



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 01:40 AM UTC

PDB ID : 9QNF / pdb_00009qnf
EMDB ID : EMD-53245
Title : Connexin-32 (Cx32) in MSP2N2 nanodiscs with POPC
Authors : Korkhov, V.M.; Lavriha, P.
Deposited on : 2025-03-25
Resolution : 3.16 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:

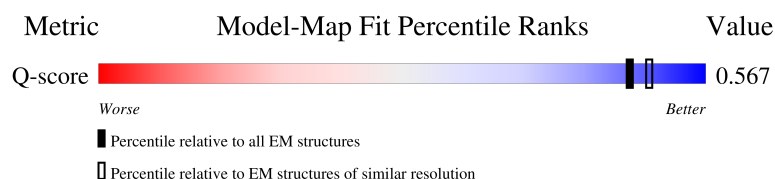
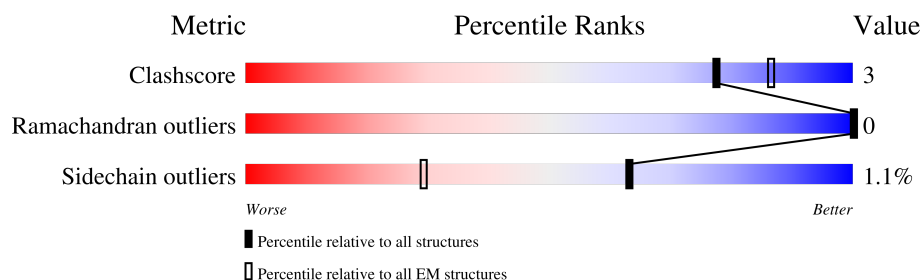
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.16 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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

Mol	Chain	Length	Quality of chain
1	A	566	
1	B	566	
1	C	566	
1	D	566	

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Mol	Chain	Length	Quality of chain
1	E	566	
1	F	566	
1	G	566	
1	H	566	
1	I	566	
1	J	566	
1	K	566	
1	L	566	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19788 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 Gap junction beta-1 protein, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	B	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	C	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	D	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	E	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	F	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	G	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	H	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	I	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	J	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	K	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		
1	L	196	Total	C	N	O	S	0	0
			1569	1041	252	261	15		

There are 612 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	ALA	-	linker	UNP P08034
A	285	ALA	-	linker	UNP P08034
A	286	ALA	-	linker	UNP P08034
A	287	LEU	-	linker	UNP P08034
A	288	GLU	-	linker	UNP P08034
A	289	VAL	-	linker	UNP P08034

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Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LEU	-	linker	UNP P08034
A	291	PHE	-	linker	UNP P08034
A	292	GLN	-	linker	UNP P08034
A	293	GLY	-	linker	UNP P08034
A	294	PRO	-	linker	UNP P08034
A	295	GLY	-	linker	UNP P08034
A	296	GLY	-	linker	UNP P08034
A	297	VAL	-	linker	UNP P08034
A	361	GLY	SER	conflict	UNP P42212
A	364	LEU	VAL	conflict	UNP P42212
A	368	ALA	SER	conflict	UNP P42212
A	499	TYR	THR	conflict	UNP P42212
A	527	LEU	HIS	conflict	UNP P42212
A	535	ALA	-	expression tag	UNP P42212
A	536	ALA	-	expression tag	UNP P42212
A	537	SER	-	expression tag	UNP P42212
A	538	ALA	-	expression tag	UNP P42212
A	539	TRP	-	expression tag	UNP P42212
A	540	SER	-	expression tag	UNP P42212
A	541	HIS	-	expression tag	UNP P42212
A	542	PRO	-	expression tag	UNP P42212
A	543	GLN	-	expression tag	UNP P42212
A	544	PHE	-	expression tag	UNP P42212
A	545	GLU	-	expression tag	UNP P42212
A	546	LYS	-	expression tag	UNP P42212
A	547	GLY	-	expression tag	UNP P42212
A	548	GLY	-	expression tag	UNP P42212
A	549	GLY	-	expression tag	UNP P42212
A	550	SER	-	expression tag	UNP P42212
A	551	GLY	-	expression tag	UNP P42212
A	552	GLY	-	expression tag	UNP P42212
A	553	GLY	-	expression tag	UNP P42212
A	554	SER	-	expression tag	UNP P42212
A	555	GLY	-	expression tag	UNP P42212
A	556	GLY	-	expression tag	UNP P42212
A	557	SER	-	expression tag	UNP P42212
A	558	ALA	-	expression tag	UNP P42212
A	559	TRP	-	expression tag	UNP P42212
A	560	SER	-	expression tag	UNP P42212
A	561	HIS	-	expression tag	UNP P42212
A	562	PRO	-	expression tag	UNP P42212
A	563	GLN	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	564	PHE	-	expression tag	UNP P42212
A	565	GLU	-	expression tag	UNP P42212
A	566	LYS	-	expression tag	UNP P42212
B	284	ALA	-	linker	UNP P08034
B	285	ALA	-	linker	UNP P08034
B	286	ALA	-	linker	UNP P08034
B	287	LEU	-	linker	UNP P08034
B	288	GLU	-	linker	UNP P08034
B	289	VAL	-	linker	UNP P08034
B	290	LEU	-	linker	UNP P08034
B	291	PHE	-	linker	UNP P08034
B	292	GLN	-	linker	UNP P08034
B	293	GLY	-	linker	UNP P08034
B	294	PRO	-	linker	UNP P08034
B	295	GLY	-	linker	UNP P08034
B	296	GLY	-	linker	UNP P08034
B	297	VAL	-	linker	UNP P08034
B	361	GLY	SER	conflict	UNP P42212
B	364	LEU	VAL	conflict	UNP P42212
B	368	ALA	SER	conflict	UNP P42212
B	499	TYR	THR	conflict	UNP P42212
B	527	LEU	HIS	conflict	UNP P42212
B	535	ALA	-	expression tag	UNP P42212
B	536	ALA	-	expression tag	UNP P42212
B	537	SER	-	expression tag	UNP P42212
B	538	ALA	-	expression tag	UNP P42212
B	539	TRP	-	expression tag	UNP P42212
B	540	SER	-	expression tag	UNP P42212
B	541	HIS	-	expression tag	UNP P42212
B	542	PRO	-	expression tag	UNP P42212
B	543	GLN	-	expression tag	UNP P42212
B	544	PHE	-	expression tag	UNP P42212
B	545	GLU	-	expression tag	UNP P42212
B	546	LYS	-	expression tag	UNP P42212
B	547	GLY	-	expression tag	UNP P42212
B	548	GLY	-	expression tag	UNP P42212
B	549	GLY	-	expression tag	UNP P42212
B	550	SER	-	expression tag	UNP P42212
B	551	GLY	-	expression tag	UNP P42212
B	552	GLY	-	expression tag	UNP P42212
B	553	GLY	-	expression tag	UNP P42212
B	554	SER	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	555	GLY	-	expression tag	UNP P42212
B	556	GLY	-	expression tag	UNP P42212
B	557	SER	-	expression tag	UNP P42212
B	558	ALA	-	expression tag	UNP P42212
B	559	TRP	-	expression tag	UNP P42212
B	560	SER	-	expression tag	UNP P42212
B	561	HIS	-	expression tag	UNP P42212
B	562	PRO	-	expression tag	UNP P42212
B	563	GLN	-	expression tag	UNP P42212
B	564	PHE	-	expression tag	UNP P42212
B	565	GLU	-	expression tag	UNP P42212
B	566	LYS	-	expression tag	UNP P42212
C	284	ALA	-	linker	UNP P08034
C	285	ALA	-	linker	UNP P08034
C	286	ALA	-	linker	UNP P08034
C	287	LEU	-	linker	UNP P08034
C	288	GLU	-	linker	UNP P08034
C	289	VAL	-	linker	UNP P08034
C	290	LEU	-	linker	UNP P08034
C	291	PHE	-	linker	UNP P08034
C	292	GLN	-	linker	UNP P08034
C	293	GLY	-	linker	UNP P08034
C	294	PRO	-	linker	UNP P08034
C	295	GLY	-	linker	UNP P08034
C	296	GLY	-	linker	UNP P08034
C	297	VAL	-	linker	UNP P08034
C	361	GLY	SER	conflict	UNP P42212
C	364	LEU	VAL	conflict	UNP P42212
C	368	ALA	SER	conflict	UNP P42212
C	499	TYR	THR	conflict	UNP P42212
C	527	LEU	HIS	conflict	UNP P42212
C	535	ALA	-	expression tag	UNP P42212
C	536	ALA	-	expression tag	UNP P42212
C	537	SER	-	expression tag	UNP P42212
C	538	ALA	-	expression tag	UNP P42212
C	539	TRP	-	expression tag	UNP P42212
C	540	SER	-	expression tag	UNP P42212
C	541	HIS	-	expression tag	UNP P42212
C	542	PRO	-	expression tag	UNP P42212
C	543	GLN	-	expression tag	UNP P42212
C	544	PHE	-	expression tag	UNP P42212
C	545	GLU	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	546	LYS	-	expression tag	UNP P42212
C	547	GLY	-	expression tag	UNP P42212
C	548	GLY	-	expression tag	UNP P42212
C	549	GLY	-	expression tag	UNP P42212
C	550	SER	-	expression tag	UNP P42212
C	551	GLY	-	expression tag	UNP P42212
C	552	GLY	-	expression tag	UNP P42212
C	553	GLY	-	expression tag	UNP P42212
C	554	SER	-	expression tag	UNP P42212
C	555	GLY	-	expression tag	UNP P42212
C	556	GLY	-	expression tag	UNP P42212
C	557	SER	-	expression tag	UNP P42212
C	558	ALA	-	expression tag	UNP P42212
C	559	TRP	-	expression tag	UNP P42212
C	560	SER	-	expression tag	UNP P42212
C	561	HIS	-	expression tag	UNP P42212
C	562	PRO	-	expression tag	UNP P42212
C	563	GLN	-	expression tag	UNP P42212
C	564	PHE	-	expression tag	UNP P42212
C	565	GLU	-	expression tag	UNP P42212
C	566	LYS	-	expression tag	UNP P42212
D	284	ALA	-	linker	UNP P08034
D	285	ALA	-	linker	UNP P08034
D	286	ALA	-	linker	UNP P08034
D	287	LEU	-	linker	UNP P08034
D	288	GLU	-	linker	UNP P08034
D	289	VAL	-	linker	UNP P08034
D	290	LEU	-	linker	UNP P08034
D	291	PHE	-	linker	UNP P08034
D	292	GLN	-	linker	UNP P08034
D	293	GLY	-	linker	UNP P08034
D	294	PRO	-	linker	UNP P08034
D	295	GLY	-	linker	UNP P08034
D	296	GLY	-	linker	UNP P08034
D	297	VAL	-	linker	UNP P08034
D	361	GLY	SER	conflict	UNP P42212
D	364	LEU	VAL	conflict	UNP P42212
D	368	ALA	SER	conflict	UNP P42212
D	499	TYR	THR	conflict	UNP P42212
D	527	LEU	HIS	conflict	UNP P42212
D	535	ALA	-	expression tag	UNP P42212
D	536	ALA	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	537	SER	-	expression tag	UNP P42212
D	538	ALA	-	expression tag	UNP P42212
D	539	TRP	-	expression tag	UNP P42212
D	540	SER	-	expression tag	UNP P42212
D	541	HIS	-	expression tag	UNP P42212
D	542	PRO	-	expression tag	UNP P42212
D	543	GLN	-	expression tag	UNP P42212
D	544	PHE	-	expression tag	UNP P42212
D	545	GLU	-	expression tag	UNP P42212
D	546	LYS	-	expression tag	UNP P42212
D	547	GLY	-	expression tag	UNP P42212
D	548	GLY	-	expression tag	UNP P42212
D	549	GLY	-	expression tag	UNP P42212
D	550	SER	-	expression tag	UNP P42212
D	551	GLY	-	expression tag	UNP P42212
D	552	GLY	-	expression tag	UNP P42212
D	553	GLY	-	expression tag	UNP P42212
D	554	SER	-	expression tag	UNP P42212
D	555	GLY	-	expression tag	UNP P42212
D	556	GLY	-	expression tag	UNP P42212
D	557	SER	-	expression tag	UNP P42212
D	558	ALA	-	expression tag	UNP P42212
D	559	TRP	-	expression tag	UNP P42212
D	560	SER	-	expression tag	UNP P42212
D	561	HIS	-	expression tag	UNP P42212
D	562	PRO	-	expression tag	UNP P42212
D	563	GLN	-	expression tag	UNP P42212
D	564	PHE	-	expression tag	UNP P42212
D	565	GLU	-	expression tag	UNP P42212
D	566	LYS	-	expression tag	UNP P42212
E	284	ALA	-	linker	UNP P08034
E	285	ALA	-	linker	UNP P08034
E	286	ALA	-	linker	UNP P08034
E	287	LEU	-	linker	UNP P08034
E	288	GLU	-	linker	UNP P08034
E	289	VAL	-	linker	UNP P08034
E	290	LEU	-	linker	UNP P08034
E	291	PHE	-	linker	UNP P08034
E	292	GLN	-	linker	UNP P08034
E	293	GLY	-	linker	UNP P08034
E	294	PRO	-	linker	UNP P08034
E	295	GLY	-	linker	UNP P08034

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Chain	Residue	Modelled	Actual	Comment	Reference
E	296	GLY	-	linker	UNP P08034
E	297	VAL	-	linker	UNP P08034
E	361	GLY	SER	conflict	UNP P42212
E	364	LEU	VAL	conflict	UNP P42212
E	368	ALA	SER	conflict	UNP P42212
E	499	TYR	THR	conflict	UNP P42212
E	527	LEU	HIS	conflict	UNP P42212
E	535	ALA	-	expression tag	UNP P42212
E	536	ALA	-	expression tag	UNP P42212
E	537	SER	-	expression tag	UNP P42212
E	538	ALA	-	expression tag	UNP P42212
E	539	TRP	-	expression tag	UNP P42212
E	540	SER	-	expression tag	UNP P42212
E	541	HIS	-	expression tag	UNP P42212
E	542	PRO	-	expression tag	UNP P42212
E	543	GLN	-	expression tag	UNP P42212
E	544	PHE	-	expression tag	UNP P42212
E	545	GLU	-	expression tag	UNP P42212
E	546	LYS	-	expression tag	UNP P42212
E	547	GLY	-	expression tag	UNP P42212
E	548	GLY	-	expression tag	UNP P42212
E	549	GLY	-	expression tag	UNP P42212
E	550	SER	-	expression tag	UNP P42212
E	551	GLY	-	expression tag	UNP P42212
E	552	GLY	-	expression tag	UNP P42212
E	553	GLY	-	expression tag	UNP P42212
E	554	SER	-	expression tag	UNP P42212
E	555	GLY	-	expression tag	UNP P42212
E	556	GLY	-	expression tag	UNP P42212
E	557	SER	-	expression tag	UNP P42212
E	558	ALA	-	expression tag	UNP P42212
E	559	TRP	-	expression tag	UNP P42212
E	560	SER	-	expression tag	UNP P42212
E	561	HIS	-	expression tag	UNP P42212
E	562	PRO	-	expression tag	UNP P42212
E	563	GLN	-	expression tag	UNP P42212
E	564	PHE	-	expression tag	UNP P42212
E	565	GLU	-	expression tag	UNP P42212
E	566	LYS	-	expression tag	UNP P42212
F	284	ALA	-	linker	UNP P08034
F	285	ALA	-	linker	UNP P08034
F	286	ALA	-	linker	UNP P08034

