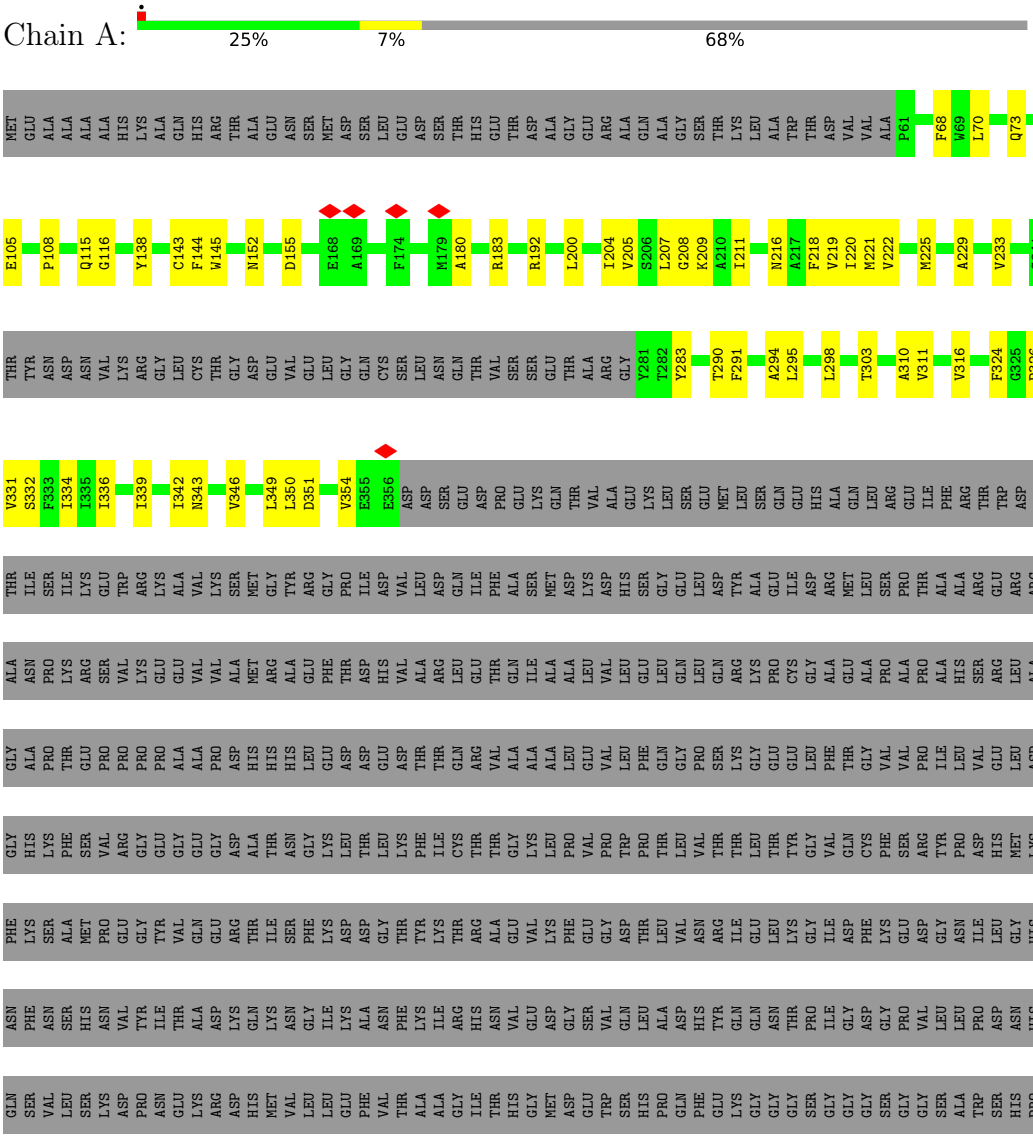
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 28 27 1	0
3	A	1	Total C O 28 27 1	0
3	D	1	Total C O 28 27 1	0
3	D	1	Total C O 28 27 1	0
3	D	1	Total C O 28 27 1	0
3	B	1	Total C O 28 27 1	0
3	B	1	Total C O 28 27 1	0
3	C	1	Total C O 28 27 1	0
3	C	1	Total C O 28 27 1	0
3	C	1	Total C O 28 27 1	0

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.

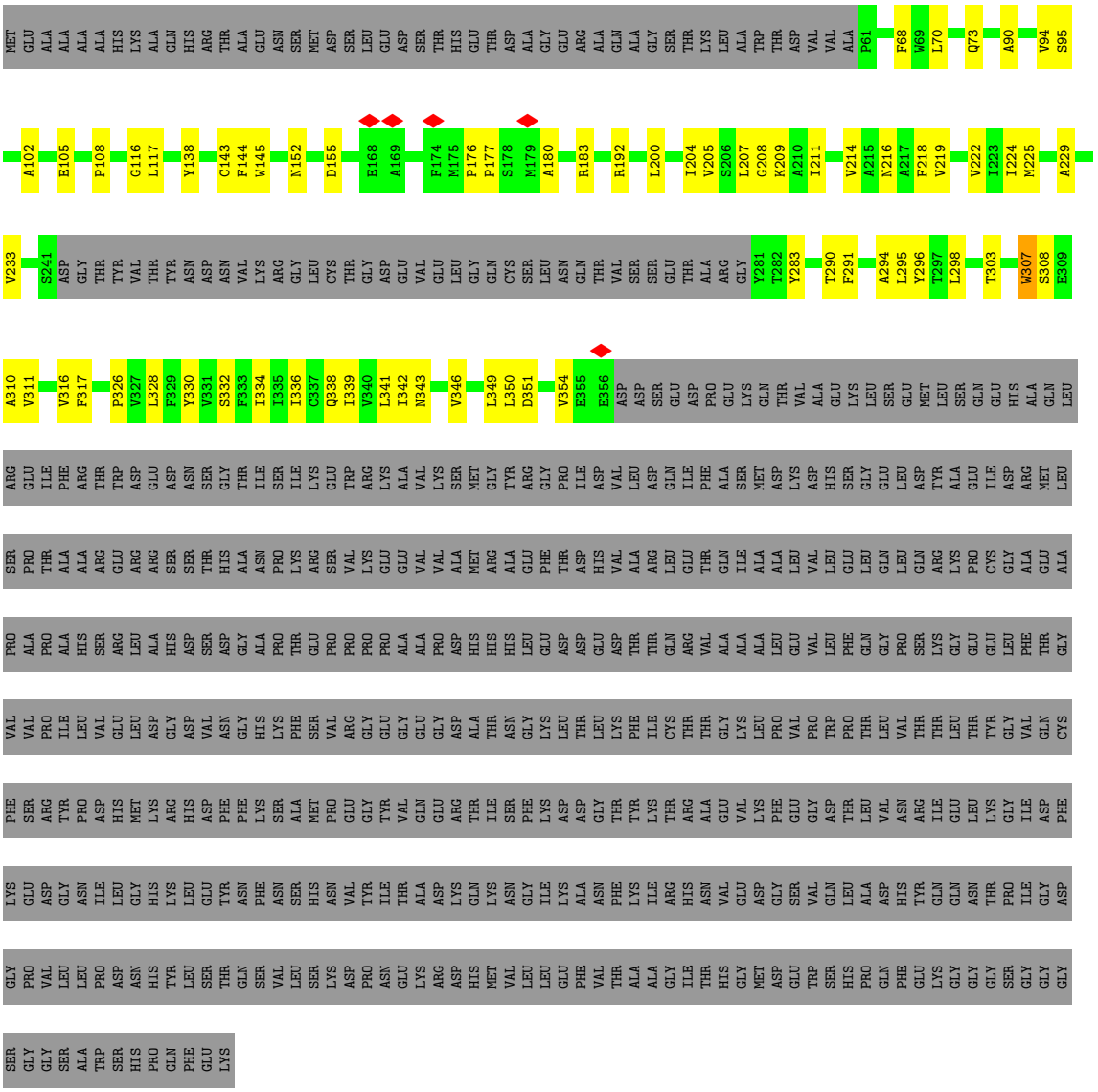
• Molecule 1: ion channel,Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment)

Chain A:



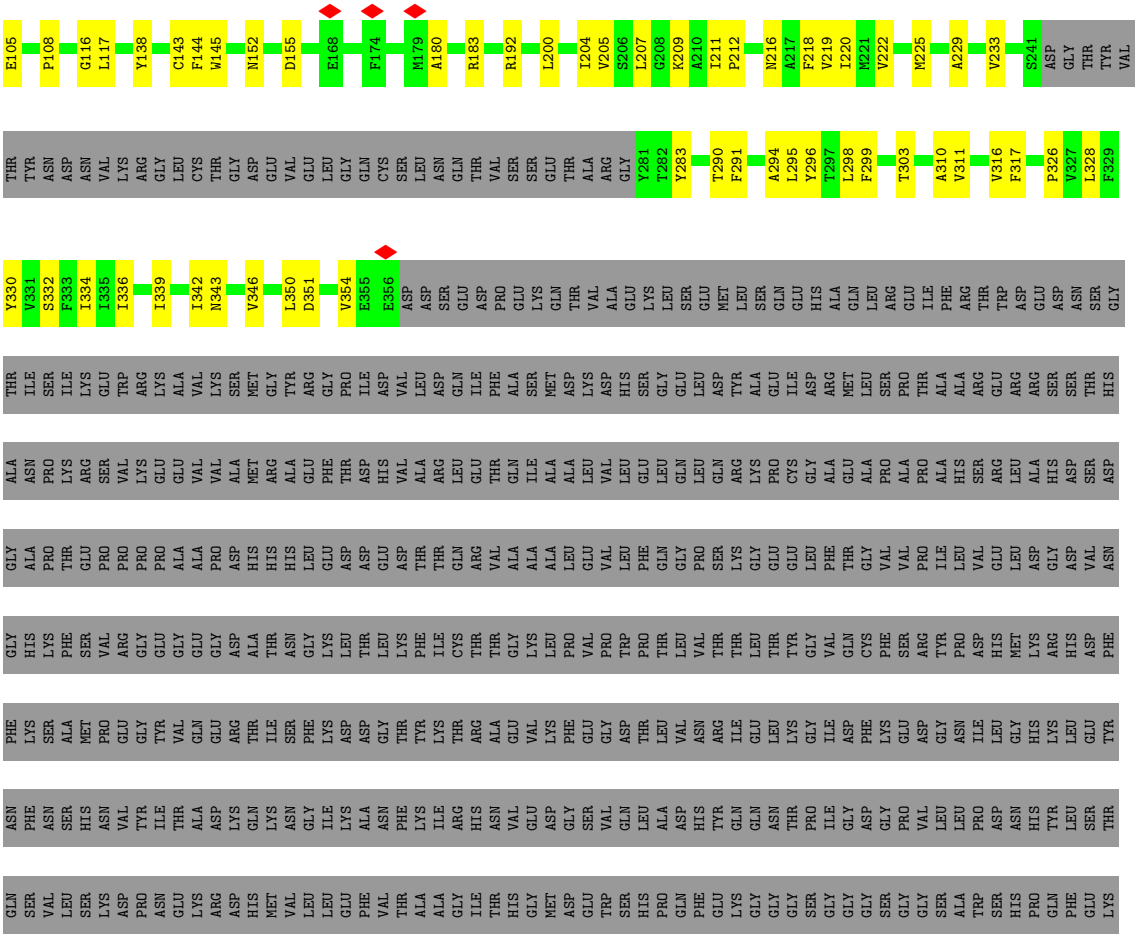
• Molecule 1: ion channel,Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment)

Chain D:



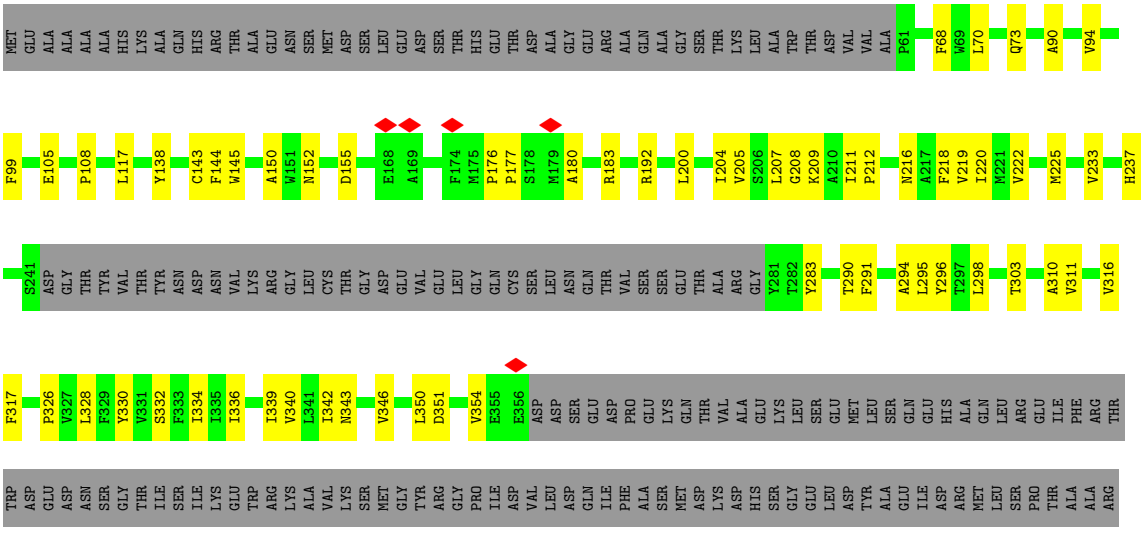
• Molecule 1: ion channel,Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment)

Chain B:



• Molecule 1: ion channel,Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment),Voltage dependent ion channel,Green fluorescent protein (Fragment)

Chain C:




GLU ARG ARG SER SER THR HIS ALA ASN PRO LYS ARG SER VAL LYS GLU GLU VAL VAL ALA MET ARG ALA GLU PHE THR ASP HIS VAL ALA ARG LEU GLU THR GLN ILE ALA ALA LEU VAL LEU GLU LEU GLN LEU GLN ARG LYS PRO CYS GLY ALA GLU ALA PRO ALA PRO ALA HIS SER
ARG LEU ALA HIS ASP SER ASP GLY ALA PRO THR GLU PRO PRO PRO PRO ALA ALA PRO ASP HIS HIS HIS LEU GLU GLU ASP ASP GLU ASP THR THR GLN ARG VAL ALA ALA ALA ALA LEU GLU VAL LEU PHE GLN GLY PRO SER LYS GLY GLU GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL
GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL ARG GLY GLU GLY GLU GLY ASP ALA THR ASN GLY LYS LEU THR LEU LYS PHE ILE CYS THR THR GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU THR TYR GLY VAL GLN CYS PHE SER ARG TYR PRO ASP
HIS MET LYS ARG HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL GLN GLU ARG THR ILE SER PHE LYS ASP ASP GLY THR TYR LYS THR ARG ALA GLU VAL LYS PHE GLU GLY ASP THR LEU VAL ASN ARG ILE GLU LEU LYS GLY ILE ASP PHE LYS GLU ASP GLY SER ILE
LEU GLY HIS LYS LEU GLU TYR ASN PHE ASN SER HIS ASN VAL TYR ILE THR ALA ASP LYS GLN LYS ASN GLY ILE LYS ALA ASN PHE LYS ILE ARG HIS ASN VAL GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO
ASP ASN HIS TYR LEU SER THR GLN SER VAL LEU SER LYS ASP PRO ASN GLU LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR HIS GLY MET ASP GLU TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP
SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81844	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)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.750	Depositor
Minimum map value	-4.127	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.423	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, 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	0.48	0/2164	0.51	0/2947
1	B	0.51	0/2164	0.54	1/2947 (0.0%)
1	C	0.51	0/2164	0.56	1/2947 (0.0%)
1	D	0.52	0/2164	0.59	3/2947 (0.1%)
All	All	0.51	0/8656	0.55	5/11788 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	307	TRP	CB-CA-C	-5.86	98.69	110.40
1	C	336	ILE	CB-CA-C	-5.77	100.06	111.60
1	B	336	ILE	CB-CA-C	-5.76	100.08	111.60
1	D	308	SER	N-CA-CB	5.70	119.05	110.50
1	D	338	GLN	CB-CA-C	-5.65	99.10	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2096	0	2065	62	0
1	B	2096	0	2065	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2096	0	2065	65	0
1	D	2096	0	2065	70	0
2	A	36	0	48	6	0
2	B	35	0	46	1	0
2	C	36	0	48	12	0
2	D	35	0	46	5	0
3	A	56	0	92	13	0
3	B	56	0	92	15	0
3	C	84	0	138	31	0
3	D	84	0	138	30	0
All	All	8806	0	8908	277	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 16.