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Chain	Residue	Modelled	Actual	Comment	Reference
F	287	LEU	-	linker	UNP P08034
F	288	GLU	-	linker	UNP P08034
F	289	VAL	-	linker	UNP P08034
F	290	LEU	-	linker	UNP P08034
F	291	PHE	-	linker	UNP P08034
F	292	GLN	-	linker	UNP P08034
F	293	GLY	-	linker	UNP P08034
F	294	PRO	-	linker	UNP P08034
F	295	GLY	-	linker	UNP P08034
F	296	GLY	-	linker	UNP P08034
F	297	VAL	-	linker	UNP P08034
F	361	GLY	SER	conflict	UNP P42212
F	364	LEU	VAL	conflict	UNP P42212
F	368	ALA	SER	conflict	UNP P42212
F	499	TYR	THR	conflict	UNP P42212
F	527	LEU	HIS	conflict	UNP P42212
F	535	ALA	-	expression tag	UNP P42212
F	536	ALA	-	expression tag	UNP P42212
F	537	SER	-	expression tag	UNP P42212
F	538	ALA	-	expression tag	UNP P42212
F	539	TRP	-	expression tag	UNP P42212
F	540	SER	-	expression tag	UNP P42212
F	541	HIS	-	expression tag	UNP P42212
F	542	PRO	-	expression tag	UNP P42212
F	543	GLN	-	expression tag	UNP P42212
F	544	PHE	-	expression tag	UNP P42212
F	545	GLU	-	expression tag	UNP P42212
F	546	LYS	-	expression tag	UNP P42212
F	547	GLY	-	expression tag	UNP P42212
F	548	GLY	-	expression tag	UNP P42212
F	549	GLY	-	expression tag	UNP P42212
F	550	SER	-	expression tag	UNP P42212
F	551	GLY	-	expression tag	UNP P42212
F	552	GLY	-	expression tag	UNP P42212
F	553	GLY	-	expression tag	UNP P42212
F	554	SER	-	expression tag	UNP P42212
F	555	GLY	-	expression tag	UNP P42212
F	556	GLY	-	expression tag	UNP P42212
F	557	SER	-	expression tag	UNP P42212
F	558	ALA	-	expression tag	UNP P42212
F	559	TRP	-	expression tag	UNP P42212
F	560	SER	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
F	561	HIS	-	expression tag	UNP P42212
F	562	PRO	-	expression tag	UNP P42212
F	563	GLN	-	expression tag	UNP P42212
F	564	PHE	-	expression tag	UNP P42212
F	565	GLU	-	expression tag	UNP P42212
F	566	LYS	-	expression tag	UNP P42212
G	284	ALA	-	linker	UNP P08034
G	285	ALA	-	linker	UNP P08034
G	286	ALA	-	linker	UNP P08034
G	287	LEU	-	linker	UNP P08034
G	288	GLU	-	linker	UNP P08034
G	289	VAL	-	linker	UNP P08034
G	290	LEU	-	linker	UNP P08034
G	291	PHE	-	linker	UNP P08034
G	292	GLN	-	linker	UNP P08034
G	293	GLY	-	linker	UNP P08034
G	294	PRO	-	linker	UNP P08034
G	295	GLY	-	linker	UNP P08034
G	296	GLY	-	linker	UNP P08034
G	297	VAL	-	linker	UNP P08034
G	361	GLY	SER	conflict	UNP P42212
G	364	LEU	VAL	conflict	UNP P42212
G	368	ALA	SER	conflict	UNP P42212
G	499	TYR	THR	conflict	UNP P42212
G	527	LEU	HIS	conflict	UNP P42212
G	535	ALA	-	expression tag	UNP P42212
G	536	ALA	-	expression tag	UNP P42212
G	537	SER	-	expression tag	UNP P42212
G	538	ALA	-	expression tag	UNP P42212
G	539	TRP	-	expression tag	UNP P42212
G	540	SER	-	expression tag	UNP P42212
G	541	HIS	-	expression tag	UNP P42212
G	542	PRO	-	expression tag	UNP P42212
G	543	GLN	-	expression tag	UNP P42212
G	544	PHE	-	expression tag	UNP P42212
G	545	GLU	-	expression tag	UNP P42212
G	546	LYS	-	expression tag	UNP P42212
G	547	GLY	-	expression tag	UNP P42212
G	548	GLY	-	expression tag	UNP P42212
G	549	GLY	-	expression tag	UNP P42212
G	550	SER	-	expression tag	UNP P42212
G	551	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
G	552	GLY	-	expression tag	UNP P42212
G	553	GLY	-	expression tag	UNP P42212
G	554	SER	-	expression tag	UNP P42212
G	555	GLY	-	expression tag	UNP P42212
G	556	GLY	-	expression tag	UNP P42212
G	557	SER	-	expression tag	UNP P42212
G	558	ALA	-	expression tag	UNP P42212
G	559	TRP	-	expression tag	UNP P42212
G	560	SER	-	expression tag	UNP P42212
G	561	HIS	-	expression tag	UNP P42212
G	562	PRO	-	expression tag	UNP P42212
G	563	GLN	-	expression tag	UNP P42212
G	564	PHE	-	expression tag	UNP P42212
G	565	GLU	-	expression tag	UNP P42212
G	566	LYS	-	expression tag	UNP P42212
H	284	ALA	-	linker	UNP P08034
H	285	ALA	-	linker	UNP P08034
H	286	ALA	-	linker	UNP P08034
H	287	LEU	-	linker	UNP P08034
H	288	GLU	-	linker	UNP P08034
H	289	VAL	-	linker	UNP P08034
H	290	LEU	-	linker	UNP P08034
H	291	PHE	-	linker	UNP P08034
H	292	GLN	-	linker	UNP P08034
H	293	GLY	-	linker	UNP P08034
H	294	PRO	-	linker	UNP P08034
H	295	GLY	-	linker	UNP P08034
H	296	GLY	-	linker	UNP P08034
H	297	VAL	-	linker	UNP P08034
H	361	GLY	SER	conflict	UNP P42212
H	364	LEU	VAL	conflict	UNP P42212
H	368	ALA	SER	conflict	UNP P42212
H	499	TYR	THR	conflict	UNP P42212
H	527	LEU	HIS	conflict	UNP P42212
H	535	ALA	-	expression tag	UNP P42212
H	536	ALA	-	expression tag	UNP P42212
H	537	SER	-	expression tag	UNP P42212
H	538	ALA	-	expression tag	UNP P42212
H	539	TRP	-	expression tag	UNP P42212
H	540	SER	-	expression tag	UNP P42212
H	541	HIS	-	expression tag	UNP P42212
H	542	PRO	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
H	543	GLN	-	expression tag	UNP P42212
H	544	PHE	-	expression tag	UNP P42212
H	545	GLU	-	expression tag	UNP P42212
H	546	LYS	-	expression tag	UNP P42212
H	547	GLY	-	expression tag	UNP P42212
H	548	GLY	-	expression tag	UNP P42212
H	549	GLY	-	expression tag	UNP P42212
H	550	SER	-	expression tag	UNP P42212
H	551	GLY	-	expression tag	UNP P42212
H	552	GLY	-	expression tag	UNP P42212
H	553	GLY	-	expression tag	UNP P42212
H	554	SER	-	expression tag	UNP P42212
H	555	GLY	-	expression tag	UNP P42212
H	556	GLY	-	expression tag	UNP P42212
H	557	SER	-	expression tag	UNP P42212
H	558	ALA	-	expression tag	UNP P42212
H	559	TRP	-	expression tag	UNP P42212
H	560	SER	-	expression tag	UNP P42212
H	561	HIS	-	expression tag	UNP P42212
H	562	PRO	-	expression tag	UNP P42212
H	563	GLN	-	expression tag	UNP P42212
H	564	PHE	-	expression tag	UNP P42212
H	565	GLU	-	expression tag	UNP P42212
H	566	LYS	-	expression tag	UNP P42212
I	284	ALA	-	linker	UNP P08034
I	285	ALA	-	linker	UNP P08034
I	286	ALA	-	linker	UNP P08034
I	287	LEU	-	linker	UNP P08034
I	288	GLU	-	linker	UNP P08034
I	289	VAL	-	linker	UNP P08034
I	290	LEU	-	linker	UNP P08034
I	291	PHE	-	linker	UNP P08034
I	292	GLN	-	linker	UNP P08034
I	293	GLY	-	linker	UNP P08034
I	294	PRO	-	linker	UNP P08034
I	295	GLY	-	linker	UNP P08034
I	296	GLY	-	linker	UNP P08034
I	297	VAL	-	linker	UNP P08034
I	361	GLY	SER	conflict	UNP P42212
I	364	LEU	VAL	conflict	UNP P42212
I	368	ALA	SER	conflict	UNP P42212
I	499	TYR	THR	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
I	527	LEU	HIS	conflict	UNP P42212
I	535	ALA	-	expression tag	UNP P42212
I	536	ALA	-	expression tag	UNP P42212
I	537	SER	-	expression tag	UNP P42212
I	538	ALA	-	expression tag	UNP P42212
I	539	TRP	-	expression tag	UNP P42212
I	540	SER	-	expression tag	UNP P42212
I	541	HIS	-	expression tag	UNP P42212
I	542	PRO	-	expression tag	UNP P42212
I	543	GLN	-	expression tag	UNP P42212
I	544	PHE	-	expression tag	UNP P42212
I	545	GLU	-	expression tag	UNP P42212
I	546	LYS	-	expression tag	UNP P42212
I	547	GLY	-	expression tag	UNP P42212
I	548	GLY	-	expression tag	UNP P42212
I	549	GLY	-	expression tag	UNP P42212
I	550	SER	-	expression tag	UNP P42212
I	551	GLY	-	expression tag	UNP P42212
I	552	GLY	-	expression tag	UNP P42212
I	553	GLY	-	expression tag	UNP P42212
I	554	SER	-	expression tag	UNP P42212
I	555	GLY	-	expression tag	UNP P42212
I	556	GLY	-	expression tag	UNP P42212
I	557	SER	-	expression tag	UNP P42212
I	558	ALA	-	expression tag	UNP P42212
I	559	TRP	-	expression tag	UNP P42212
I	560	SER	-	expression tag	UNP P42212
I	561	HIS	-	expression tag	UNP P42212
I	562	PRO	-	expression tag	UNP P42212
I	563	GLN	-	expression tag	UNP P42212
I	564	PHE	-	expression tag	UNP P42212
I	565	GLU	-	expression tag	UNP P42212
I	566	LYS	-	expression tag	UNP P42212
J	284	ALA	-	linker	UNP P08034
J	285	ALA	-	linker	UNP P08034
J	286	ALA	-	linker	UNP P08034
J	287	LEU	-	linker	UNP P08034
J	288	GLU	-	linker	UNP P08034
J	289	VAL	-	linker	UNP P08034
J	290	LEU	-	linker	UNP P08034
J	291	PHE	-	linker	UNP P08034
J	292	GLN	-	linker	UNP P08034

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Chain	Residue	Modelled	Actual	Comment	Reference
J	293	GLY	-	linker	UNP P08034
J	294	PRO	-	linker	UNP P08034
J	295	GLY	-	linker	UNP P08034
J	296	GLY	-	linker	UNP P08034
J	297	VAL	-	linker	UNP P08034
J	361	GLY	SER	conflict	UNP P42212
J	364	LEU	VAL	conflict	UNP P42212
J	368	ALA	SER	conflict	UNP P42212
J	499	TYR	THR	conflict	UNP P42212
J	527	LEU	HIS	conflict	UNP P42212
J	535	ALA	-	expression tag	UNP P42212
J	536	ALA	-	expression tag	UNP P42212
J	537	SER	-	expression tag	UNP P42212
J	538	ALA	-	expression tag	UNP P42212
J	539	TRP	-	expression tag	UNP P42212
J	540	SER	-	expression tag	UNP P42212
J	541	HIS	-	expression tag	UNP P42212
J	542	PRO	-	expression tag	UNP P42212
J	543	GLN	-	expression tag	UNP P42212
J	544	PHE	-	expression tag	UNP P42212
J	545	GLU	-	expression tag	UNP P42212
J	546	LYS	-	expression tag	UNP P42212
J	547	GLY	-	expression tag	UNP P42212
J	548	GLY	-	expression tag	UNP P42212
J	549	GLY	-	expression tag	UNP P42212
J	550	SER	-	expression tag	UNP P42212
J	551	GLY	-	expression tag	UNP P42212
J	552	GLY	-	expression tag	UNP P42212
J	553	GLY	-	expression tag	UNP P42212
J	554	SER	-	expression tag	UNP P42212
J	555	GLY	-	expression tag	UNP P42212
J	556	GLY	-	expression tag	UNP P42212
J	557	SER	-	expression tag	UNP P42212
J	558	ALA	-	expression tag	UNP P42212
J	559	TRP	-	expression tag	UNP P42212
J	560	SER	-	expression tag	UNP P42212
J	561	HIS	-	expression tag	UNP P42212
J	562	PRO	-	expression tag	UNP P42212
J	563	GLN	-	expression tag	UNP P42212
J	564	PHE	-	expression tag	UNP P42212
J	565	GLU	-	expression tag	UNP P42212
J	566	LYS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
K	284	ALA	-	linker	UNP P08034
K	285	ALA	-	linker	UNP P08034
K	286	ALA	-	linker	UNP P08034
K	287	LEU	-	linker	UNP P08034
K	288	GLU	-	linker	UNP P08034
K	289	VAL	-	linker	UNP P08034
K	290	LEU	-	linker	UNP P08034
K	291	PHE	-	linker	UNP P08034
K	292	GLN	-	linker	UNP P08034
K	293	GLY	-	linker	UNP P08034
K	294	PRO	-	linker	UNP P08034
K	295	GLY	-	linker	UNP P08034
K	296	GLY	-	linker	UNP P08034
K	297	VAL	-	linker	UNP P08034
K	361	GLY	SER	conflict	UNP P42212
K	364	LEU	VAL	conflict	UNP P42212
K	368	ALA	SER	conflict	UNP P42212
K	499	TYR	THR	conflict	UNP P42212
K	527	LEU	HIS	conflict	UNP P42212
K	535	ALA	-	expression tag	UNP P42212
K	536	ALA	-	expression tag	UNP P42212
K	537	SER	-	expression tag	UNP P42212
K	538	ALA	-	expression tag	UNP P42212
K	539	TRP	-	expression tag	UNP P42212
K	540	SER	-	expression tag	UNP P42212
K	541	HIS	-	expression tag	UNP P42212
K	542	PRO	-	expression tag	UNP P42212
K	543	GLN	-	expression tag	UNP P42212
K	544	PHE	-	expression tag	UNP P42212
K	545	GLU	-	expression tag	UNP P42212
K	546	LYS	-	expression tag	UNP P42212
K	547	GLY	-	expression tag	UNP P42212
K	548	GLY	-	expression tag	UNP P42212
K	549	GLY	-	expression tag	UNP P42212
K	550	SER	-	expression tag	UNP P42212
K	551	GLY	-	expression tag	UNP P42212
K	552	GLY	-	expression tag	UNP P42212
K	553	GLY	-	expression tag	UNP P42212
K	554	SER	-	expression tag	UNP P42212
K	555	GLY	-	expression tag	UNP P42212
K	556	GLY	-	expression tag	UNP P42212
K	557	SER	-	expression tag	UNP P42212

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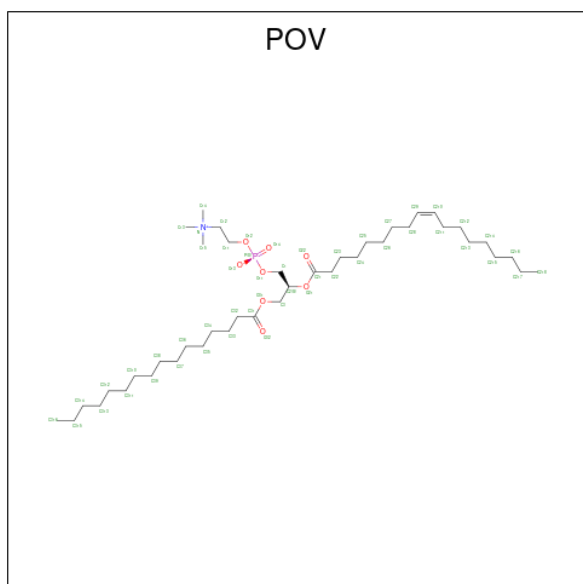
Chain	Residue	Modelled	Actual	Comment	Reference
K	558	ALA	-	expression tag	UNP P42212
K	559	TRP	-	expression tag	UNP P42212
K	560	SER	-	expression tag	UNP P42212
K	561	HIS	-	expression tag	UNP P42212
K	562	PRO	-	expression tag	UNP P42212
K	563	GLN	-	expression tag	UNP P42212
K	564	PHE	-	expression tag	UNP P42212
K	565	GLU	-	expression tag	UNP P42212
K	566	LYS	-	expression tag	UNP P42212
L	284	ALA	-	linker	UNP P08034
L	285	ALA	-	linker	UNP P08034
L	286	ALA	-	linker	UNP P08034
L	287	LEU	-	linker	UNP P08034
L	288	GLU	-	linker	UNP P08034
L	289	VAL	-	linker	UNP P08034
L	290	LEU	-	linker	UNP P08034
L	291	PHE	-	linker	UNP P08034
L	292	GLN	-	linker	UNP P08034
L	293	GLY	-	linker	UNP P08034
L	294	PRO	-	linker	UNP P08034
L	295	GLY	-	linker	UNP P08034
L	296	GLY	-	linker	UNP P08034
L	297	VAL	-	linker	UNP P08034
L	361	GLY	SER	conflict	UNP P42212
L	364	LEU	VAL	conflict	UNP P42212
L	368	ALA	SER	conflict	UNP P42212
L	499	TYR	THR	conflict	UNP P42212
L	527	LEU	HIS	conflict	UNP P42212
L	535	ALA	-	expression tag	UNP P42212
L	536	ALA	-	expression tag	UNP P42212
L	537	SER	-	expression tag	UNP P42212
L	538	ALA	-	expression tag	UNP P42212
L	539	TRP	-	expression tag	UNP P42212
L	540	SER	-	expression tag	UNP P42212
L	541	HIS	-	expression tag	UNP P42212
L	542	PRO	-	expression tag	UNP P42212
L	543	GLN	-	expression tag	UNP P42212
L	544	PHE	-	expression tag	UNP P42212
L	545	GLU	-	expression tag	UNP P42212
L	546	LYS	-	expression tag	UNP P42212
L	547	GLY	-	expression tag	UNP P42212
L	548	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
L	549	GLY	-	expression tag	UNP P42212
L	550	SER	-	expression tag	UNP P42212
L	551	GLY	-	expression tag	UNP P42212
L	552	GLY	-	expression tag	UNP P42212
L	553	GLY	-	expression tag	UNP P42212
L	554	SER	-	expression tag	UNP P42212
L	555	GLY	-	expression tag	UNP P42212
L	556	GLY	-	expression tag	UNP P42212
L	557	SER	-	expression tag	UNP P42212
L	558	ALA	-	expression tag	UNP P42212
L	559	TRP	-	expression tag	UNP P42212
L	560	SER	-	expression tag	UNP P42212
L	561	HIS	-	expression tag	UNP P42212
L	562	PRO	-	expression tag	UNP P42212
L	563	GLN	-	expression tag	UNP P42212
L	564	PHE	-	expression tag	UNP P42212
L	565	GLU	-	expression tag	UNP P42212
L	566	LYS	-	expression tag	UNP P42212

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



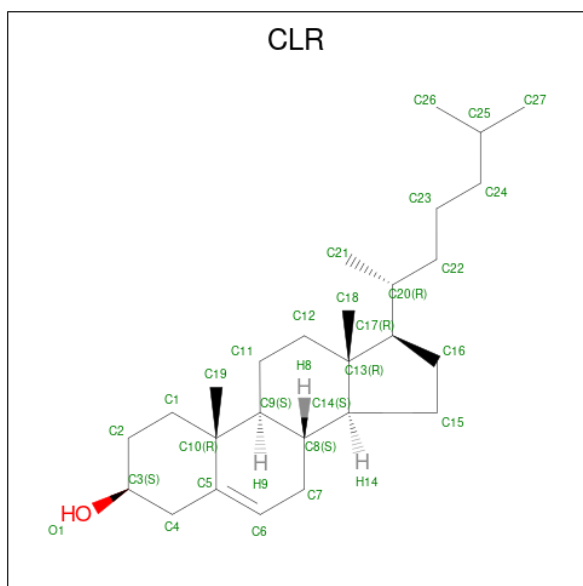
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	K	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).

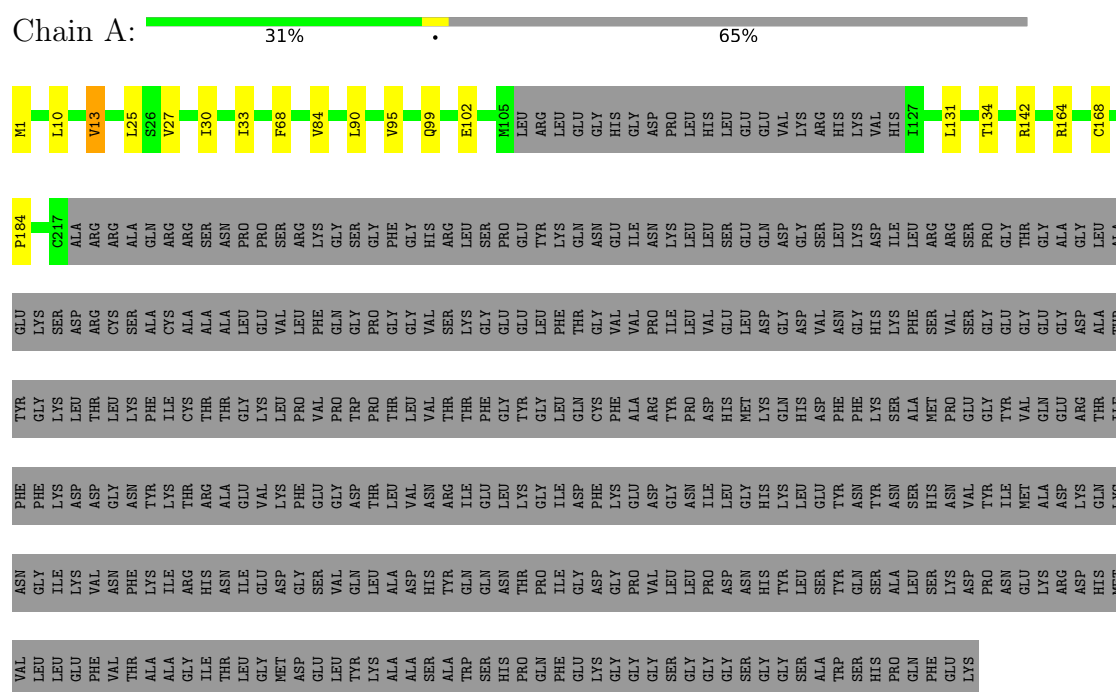


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	E	1	Total	C	O	0
			28	27	1	
3	F	1	Total	C	O	0
			28	27	1	
3	G	1	Total	C	O	0
			28	27	1	
3	H	1	Total	C	O	0
			28	27	1	
3	I	1	Total	C	O	0
			28	27	1	
3	J	1	Total	C	O	0
			28	27	1	
3	K	1	Total	C	O	0
			28	27	1	
3	L	1	Total	C	O	0
			28	27	1	

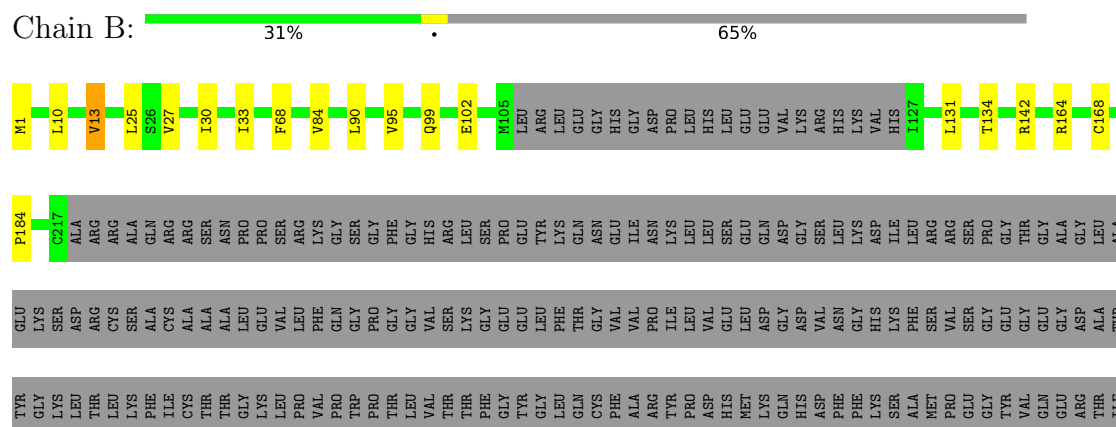
3 Residue-property plots [i](#)

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: Gap junction beta-1 protein, Green fluorescent protein



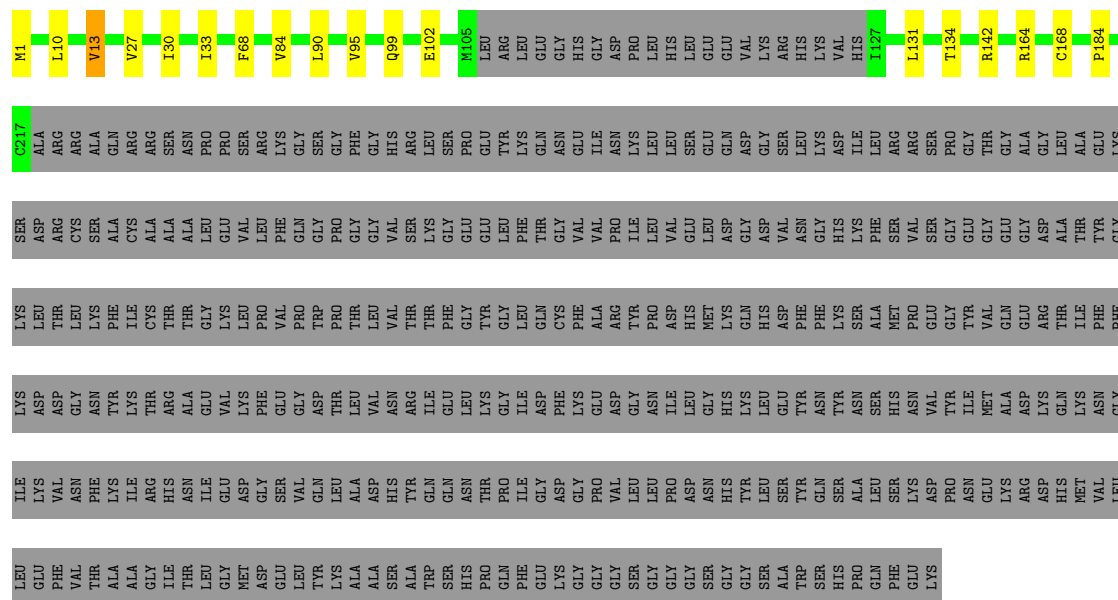
- Molecule 1: Gap junction beta-1 protein, Green fluorescent protein



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

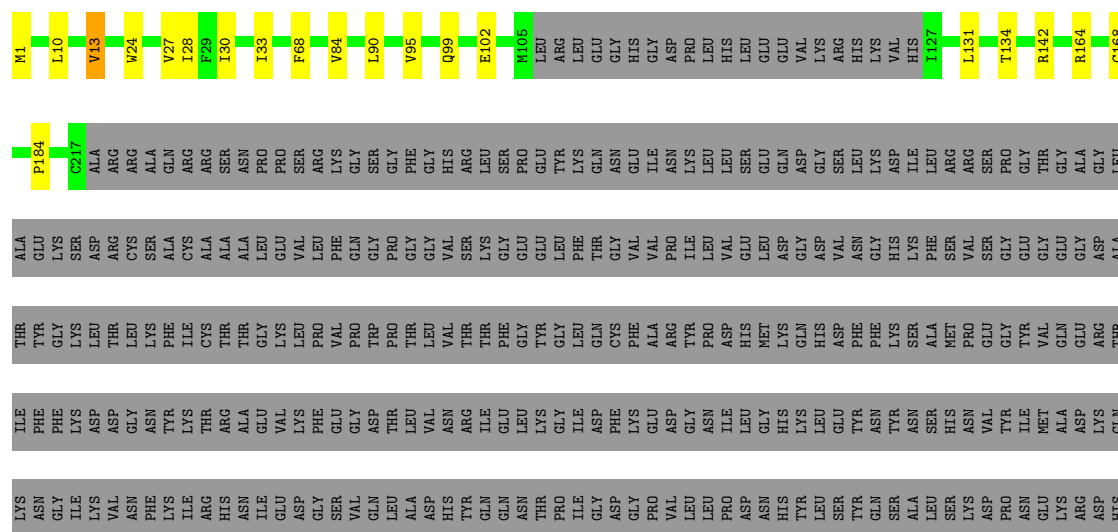
- Molecule 1: Gap junction beta-1 protein, Green fluorescent protein.

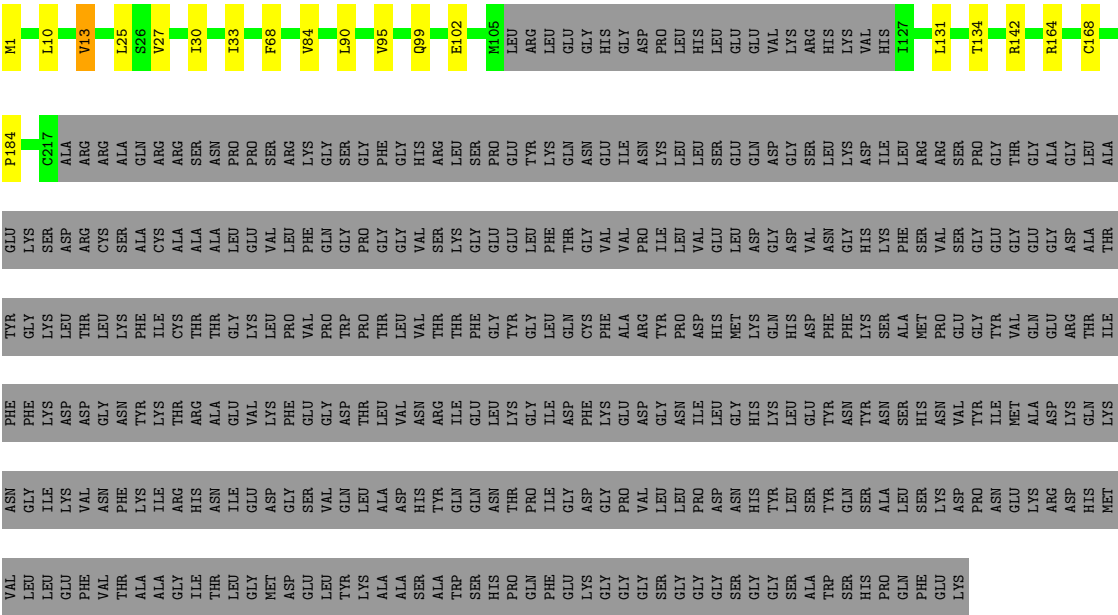
Chain C:  31% . 65%



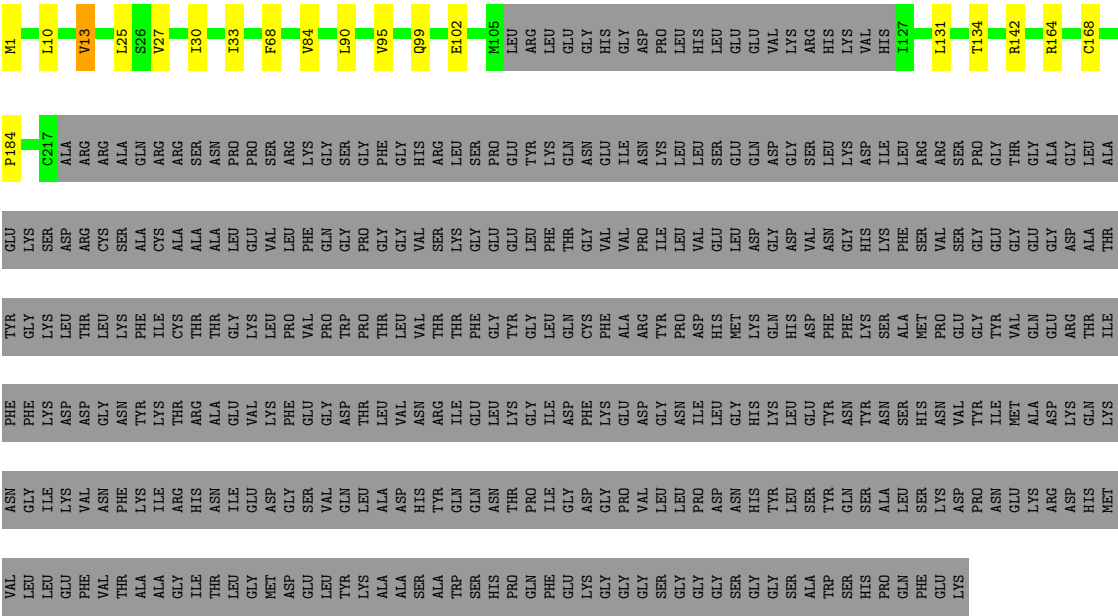
- Molecule 1: Gap junction beta-1 protein, Green fluorescent protein

Chain D: 31% 1% 65%

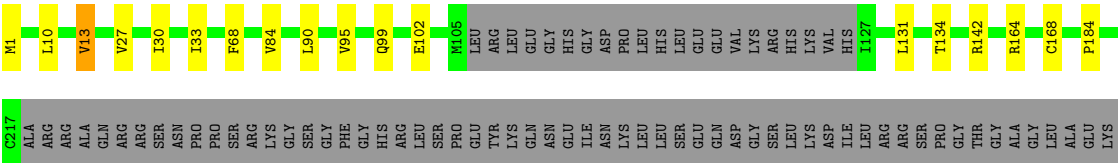




• Molecule 1: Gap junction beta-1 protein,Green fluorescent protein

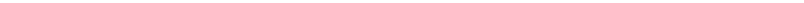


• Molecule 1: Gap junction beta-1 protein,Green fluorescent protein



[illegible]

- Molecule 1: Gap junction beta-1 protein, Green fluorescent protein

Chain J:  31% . 65%

VAL	ASN	PHE	TYR	GLU	P184
LEU	GLY	PHE	GLY	LYS	R2
LEU	IIE	LYS	LYS	SER	W3
GLU	LYS	ASP	LEU	ASP	L10
PHE	VAL	ASP	THR	ARG	V13
VAL	ASN	GLY	LEU	CYS	V27
THR	PHE	ASN	LYS	SER	I30
THR	LYS	TYR	PHE	ALA	I33
ALA	IIE	ALA	ALA	GLN	F68
GLY	ARG	THR	CYS	ARG	V84
ILE	HIS	ARG	THR	ALA	L90
THR	ASN	ALA	THR	ASN	V95
LEU	IIE	GLU	GLY	PRO	Q99
GLY	GLU	VAL	VAL	PHE	E102
LEU	VAL	GLY	PRO	GLN	M105
TYR	GLN	ASP	TRP	GLY	LEU
LYS	LEU	THR	PRO	PHO	ARG
THR	GLN	LEU	THR	GLY	LEU
HIS	GLN	GLU	PHE	GLY	GLY
PRO	THR	LEU	LEU	GLU	HIS
GLN	THR	LYS	GLY	LEU	GLY
PHE	IIE	IIE	LEU	PHE	ASP
GLU	GLY	ASP	GLN	THR	PRO
LYS	GLY	PHE	CYS	GLY	LEU
GLY	PRO	GLU	PHE	VAL	HIS
GLY	GLY	GLU	ALA	VAL	GLY
GLY	VAL	ASP	ARG	PRO	ASN
SER	LEU	GLY	TYR	IIE	LYS
GLY	LEU	ASN	PRO	LEU	LEU
GLY	PHO	IIE	ASP	VAL	HIS
GLY	GLY	LEU	HIS	SER	LEU
SER	ASN	GLY	MET	GLY	GLU
GLY	HIS	HIS	LYS	ASP	GLU
GLY	TYR	LYS	GLN	GLY	VAL
SER	LEU	LEU	ASP	GLY	LYS
THR	ALA	GLU	HIS	GLY	ARG
TRP	TYR	THR	ASP	VAL	HIS
LYS	ASN	THR	PHE	GLY	VAL
GLU	GLN	ASN	GLY	LYS	ASP
GLU	ASP	SER	ALA	PHE	HIS
GLU	SER	HIS	MET	LEU	ARG
LYS	PRO	VAL	PRO	VAL	LEU
LYS	ASP	THR	GLY	SER	GLY
LYS	ASN	TYR	TYR	GLY	THR
ILE	ASN	IIE	ILE	GLU	GLY
MET	GLU	MET	VAL	GLY	THR
LYS	LYS	ALA	GLN	GLU	GLY
ASP	ARG	ASP	ARG	GLY	ALA
ASP	ASP	LYS	GLU	ASP	LYS
HIS	THR	GLN	THR	ALA	LEU
MET	THR	LYS	THR	THR	ALA

- Molecule 1: Gap junction beta-1 protein, Green fluorescent protein

Chain K:  31% . 65%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	80708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0022	Depositor
Map size (Å)	249.84033, 249.84033, 249.84033	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6506259, 0.6506259, 0.6506259	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.10	0/1612	0.23	0/2200
1	B	0.10	0/1612	0.23	0/2200
1	C	0.10	0/1612	0.23	0/2200
1	D	0.10	0/1612	0.23	0/2200
1	E	0.10	0/1612	0.23	0/2200
1	F	0.10	0/1612	0.23	0/2200
1	G	0.10	0/1612	0.23	0/2200
1	H	0.10	0/1612	0.23	0/2200
1	I	0.10	0/1612	0.23	0/2200
1	J	0.10	0/1612	0.23	0/2200
1	K	0.10	0/1612	0.23	0/2200
1	L	0.10	0/1612	0.23	0/2200
All	All	0.10	0/19344	0.23	0/26400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1569	0	1598	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1569	0	1598	11	0
1	C	1569	0	1598	10	0
1	D	1569	0	1598	11	0
1	E	1569	0	1598	10	0
1	F	1569	0	1598	11	0
1	G	1569	0	1598	11	0
1	H	1569	0	1598	11	0
1	I	1569	0	1598	10	0
1	J	1569	0	1598	11	0
1	K	1569	0	1598	11	0
1	L	1569	0	1598	11	0
2	A	104	0	164	3	0
2	B	52	0	82	1	0
2	C	52	0	82	1	0
2	D	52	0	82	1	0
2	E	52	0	82	1	0
2	G	52	0	82	2	0
2	H	104	0	164	2	0
2	I	52	0	82	1	0
2	J	52	0	82	1	0
2	K	52	0	82	1	0
3	A	28	0	46	0	0
3	B	28	0	46	0	0
3	C	28	0	46	0	0
3	D	28	0	46	0	0
3	E	28	0	46	0	0
3	F	28	0	46	0	0
3	G	28	0	46	1	0
3	H	28	0	46	0	0
3	I	28	0	46	0	0
3	J	28	0	46	0	0
3	K	28	0	46	0	0
3	L	28	0	46	0	0
All	All	19788	0	20712	119	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 3.