All (277) 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)
3:B:903:CLR:H222	3:B:903:CLR:H272	1.45	0.98
1:C:208:GLY:HA3	2:C:901:POV:H22	1.50	0.93
1:D:143:CYS:O	1:D:145:TRP:CE3	2.22	0.91
3:C:902:CLR:H183	3:C:902:CLR:H212	1.49	0.91
3:D:904:CLR:C16	3:D:904:CLR:H232	2.01	0.91
1:A:143:CYS:O	1:A:145:TRP:CE3	2.24	0.91
3:D:904:CLR:H183	3:D:904:CLR:H212	1.53	0.89
1:C:143:CYS:O	1:C:145:TRP:CE3	2.26	0.89
1:D:307:TRP:O	1:D:307:TRP:CE3	2.26	0.88
1:B:339:ILE:O	1:B:343:ASN:ND2	2.12	0.82
1:B:143:CYS:O	1:B:145:TRP:CE3	2.33	0.81
1:D:102:ALA:HB1	3:D:902:CLR:H151	1.60	0.80
1:D:222:VAL:HG22	3:D:903:CLR:H242	1.66	0.77
1:A:218:PHE:CD1	3:A:903:CLR:H271	2.22	0.74
3:C:903:CLR:H121	3:C:903:CLR:H212	1.69	0.74
3:D:904:CLR:H232	3:D:904:CLR:H161	1.69	0.74
3:A:903:CLR:H212	3:A:903:CLR:H121	1.69	0.73
1:D:105:GLU:HB2	1:B:291:PHE:HB3	1.70	0.73
1:D:326:PRO:O	1:D:330:TYR:HD2	1.71	0.73
1:C:326:PRO:O	1:C:330:TYR:HD2	1.71	0.73
1:D:208:GLY:CA	2:D:901:POV:H23A	2.19	0.73
1:A:326:PRO:O	1:A:330:TYR:HD2	1.71	0.72
1:B:326:PRO:O	1:B:330:TYR:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ALA:CB	3:D:902:CLR:H151	2.18	0.72
1:D:224:ILE:HD12	1:D:341:LEU:HD11	1.71	0.72
1:C:218:PHE:CD1	3:C:903:CLR:H271	2.25	0.72
3:B:902:CLR:H212	3:B:902:CLR:H121	1.69	0.71
3:C:902:CLR:C21	3:C:902:CLR:H121	2.21	0.71
1:B:218:PHE:CD1	3:B:902:CLR:H271	2.26	0.70
1:D:208:GLY:HA3	2:D:901:POV:H23A	1.73	0.70
3:D:903:CLR:H121	3:D:903:CLR:H212	1.72	0.70
3:D:904:CLR:H212	3:D:904:CLR:H121	1.73	0.70
3:D:904:CLR:H121	3:D:904:CLR:C21	2.22	0.69
1:C:208:GLY:HA3	2:C:901:POV:C22	2.22	0.69
1:A:105:GLU:HB2	1:C:291:PHE:HB3	1.73	0.69
1:A:200:LEU:HD21	1:C:219:VAL:HG13	1.76	0.68
3:C:902:CLR:H232	3:C:902:CLR:H161	1.74	0.67
1:C:346:VAL:O	1:C:350:LEU:HG	1.95	0.67
1:D:334:ILE:HG21	1:C:303:THR:HG21	1.76	0.67
1:B:346:VAL:O	1:B:350:LEU:HG	1.95	0.67
1:A:334:ILE:HG21	1:B:303:THR:HG21	1.74	0.67
1:A:346:VAL:O	1:A:350:LEU:HG	1.95	0.66
1:D:346:VAL:O	1:D:350:LEU:HG	1.95	0.66
1:B:222:VAL:HG22	3:B:902:CLR:H241	1.78	0.66
1:D:307:TRP:O	1:D:307:TRP:HE3	1.78	0.66
3:B:903:CLR:H272	3:B:903:CLR:C22	2.14	0.66
1:D:291:PHE:HB3	1:C:105:GLU:HB2	1.78	0.66
1:A:219:VAL:HG13	1:B:200:LEU:HD21	1.78	0.65
3:B:903:CLR:H121	3:B:903:CLR:H212	1.79	0.64
1:C:222:VAL:HG22	3:C:903:CLR:H241	1.80	0.64
1:A:291:PHE:HB3	1:B:105:GLU:HB2	1.81	0.63
1:B:222:VAL:CG2	3:B:902:CLR:H241	2.29	0.63
1:D:200:LEU:HD21	1:B:219:VAL:HG13	1.81	0.63
1:D:219:VAL:HG13	1:C:200:LEU:HD21	1.80	0.63
1:C:222:VAL:CG2	3:C:903:CLR:H241	2.29	0.62
1:D:222:VAL:CG2	3:D:903:CLR:H242	2.29	0.62
1:A:303:THR:HG21	1:C:334:ILE:HG21	1.80	0.62
1:A:290:THR:HG22	1:B:108:PRO:HG3	1.82	0.62
1:D:218:PHE:CD1	3:D:903:CLR:C26	2.82	0.62
1:C:208:GLY:CA	2:C:901:POV:H22	2.29	0.62
1:B:68:PHE:HA	1:B:73:GLN:NE2	2.16	0.61
1:C:233:VAL:O	1:C:237:HIS:HB3	1.99	0.61
1:A:68:PHE:HA	1:A:73:GLN:NE2	2.16	0.61
1:D:68:PHE:HA	1:D:73:GLN:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:PHE:HA	1:C:73:GLN:NE2	2.16	0.61
1:A:216:ASN:HA	1:A:219:VAL:HG12	1.82	0.60
1:A:222:VAL:CG2	3:A:903:CLR:H241	2.32	0.60
1:D:307:TRP:O	1:D:307:TRP:CD2	2.54	0.59
1:A:218:PHE:CD1	3:A:903:CLR:C27	2.85	0.59
3:C:902:CLR:H232	3:C:902:CLR:C16	2.30	0.59
1:D:205:VAL:O	1:D:209:LYS:HG2	2.03	0.59
1:B:205:VAL:O	1:B:209:LYS:HG2	2.02	0.59
3:C:902:CLR:H212	3:C:902:CLR:H121	1.85	0.58
1:A:205:VAL:O	1:A:209:LYS:HG2	2.03	0.58
3:D:903:CLR:H121	3:D:903:CLR:C21	2.32	0.58
1:C:117:LEU:HD21	3:C:902:CLR:H12	1.85	0.58
3:D:904:CLR:H232	3:D:904:CLR:H162	1.86	0.58
1:C:205:VAL:O	1:C:209:LYS:HG2	2.03	0.58
1:A:222:VAL:HG22	3:A:903:CLR:H241	1.86	0.57
1:C:218:PHE:CD1	3:C:903:CLR:C27	2.86	0.57
3:C:902:CLR:H121	3:C:902:CLR:H213	1.87	0.57
1:D:303:THR:HG21	1:B:334:ILE:HG21	1.85	0.57
1:D:207:LEU:O	1:D:211:ILE:HG12	2.05	0.57
1:A:208:GLY:CA	2:A:901:POV:H24A	2.35	0.56
1:D:336:ILE:HG23	2:C:901:POV:H315	1.87	0.56
3:D:904:CLR:H183	3:D:904:CLR:C21	2.28	0.56
1:B:218:PHE:CD1	3:B:902:CLR:C27	2.89	0.55
1:D:290:THR:HG22	1:C:108:PRO:HG3	1.89	0.55
3:C:902:CLR:C16	3:C:902:CLR:C23	2.85	0.55
1:D:95:SER:HB2	3:D:902:CLR:H241	1.89	0.54
1:B:326:PRO:O	1:B:330:TYR:CD2	2.59	0.54
1:C:209:LYS:O	1:C:212:PRO:HD2	2.08	0.53
1:D:108:PRO:HG3	1:B:290:THR:HG22	1.90	0.53
1:C:99:PHE:CE1	3:C:902:CLR:H122	2.43	0.53
1:C:117:LEU:CD2	3:C:902:CLR:H12	2.37	0.53
1:D:144:PHE:HB2	1:D:152:ASN:HB3	1.91	0.53
1:A:144:PHE:HB2	1:A:152:ASN:HB3	1.91	0.53
1:D:224:ILE:HD11	2:C:901:POV:H312	1.90	0.53
1:A:219:VAL:CG1	1:B:200:LEU:HD21	2.39	0.53
1:A:155:ASP:OD1	1:A:192:ARG:HD2	2.09	0.52
1:C:144:PHE:HB2	1:C:152:ASN:HB3	1.91	0.52
1:D:155:ASP:OD1	1:D:192:ARG:HD2	2.09	0.52
1:D:216:ASN:HA	1:D:219:VAL:HG12	1.90	0.52
1:B:144:PHE:HB2	1:B:152:ASN:HB3	1.91	0.52
1:A:326:PRO:O	1:A:330:TYR:CD2	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:902:CLR:H183	3:C:902:CLR:C21	2.28	0.52
1:A:200:LEU:O	1:A:204:ILE:HG12	2.10	0.52
1:D:200:LEU:O	1:D:204:ILE:HG12	2.10	0.52
1:B:155:ASP:OD1	1:B:192:ARG:HD2	2.09	0.52
1:B:328:LEU:O	1:B:332:SER:OG	2.25	0.51
1:C:155:ASP:OD1	1:C:192:ARG:HD2	2.09	0.51
1:B:200:LEU:O	1:B:204:ILE:HG12	2.10	0.51
1:B:180:ALA:HA	1:B:183:ARG:HE	1.76	0.51
1:C:326:PRO:O	1:C:330:TYR:CD2	2.59	0.51
1:D:180:ALA:HA	1:D:183:ARG:HE	1.76	0.51
1:B:216:ASN:HA	1:B:219:VAL:HG12	1.92	0.50
1:C:200:LEU:O	1:C:204:ILE:HG12	2.10	0.50
1:C:218:PHE:HD1	3:C:903:CLR:H271	1.76	0.50
3:C:902:CLR:H212	3:C:902:CLR:C18	2.23	0.50
1:A:180:ALA:HA	1:A:183:ARG:HE	1.76	0.50
1:D:224:ILE:CD1	1:D:341:LEU:HD11	2.39	0.50
1:C:342:ILE:O	1:C:346:VAL:HG23	2.12	0.50
1:A:350:LEU:HD13	1:C:350:LEU:HD12	1.94	0.50
1:D:350:LEU:HD13	1:B:350:LEU:HD12	1.94	0.50
3:D:904:CLR:H212	3:D:904:CLR:C18	2.25	0.50
1:C:216:ASN:HA	1:C:219:VAL:HG12	1.92	0.50
1:C:180:ALA:HA	1:C:183:ARG:HE	1.76	0.50
3:D:904:CLR:C21	3:D:904:CLR:C12	2.86	0.49
1:A:342:ILE:O	1:A:346:VAL:HG23	2.12	0.49
1:D:342:ILE:O	1:D:346:VAL:HG23	2.12	0.49
1:B:342:ILE:O	1:B:346:VAL:HG23	2.12	0.49
1:C:328:LEU:O	1:C:332:SER:OG	2.25	0.49
1:D:326:PRO:O	1:D:330:TYR:CD2	2.59	0.49
1:D:350:LEU:HD12	1:C:350:LEU:HD13	1.95	0.49
1:A:208:GLY:HA2	2:A:901:POV:H24A	1.95	0.49
3:A:903:CLR:H121	3:A:903:CLR:C21	2.42	0.49
1:A:200:LEU:HD21	1:C:219:VAL:CG1	2.40	0.49
1:A:354:VAL:HG12	1:C:351:ASP:HB2	1.95	0.48
1:D:218:PHE:CD1	3:D:903:CLR:H261	2.48	0.48
3:D:903:CLR:H212	3:D:903:CLR:H183	1.93	0.48
1:B:222:VAL:HG22	3:B:902:CLR:C24	2.42	0.48
1:D:208:GLY:HA2	2:D:901:POV:H23A	1.95	0.48
1:D:229:ALA:O	1:D:233:VAL:HG23	2.14	0.48
1:B:209:LYS:O	1:B:212:PRO:HD2	2.14	0.48
3:C:904:CLR:H162	3:C:904:CLR:H221	1.47	0.48
1:A:350:LEU:HD12	1:B:350:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:903:CLR:H272	3:D:903:CLR:H231	1.68	0.47
1:C:222:VAL:HG22	3:C:903:CLR:C24	2.43	0.47
3:C:904:CLR:H272	3:C:904:CLR:H231	1.54	0.47
1:A:208:GLY:HA3	2:A:901:POV:H22	1.95	0.47
1:D:219:VAL:CG1	1:C:200:LEU:HD21	2.43	0.47
1:A:225:MET:HE2	1:A:295:LEU:CD1	2.45	0.47
3:B:902:CLR:H121	3:B:902:CLR:C21	2.41	0.47
1:A:70:LEU:HD23	1:A:138:TYR:CE2	2.50	0.47
3:D:904:CLR:H272	3:D:904:CLR:H221	1.97	0.47
2:A:901:POV:H31F	1:C:340:VAL:HG21	1.97	0.46
1:A:108:PRO:HG3	1:C:290:THR:HG22	1.98	0.46
1:D:224:ILE:HD12	1:D:341:LEU:CD1	2.43	0.46
1:A:351:ASP:HB2	1:B:354:VAL:HG12	1.98	0.46
1:D:350:LEU:O	1:D:354:VAL:HG13	2.16	0.46
2:C:901:POV:H35	2:C:901:POV:H32A	1.59	0.46
1:A:229:ALA:O	1:A:233:VAL:HG23	2.15	0.46
1:C:350:LEU:O	1:C:354:VAL:HG13	2.16	0.46
3:C:902:CLR:H212	3:C:902:CLR:C12	2.45	0.46
1:D:70:LEU:HD23	1:D:138:TYR:CE2	2.50	0.46
1:C:218:PHE:HD1	3:C:903:CLR:C27	2.28	0.46
1:C:233:VAL:HG21	1:C:291:PHE:HA	1.98	0.46
2:C:901:POV:H31E	2:C:901:POV:H27	1.98	0.46
3:D:904:CLR:H212	3:D:904:CLR:C12	2.37	0.45
1:C:70:LEU:HD23	1:C:138:TYR:CE2	2.50	0.45
1:B:70:LEU:HD23	1:B:138:TYR:CE2	2.50	0.45
2:A:901:POV:H1	2:A:901:POV:O22	2.16	0.45
2:A:901:POV:H310	3:C:904:CLR:H273	1.98	0.45
1:B:296:TYR:HB2	3:B:902:CLR:H72	1.98	0.45
1:B:350:LEU:O	1:B:354:VAL:HG13	2.16	0.45
2:C:901:POV:H310	2:C:901:POV:H313	1.41	0.45
1:D:143:CYS:O	1:D:145:TRP:CZ3	2.66	0.45
1:D:200:LEU:HD22	1:B:220:ILE:HG13	1.98	0.45
1:D:354:VAL:HG12	1:B:351:ASP:HB2	1.97	0.45
1:D:328:LEU:O	1:D:332:SER:OG	2.25	0.45
1:C:143:CYS:O	1:C:145:TRP:CZ3	2.69	0.45
1:C:296:TYR:HB2	3:C:903:CLR:H72	1.97	0.45
1:A:324:PHE:CD2	3:B:902:CLR:H192	2.52	0.45
3:A:902:CLR:H211	3:A:902:CLR:H232	1.50	0.45
1:D:351:ASP:HB2	1:C:354:VAL:HG12	1.98	0.45
1:A:350:LEU:O	1:A:354:VAL:HG13	2.16	0.45
1:D:294:ALA:O	1:D:298:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:O	1:A:298:LEU:HG	2.17	0.45
1:B:294:ALA:O	1:B:298:LEU:HG	2.17	0.45
1:C:294:ALA:O	1:C:298:LEU:HG	2.17	0.44
3:C:902:CLR:H8	3:C:902:CLR:H191	1.77	0.44
3:C:903:CLR:H121	3:C:903:CLR:C21	2.41	0.44
1:D:200:LEU:HD21	1:B:219:VAL:CG1	2.46	0.44
1:A:218:PHE:HD1	3:A:903:CLR:C27	2.30	0.44
1:A:220:ILE:HG13	1:B:200:LEU:HD22	2.00	0.44
1:A:221:MET:HE2	1:A:221:MET:HB2	1.84	0.44
3:D:904:CLR:H191	3:D:904:CLR:H8	1.74	0.44
3:C:902:CLR:C21	3:C:902:CLR:C12	2.86	0.44
1:D:296:TYR:HB2	3:D:903:CLR:H72	2.00	0.44
1:D:68:PHE:HA	1:D:73:GLN:HE21	1.83	0.44
1:A:207:LEU:O	1:A:211:ILE:HG12	2.18	0.44
1:A:336:ILE:HG23	2:B:901:POV:H311	2.00	0.44
2:D:901:POV:H32	2:D:901:POV:H35	1.88	0.44
1:C:68:PHE:HA	1:C:73:GLN:HE21	1.83	0.43
3:C:902:CLR:C16	3:C:902:CLR:C24	2.95	0.43
1:D:350:LEU:HD13	1:B:350:LEU:CD1	2.49	0.43
1:C:207:LEU:O	1:C:211:ILE:HG12	2.18	0.43
1:D:349:LEU:HD12	1:D:349:LEU:HA	1.89	0.43
2:C:901:POV:H36A	2:C:901:POV:H32	1.99	0.43
1:A:350:LEU:HD13	1:C:350:LEU:CD1	2.48	0.43
1:D:70:LEU:HD13	1:D:73:GLN:OE1	2.19	0.43
1:A:68:PHE:HA	1:A:73:GLN:HE21	1.83	0.43
1:B:207:LEU:O	1:B:211:ILE:HG12	2.18	0.43
1:C:70:LEU:HD13	1:C:73:GLN:OE1	2.19	0.43
1:A:115:GLN:O	1:A:116:GLY:C	2.57	0.43
1:A:328:LEU:O	1:A:332:SER:OG	2.25	0.43
1:C:225:MET:HE2	1:C:295:LEU:CD1	2.49	0.43
1:A:200:LEU:HD22	1:C:220:ILE:HG13	2.01	0.43
1:A:349:LEU:HD23	1:C:343:ASN:HB2	2.01	0.43
2:D:901:POV:H311	3:B:903:CLR:C26	2.49	0.43
3:D:903:CLR:H41	1:B:317:PHE:CE1	2.53	0.43
3:D:903:CLR:C21	3:D:903:CLR:C12	2.94	0.43
1:B:229:ALA:O	1:B:233:VAL:HG23	2.18	0.43
1:B:311:VAL:HG12	1:B:316:VAL:HG21	2.01	0.43
1:C:225:MET:HE2	1:C:295:LEU:HD12	2.01	0.43
1:D:311:VAL:HG12	1:D:316:VAL:HG21	2.01	0.42
1:D:225:MET:HE2	1:D:295:LEU:CD1	2.49	0.42
1:B:90:ALA:O	1:B:94:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:O	1:A:94:VAL:HG23	2.19	0.42
1:A:311:VAL:HG12	1:A:316:VAL:HG21	2.01	0.42
1:D:218:PHE:HD1	3:D:903:CLR:H261	1.83	0.42
1:B:218:PHE:HD1	3:B:902:CLR:C27	2.30	0.42
1:C:311:VAL:HG12	1:C:316:VAL:HG21	2.01	0.42
1:D:339:ILE:O	1:D:343:ASN:ND2	2.52	0.42
1:C:339:ILE:O	1:C:343:ASN:ND2	2.52	0.42
1:B:68:PHE:HA	1:B:73:GLN:HE21	1.83	0.42
1:A:225:MET:HE2	1:A:295:LEU:HD12	2.00	0.42
1:A:283:TYR:OH	1:A:310:ALA:HB2	2.19	0.42
3:A:902:CLR:H8	3:A:902:CLR:H191	1.76	0.42
1:C:90:ALA:O	1:C:94:VAL:HG23	2.19	0.42
1:A:70:LEU:HD13	1:A:73:GLN:OE1	2.19	0.42
1:D:176:PRO:HA	1:D:177:PRO:HD3	1.96	0.42
3:D:904:CLR:H272	3:D:904:CLR:C22	2.49	0.42
1:A:339:ILE:O	1:A:343:ASN:ND2	2.52	0.42
1:D:225:MET:HE2	1:D:295:LEU:HD12	2.02	0.42
3:D:904:CLR:H121	3:D:904:CLR:H213	2.00	0.42
1:B:70:LEU:HD13	1:B:73:GLN:OE1	2.19	0.42
1:B:218:PHE:HD1	3:B:902:CLR:H271	1.77	0.42
3:C:902:CLR:C24	3:C:902:CLR:H162	2.50	0.42
3:A:902:CLR:H192	3:A:902:CLR:H22	1.84	0.42
1:C:283:TYR:OH	1:C:310:ALA:HB2	2.19	0.42
1:A:143:CYS:O	1:A:145:TRP:CZ3	2.68	0.41
1:D:90:ALA:O	1:D:94:VAL:HG23	2.19	0.41
1:B:283:TYR:OH	1:B:310:ALA:HB2	2.19	0.41
1:B:334:ILE:HD13	1:B:334:ILE:HA	1.93	0.41
1:C:176:PRO:HA	1:C:177:PRO:HD3	1.96	0.41
1:A:331:VAL:HG22	1:B:299:PHE:CE2	2.55	0.41
2:C:901:POV:O22	2:C:901:POV:H1	2.20	0.41
3:A:902:CLR:H8	3:A:902:CLR:H182	1.77	0.41
1:D:350:LEU:CD1	1:C:350:LEU:HD13	2.51	0.41
1:B:225:MET:HE2	1:B:295:LEU:CD1	2.50	0.41
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.90	0.41
1:D:349:LEU:HD23	1:B:343:ASN:HB2	2.03	0.41
1:A:222:VAL:HG22	3:A:903:CLR:C24	2.49	0.41
1:C:150:ALA:HB1	2:C:901:POV:O32	2.20	0.41
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.89	0.41
1:D:283:TYR:OH	1:D:310:ALA:HB2	2.20	0.41
1:D:317:PHE:CE1	3:C:903:CLR:H41	2.56	0.41
2:C:901:POV:H26	2:C:901:POV:H23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLY:O	1:D:117:LEU:C	2.58	0.41
3:D:904:CLR:H193	3:D:904:CLR:H111	1.91	0.41
1:B:180:ALA:HA	1:B:183:ARG:NE	2.36	0.40
1:B:225:MET:HE3	1:B:225:MET:HB3	1.72	0.40
1:B:116:GLY:O	1:B:117:LEU:C	2.56	0.40
1:D:214:VAL:HG21	1:D:349:LEU:HD13	2.03	0.40
1:A:180:ALA:HA	1:A:183:ARG:NE	2.36	0.40
3:A:903:CLR:H41	1:C:317:PHE:CE1	2.57	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	253/803 (32%)	228 (90%)	25 (10%)	0	100	100
1	B	253/803 (32%)	235 (93%)	18 (7%)	0	100	100
1	C	253/803 (32%)	232 (92%)	21 (8%)	0	100	100
1	D	253/803 (32%)	233 (92%)	20 (8%)	0	100	100
All	All	1012/3212 (32%)	928 (92%)	84 (8%)	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	216/679 (32%)	216 (100%)	0	100	100
1	B	216/679 (32%)	216 (100%)	0	100	100
1	C	216/679 (32%)	216 (100%)	0	100	100
1	D	216/679 (32%)	216 (100%)	0	100	100
All	All	864/2716 (32%)	864 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	126	ASN
1	A	184	ASN
1	A	343	ASN
1	D	72	HIS
1	D	126	ASN
1	D	343	ASN
1	B	72	HIS
1	B	126	ASN
1	C	72	HIS
1	C	126	ASN
1	C	343	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 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	$\#\|Z\| > 2$
3	CLR	C	904	-	31,31,31	1.10	3 (9%)	48,48,48	1.66	10 (20%)
3	CLR	A	903	-	31,31,31	1.15	3 (9%)	48,48,48	1.93	12 (25%)
3	CLR	D	903	-	31,31,31	1.12	2 (6%)	48,48,48	1.91	13 (27%)
3	CLR	C	902	-	31,31,31	1.01	2 (6%)	48,48,48	1.97	12 (25%)
3	CLR	D	904	-	31,31,31	1.17	3 (9%)	48,48,48	1.93	15 (31%)
2	POV	D	901	-	34,34,51	1.12	2 (5%)	38,39,59	1.22	4 (10%)
2	POV	B	901	-	34,34,51	1.13	2 (5%)	38,39,59	1.32	5 (13%)
3	CLR	C	903	-	31,31,31	1.15	1 (3%)	48,48,48	1.92	12 (25%)
2	POV	C	901	-	35,35,51	1.08	2 (5%)	39,40,59	1.33	5 (12%)
3	CLR	B	903	-	31,31,31	1.17	3 (9%)	48,48,48	1.96	17 (35%)
3	CLR	D	902	-	31,31,31	1.11	2 (6%)	48,48,48	2.14	15 (31%)
2	POV	A	901	-	35,35,51	1.11	2 (5%)	39,40,59	1.23	4 (10%)
3	CLR	B	902	-	31,31,31	1.15	1 (3%)	48,48,48	1.92	12 (25%)
3	CLR	A	902	-	31,31,31	1.20	3 (9%)	48,48,48	1.97	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	C	904	-	-	10/10/68/68	0/4/4/4
3	CLR	A	903	-	-	3/10/68/68	0/4/4/4
3	CLR	D	903	-	-	7/10/68/68	0/4/4/4
3	CLR	C	902	-	-	8/10/68/68	0/4/4/4
3	CLR	D	904	-	-	7/10/68/68	0/4/4/4
2	POV	D	901	-	-	18/36/36/55	-
2	POV	B	901	-	-	16/36/36/55	-
3	CLR	C	903	-	-	3/10/68/68	0/4/4/4
2	POV	C	901	-	-	20/37/37/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	B	903	-	-	3/10/68/68	0/4/4/4
3	CLR	D	902	-	-	7/10/68/68	0/4/4/4
2	POV	A	901	-	-	18/37/37/55	-
3	CLR	B	902	-	-	3/10/68/68	0/4/4/4
3	CLR	A	902	-	-	9/10/68/68	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	POV	O31-C31	4.25	1.45	1.33
2	D	901	POV	O31-C31	4.19	1.45	1.33
2	B	901	POV	O21-C21	4.18	1.46	1.34
2	B	901	POV	O31-C31	4.15	1.45	1.33
2	D	901	POV	O21-C21	4.04	1.45	1.34
2	A	901	POV	O21-C21	4.04	1.45	1.34
2	C	901	POV	O31-C31	3.98	1.45	1.33
2	C	901	POV	O21-C21	3.98	1.45	1.34
3	B	902	CLR	C13-C14	-2.76	1.49	1.55
3	C	903	CLR	C13-C14	-2.76	1.49	1.55
3	A	903	CLR	C13-C14	-2.74	1.49	1.55
3	D	903	CLR	C13-C14	-2.74	1.49	1.55
3	C	902	CLR	C13-C14	-2.57	1.50	1.55
3	D	902	CLR	C13-C14	-2.55	1.50	1.55
3	A	902	CLR	C13-C14	-2.49	1.50	1.55
3	C	904	CLR	C10-C9	-2.48	1.51	1.56
3	B	903	CLR	C13-C14	-2.48	1.50	1.55
3	A	902	CLR	C10-C9	-2.45	1.51	1.56
3	D	904	CLR	C10-C9	-2.40	1.52	1.56
3	C	904	CLR	C19-C10	-2.37	1.50	1.54
3	D	904	CLR	C13-C14	-2.36	1.50	1.55
3	C	902	CLR	C10-C9	-2.28	1.52	1.56
3	C	904	CLR	C13-C14	-2.26	1.50	1.55
3	B	903	CLR	C10-C9	-2.25	1.52	1.56
3	D	902	CLR	C10-C9	-2.18	1.52	1.56
3	B	903	CLR	C20-C17	-2.09	1.50	1.54
3	D	904	CLR	C20-C17	-2.08	1.50	1.54
3	A	902	CLR	C20-C17	-2.04	1.50	1.54
3	D	903	CLR	C18-C13	-2.03	1.50	1.54
3	A	903	CLR	C18-C13	-2.01	1.50	1.54
3	A	903	CLR	C20-C17	-2.00	1.50	1.54