All (119) 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)
1:D:84:VAL:HG13	1:D:142:ARG:HG3	1.89	0.55
1:J:84:VAL:HG13	1:J:142:ARG:HG3	1.89	0.54
1:C:84:VAL:HG13	1:C:142:ARG:HG3	1.89	0.54
1:A:84:VAL:HG13	1:A:142:ARG:HG3	1.89	0.54
1:G:84:VAL:HG13	1:G:142:ARG:HG3	1.89	0.54
1:K:84:VAL:HG13	1:K:142:ARG:HG3	1.90	0.54
1:F:84:VAL:HG13	1:F:142:ARG:HG3	1.89	0.54
1:I:84:VAL:HG13	1:I:142:ARG:HG3	1.89	0.54
1:E:84:VAL:HG13	1:E:142:ARG:HG3	1.90	0.53
1:L:84:VAL:HG13	1:L:142:ARG:HG3	1.89	0.53
1:B:84:VAL:HG13	1:B:142:ARG:HG3	1.90	0.52
1:H:84:VAL:HG13	1:H:142:ARG:HG3	1.90	0.52
1:G:164:ARG:HG2	1:G:184:PRO:HG2	1.95	0.49
1:E:164:ARG:HG2	1:E:184:PRO:HG2	1.96	0.48
1:A:164:ARG:HG2	1:A:184:PRO:HG2	1.96	0.48
1:K:164:ARG:HG2	1:K:184:PRO:HG2	1.96	0.47
1:H:164:ARG:HG2	1:H:184:PRO:HG2	1.96	0.47
1:F:164:ARG:HG2	1:F:184:PRO:HG2	1.97	0.47
1:F:68:PHE:HE2	1:F:168:CYS:HB2	1.79	0.47
1:B:164:ARG:HG2	1:B:184:PRO:HG2	1.96	0.47
1:D:164:ARG:HG2	1:D:184:PRO:HG2	1.96	0.46
1:I:68:PHE:HE2	1:I:168:CYS:HB2	1.80	0.46
1:J:68:PHE:HE2	1:J:168:CYS:HB2	1.80	0.46
1:J:164:ARG:HG2	1:J:184:PRO:HG2	1.96	0.46
2:B:602:POV:H3	1:C:1:MET:HA	1.98	0.45
1:L:164:ARG:HG2	1:L:184:PRO:HG2	1.98	0.45
1:L:99:GLN:O	1:L:102:GLU:HG3	2.17	0.45
1:C:164:ARG:HG2	1:C:184:PRO:HG2	1.97	0.45
1:A:68:PHE:HE2	1:A:168:CYS:HB2	1.81	0.45
1:D:68:PHE:HE2	1:D:168:CYS:HB2	1.81	0.45
1:F:99:GLN:O	1:F:102:GLU:HG3	2.17	0.45
1:B:99:GLN:O	1:B:102:GLU:HG3	2.17	0.45
1:G:99:GLN:O	1:G:102:GLU:HG3	2.17	0.45
1:H:99:GLN:O	1:H:102:GLU:HG3	2.17	0.45
1:A:99:GLN:O	1:A:102:GLU:HG3	2.17	0.45
1:I:99:GLN:O	1:I:102:GLU:HG3	2.17	0.45
1:K:27:VAL:HG21	1:L:90:LEU:HD23	1.99	0.45
2:A:602:POV:H3	1:B:1:MET:HA	1.98	0.45
1:C:99:GLN:O	1:C:102:GLU:HG3	2.17	0.45
1:L:68:PHE:HE2	1:L:168:CYS:HB2	1.81	0.45
1:I:164:ARG:HG2	1:I:184:PRO:HG2	1.98	0.45
1:K:99:GLN:O	1:K:102:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLN:O	1:E:102:GLU:HG3	2.17	0.44
1:C:68:PHE:HE2	1:C:168:CYS:HB2	1.82	0.44
1:E:68:PHE:HE2	1:E:168:CYS:HB2	1.82	0.44
1:H:27:VAL:HG21	1:I:90:LEU:HD23	2.00	0.44
1:B:27:VAL:HG21	1:C:90:LEU:HD23	2.00	0.44
1:H:68:PHE:HE2	1:H:168:CYS:HB2	1.83	0.44
1:G:68:PHE:HE2	1:G:168:CYS:HB2	1.82	0.44
1:K:68:PHE:HE2	1:K:168:CYS:HB2	1.82	0.44
1:A:1:MET:HA	2:A:601:POV:H3	1.99	0.44
1:J:99:GLN:O	1:J:102:GLU:HG3	2.17	0.43
1:D:99:GLN:O	1:D:102:GLU:HG3	2.17	0.43
1:G:27:VAL:HG21	1:H:90:LEU:HD23	2.00	0.43
1:B:68:PHE:HE2	1:B:168:CYS:HB2	1.84	0.43
1:J:27:VAL:HG21	1:K:90:LEU:HD23	2.00	0.43
1:D:27:VAL:HG21	1:E:90:LEU:HD23	2.00	0.43
1:E:27:VAL:HG21	1:F:90:LEU:HD23	2.01	0.43
2:E:602:POV:H3	1:F:1:MET:HA	2.00	0.43
1:G:90:LEU:HD23	1:L:27:VAL:HG21	2.00	0.43
1:I:27:VAL:HG21	1:J:90:LEU:HD23	2.00	0.43
2:D:602:POV:H3	1:E:1:MET:HA	1.99	0.43
2:H:603:POV:H3	1:I:1:MET:HA	2.01	0.43
2:K:602:POV:H3	1:L:1:MET:HA	1.99	0.43
2:C:602:POV:H3	1:D:1:MET:HA	2.00	0.43
1:C:27:VAL:HG21	1:D:90:LEU:HD23	2.00	0.43
2:J:602:POV:H3	1:K:1:MET:HA	1.99	0.43
1:L:10:LEU:HD11	1:L:30:ILE:HD11	2.01	0.42
1:F:10:LEU:HD11	1:F:30:ILE:HD11	2.01	0.42
1:H:1:MET:HA	2:H:602:POV:H3	2.00	0.42
1:K:10:LEU:HD11	1:K:30:ILE:HD11	2.01	0.42
1:E:10:LEU:HD11	1:E:30:ILE:HD11	2.02	0.42
1:A:27:VAL:HG21	1:B:90:LEU:HD23	2.01	0.42
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.93	0.42
1:D:13:VAL:HB	1:D:95:VAL:HG11	2.02	0.42
1:H:25:LEU:HD23	1:H:25:LEU:HA	1.93	0.42
1:G:1:MET:HA	2:G:601:POV:H3	2.01	0.42
1:I:13:VAL:HB	1:I:95:VAL:HG11	2.02	0.42
1:C:131:LEU:HA	1:C:134:THR:HG22	2.02	0.42
1:I:131:LEU:HA	1:I:134:THR:HG22	2.02	0.42
1:J:13:VAL:HB	1:J:95:VAL:HG11	2.02	0.42
2:A:601:POV:H31G	2:A:601:POV:H31D	1.92	0.42
1:D:10:LEU:HD11	1:D:30:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:VAL:HB	1:E:95:VAL:HG11	2.01	0.42
1:A:90:LEU:HD23	1:F:27:VAL:HG21	2.01	0.42
1:J:10:LEU:HD11	1:J:30:ILE:HD11	2.02	0.42
1:C:13:VAL:HB	1:C:95:VAL:HG11	2.02	0.42
1:G:13:VAL:HB	1:G:95:VAL:HG11	2.02	0.42
2:I:602:POV:H3	1:J:1:MET:HA	2.01	0.42
1:B:13:VAL:HB	1:B:95:VAL:HG11	2.02	0.41
1:A:13:VAL:HB	1:A:95:VAL:HG11	2.02	0.41
1:B:131:LEU:HA	1:B:134:THR:HG22	2.02	0.41
1:H:13:VAL:HB	1:H:95:VAL:HG11	2.02	0.41
1:H:131:LEU:HA	1:H:134:THR:HG22	2.02	0.41
1:D:131:LEU:HA	1:D:134:THR:HG22	2.02	0.41
1:J:131:LEU:HA	1:J:134:THR:HG22	2.02	0.41
1:K:13:VAL:HB	1:K:95:VAL:HG11	2.02	0.41
1:A:10:LEU:HD11	1:A:30:ILE:HD11	2.02	0.41
1:C:10:LEU:HD11	1:C:30:ILE:HD11	2.01	0.41
1:F:131:LEU:HD13	1:F:131:LEU:HA	1.94	0.41
1:G:25:LEU:HD23	1:G:25:LEU:HA	1.92	0.41
1:L:13:VAL:HB	1:L:95:VAL:HG11	2.02	0.41
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.93	0.41
1:A:131:LEU:HA	1:A:134:THR:HG22	2.02	0.41
1:B:10:LEU:HD11	1:B:30:ILE:HD11	2.02	0.41
2:G:601:POV:H31G	2:G:601:POV:H31D	1.93	0.41
1:G:10:LEU:HD11	1:G:30:ILE:HD11	2.02	0.41
1:I:10:LEU:HD11	1:I:30:ILE:HD11	2.01	0.41
1:F:13:VAL:HB	1:F:95:VAL:HG11	2.03	0.41
1:F:131:LEU:HA	1:F:134:THR:HG22	2.02	0.41
1:G:131:LEU:HA	1:G:134:THR:HG22	2.02	0.41
1:H:10:LEU:HD11	1:H:30:ILE:HD11	2.02	0.41
1:L:131:LEU:HD13	1:L:131:LEU:HA	1.94	0.41
1:K:131:LEU:HA	1:K:134:THR:HG22	2.02	0.41
1:D:24:TRP:O	1:D:28:ILE:HG12	2.22	0.40
1:L:131:LEU:HA	1:L:134:THR:HG22	2.02	0.40
1:E:131:LEU:HA	1:E:134:THR:HG22	2.02	0.40
3:G:602:CLR:H162	3:G:602:CLR:H222	1.92	0.40
1:J:3:TRP:NE1	1:K:12:GLY:HA2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	B	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	C	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	D	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	E	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	F	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	G	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	H	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	I	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	J	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	K	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
1	L	192/566 (34%)	190 (99%)	2 (1%)	0	100	100
All	All	2304/6792 (34%)	2280 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	B	176/482 (36%)	174 (99%)	2 (1%)	65	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	D	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	E	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	F	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	G	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	H	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	I	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	J	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	K	176/482 (36%)	174 (99%)	2 (1%)	65	75
1	L	176/482 (36%)	174 (99%)	2 (1%)	65	75
All	All	2112/5784 (36%)	2088 (99%)	24 (1%)	63	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	33	ILE
1	B	13	VAL
1	B	33	ILE
1	C	13	VAL
1	C	33	ILE
1	D	13	VAL
1	D	33	ILE
1	E	13	VAL
1	E	33	ILE
1	F	13	VAL
1	F	33	ILE
1	G	13	VAL
1	G	33	ILE
1	H	13	VAL
1	H	33	ILE
1	I	13	VAL
1	I	33	ILE
1	J	13	VAL
1	J	33	ILE
1	K	13	VAL
1	K	33	ILE
1	L	13	VAL
1	L	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	100	HIS
1	B	16	HIS
1	B	94	HIS
1	B	100	HIS
1	C	94	HIS
1	C	100	HIS
1	D	16	HIS
1	D	94	HIS
1	D	100	HIS
1	E	94	HIS
1	E	100	HIS
1	F	100	HIS
1	G	94	HIS
1	G	100	HIS
1	H	16	HIS
1	H	94	HIS
1	H	100	HIS
1	I	16	HIS
1	I	100	HIS
1	J	100	HIS
1	K	16	HIS
1	K	94	HIS
1	K	100	HIS
1	L	16	HIS
1	L	94	HIS
1	L	100	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

24 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	K	601	-	31,31,31	0.35	0	48,48,48	0.48	0
2	POV	J	602	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	A	601	-	51,51,51	0.50	0	57,59,59	0.47	0
3	CLR	E	601	-	31,31,31	0.35	0	48,48,48	0.48	0
2	POV	G	601	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	H	603	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	A	602	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	B	602	-	51,51,51	0.50	0	57,59,59	0.46	0
3	CLR	I	601	-	31,31,31	0.35	0	48,48,48	0.49	0
2	POV	K	602	-	51,51,51	0.50	0	57,59,59	0.47	0
3	CLR	L	601	-	31,31,31	0.35	0	48,48,48	0.48	0
2	POV	C	602	-	51,51,51	0.50	0	57,59,59	0.47	0
3	CLR	D	601	-	31,31,31	0.35	0	48,48,48	0.48	0
3	CLR	F	601	-	31,31,31	0.35	0	48,48,48	0.48	0
3	CLR	J	601	-	31,31,31	0.35	0	48,48,48	0.48	0
3	CLR	A	603	-	31,31,31	0.35	0	48,48,48	0.48	0
3	CLR	B	601	-	31,31,31	0.35	0	48,48,48	0.48	0
2	POV	E	602	-	51,51,51	0.50	0	57,59,59	0.47	0
3	CLR	G	602	-	31,31,31	0.35	0	48,48,48	0.48	0
2	POV	H	602	-	51,51,51	0.50	0	57,59,59	0.47	0
2	POV	I	602	-	51,51,51	0.50	0	57,59,59	0.47	0
3	CLR	C	601	-	31,31,31	0.35	0	48,48,48	0.48	0
3	CLR	H	601	-	31,31,31	0.36	0	48,48,48	0.49	0
2	POV	D	602	-	51,51,51	0.50	0	57,59,59	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	K	601	-	-	5/10/68/68	0/4/4/4
2	POV	J	602	-	-	19/55/55/55	-
2	POV	A	601	-	-	19/55/55/55	-
3	CLR	E	601	-	-	5/10/68/68	0/4/4/4
2	POV	G	601	-	-	18/55/55/55	-
2	POV	H	603	-	-	17/55/55/55	-
2	POV	A	602	-	-	17/55/55/55	-
2	POV	B	602	-	-	18/55/55/55	-
3	CLR	I	601	-	-	5/10/68/68	0/4/4/4
2	POV	K	602	-	-	20/55/55/55	-
3	CLR	L	601	-	-	5/10/68/68	0/4/4/4
2	POV	C	602	-	-	17/55/55/55	-
3	CLR	D	601	-	-	5/10/68/68	0/4/4/4
3	CLR	F	601	-	-	5/10/68/68	0/4/4/4
3	CLR	J	601	-	-	5/10/68/68	0/4/4/4
3	CLR	A	603	-	-	5/10/68/68	0/4/4/4
3	CLR	B	601	-	-	5/10/68/68	0/4/4/4
2	POV	E	602	-	-	20/55/55/55	-
3	CLR	G	602	-	-	5/10/68/68	0/4/4/4
2	POV	H	602	-	-	17/55/55/55	-
2	POV	I	602	-	-	18/55/55/55	-
3	CLR	C	601	-	-	5/10/68/68	0/4/4/4
3	CLR	H	601	-	-	5/10/68/68	0/4/4/4
2	POV	D	602	-	-	17/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (277) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	POV	C11-O12-P-O11
2	A	601	POV	C11-O12-P-O13
2	A	601	POV	C12-C11-O12-P
2	A	602	POV	C11-O12-P-O11
2	A	602	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	602	POV	C12-C11-O12-P
2	B	602	POV	C11-O12-P-O11
2	B	602	POV	C11-O12-P-O13
2	B	602	POV	C12-C11-O12-P
2	C	602	POV	C11-O12-P-O11
2	C	602	POV	C11-O12-P-O13
2	C	602	POV	C12-C11-O12-P
2	D	602	POV	C11-O12-P-O11
2	D	602	POV	C11-O12-P-O13
2	D	602	POV	C12-C11-O12-P
2	E	602	POV	C11-O12-P-O11
2	E	602	POV	C11-O12-P-O13
2	E	602	POV	C12-C11-O12-P
2	G	601	POV	C11-O12-P-O11
2	G	601	POV	C11-O12-P-O13
2	G	601	POV	C12-C11-O12-P
2	H	602	POV	C11-O12-P-O11
2	H	602	POV	C11-O12-P-O13
2	H	602	POV	C12-C11-O12-P
2	H	603	POV	C11-O12-P-O11
2	H	603	POV	C11-O12-P-O13
2	H	603	POV	C12-C11-O12-P
2	I	602	POV	C11-O12-P-O11
2	I	602	POV	C11-O12-P-O13
2	I	602	POV	C12-C11-O12-P
2	J	602	POV	C11-O12-P-O11
2	J	602	POV	C11-O12-P-O13
2	J	602	POV	C12-C11-O12-P
2	K	602	POV	C11-O12-P-O11
2	K	602	POV	C11-O12-P-O13
2	K	602	POV	C12-C11-O12-P
2	G	601	POV	C22-C23-C24-C25
2	A	601	POV	C22-C23-C24-C25
2	B	602	POV	C22-C23-C24-C25
2	A	602	POV	C22-C23-C24-C25
2	H	603	POV	C22-C23-C24-C25
2	I	602	POV	C22-C23-C24-C25
2	K	602	POV	C22-C23-C24-C25
2	C	602	POV	C22-C23-C24-C25
2	E	602	POV	C22-C23-C24-C25
2	D	602	POV	C22-C23-C24-C25
2	H	602	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	J	602	POV	C22-C23-C24-C25
2	H	603	POV	C36-C37-C38-C39
2	C	602	POV	C36-C37-C38-C39
2	B	602	POV	C36-C37-C38-C39
2	E	602	POV	C36-C37-C38-C39
2	I	602	POV	C36-C37-C38-C39
2	A	602	POV	C210-C211-C212-C213
2	A	601	POV	C36-C37-C38-C39
2	G	601	POV	C36-C37-C38-C39
2	D	602	POV	C36-C37-C38-C39
2	K	602	POV	C36-C37-C38-C39
2	H	602	POV	C36-C37-C38-C39
2	J	602	POV	C36-C37-C38-C39
2	A	602	POV	C36-C37-C38-C39
2	A	601	POV	C210-C211-C212-C213
2	A	601	POV	C24-C25-C26-C27
2	A	602	POV	C31-C32-C33-C34
2	D	602	POV	C210-C211-C212-C213
2	G	601	POV	C210-C211-C212-C213
2	H	603	POV	C210-C211-C212-C213
2	J	602	POV	C210-C211-C212-C213
2	G	601	POV	C31-C32-C33-C34
2	G	601	POV	C24-C25-C26-C27
2	A	601	POV	C31-C32-C33-C34
2	A	601	POV	C312-C313-C314-C315
2	E	602	POV	C312-C313-C314-C315
2	K	602	POV	C312-C313-C314-C315
2	G	601	POV	C312-C313-C314-C315
2	J	602	POV	C31-C32-C33-C34
2	K	602	POV	C31-C32-C33-C34
2	B	602	POV	C312-C313-C314-C315
2	H	603	POV	C312-C313-C314-C315
2	A	602	POV	C312-C313-C314-C315
2	J	602	POV	C312-C313-C314-C315
2	B	602	POV	C210-C211-C212-C213
2	C	602	POV	C210-C211-C212-C213
2	E	602	POV	C210-C211-C212-C213
2	H	602	POV	C210-C211-C212-C213
2	I	602	POV	C210-C211-C212-C213
2	K	602	POV	C210-C211-C212-C213
2	H	602	POV	C312-C313-C314-C315
2	I	602	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
2	C	602	POV	C312-C313-C314-C315
2	D	602	POV	C312-C313-C314-C315
2	B	602	POV	C31-C32-C33-C34
2	H	602	POV	C31-C32-C33-C34
2	C	602	POV	C24-C25-C26-C27
2	I	602	POV	C31-C32-C33-C34
2	I	602	POV	C24-C25-C26-C27
2	H	603	POV	C24-C25-C26-C27
2	E	602	POV	C31-C32-C33-C34
2	H	602	POV	C24-C25-C26-C27
2	D	602	POV	C31-C32-C33-C34
2	H	603	POV	C31-C32-C33-C34
2	B	602	POV	C24-C25-C26-C27
2	A	602	POV	C24-C25-C26-C27
2	E	602	POV	C24-C25-C26-C27
2	K	602	POV	C24-C25-C26-C27
2	D	602	POV	C24-C25-C26-C27
2	C	602	POV	C31-C32-C33-C34
2	J	602	POV	C24-C25-C26-C27
3	B	601	CLR	C13-C17-C20-C22
2	A	601	POV	O21-C2-C3-O31
2	A	602	POV	O21-C2-C3-O31
2	B	602	POV	O21-C2-C3-O31
2	C	602	POV	O21-C2-C3-O31
2	D	602	POV	O21-C2-C3-O31
2	E	602	POV	O21-C2-C3-O31
2	G	601	POV	O21-C2-C3-O31
2	H	602	POV	O21-C2-C3-O31
2	H	603	POV	O21-C2-C3-O31
2	I	602	POV	O21-C2-C3-O31
2	J	602	POV	O21-C2-C3-O31
2	K	602	POV	O21-C2-C3-O31
3	F	601	CLR	C13-C17-C20-C22
3	B	601	CLR	C13-C17-C20-C21
3	F	601	CLR	C13-C17-C20-C21
3	D	601	CLR	C13-C17-C20-C22
3	C	601	CLR	C13-C17-C20-C22
3	E	601	CLR	C13-C17-C20-C22
2	A	601	POV	O11-C1-C2-C3
2	A	602	POV	O11-C1-C2-C3
2	C	602	POV	O11-C1-C2-C3
2	D	602	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	E	602	POV	O11-C1-C2-C3
2	G	601	POV	O11-C1-C2-C3
2	H	602	POV	O11-C1-C2-C3
2	H	603	POV	O11-C1-C2-C3
2	I	602	POV	O11-C1-C2-C3
2	J	602	POV	O11-C1-C2-C3
2	K	602	POV	O11-C1-C2-C3
3	D	601	CLR	C13-C17-C20-C21
3	I	601	CLR	C13-C17-C20-C22
3	A	603	CLR	C13-C17-C20-C21
3	C	601	CLR	C13-C17-C20-C21
3	E	601	CLR	C13-C17-C20-C21
3	G	602	CLR	C13-C17-C20-C21
3	H	601	CLR	C13-C17-C20-C21
3	I	601	CLR	C13-C17-C20-C21
3	J	601	CLR	C13-C17-C20-C21
3	K	601	CLR	C13-C17-C20-C21
3	L	601	CLR	C13-C17-C20-C21
3	A	603	CLR	C13-C17-C20-C22
3	J	601	CLR	C13-C17-C20-C22
2	C	602	POV	O11-C1-C2-O21
2	D	602	POV	O11-C1-C2-O21
2	H	602	POV	O11-C1-C2-O21
2	I	602	POV	O11-C1-C2-O21
3	G	602	CLR	C13-C17-C20-C22
3	H	601	CLR	C13-C17-C20-C22
3	L	601	CLR	C13-C17-C20-C22
3	K	601	CLR	C13-C17-C20-C22
2	A	601	POV	O12-C11-C12-N
2	A	602	POV	O12-C11-C12-N
2	B	602	POV	O12-C11-C12-N
2	C	602	POV	O12-C11-C12-N
2	D	602	POV	O12-C11-C12-N
2	E	602	POV	O12-C11-C12-N
2	G	601	POV	O12-C11-C12-N
2	H	602	POV	O12-C11-C12-N
2	H	603	POV	O12-C11-C12-N
2	I	602	POV	O12-C11-C12-N
2	J	602	POV	O12-C11-C12-N
2	K	602	POV	O12-C11-C12-N
2	A	602	POV	C211-C212-C213-C214
2	E	602	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
2	K	602	POV	C211-C212-C213-C214
3	B	601	CLR	C16-C17-C20-C21
2	A	601	POV	C211-C212-C213-C214
3	F	601	CLR	C16-C17-C20-C21
2	B	602	POV	O11-C1-C2-C3
2	B	602	POV	C211-C212-C213-C214
2	J	602	POV	C211-C212-C213-C214
3	B	601	CLR	C16-C17-C20-C22
3	F	601	CLR	C16-C17-C20-C22
2	A	601	POV	O11-C1-C2-O21
2	A	602	POV	O11-C1-C2-O21
2	B	602	POV	O11-C1-C2-O21
2	E	602	POV	O11-C1-C2-O21
2	G	601	POV	O11-C1-C2-O21
2	H	603	POV	O11-C1-C2-O21
2	J	602	POV	O11-C1-C2-O21
2	K	602	POV	O11-C1-C2-O21
3	D	601	CLR	C16-C17-C20-C22
3	D	601	CLR	C16-C17-C20-C21
2	A	602	POV	C1-C2-C3-O31
2	B	602	POV	C1-C2-C3-O31
2	E	602	POV	C1-C2-C3-O31
2	G	601	POV	C1-C2-C3-O31
2	I	602	POV	C1-C2-C3-O31
2	K	602	POV	C1-C2-C3-O31
2	C	602	POV	C35-C36-C37-C38
3	C	601	CLR	C16-C17-C20-C22
3	E	601	CLR	C16-C17-C20-C22
3	I	601	CLR	C16-C17-C20-C22
3	C	601	CLR	C16-C17-C20-C21
3	E	601	CLR	C16-C17-C20-C21
2	H	603	POV	C211-C212-C213-C214
2	H	602	POV	C211-C212-C213-C214
2	H	602	POV	C35-C36-C37-C38
2	D	602	POV	C35-C36-C37-C38
3	A	603	CLR	C16-C17-C20-C22
3	G	602	CLR	C16-C17-C20-C22
3	H	601	CLR	C16-C17-C20-C22
3	J	601	CLR	C16-C17-C20-C22
3	L	601	CLR	C16-C17-C20-C22
2	A	601	POV	C2-C1-O11-P
2	A	602	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
2	B	602	POV	C2-C1-O11-P
2	C	602	POV	C2-C1-O11-P
2	D	602	POV	C2-C1-O11-P
2	E	602	POV	C2-C1-O11-P
2	G	601	POV	C2-C1-O11-P
2	H	602	POV	C2-C1-O11-P
2	H	603	POV	C2-C1-O11-P
2	I	602	POV	C2-C1-O11-P
2	J	602	POV	C2-C1-O11-P
2	K	602	POV	C2-C1-O11-P
2	G	601	POV	C211-C212-C213-C214
3	K	601	CLR	C16-C17-C20-C22
2	A	601	POV	C35-C36-C37-C38
3	I	601	CLR	C16-C17-C20-C21
2	D	602	POV	C211-C212-C213-C214
2	I	602	POV	C211-C212-C213-C214
2	H	603	POV	C35-C36-C37-C38
2	B	602	POV	C35-C36-C37-C38
2	I	602	POV	C35-C36-C37-C38
2	A	602	POV	C35-C36-C37-C38
3	A	603	CLR	C16-C17-C20-C21
2	C	602	POV	C211-C212-C213-C214
2	G	601	POV	C35-C36-C37-C38
3	J	601	CLR	C16-C17-C20-C21
3	L	601	CLR	C16-C17-C20-C21
2	J	602	POV	C35-C36-C37-C38
2	A	601	POV	C1-C2-C3-O31
2	C	602	POV	C1-C2-C3-O31
2	D	602	POV	C1-C2-C3-O31
2	H	602	POV	C1-C2-C3-O31
2	H	603	POV	C1-C2-C3-O31
2	J	602	POV	C1-C2-C3-O31
3	G	602	CLR	C16-C17-C20-C21
3	H	601	CLR	C16-C17-C20-C21
2	K	602	POV	C35-C36-C37-C38
3	K	601	CLR	C16-C17-C20-C21
2	E	602	POV	C35-C36-C37-C38
3	D	601	CLR	C20-C22-C23-C24
3	G	602	CLR	C20-C22-C23-C24
3	A	603	CLR	C20-C22-C23-C24
3	H	601	CLR	C20-C22-C23-C24
3	C	601	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	B	601	CLR	C20-C22-C23-C24
3	J	601	CLR	C20-C22-C23-C24
3	E	601	CLR	C20-C22-C23-C24
3	I	601	CLR	C20-C22-C23-C24
3	F	601	CLR	C20-C22-C23-C24
3	K	601	CLR	C20-C22-C23-C24
2	E	602	POV	C310-C311-C312-C313
3	L	601	CLR	C20-C22-C23-C24
2	A	601	POV	C313-C314-C315-C316
2	J	602	POV	C310-C311-C312-C313
2	K	602	POV	C313-C314-C315-C316
2	K	602	POV	C310-C311-C312-C313
2	E	602	POV	C313-C314-C315-C316
2	A	601	POV	O31-C31-C32-C33
2	G	601	POV	O31-C31-C32-C33
2	J	602	POV	C313-C314-C315-C316
2	K	602	POV	O31-C31-C32-C33
2	E	602	POV	O31-C31-C32-C33
2	B	602	POV	O31-C31-C32-C33
2	I	602	POV	O31-C31-C32-C33

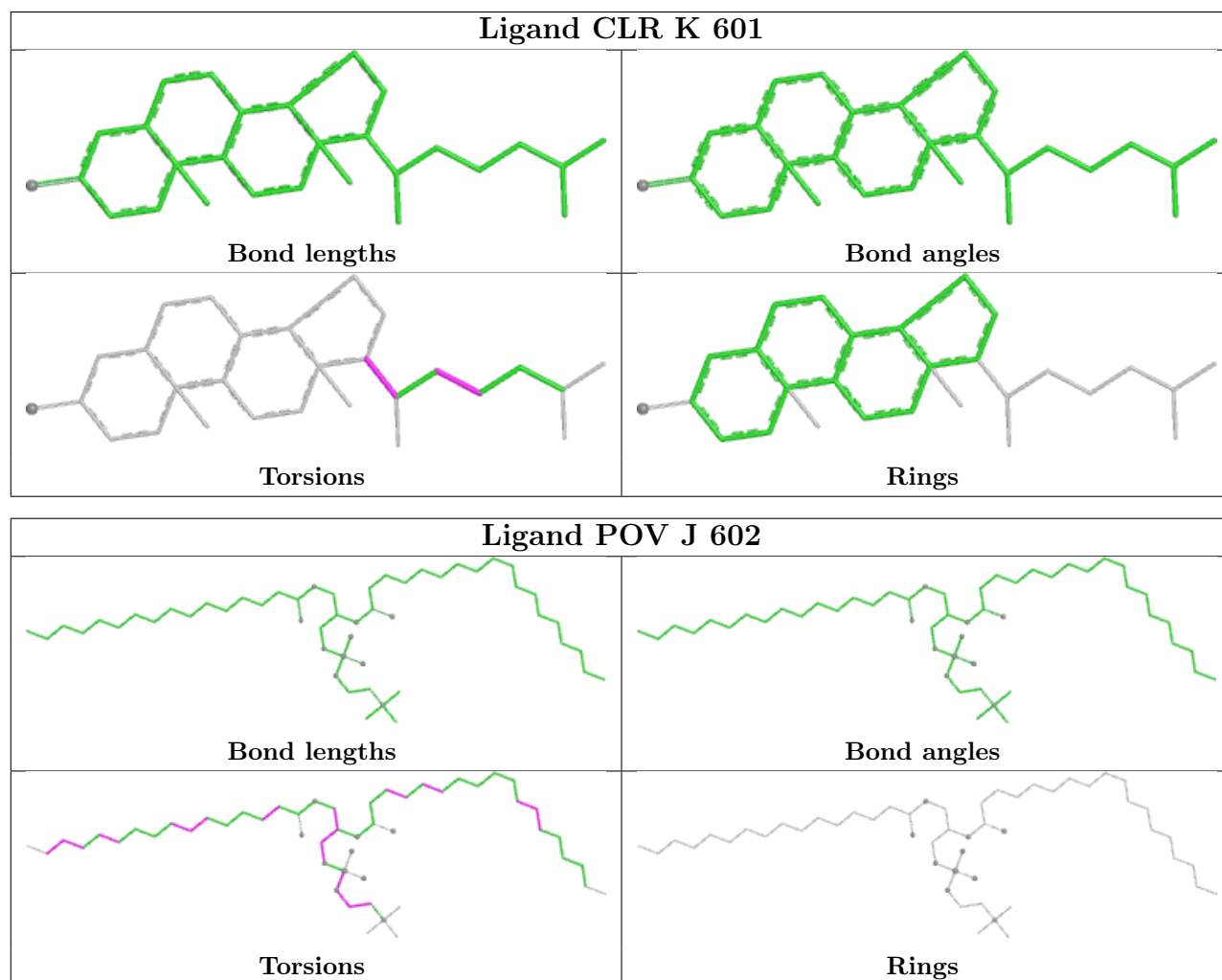
There are no ring outliers.

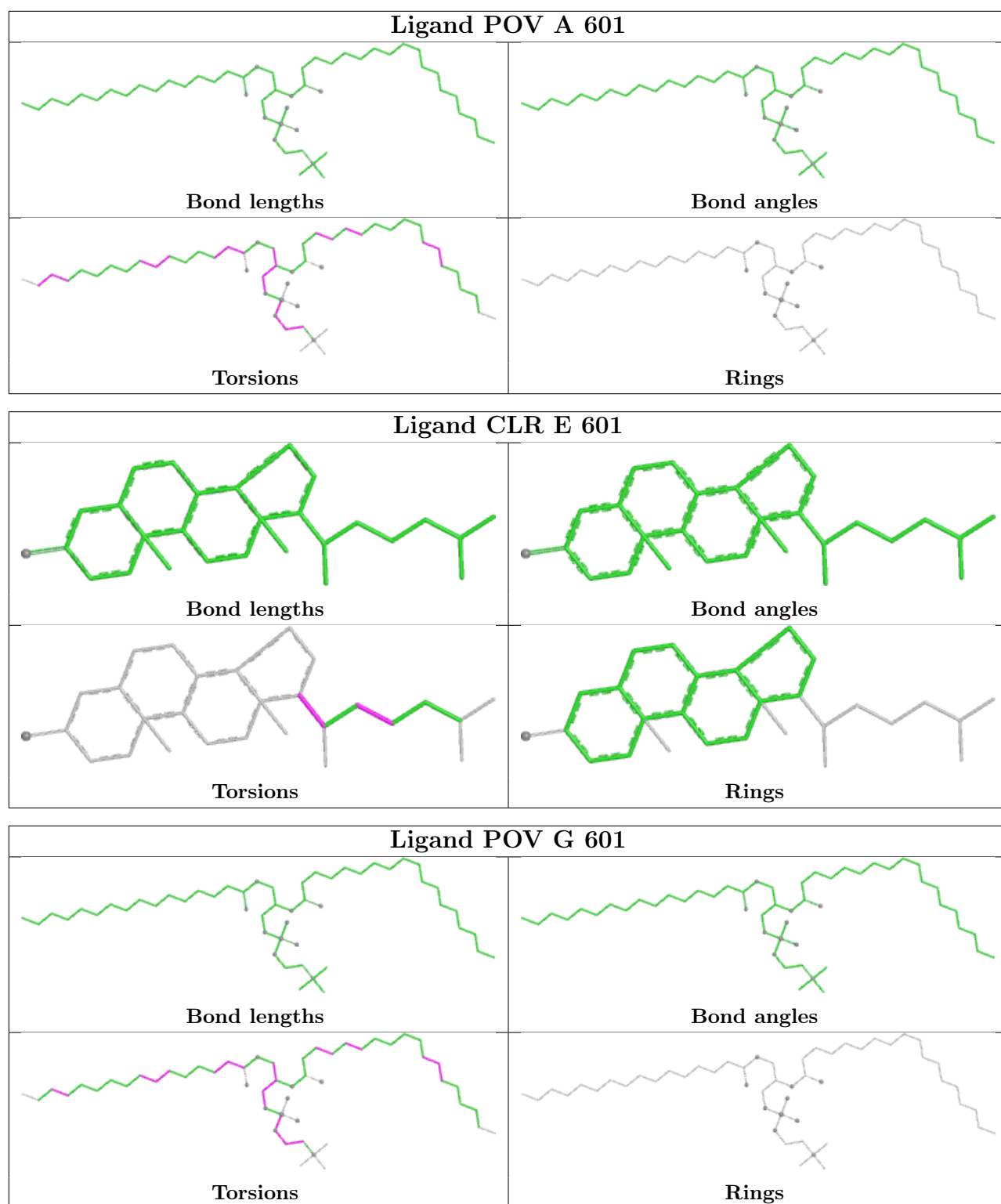
13 monomers are involved in 15 short contacts:

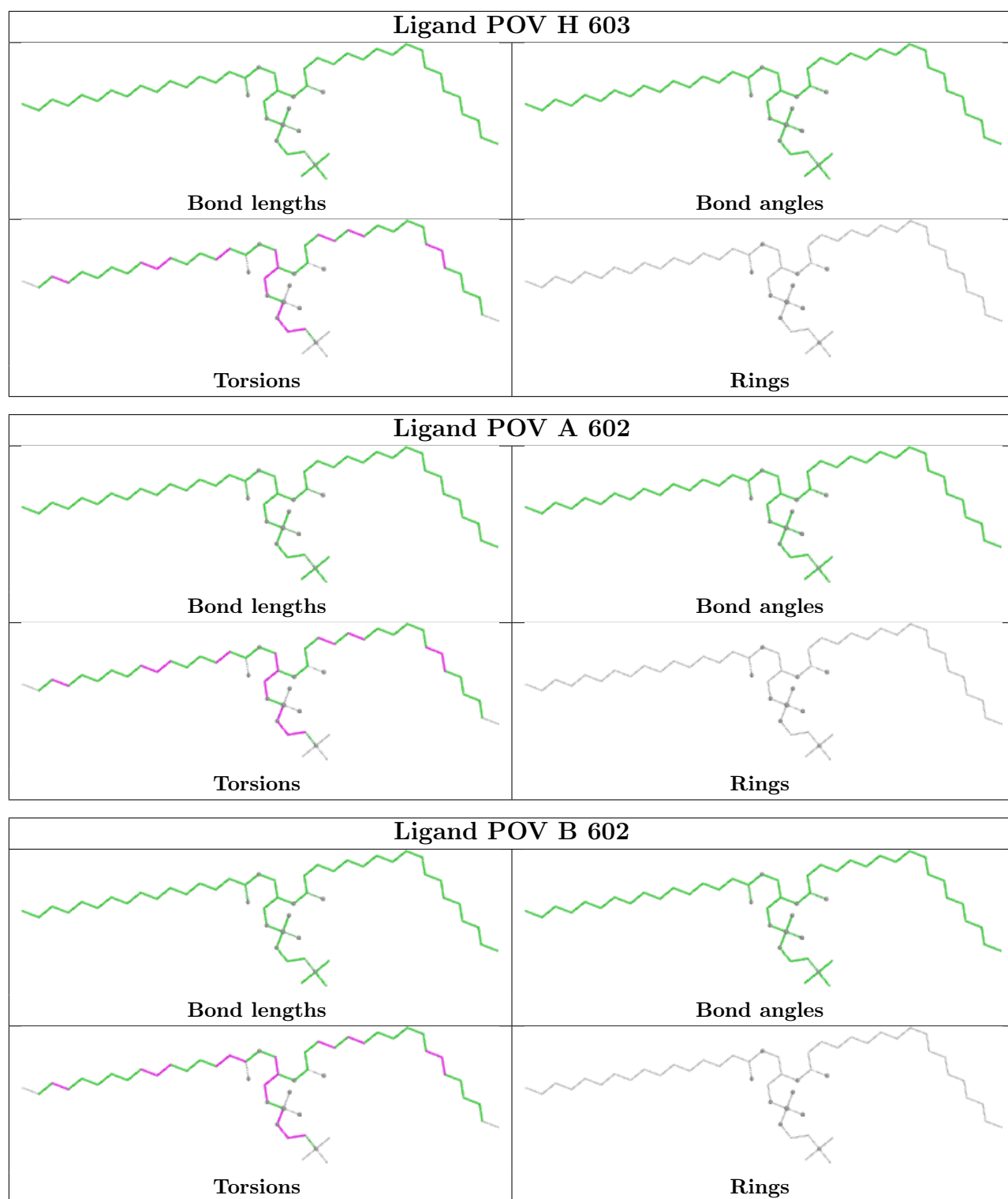
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	602	POV	1	0
2	A	601	POV	2	0
2	G	601	POV	2	0
2	H	603	POV	1	0
2	A	602	POV	1	0
2	B	602	POV	1	0
2	K	602	POV	1	0
2	C	602	POV	1	0
2	E	602	POV	1	0
3	G	602	CLR	1	0
2	H	602	POV	1	0
2	I	602	POV	1	0
2	D	602	POV	1	0