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	902	CLR	C13-C14-C8	-5.88	105.67	114.38
3	A	903	CLR	C4-C5-C10	5.60	123.86	116.42
3	B	902	CLR	C4-C5-C10	5.59	123.84	116.42
3	C	903	CLR	C4-C5-C10	5.53	123.77	116.42
3	D	903	CLR	C4-C5-C10	5.46	123.67	116.42
3	D	902	CLR	C13-C17-C20	-4.99	111.68	119.49
3	C	902	CLR	C13-C17-C20	-4.80	111.98	119.49
3	D	904	CLR	C13-C17-C20	-4.78	112.00	119.49
2	B	901	POV	O21-C21-C22	4.78	121.79	111.50
3	C	902	CLR	C1-C10-C9	4.75	115.37	108.73
3	D	902	CLR	C7-C8-C9	4.66	115.36	109.71
3	C	902	CLR	C7-C6-C5	-4.65	116.47	125.06
3	D	903	CLR	C8-C7-C6	-4.65	106.05	112.73
3	A	903	CLR	C8-C7-C6	-4.65	106.05	112.73
2	C	901	POV	O21-C21-C22	4.62	121.45	111.50
3	C	903	CLR	C8-C7-C6	-4.60	106.12	112.73
3	B	902	CLR	C8-C7-C6	-4.60	106.12	112.73
3	B	903	CLR	C1-C10-C9	4.58	115.12	108.73
2	A	901	POV	O21-C21-C22	4.49	121.18	111.50
3	A	902	CLR	C13-C17-C20	-4.47	112.48	119.49
3	C	904	CLR	C3-C4-C5	-4.27	104.78	112.03
3	D	902	CLR	C7-C6-C5	-4.23	117.25	125.06
3	D	904	CLR	C1-C10-C9	4.22	114.62	108.73
2	D	901	POV	O21-C21-C22	4.21	120.57	111.50
3	A	902	CLR	C1-C10-C9	4.18	114.57	108.73
3	D	902	CLR	C14-C8-C9	-4.14	103.55	109.09
3	C	903	CLR	C19-C10-C9	-4.05	106.85	111.68
3	A	903	CLR	C19-C10-C9	-4.04	106.86	111.68
3	B	902	CLR	C19-C10-C9	-4.00	106.91	111.68
3	A	902	CLR	C4-C5-C10	3.96	121.68	116.42
3	B	903	CLR	C13-C17-C20	-3.95	113.31	119.49
3	C	904	CLR	C2-C3-C4	-3.94	104.91	110.31
3	D	903	CLR	C4-C5-C6	-3.92	114.96	120.61
3	C	902	CLR	C4-C5-C10	3.89	121.59	116.42
3	A	903	CLR	C4-C5-C6	-3.87	115.04	120.61
3	D	904	CLR	C10-C9-C8	-3.86	106.94	112.73
3	A	902	CLR	C10-C9-C8	-3.85	106.96	112.73
3	C	903	CLR	C4-C5-C6	-3.81	115.11	120.61
3	D	903	CLR	C19-C10-C9	-3.81	107.13	111.68
3	B	902	CLR	C4-C5-C6	-3.81	115.12	120.61
3	B	903	CLR	C10-C9-C8	-3.78	107.06	112.73
3	A	902	CLR	C13-C14-C8	-3.73	108.86	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	CLR	C13-C14-C8	-3.73	108.86	114.38
3	D	904	CLR	C11-C12-C13	-3.71	106.42	112.78
3	B	903	CLR	C7-C6-C5	-3.68	118.28	125.06
3	B	903	CLR	C4-C5-C10	3.66	121.28	116.42
3	D	904	CLR	C4-C5-C10	3.61	121.22	116.42
3	D	904	CLR	C13-C14-C8	-3.60	109.05	114.38
3	C	902	CLR	C10-C5-C6	-3.54	117.49	122.90
3	C	902	CLR	C11-C12-C13	-3.53	106.72	112.78
3	A	902	CLR	C7-C6-C5	-3.48	118.64	125.06
3	D	903	CLR	C2-C3-C4	-3.45	105.57	110.31
3	C	904	CLR	C11-C12-C13	-3.44	106.88	112.78
3	C	904	CLR	C4-C5-C10	3.43	120.97	116.42
3	C	903	CLR	C2-C3-C4	-3.39	105.65	110.31
3	B	902	CLR	C2-C3-C4	-3.39	105.66	110.31
3	B	903	CLR	C13-C14-C8	-3.38	109.37	114.38
3	D	902	CLR	C4-C5-C10	3.38	120.90	116.42
3	A	903	CLR	C2-C3-C4	-3.37	105.68	110.31
3	A	902	CLR	C10-C5-C6	-3.25	117.93	122.90
3	B	903	CLR	C10-C5-C6	-3.24	117.95	122.90
3	D	904	CLR	C10-C5-C6	-3.10	118.15	122.90
3	C	903	CLR	C11-C12-C13	-3.07	107.51	112.78
3	C	902	CLR	C10-C9-C8	-3.06	108.14	112.73
3	D	902	CLR	C1-C10-C9	3.06	113.00	108.73
3	B	902	CLR	C11-C12-C13	-3.05	107.55	112.78
2	C	901	POV	C2-O21-C21	-3.03	110.32	117.79
3	D	904	CLR	C7-C6-C5	-3.03	119.48	125.06
3	C	904	CLR	C19-C10-C9	-3.01	108.09	111.68
3	A	903	CLR	C11-C12-C13	-3.01	107.61	112.78
3	A	902	CLR	C11-C12-C13	-2.99	107.65	112.78
3	D	903	CLR	C21-C20-C17	-2.95	108.41	112.92
3	B	903	CLR	C1-C2-C3	2.94	114.24	110.47
3	D	904	CLR	C19-C10-C9	-2.92	108.20	111.68
3	D	902	CLR	C8-C7-C6	-2.89	108.57	112.73
3	D	903	CLR	C11-C12-C13	-2.86	107.88	112.78
3	A	902	CLR	C19-C10-C9	-2.85	108.28	111.68
3	D	904	CLR	C21-C20-C17	-2.85	108.56	112.92
2	A	901	POV	C2-O21-C21	-2.84	110.80	117.79
3	B	903	CLR	C19-C10-C9	-2.82	108.32	111.68
3	C	904	CLR	C21-C20-C17	-2.82	108.60	112.92
2	B	901	POV	O31-C31-C32	2.79	120.65	111.91
3	B	903	CLR	C21-C20-C17	-2.78	108.67	112.92
3	D	902	CLR	C17-C13-C14	2.73	103.30	100.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	CLR	C8-C7-C6	-2.72	108.82	112.73
3	C	904	CLR	C1-C10-C9	2.70	112.50	108.73
3	B	903	CLR	C15-C14-C8	-2.69	114.66	119.08
3	A	902	CLR	C17-C13-C14	2.67	103.24	100.07
2	C	901	POV	O31-C31-C32	2.65	120.21	111.91
3	A	903	CLR	C7-C6-C5	-2.64	120.20	125.06
3	B	902	CLR	C7-C6-C5	-2.62	120.23	125.06
3	C	902	CLR	C9-C10-C5	-2.61	105.56	109.65
3	D	902	CLR	C21-C20-C17	-2.61	108.93	112.92
3	C	903	CLR	C7-C6-C5	-2.60	120.26	125.06
3	D	902	CLR	C10-C5-C6	-2.57	118.98	122.90
3	A	902	CLR	C15-C14-C8	-2.55	114.89	119.08
3	D	904	CLR	C1-C2-C3	2.54	113.73	110.47
3	D	903	CLR	C7-C6-C5	-2.54	120.38	125.06
3	C	903	CLR	C13-C14-C8	-2.51	110.66	114.38
3	B	902	CLR	C21-C20-C17	-2.50	109.10	112.92
3	A	903	CLR	C13-C14-C8	-2.49	110.69	114.38
3	B	902	CLR	C13-C14-C8	-2.49	110.70	114.38
3	A	903	CLR	C21-C20-C17	-2.48	109.12	112.92
3	A	902	CLR	C1-C2-C3	2.48	113.65	110.47
3	C	903	CLR	C21-C20-C17	-2.48	109.13	112.92
3	B	903	CLR	C1-C10-C5	-2.47	104.24	108.75
3	D	904	CLR	C17-C13-C14	2.44	102.97	100.07
3	A	903	CLR	C15-C14-C8	-2.42	115.10	119.08
3	B	902	CLR	C15-C14-C8	-2.41	115.10	119.08
3	C	903	CLR	C15-C14-C8	-2.41	115.12	119.08
3	C	902	CLR	C17-C13-C14	2.40	102.92	100.07
3	C	903	CLR	C13-C17-C20	-2.40	115.73	119.49
3	B	902	CLR	C13-C17-C20	-2.39	115.75	119.49
3	D	903	CLR	C15-C14-C8	-2.38	115.16	119.08
2	D	901	POV	O31-C31-C32	2.38	119.38	111.91
3	A	903	CLR	C13-C17-C20	-2.36	115.79	119.49
3	B	903	CLR	C11-C12-C13	-2.34	108.76	112.78
3	D	903	CLR	C13-C14-C8	-2.34	110.92	114.38
2	B	901	POV	O13-P-O14	2.31	119.71	110.68
3	C	904	CLR	C10-C5-C6	-2.30	119.39	122.90
3	D	902	CLR	C2-C1-C10	-2.29	107.79	112.74
3	A	902	CLR	C2-C1-C10	-2.28	107.81	112.74
3	B	903	CLR	C17-C13-C14	2.27	102.77	100.07
3	D	903	CLR	C12-C13-C17	2.26	119.95	116.57
3	C	902	CLR	C19-C10-C9	-2.25	109.00	111.68
2	A	901	POV	O31-C31-C32	2.22	118.88	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	903	CLR	C23-C22-C20	-2.21	108.68	115.03
3	D	902	CLR	C11-C12-C13	-2.21	109.00	112.78
3	A	902	CLR	C1-C10-C5	-2.20	104.73	108.75
3	D	903	CLR	C13-C17-C20	-2.19	116.06	119.49
2	C	901	POV	O21-C21-O22	-2.19	118.41	123.70
2	C	901	POV	O13-P-O14	2.17	119.17	110.68
2	B	901	POV	O21-C21-O22	-2.16	118.47	123.70
3	A	903	CLR	C12-C13-C17	2.15	119.79	116.57
2	D	901	POV	O13-P-O14	2.15	119.09	110.68
3	B	902	CLR	C12-C13-C17	2.15	119.78	116.57
3	D	903	CLR	C1-C10-C9	2.15	111.72	108.73
3	D	904	CLR	C1-C10-C5	-2.15	104.83	108.75
2	A	901	POV	O13-P-O14	2.14	119.05	110.68
3	D	904	CLR	C15-C14-C8	-2.13	115.57	119.08
3	D	904	CLR	C2-C1-C10	-2.13	108.13	112.74
2	D	901	POV	C2-O21-C21	-2.12	112.56	117.79
3	C	903	CLR	C12-C13-C17	2.12	119.75	116.57
3	A	902	CLR	C7-C8-C9	2.09	112.25	109.71
3	D	902	CLR	C15-C14-C13	2.08	106.35	103.84
3	B	903	CLR	C2-C1-C10	-2.08	108.24	112.74
2	B	901	POV	O31-C31-O32	-2.08	118.35	123.59
3	C	904	CLR	C13-C17-C20	-2.05	116.27	119.49
3	B	903	CLR	C7-C8-C9	2.05	112.20	109.71
3	C	904	CLR	C7-C8-C14	-2.04	107.94	110.91
3	D	902	CLR	C16-C17-C20	-2.04	108.99	112.15