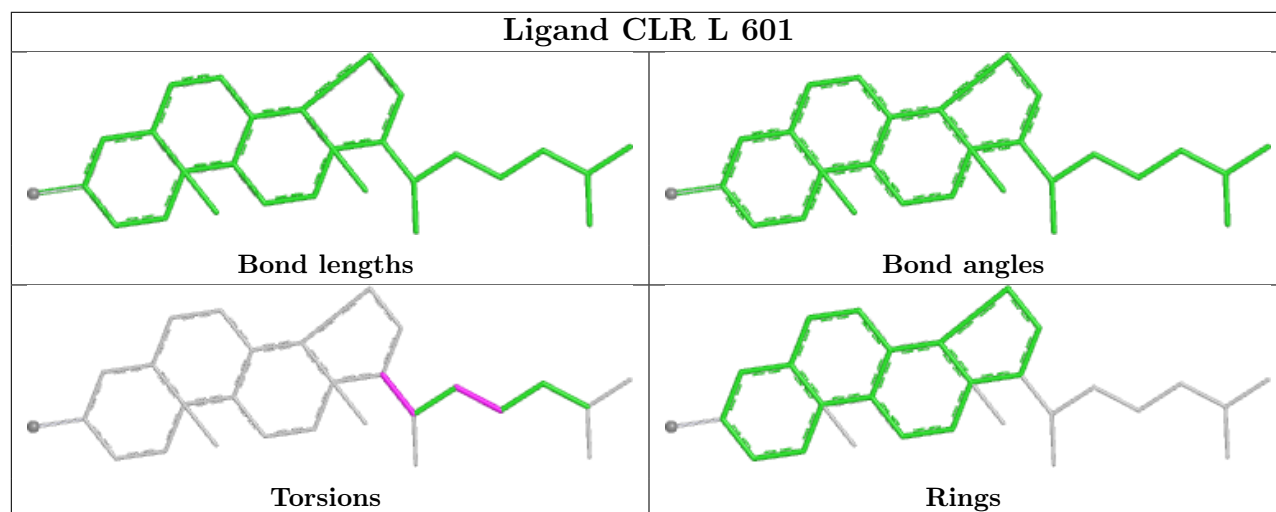
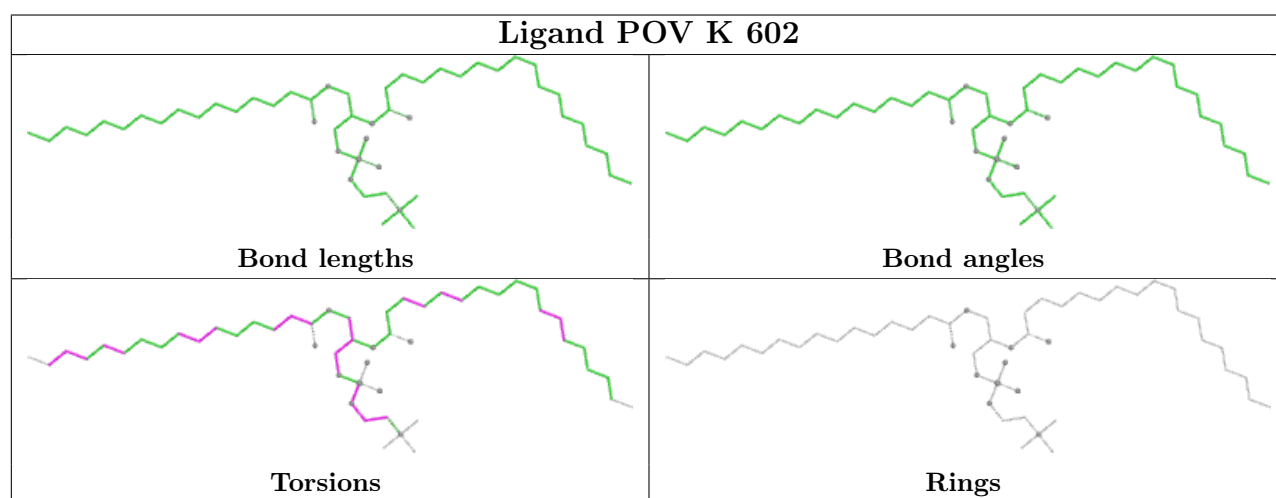
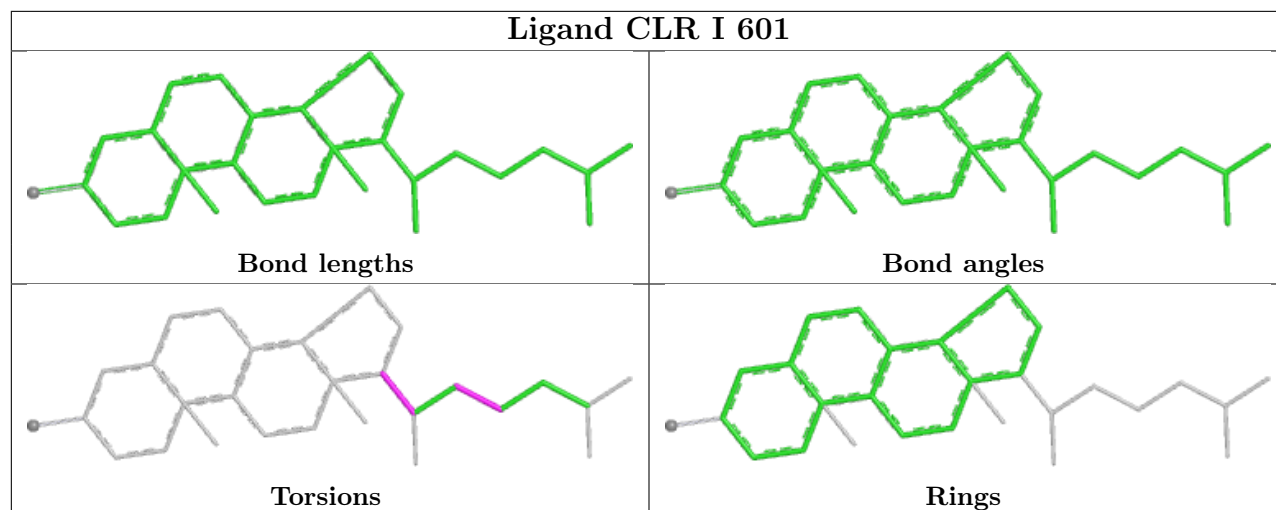
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

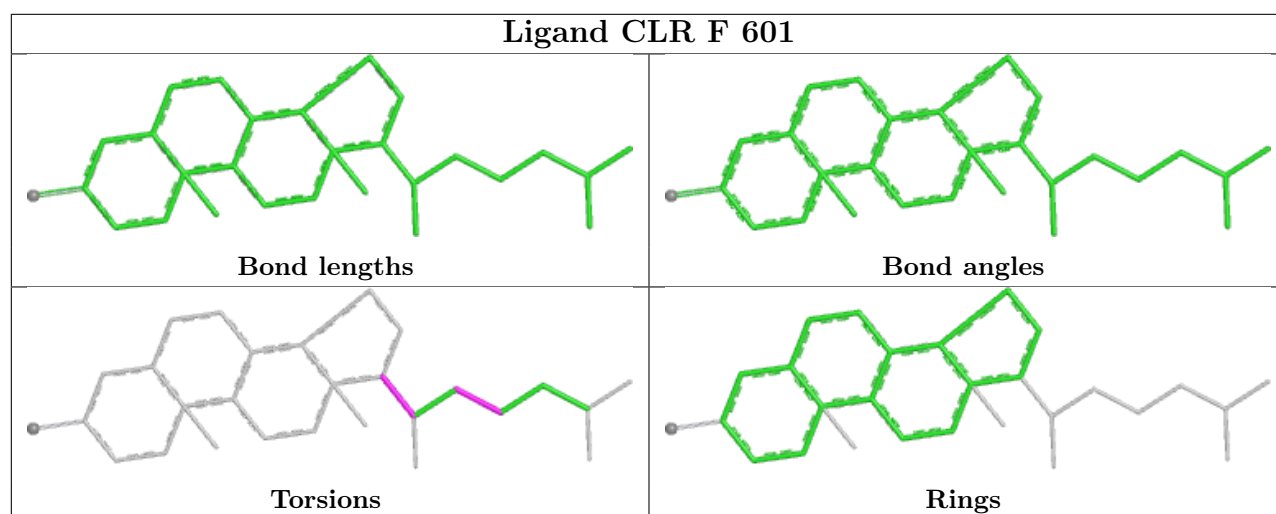
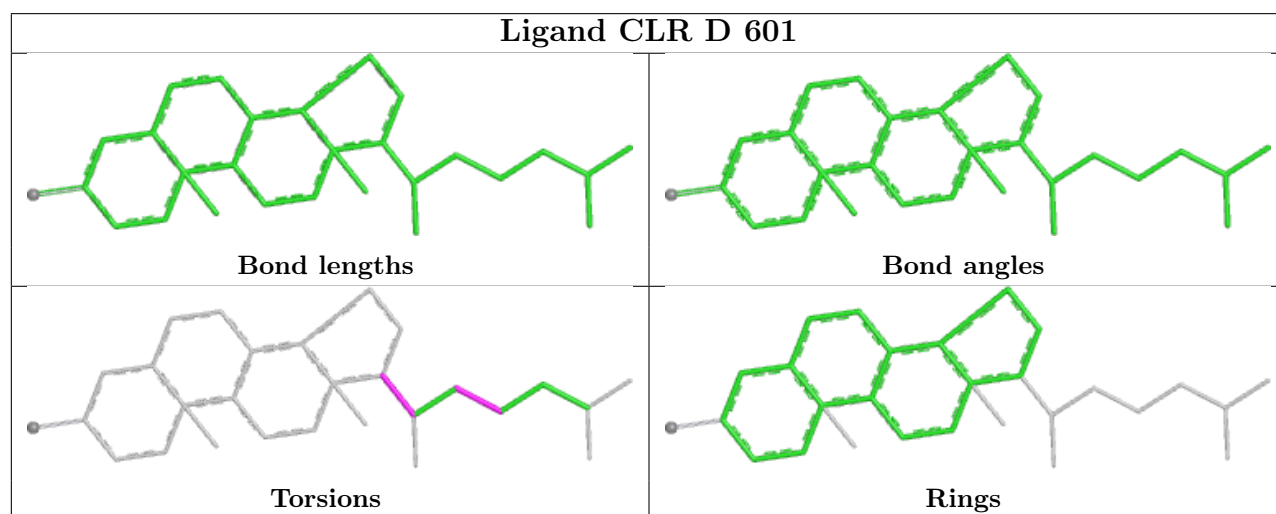
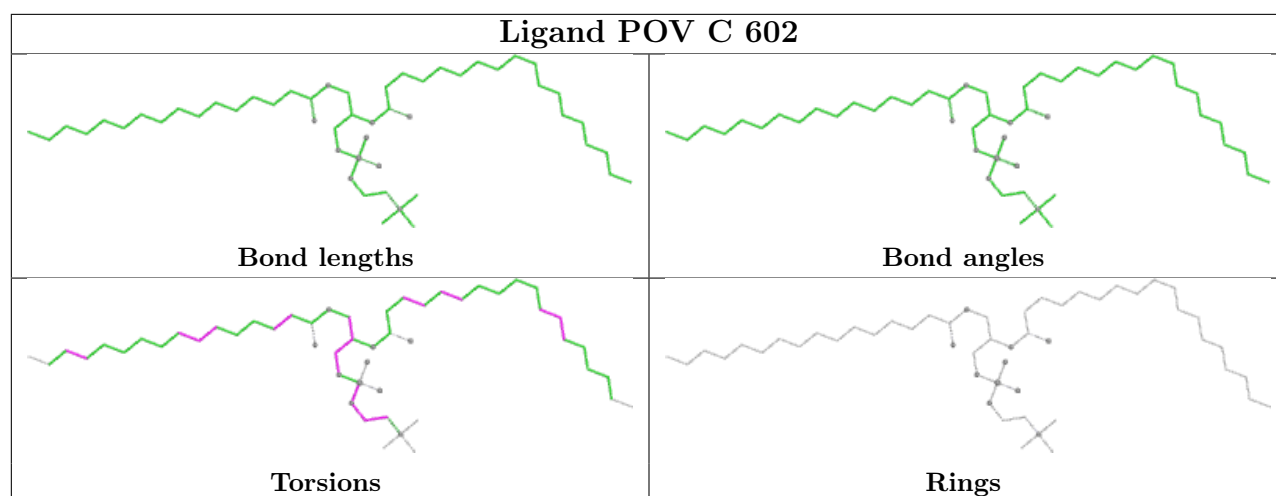
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

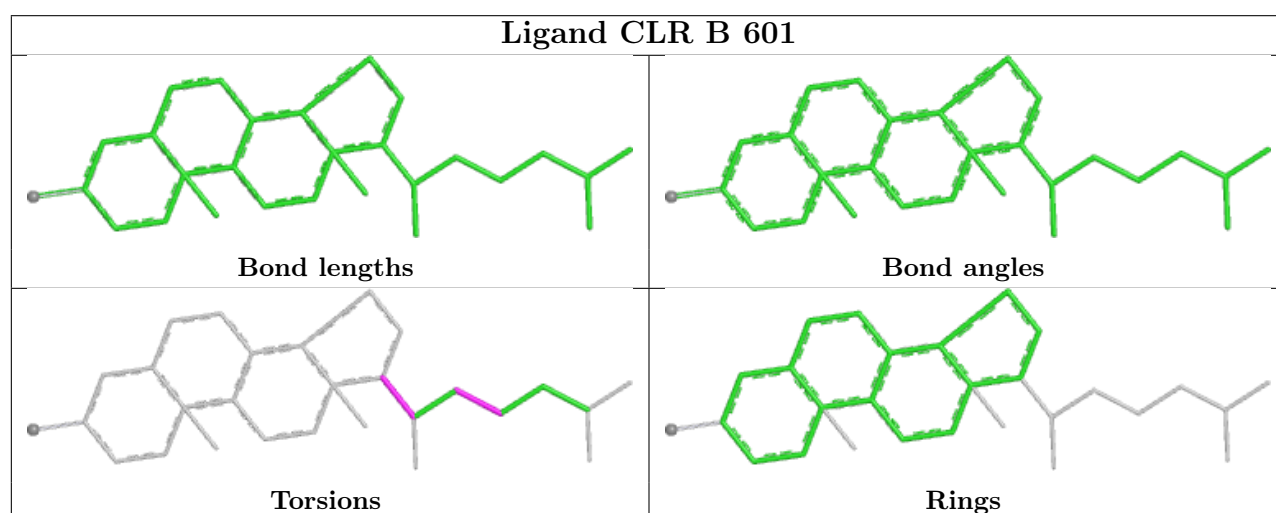
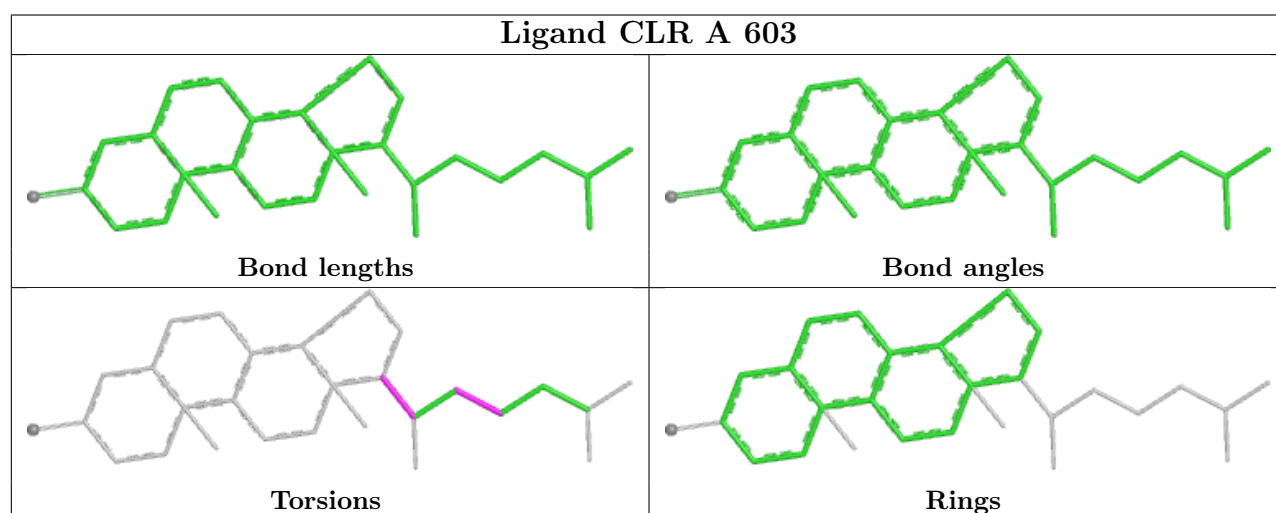
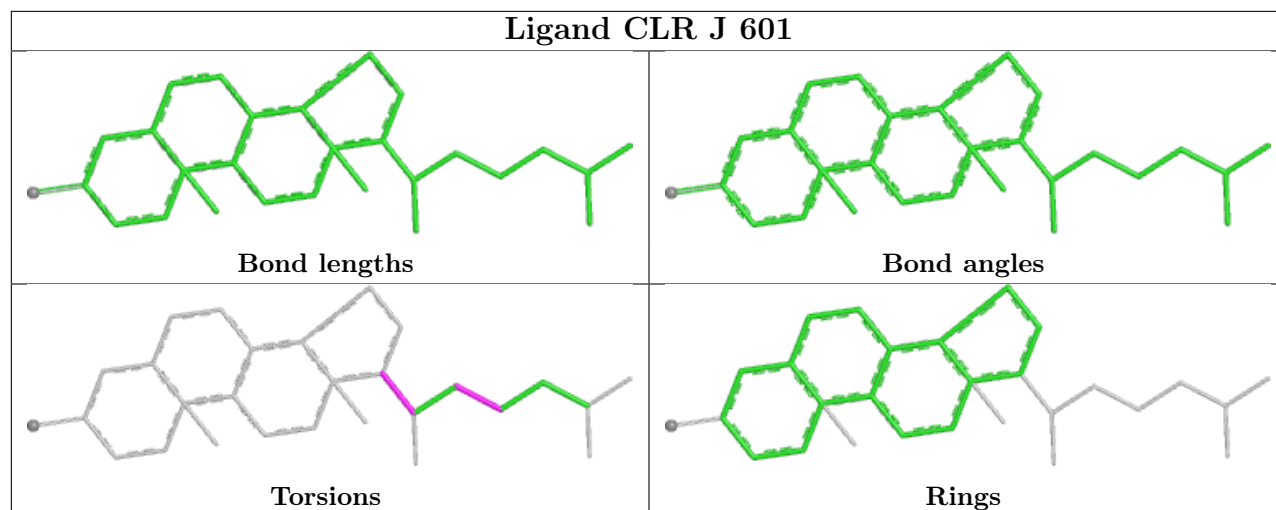


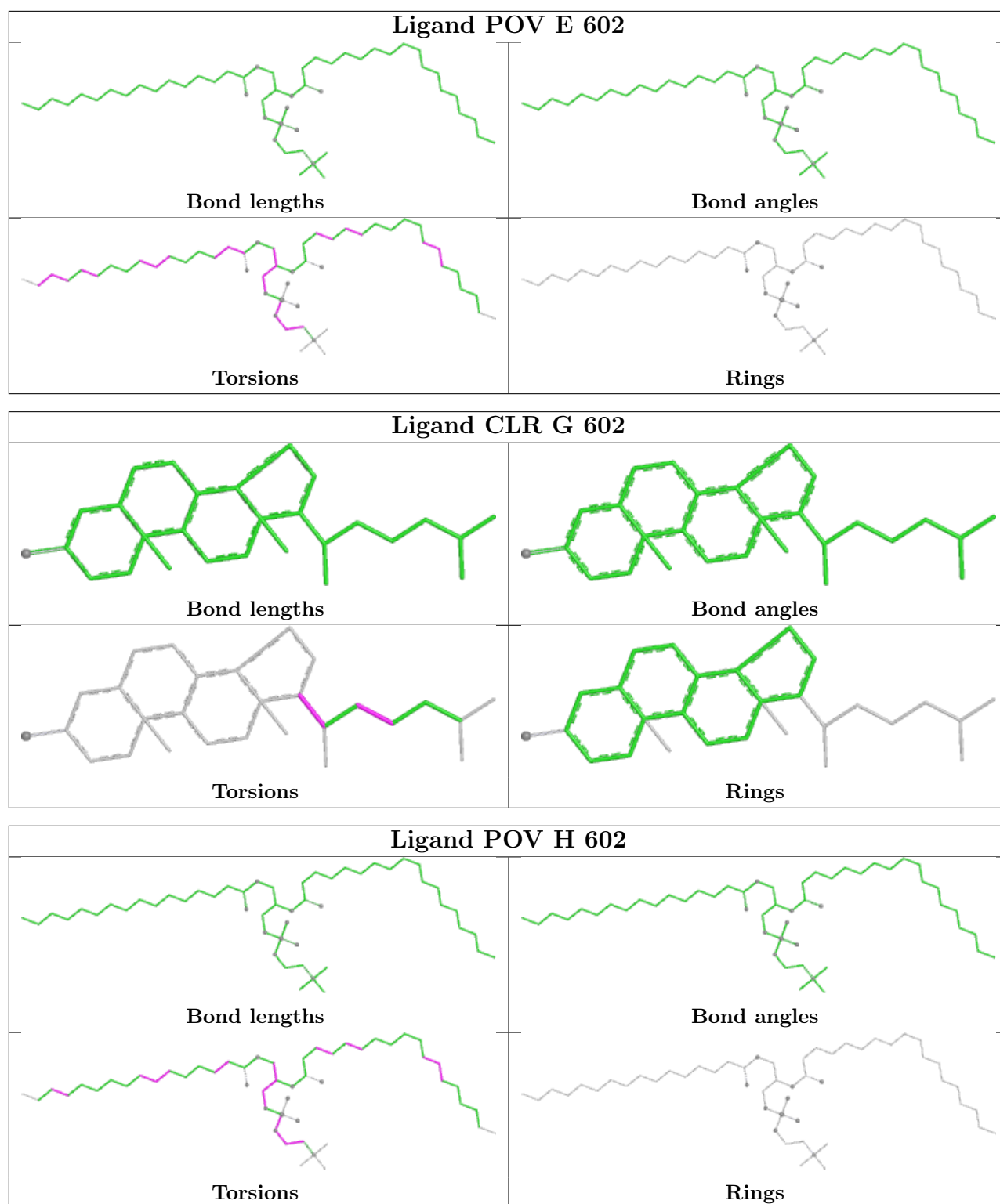


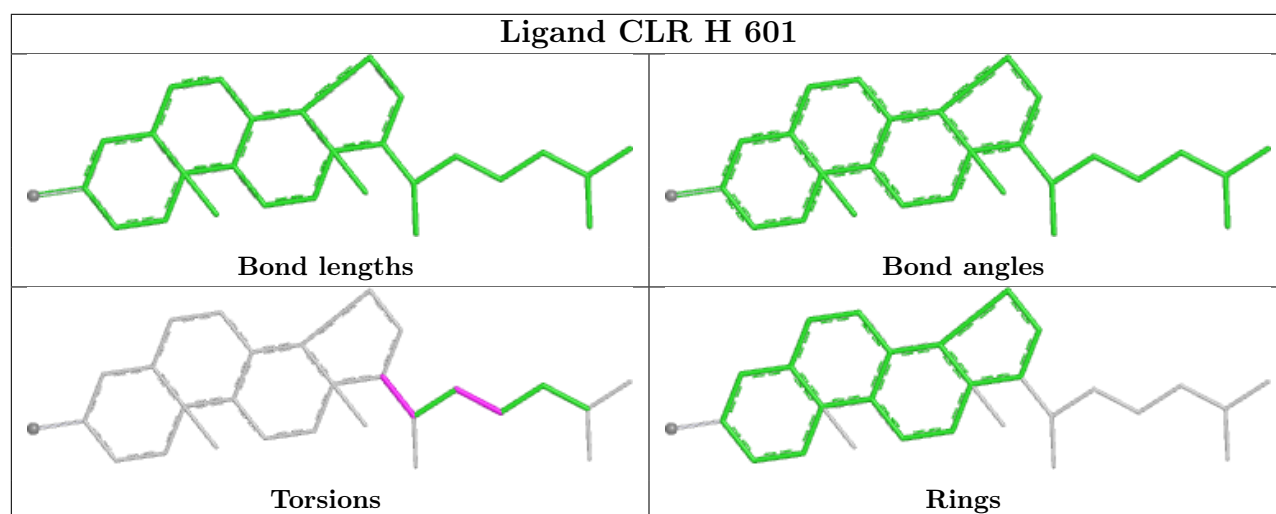
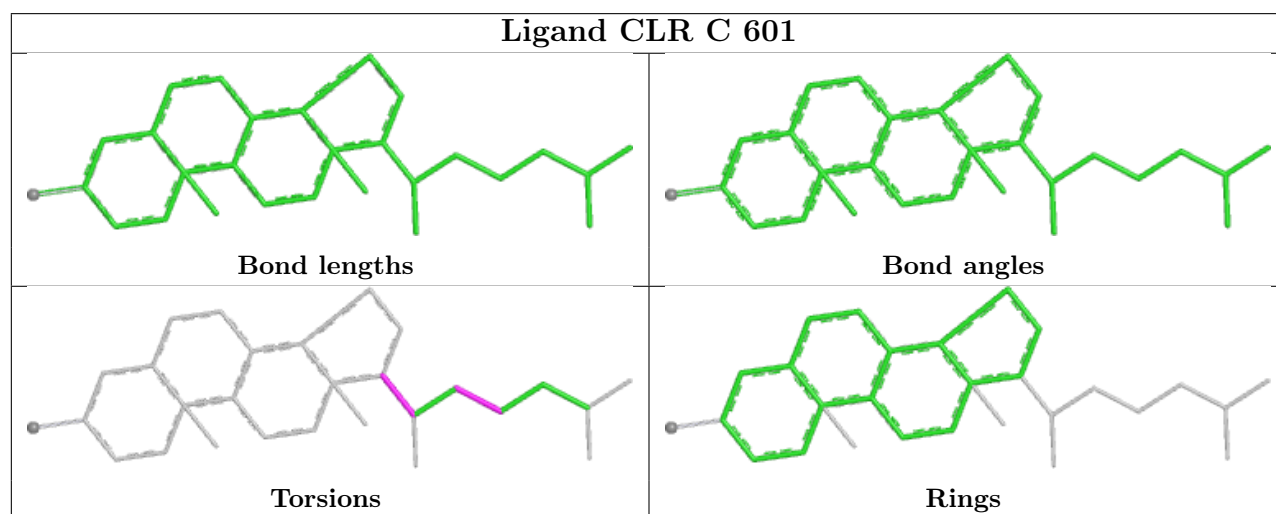
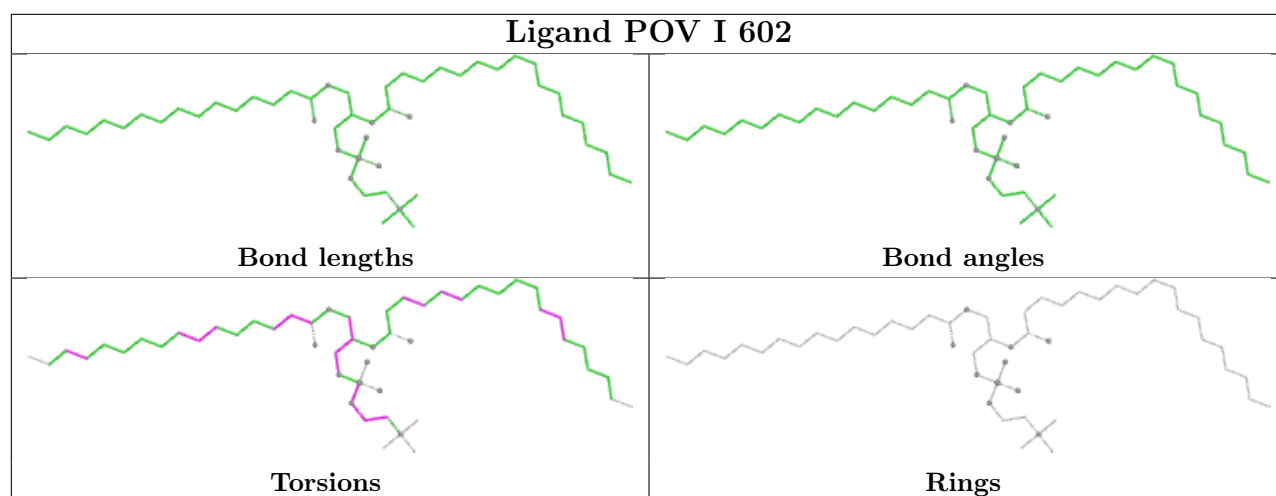


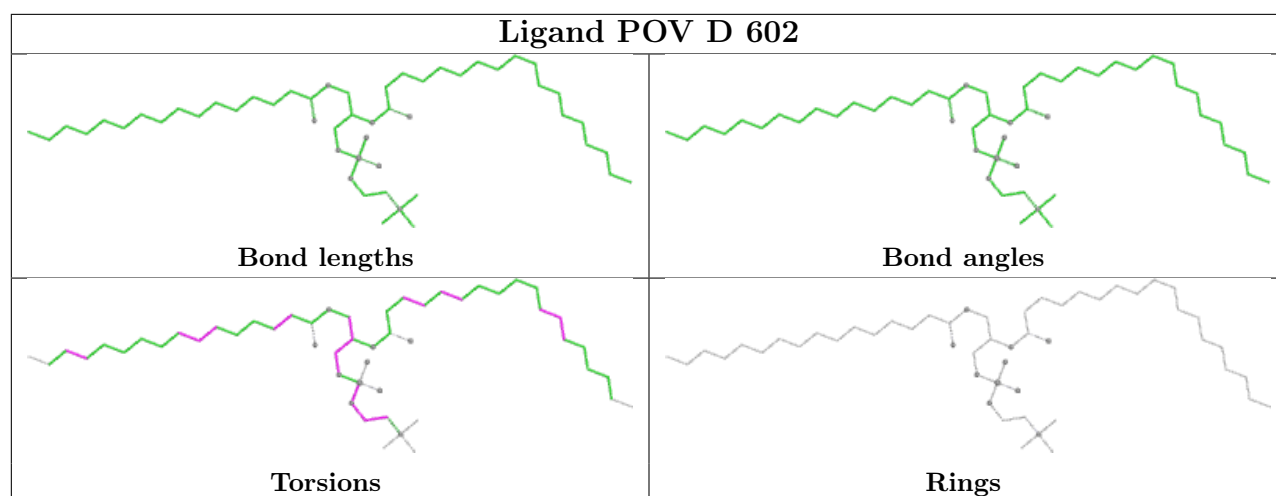












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

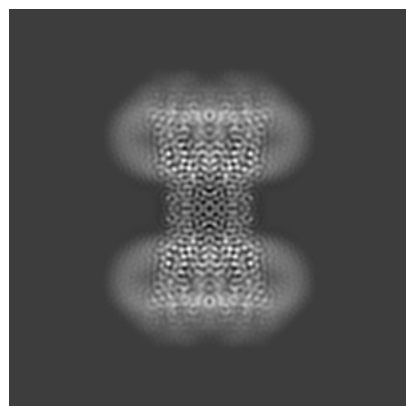
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53245. These allow visual inspection of the internal detail of the map and identification of artifacts.

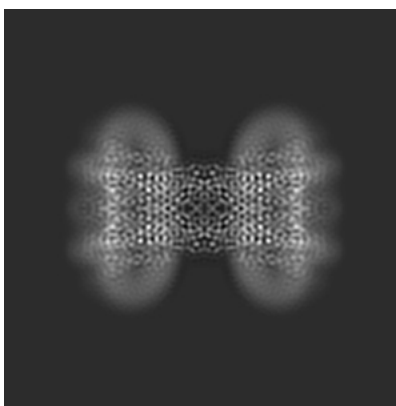
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

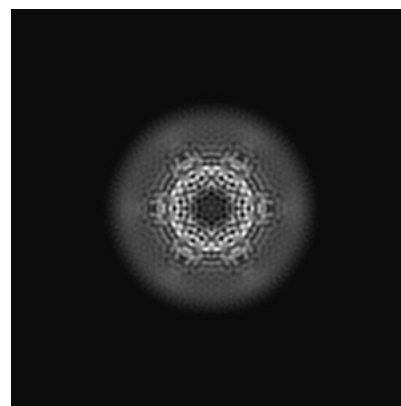
6.1.1 Primary map



X

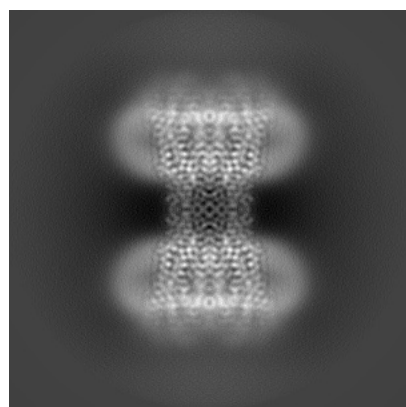


Y

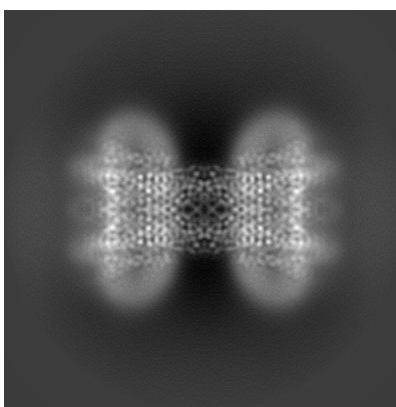


Z

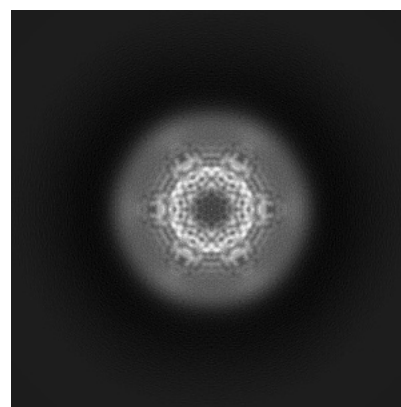
6.1.2 Raw map



X



Y

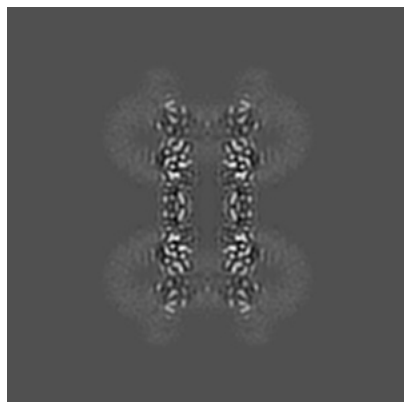


Z

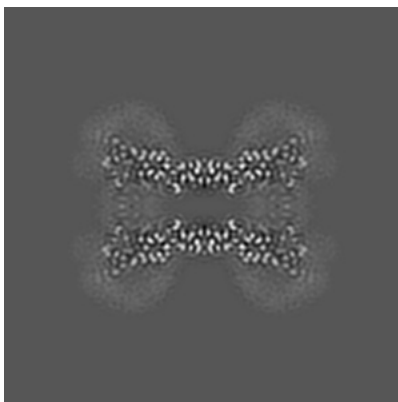
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

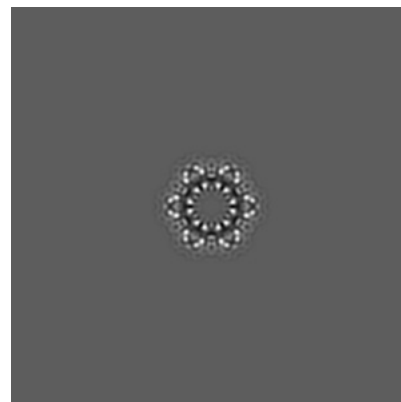
6.2.1 Primary map



X Index: 192

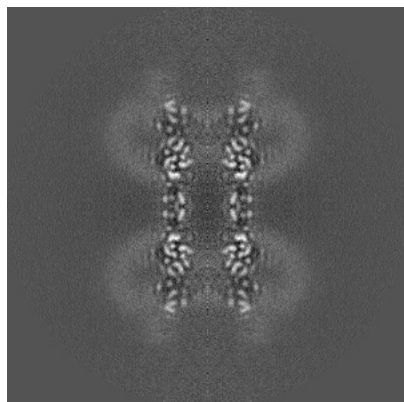


Y Index: 192

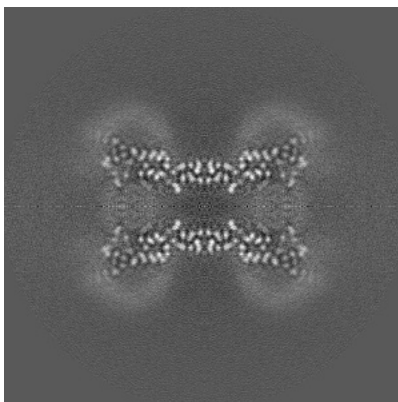


Z Index: 192

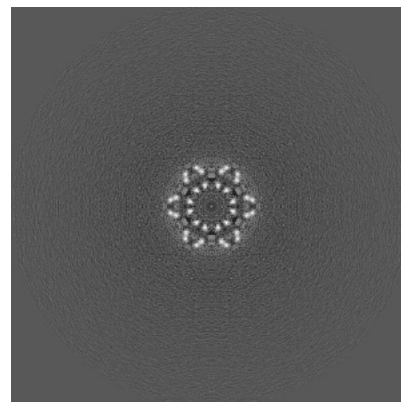
6.2.2 Raw map



X Index: 192



Y Index: 192

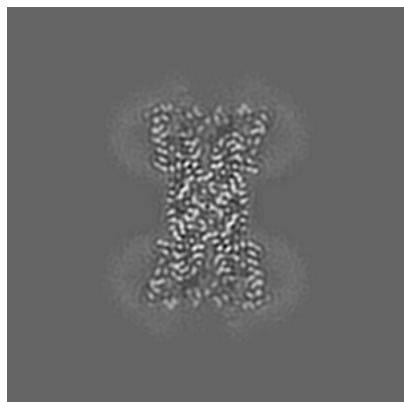


Z Index: 192

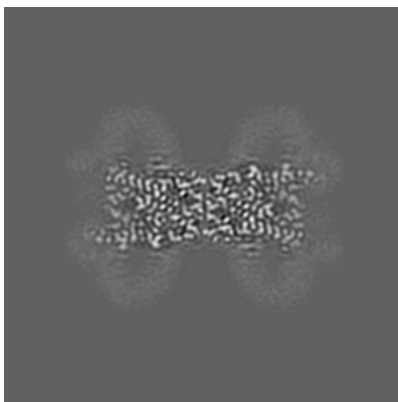
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

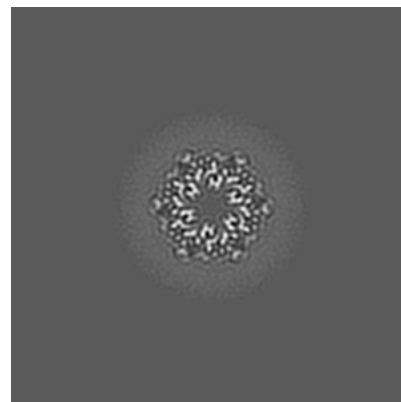
6.3.1 Primary map



X Index: 213

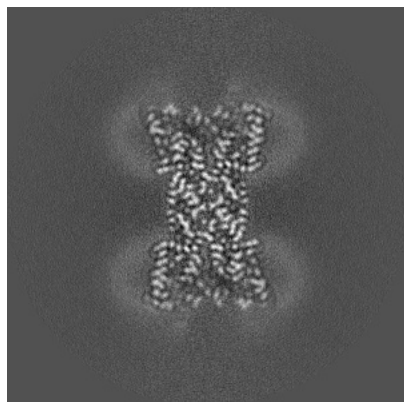


Y Index: 167

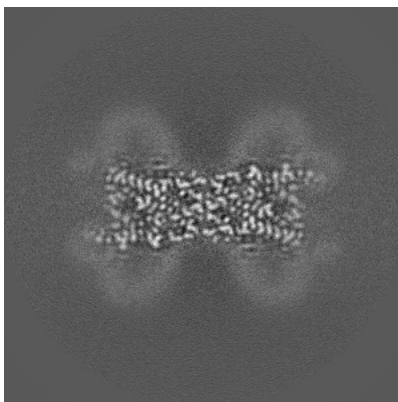


Z Index: 231

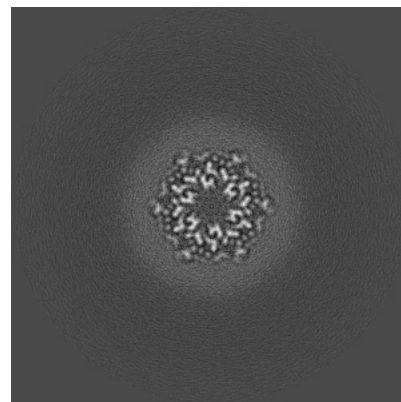
6.3.2 Raw map



X Index: 171



Y Index: 167

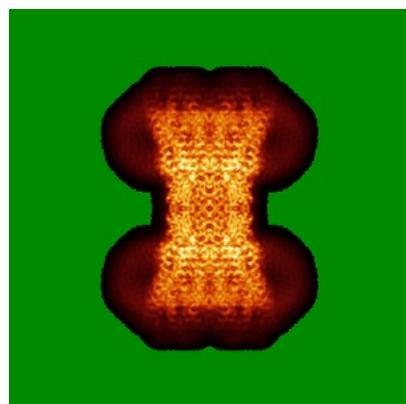


Z Index: 153

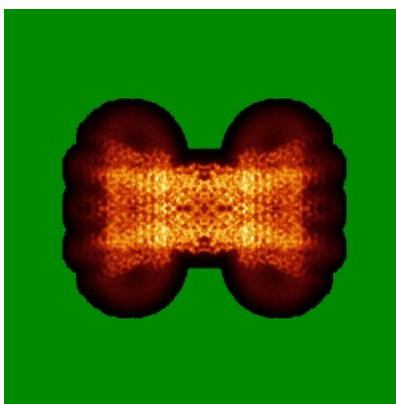
The images above show the largest variance slices of the map in three orthogonal directions.