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	904	CLR	C13-C17-C20-C21
3	C	904	CLR	C13-C17-C20-C22
3	C	904	CLR	C16-C17-C20-C22
2	A	901	POV	O32-C31-O31-C3
2	D	901	POV	O32-C31-O31-C3
2	C	901	POV	O32-C31-O31-C3
2	A	901	POV	C32-C31-O31-C3
2	D	901	POV	C32-C31-O31-C3
2	C	901	POV	C32-C31-O31-C3
3	C	904	CLR	C16-C17-C20-C21
3	D	902	CLR	C21-C20-C22-C23
3	C	904	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	D	901	POV	C32-C33-C34-C35
3	A	902	CLR	C13-C17-C20-C21
3	A	902	CLR	C13-C17-C20-C22
3	D	903	CLR	C17-C20-C22-C23
2	C	901	POV	C310-C311-C312-C313
2	C	901	POV	C32-C33-C34-C35
3	A	902	CLR	C21-C20-C22-C23
3	D	903	CLR	C21-C20-C22-C23
3	D	902	CLR	C17-C20-C22-C23
3	B	903	CLR	C21-C20-C22-C23
3	C	902	CLR	C16-C17-C20-C22
2	C	901	POV	C21-C22-C23-C24
2	B	901	POV	C22-C21-O21-C2
3	C	904	CLR	C20-C22-C23-C24
3	C	904	CLR	C17-C20-C22-C23
3	D	903	CLR	C20-C22-C23-C24
3	A	902	CLR	C20-C22-C23-C24
2	A	901	POV	C21-C22-C23-C24
3	D	903	CLR	C22-C23-C24-C25
3	C	904	CLR	C22-C23-C24-C25
2	A	901	POV	C22-C21-O21-C2
2	D	901	POV	C22-C21-O21-C2
3	C	902	CLR	C22-C23-C24-C25
2	D	901	POV	O22-C21-O21-C2
2	B	901	POV	O22-C21-O21-C2
3	A	902	CLR	C23-C24-C25-C27
2	B	901	POV	C37-C38-C39-C310
2	C	901	POV	C311-C312-C313-C314
2	D	901	POV	C310-C311-C312-C313
2	C	901	POV	C312-C313-C314-C315
2	A	901	POV	O22-C21-O21-C2
2	D	901	POV	C39-C310-C311-C312
2	B	901	POV	C312-C313-C314-C315
2	C	901	POV	C35-C36-C37-C38
3	A	903	CLR	C23-C24-C25-C27
3	D	903	CLR	C23-C24-C25-C26
3	C	903	CLR	C23-C24-C25-C27
2	B	901	POV	C310-C311-C312-C313
2	B	901	POV	C22-C23-C24-C25
3	A	902	CLR	C23-C24-C25-C26
3	A	903	CLR	C23-C24-C25-C26
3	B	902	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	B	902	CLR	C23-C24-C25-C27
3	C	902	CLR	C23-C24-C25-C26
3	C	902	CLR	C23-C24-C25-C27
2	D	901	POV	C22-C23-C24-C25
3	D	904	CLR	C20-C22-C23-C24
3	D	904	CLR	C23-C24-C25-C26
3	C	903	CLR	C23-C24-C25-C26
2	A	901	POV	C35-C36-C37-C38
2	A	901	POV	C22-C23-C24-C25
2	C	901	POV	C37-C38-C39-C310
3	D	904	CLR	C16-C17-C20-C22
2	C	901	POV	C22-C21-O21-C2
2	B	901	POV	O21-C2-C3-O31
2	A	901	POV	C23-C24-C25-C26
2	C	901	POV	C33-C34-C35-C36
2	C	901	POV	O22-C21-O21-C2
2	A	901	POV	C311-C310-C39-C38
2	D	901	POV	C23-C24-C25-C26
2	C	901	POV	C36-C37-C38-C39
3	A	902	CLR	C16-C17-C20-C21
3	C	902	CLR	C13-C17-C20-C21
2	A	901	POV	C311-C312-C313-C314
2	D	901	POV	C1-C2-C3-O31
2	C	901	POV	C1-C2-C3-O31
3	C	903	CLR	C22-C23-C24-C25
3	A	903	CLR	C22-C23-C24-C25
2	A	901	POV	C34-C35-C36-C37
3	C	902	CLR	C16-C17-C20-C21
3	B	902	CLR	C22-C23-C24-C25
2	D	901	POV	C311-C312-C313-C314
2	A	901	POV	C24-C25-C26-C27
2	C	901	POV	C22-C23-C24-C25
3	D	902	CLR	C13-C17-C20-C21
3	A	902	CLR	C16-C17-C20-C22
2	A	901	POV	C313-C314-C315-C316
2	B	901	POV	C32-C31-O31-C3
2	B	901	POV	C1-C2-C3-O31
2	D	901	POV	C312-C313-C314-C315
3	D	903	CLR	C23-C24-C25-C27
2	C	901	POV	O21-C21-C22-C23
3	D	902	CLR	C13-C17-C20-C22
3	C	904	CLR	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
3	D	904	CLR	C23-C24-C25-C27
2	C	901	POV	C313-C314-C315-C316
3	B	903	CLR	C23-C24-C25-C27
2	D	901	POV	C35-C36-C37-C38
2	B	901	POV	O32-C31-O31-C3
2	D	901	POV	O21-C2-C3-O31
2	C	901	POV	O21-C2-C3-O31
2	B	901	POV	C39-C310-C311-C312
2	A	901	POV	C310-C311-C312-C313
2	B	901	POV	C34-C35-C36-C37
2	A	901	POV	C31-C32-C33-C34
3	D	904	CLR	C22-C23-C24-C25
2	B	901	POV	O31-C31-C32-C33
3	D	904	CLR	C21-C20-C22-C23
2	C	901	POV	C23-C24-C25-C26
3	D	903	CLR	C16-C17-C20-C22
3	C	904	CLR	C23-C24-C25-C26
2	A	901	POV	C32-C33-C34-C35
3	D	902	CLR	C16-C17-C20-C22
2	A	901	POV	C39-C310-C311-C312
2	B	901	POV	C36-C37-C38-C39
3	D	904	CLR	C16-C17-C20-C21
3	B	903	CLR	C23-C24-C25-C26
3	C	902	CLR	C21-C20-C22-C23
3	C	902	CLR	C17-C20-C22-C23
2	B	901	POV	O21-C21-C22-C23
2	D	901	POV	C36-C37-C38-C39
2	D	901	POV	O11-C1-C2-O21
2	A	901	POV	C37-C38-C39-C310
2	B	901	POV	C313-C314-C315-C316
2	D	901	POV	C33-C34-C35-C36
2	C	901	POV	O22-C21-C22-C23
3	A	902	CLR	C22-C23-C24-C25
2	D	901	POV	O11-C1-C2-C3
3	D	902	CLR	C22-C23-C24-C25
3	D	902	CLR	C16-C17-C20-C21

There are no ring outliers.

14 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	904	CLR	3	0

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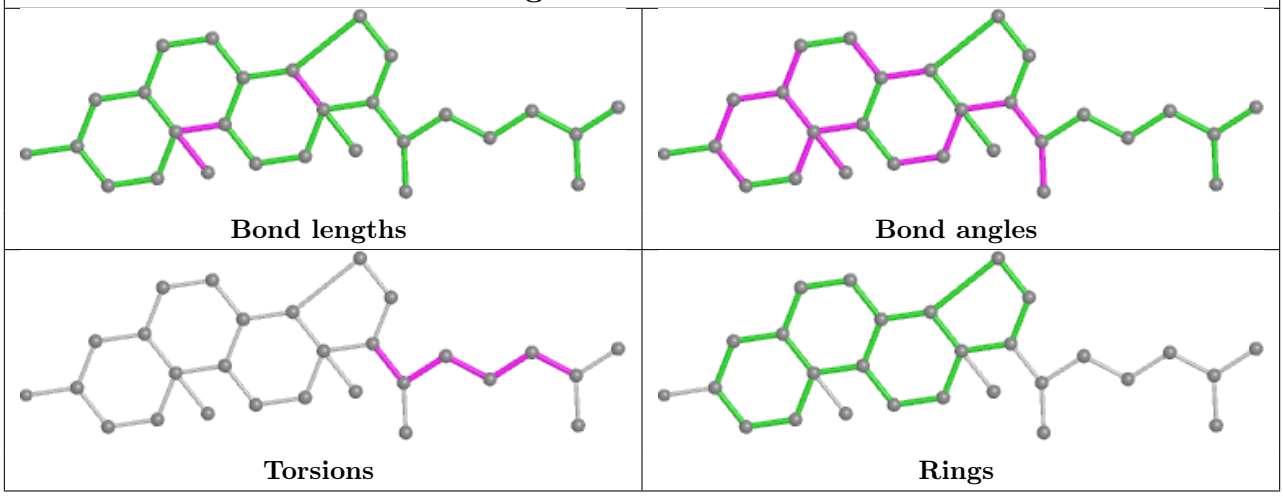
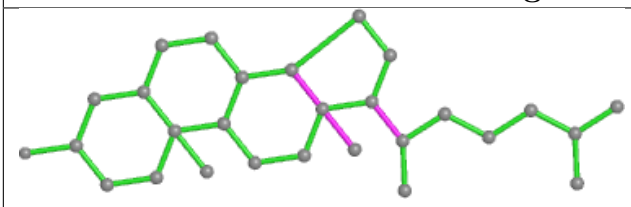
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	CLR	9	0
3	D	903	CLR	12	0
3	C	902	CLR	17	0
3	D	904	CLR	15	0
2	D	901	POV	5	0
2	B	901	POV	1	0
3	C	903	CLR	11	0
2	C	901	POV	12	0
3	B	903	CLR	4	0
3	D	902	CLR	3	0
2	A	901	POV	6	0
3	B	902	CLR	11	0
3	A	902	CLR	4	0

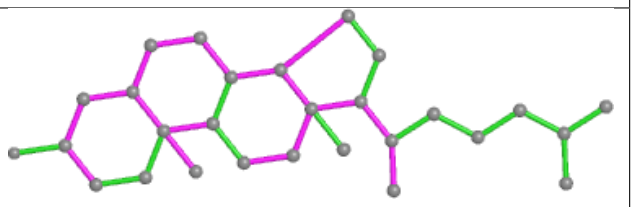
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

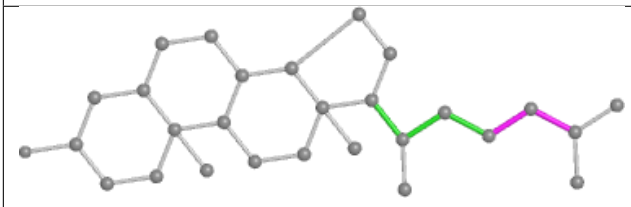
Ligand CLR C 904

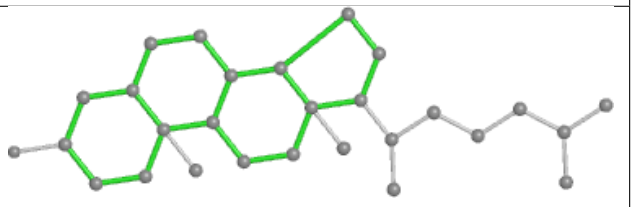


Ligand CLR A 903

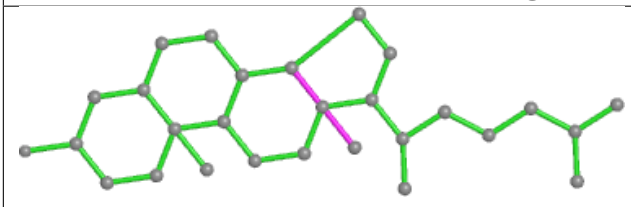

Bond lengths

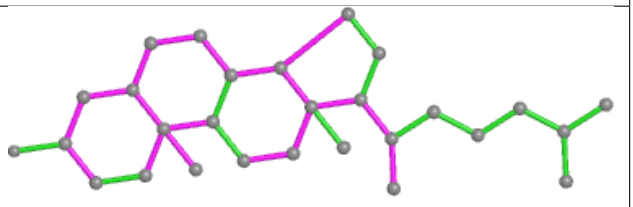

Bond angles

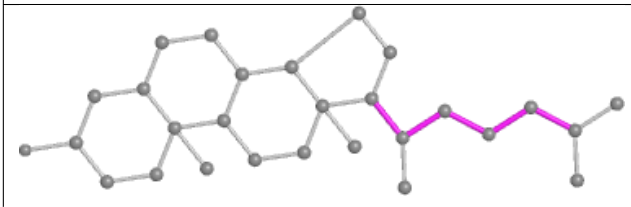

Torsions


Rings

Ligand CLR D 903


Bond lengths


Bond angles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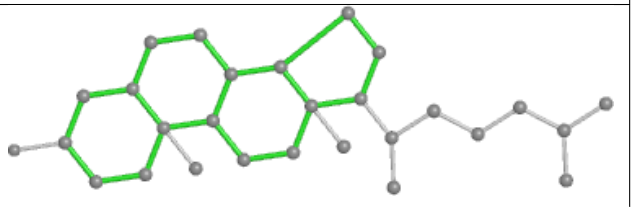
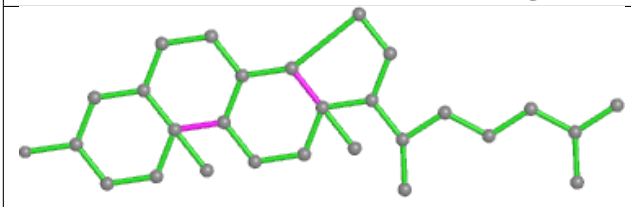
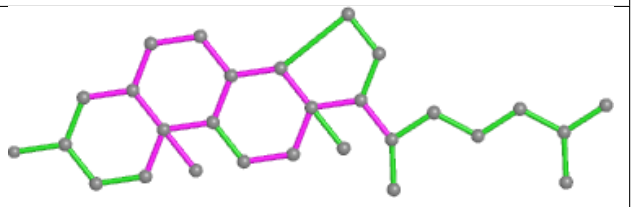
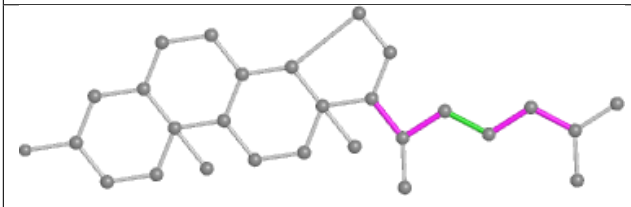

Rings

Ligand CLR C 902


Bond lengths


Bond angles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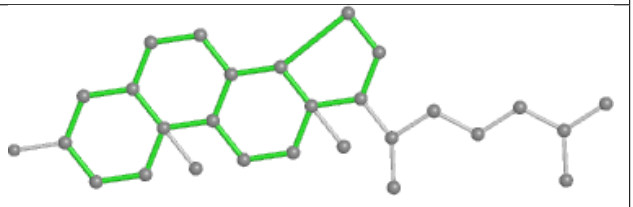
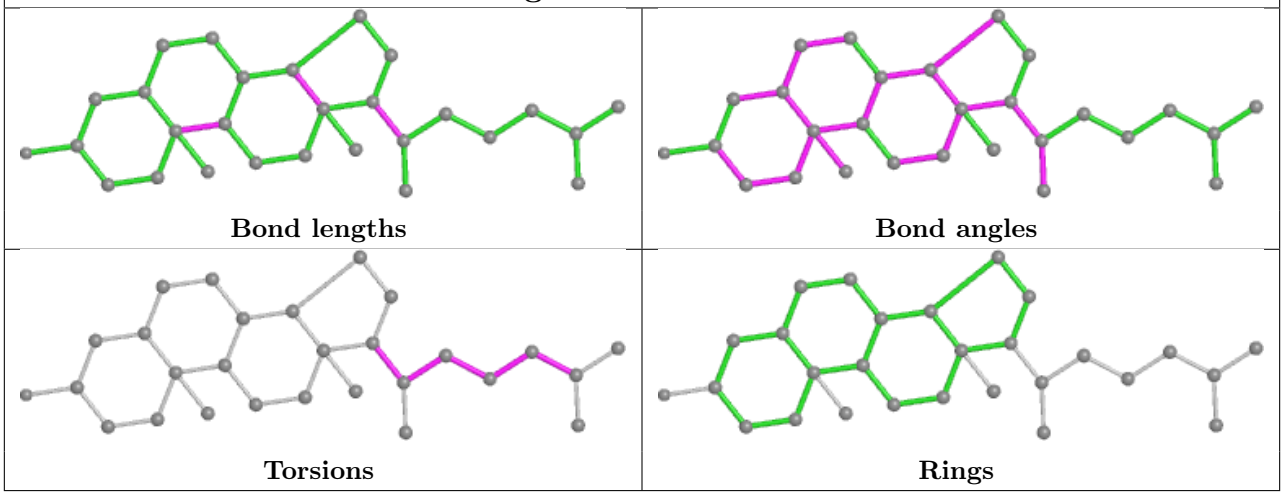
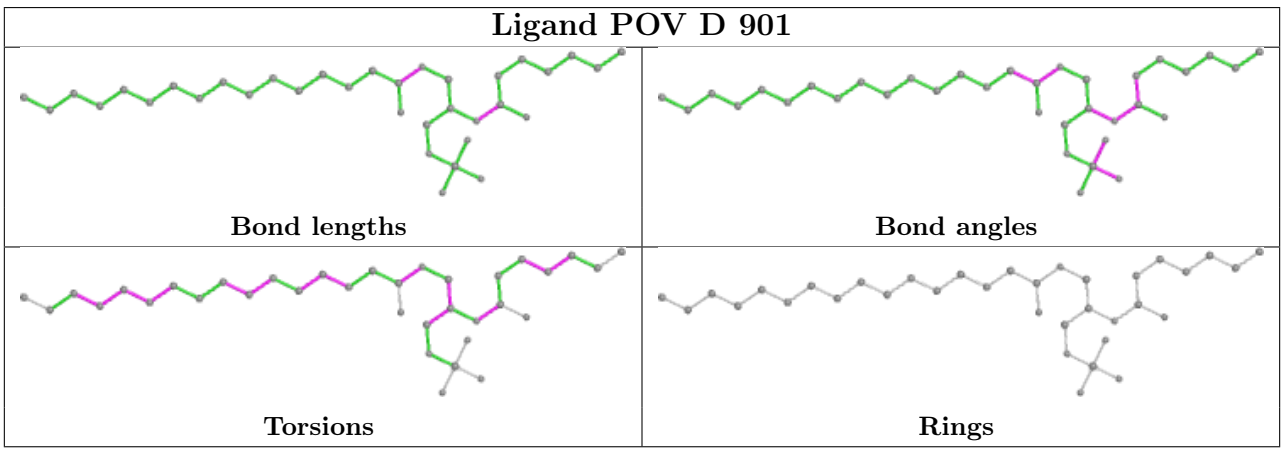

Rings

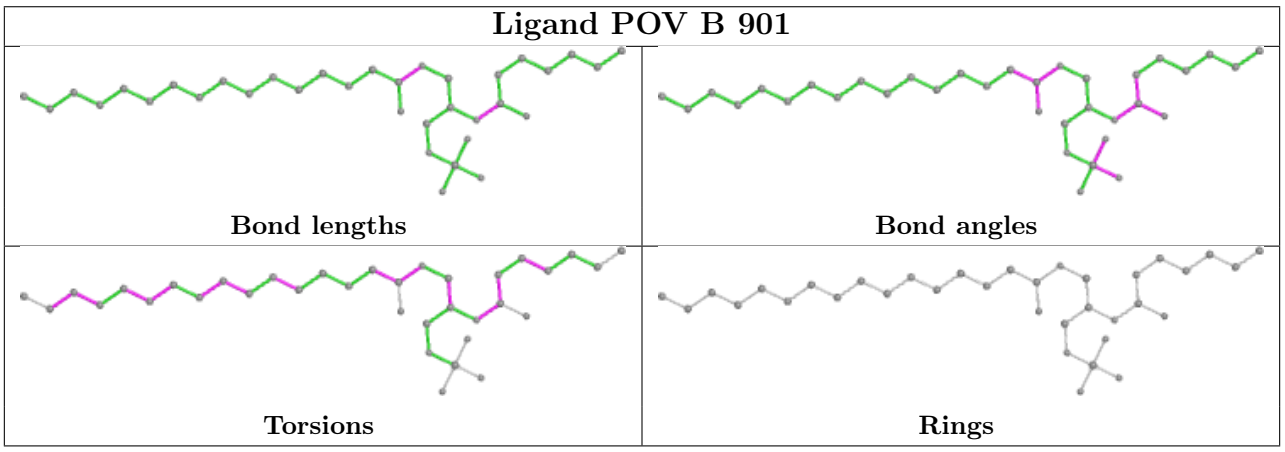
Ligand CLR D 904



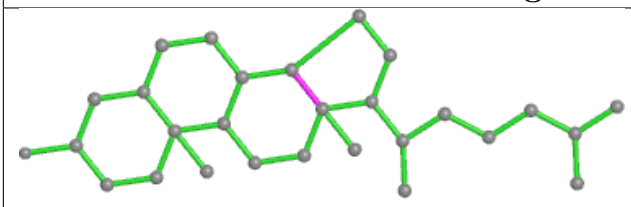
Ligand POV D 901

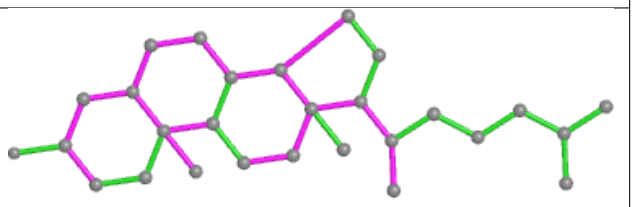


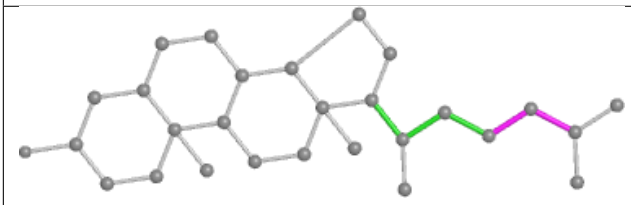
Ligand POV B 901

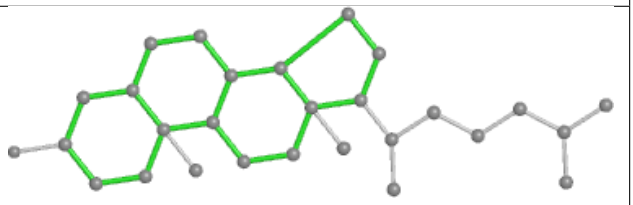


Ligand CLR C 903

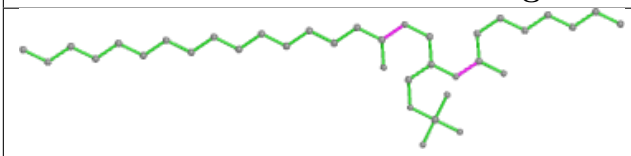

Bond lengths

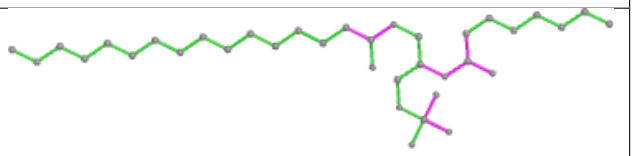

Bond angles

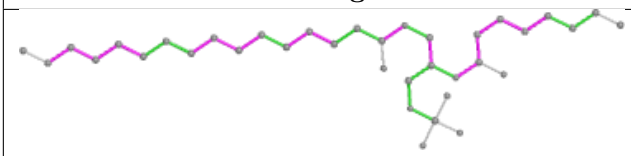

Torsions


Rings

Ligand POV C 901

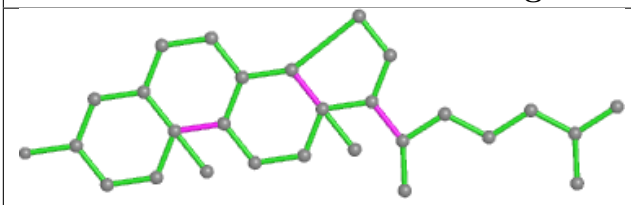

Bond lengths

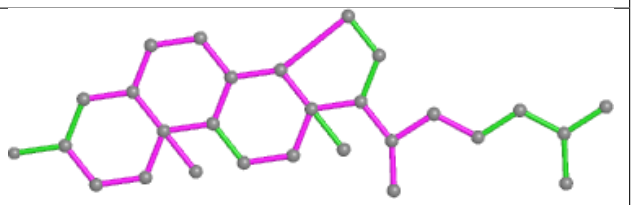

Bond angles

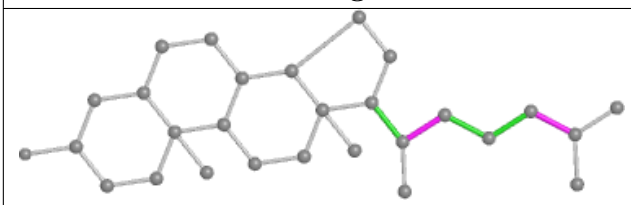

Torsions

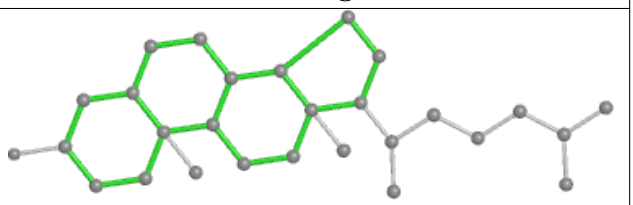

Rings

Ligand CLR B 903

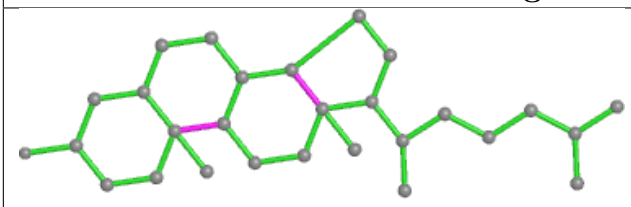

Bond lengths

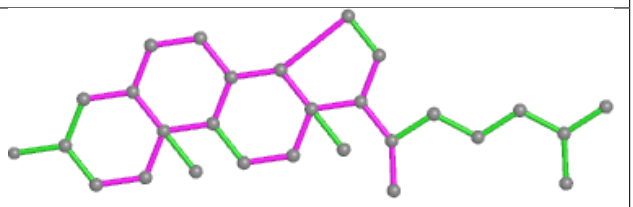

Bond angles

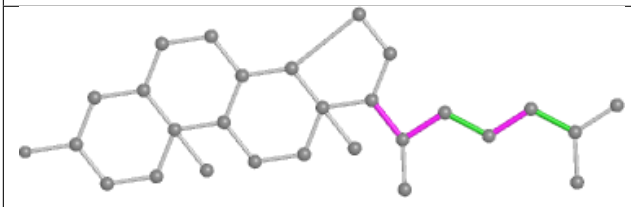

Torsions

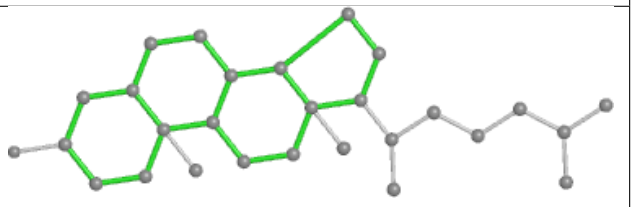

Rings

Ligand CLR D 902

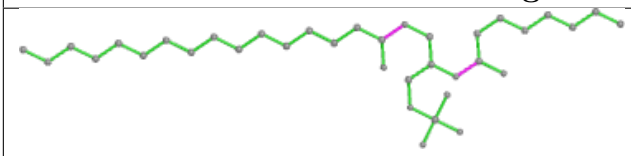

Bond lengths

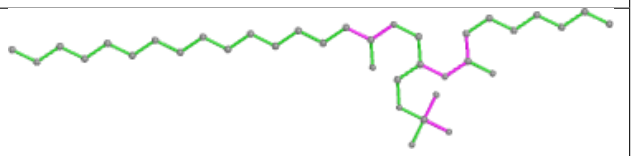

Bond angles

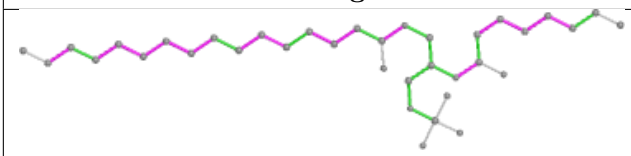

Torsions


Rings

Ligand POV A 901

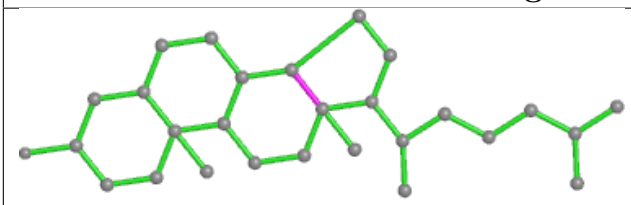

Bond lengths

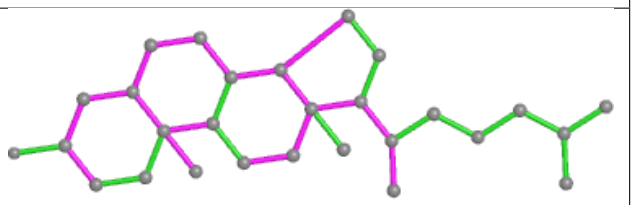

Bond angles

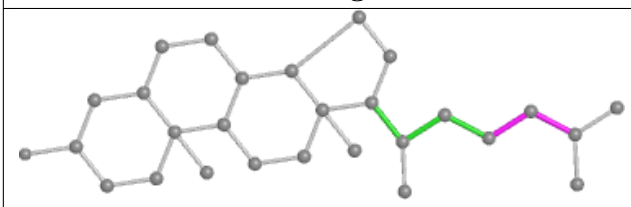

Torsions

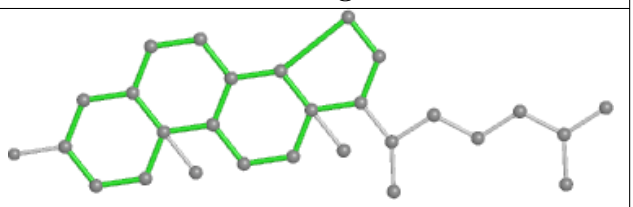

Rings

Ligand CLR B 902

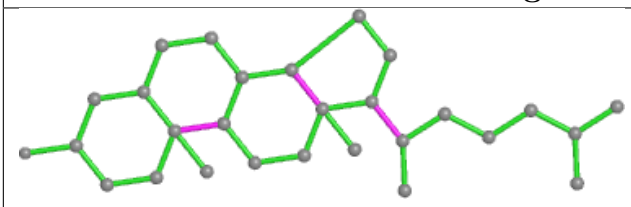

Bond lengths


Bond angles

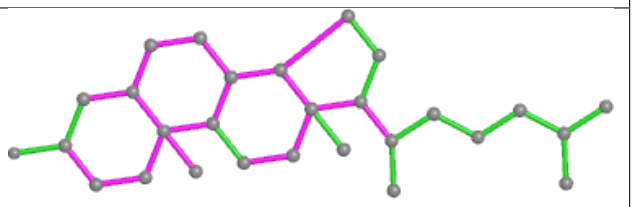

Torsions


Rings

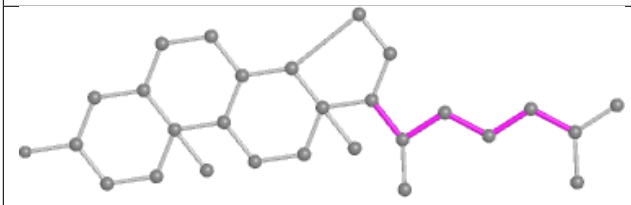
Ligand CLR A 902



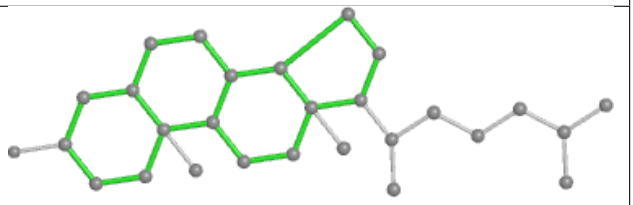
Bond lengths



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.

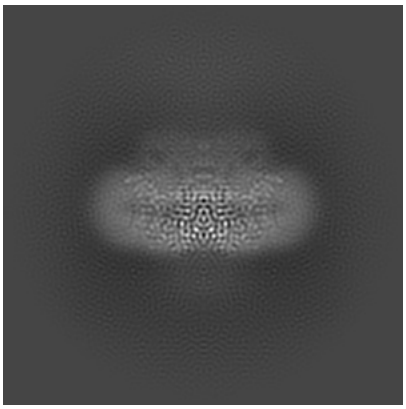
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36042. These allow visual inspection of the internal detail of the map and identification of artifacts.

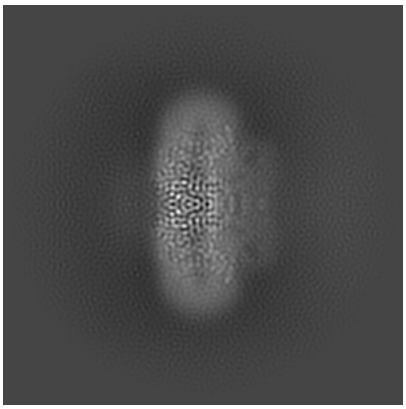
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

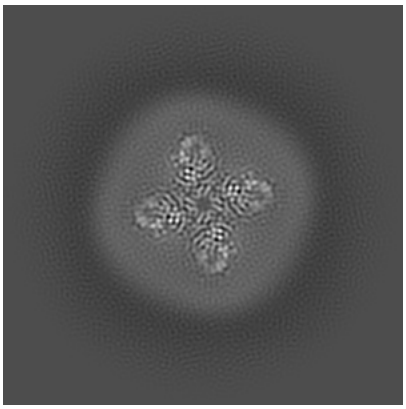
6.1.1 Primary map



X

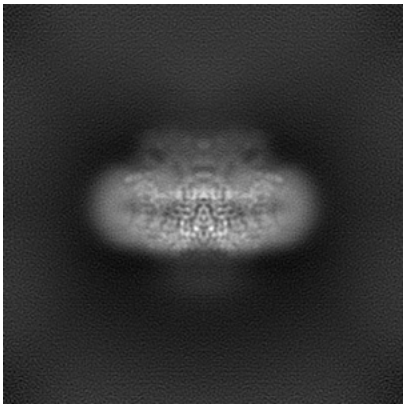


Y

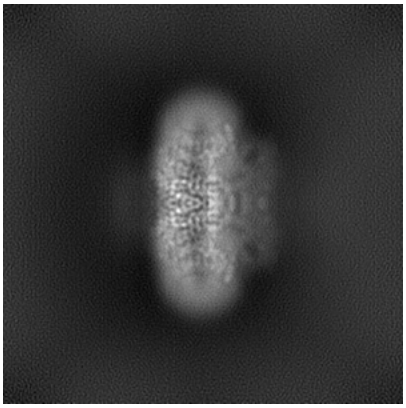


Z

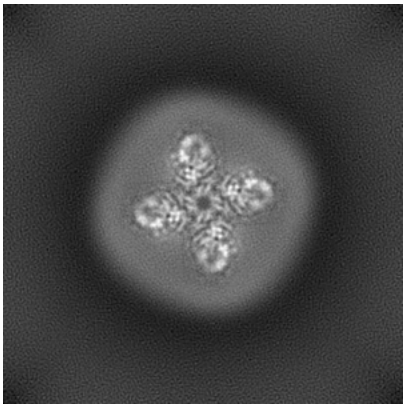
6.1.2 Raw map



X



Y

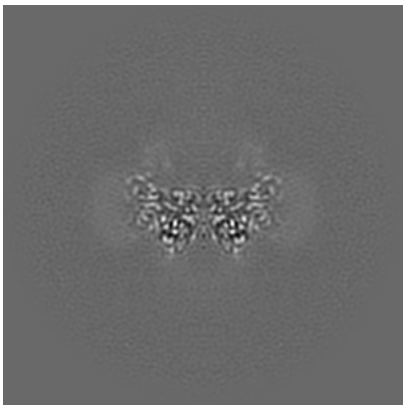


Z

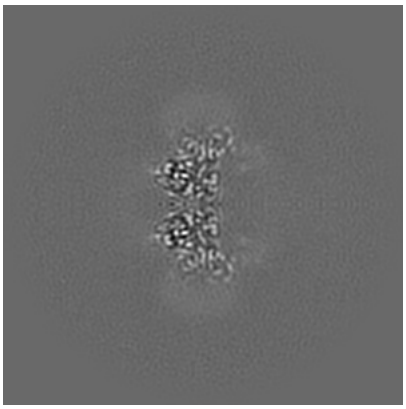
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

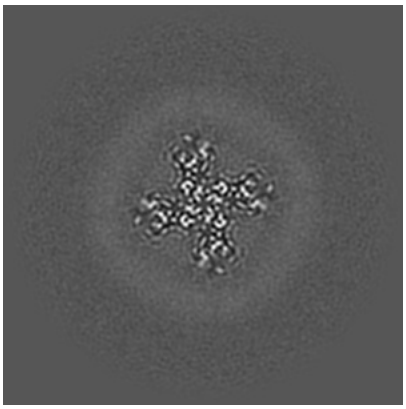
6.2.1 Primary map



X Index: 128

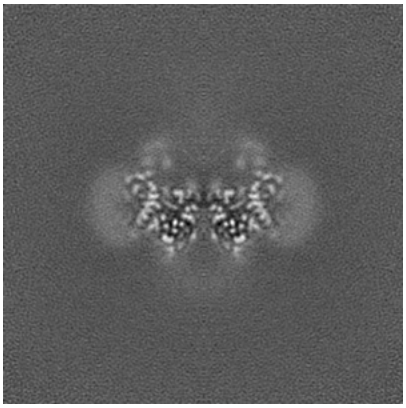


Y Index: 128

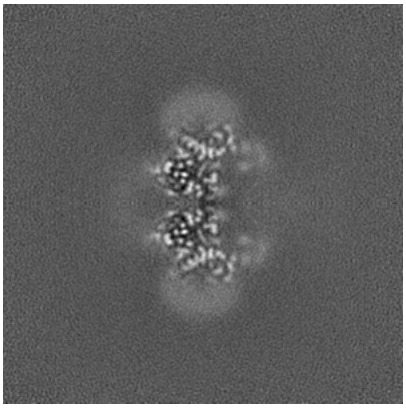


Z Index: 128

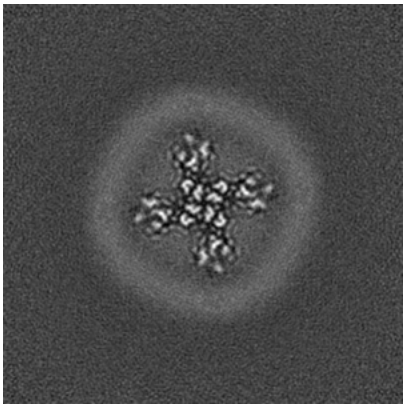
6.2.2 Raw map



X Index: 128



Y Index: 128

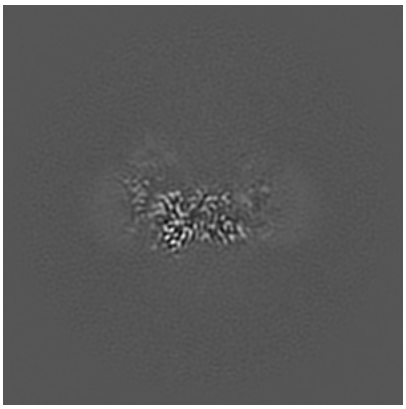


Z Index: 128

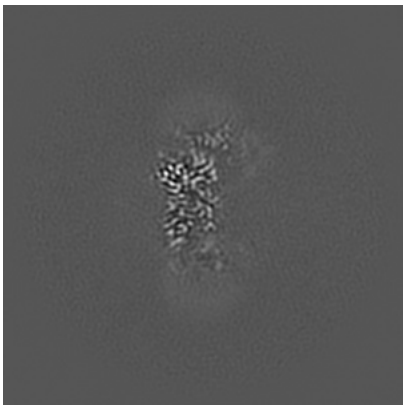
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

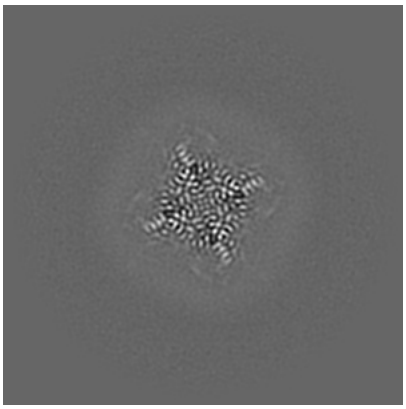
6.3.1 Primary map



X Index: 134

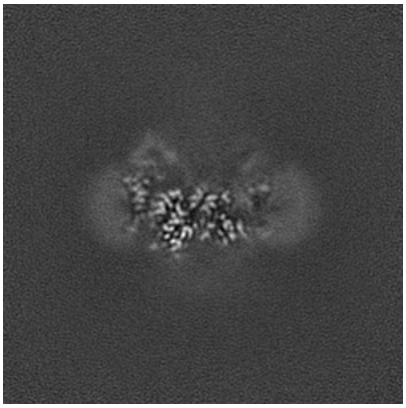


Y Index: 134

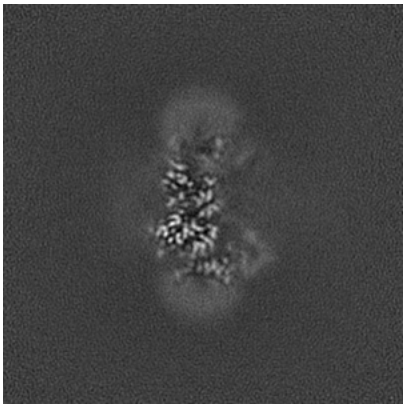


Z Index: 109

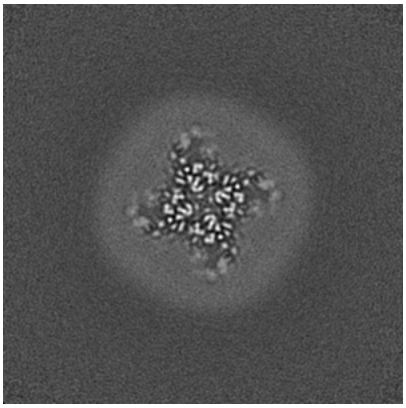
6.3.2 Raw map



X Index: 134



Y Index: 122

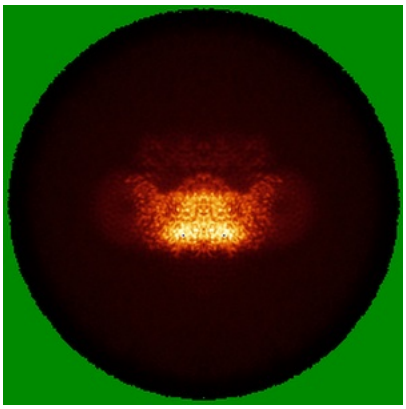


Z Index: 111

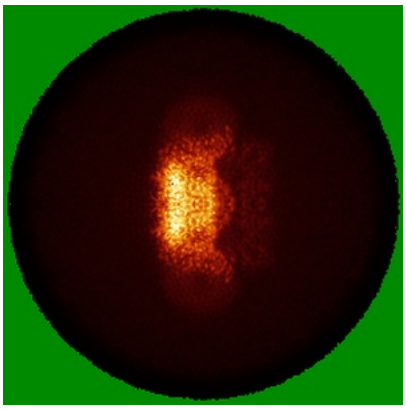
The images above show the largest variance slices of the map in three orthogonal directions.

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

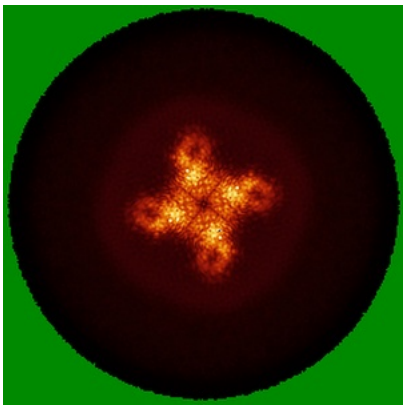
6.4.1 Primary map



X

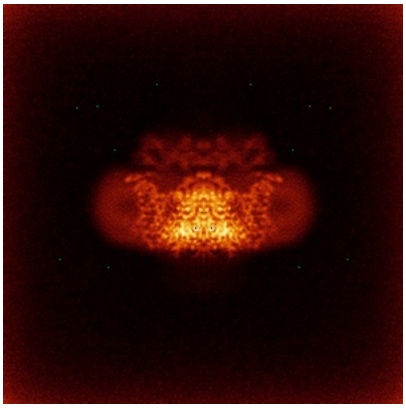


Y

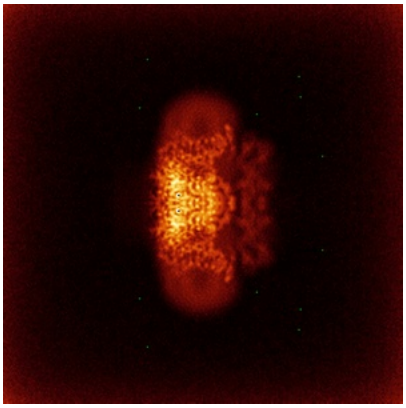


Z

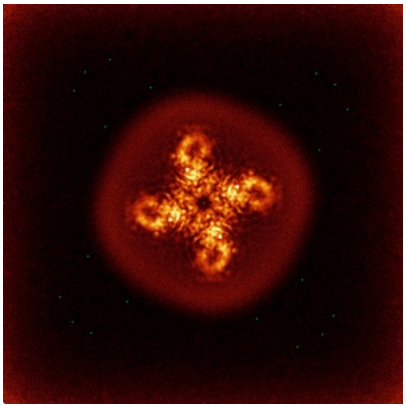
6.4.2 Raw map



X



Y

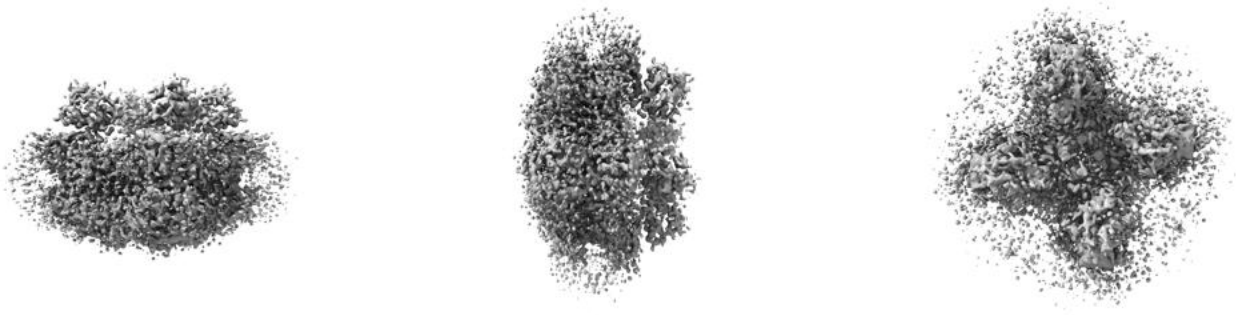


Z

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)

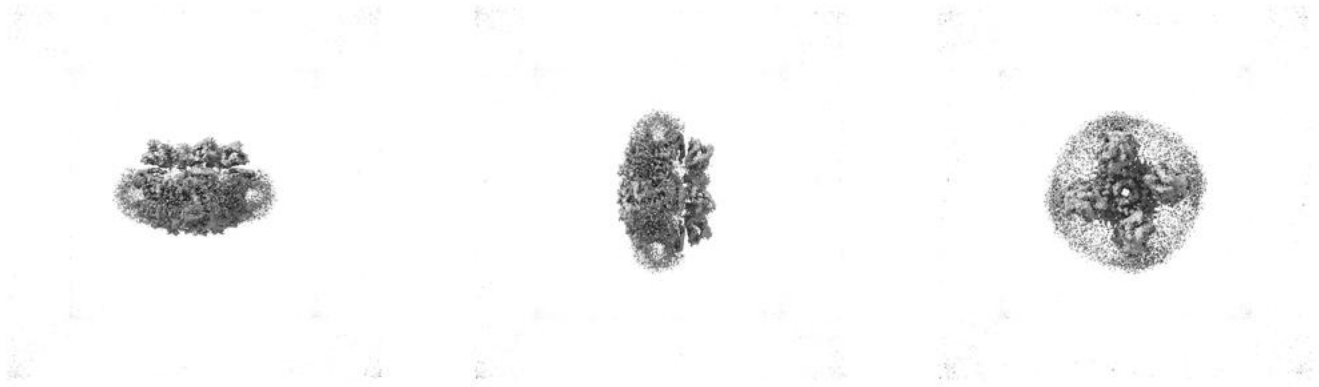
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.423. 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.

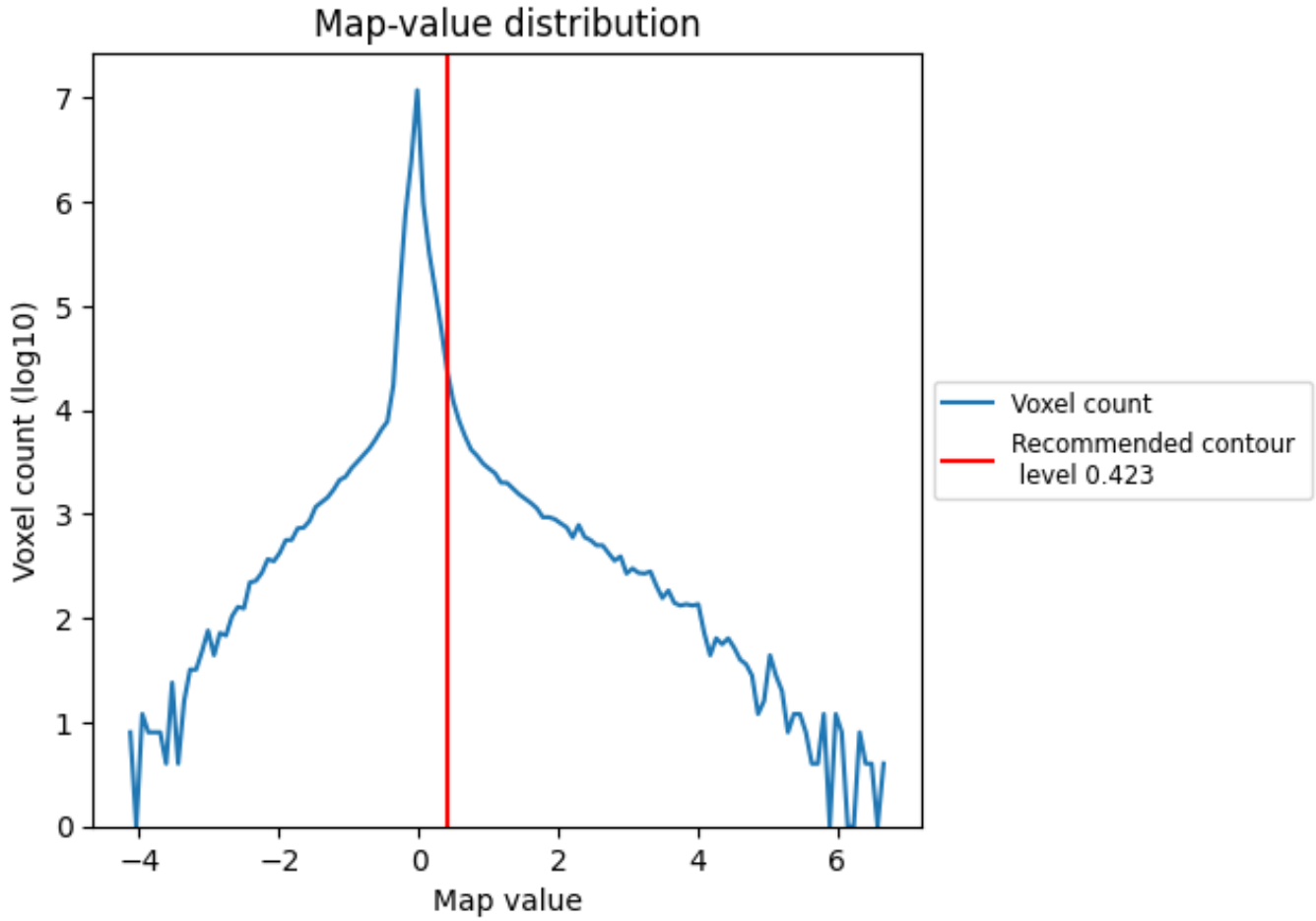
6.6 Mask visualisation (i)

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

7 Map analysis

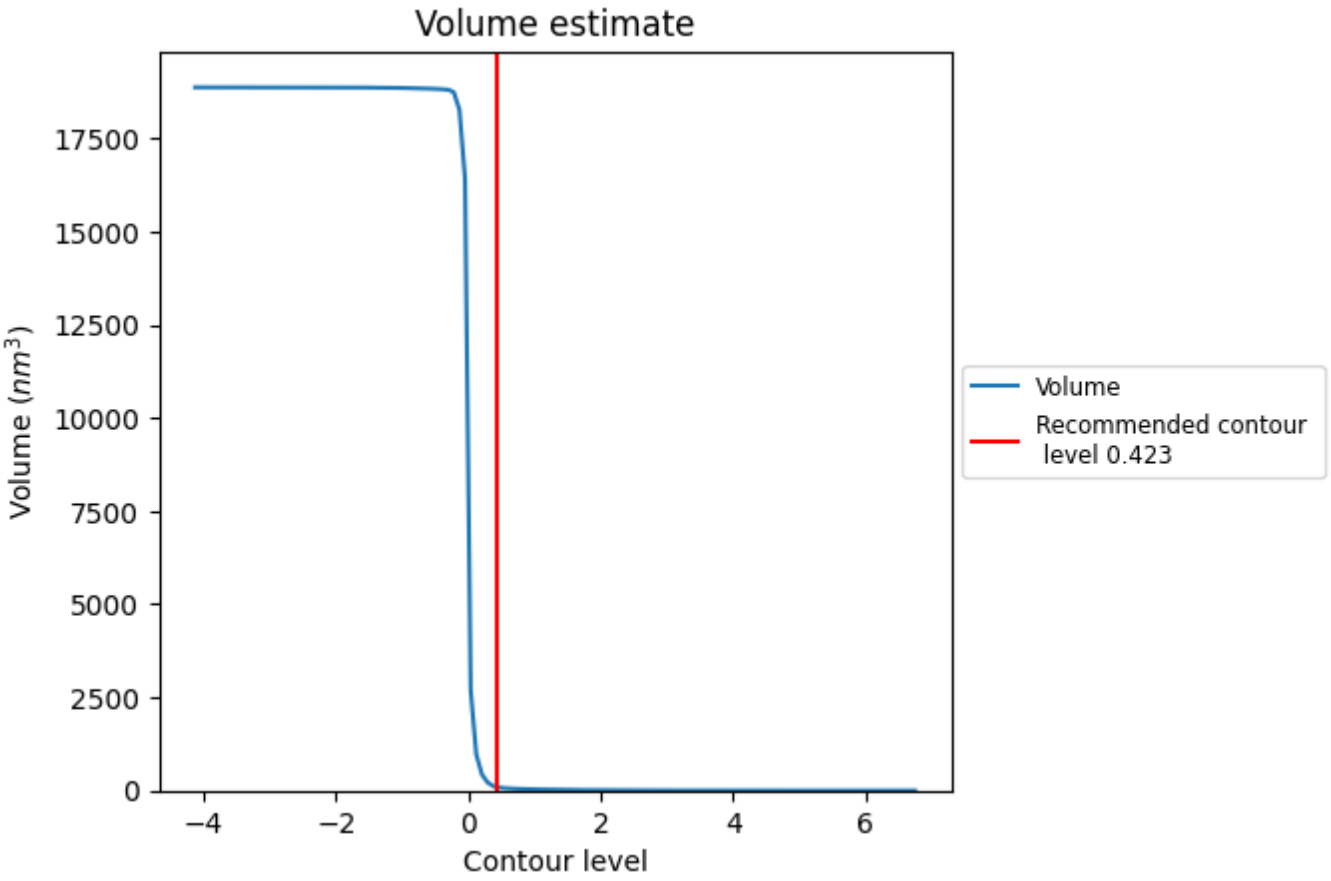
This section contains the results of statistical analysis of the map.

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.

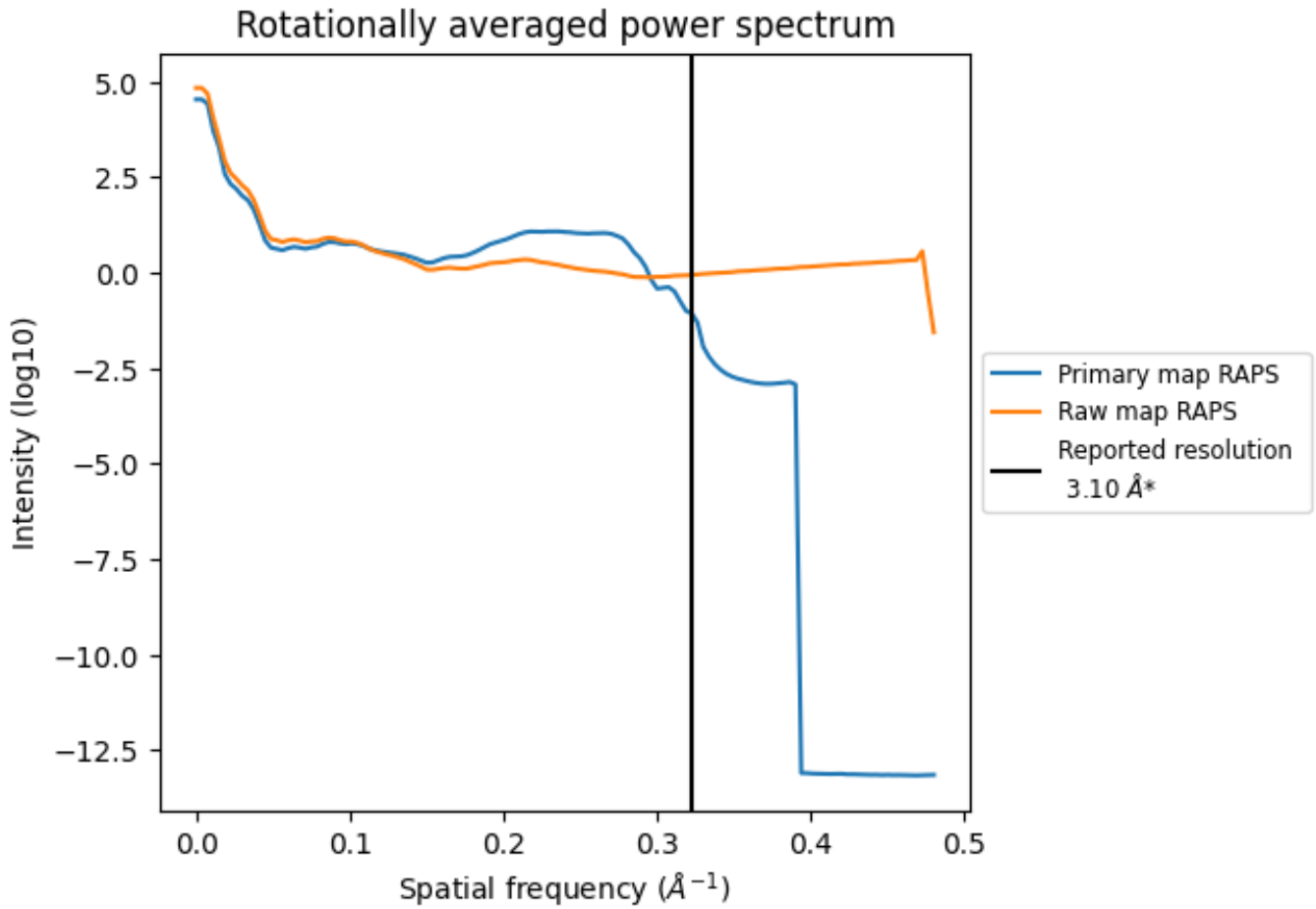
7.2 Volume estimate



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

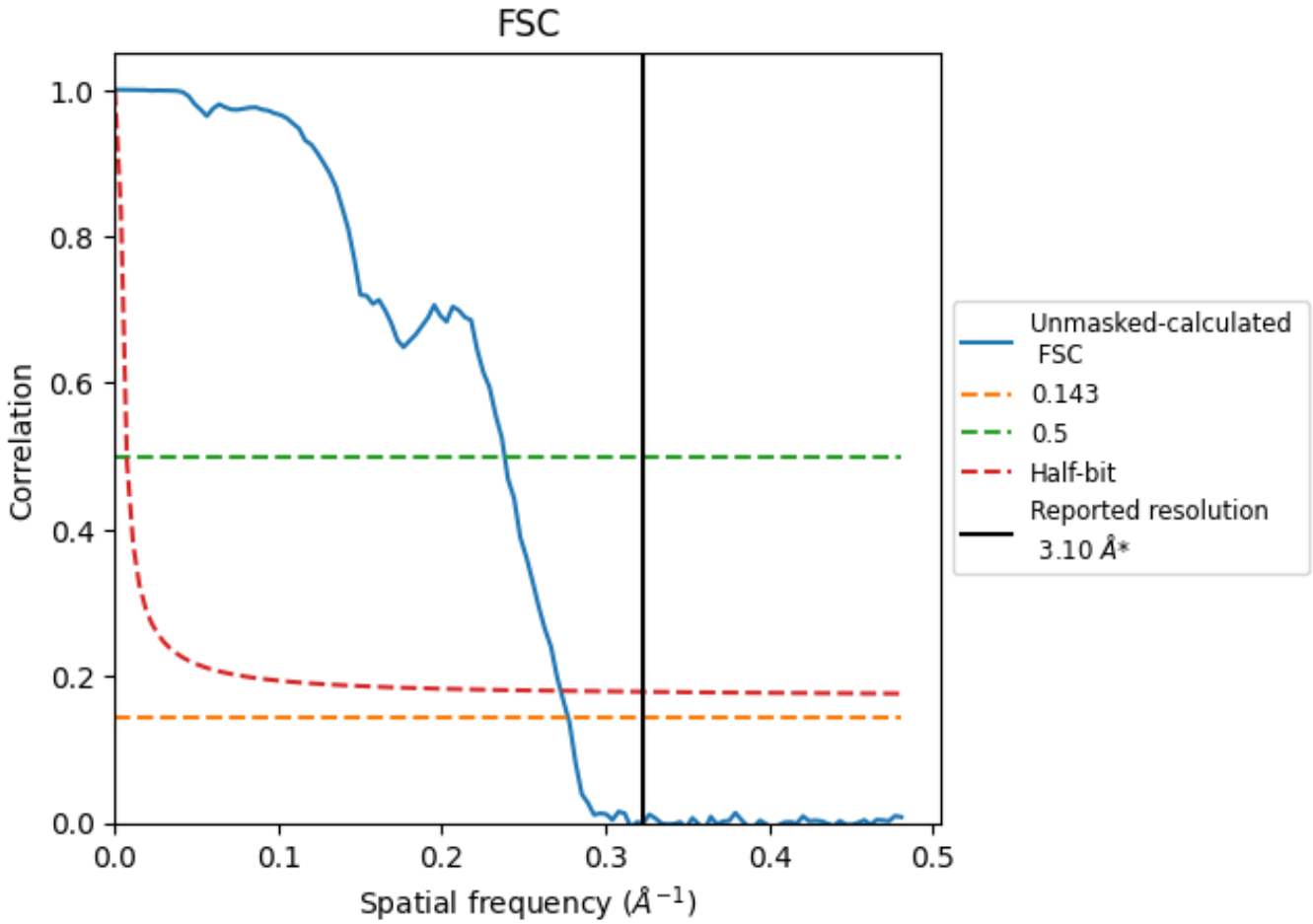


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

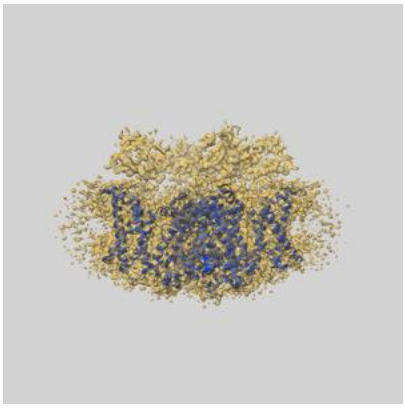
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.20	3.67

*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 3.61 differs from the reported value 3.1 by more than 10 %

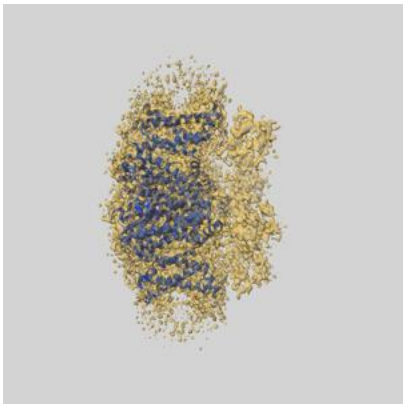
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36042 and PDB model 8J7M. Per-residue inclusion information can be found in section 3 on page 10.

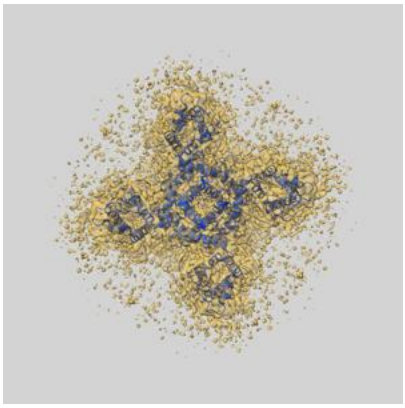
9.1 Map-model overlay



X



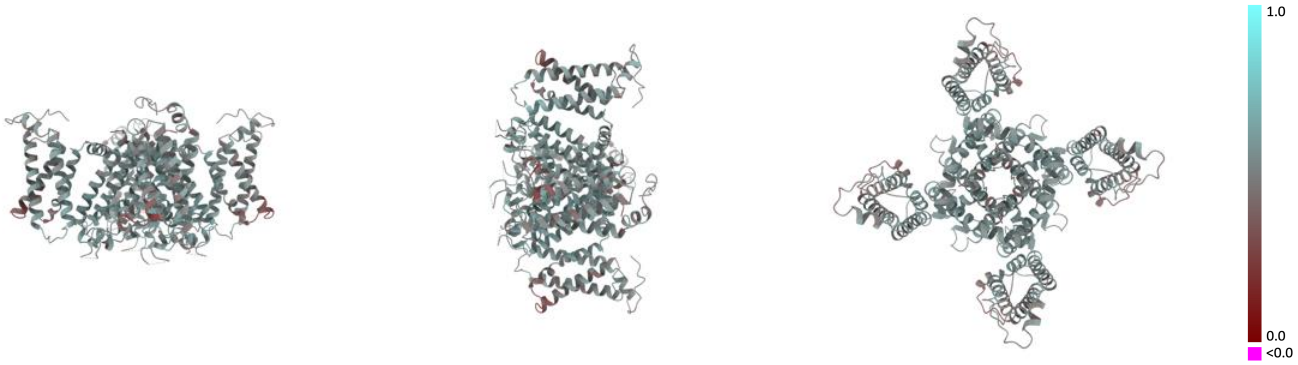
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.423 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

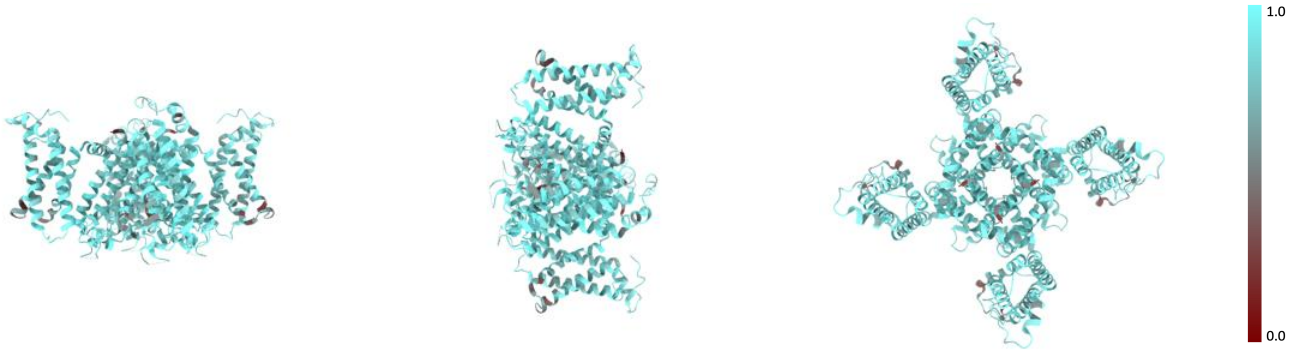
9.2 Q-score mapped to coordinate model



X Y Z

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

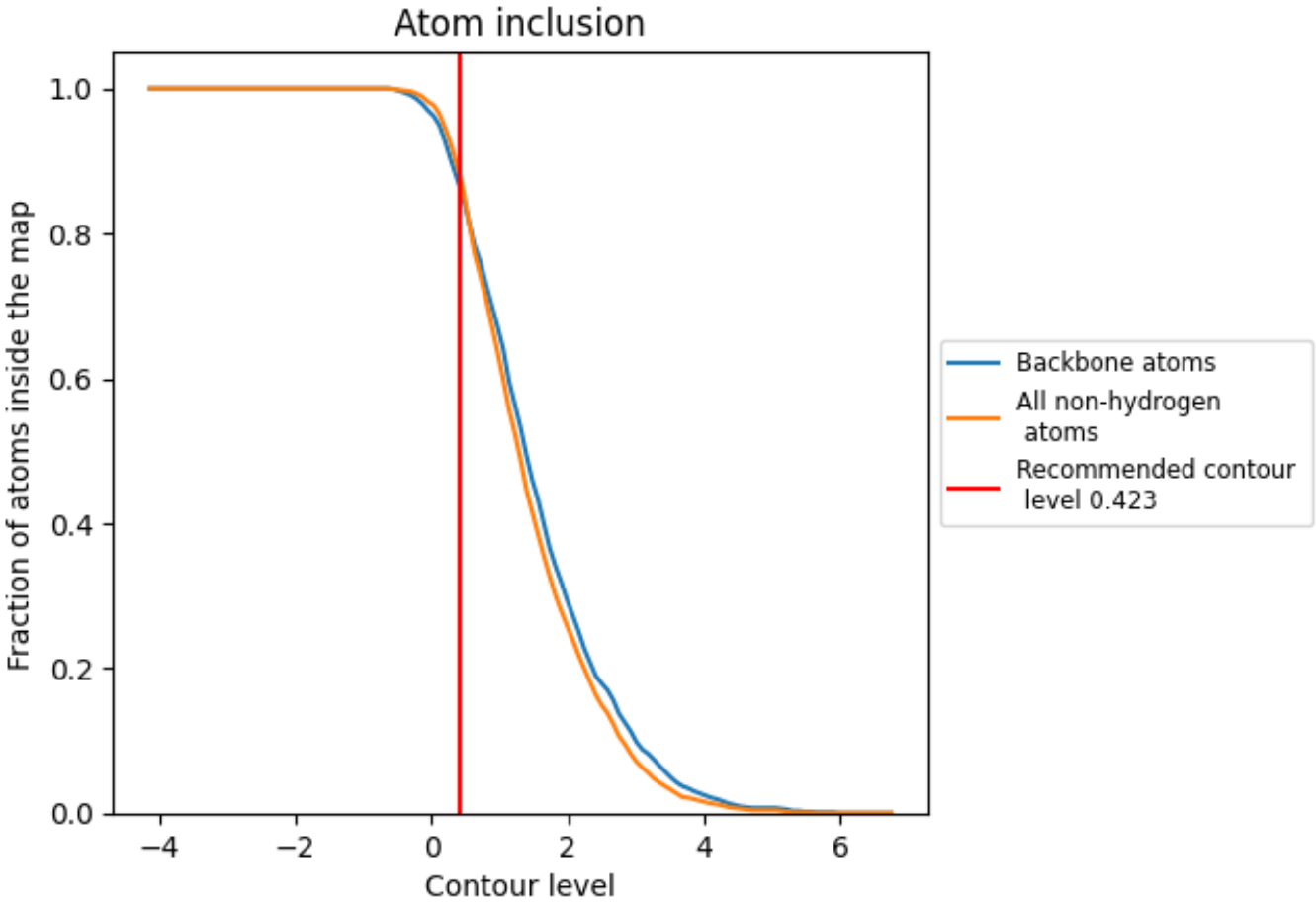
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.423).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.423) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.5300
A	0.8780	0.5300
B	0.8800	0.5290
C	0.8800	0.5290
D	0.8780	0.5310