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

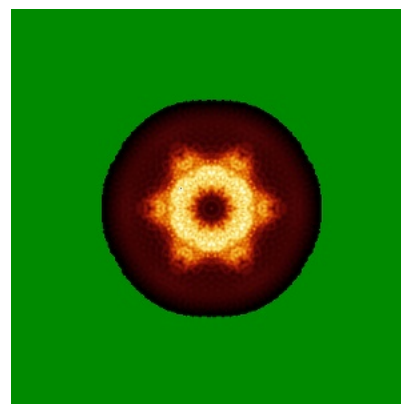
6.4.1 Primary map



X

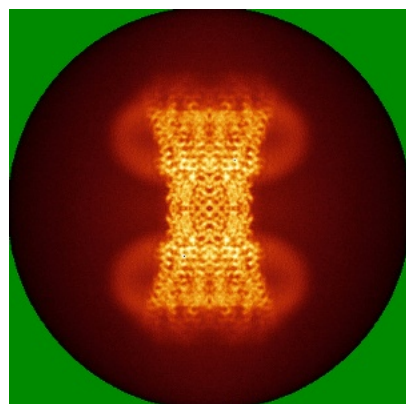


Y

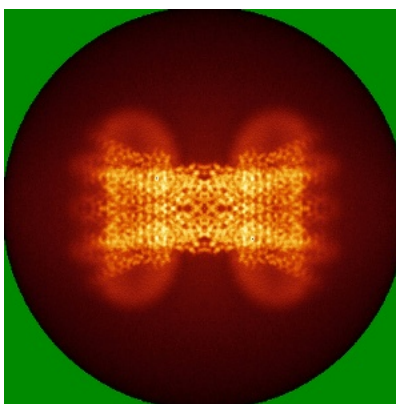


Z

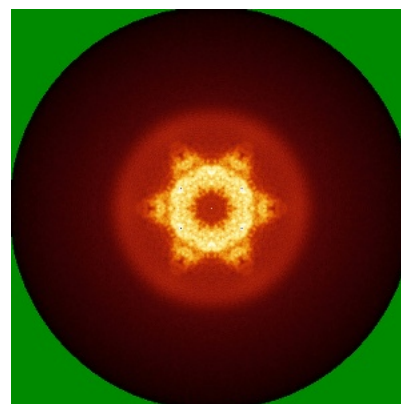
6.4.2 Raw map



X



Y

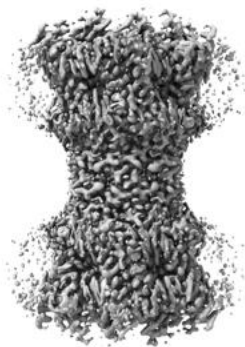


Z

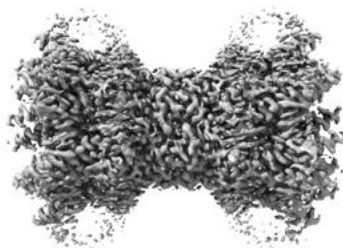
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



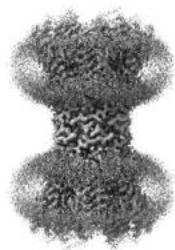
Y



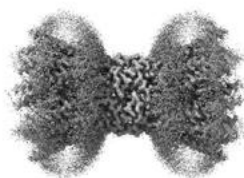
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

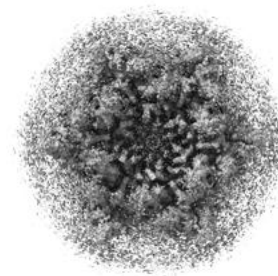
6.5.2 Raw map



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.

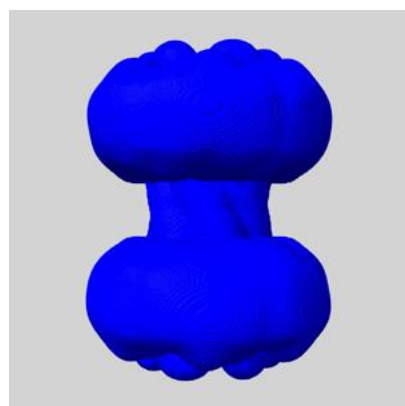
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

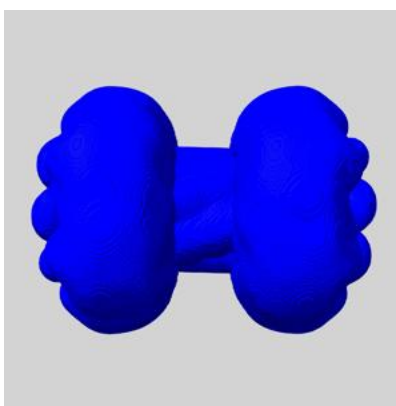
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

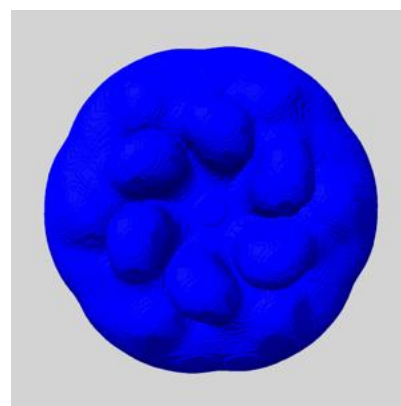
6.6.1 emd_53245_msk_1.map [i](#)



X



Y

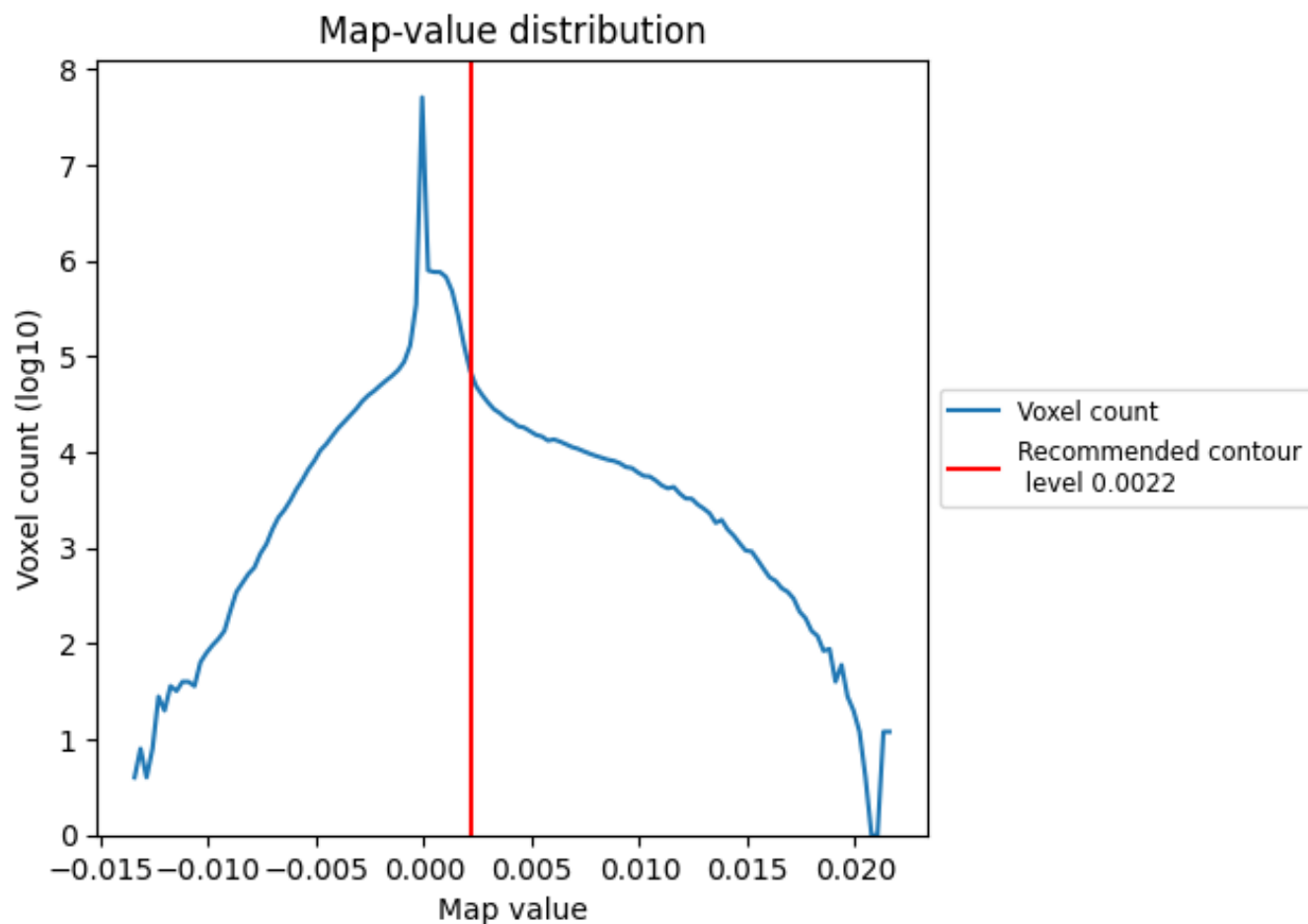


Z

7 Map analysis [i](#)

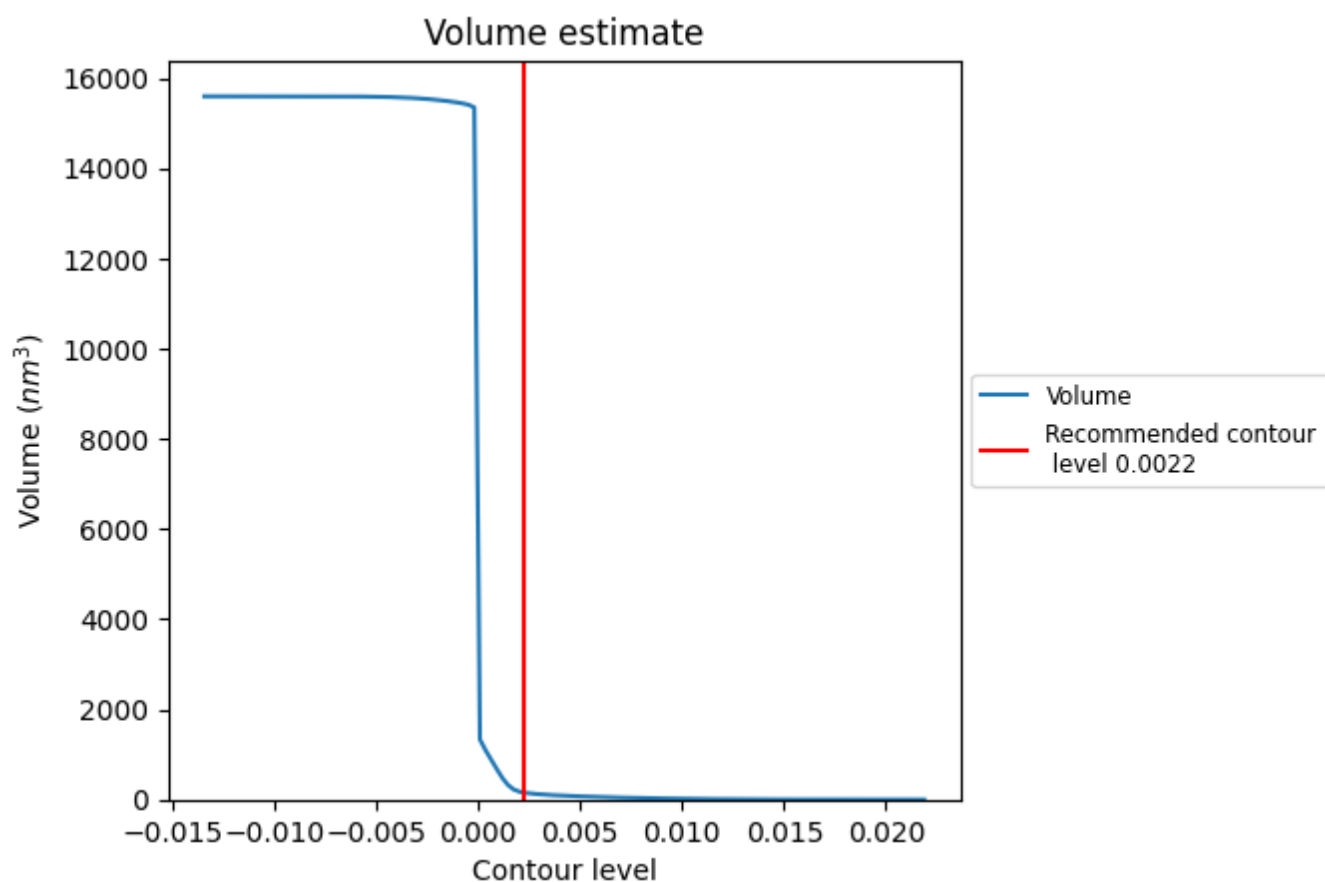
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

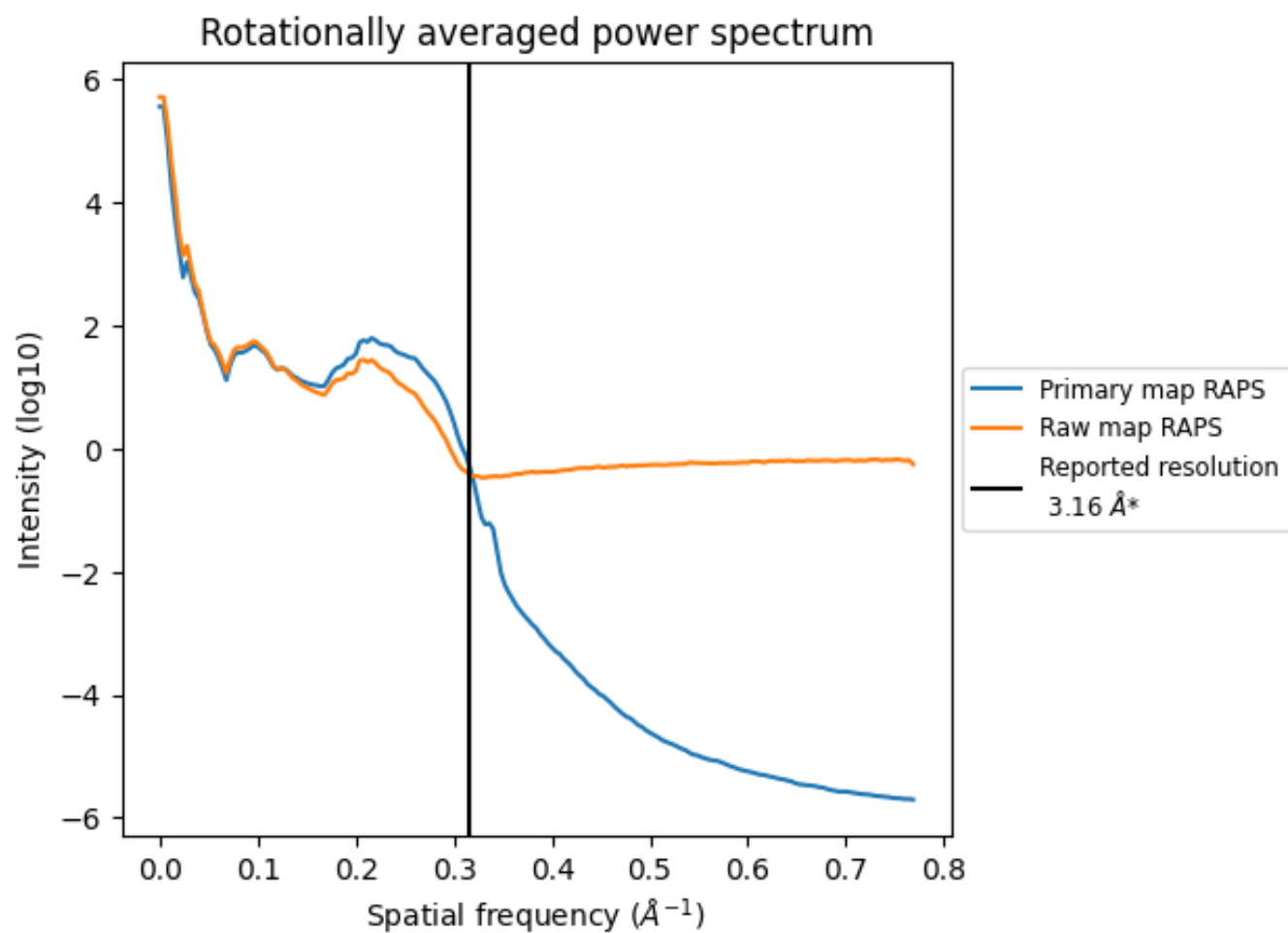
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

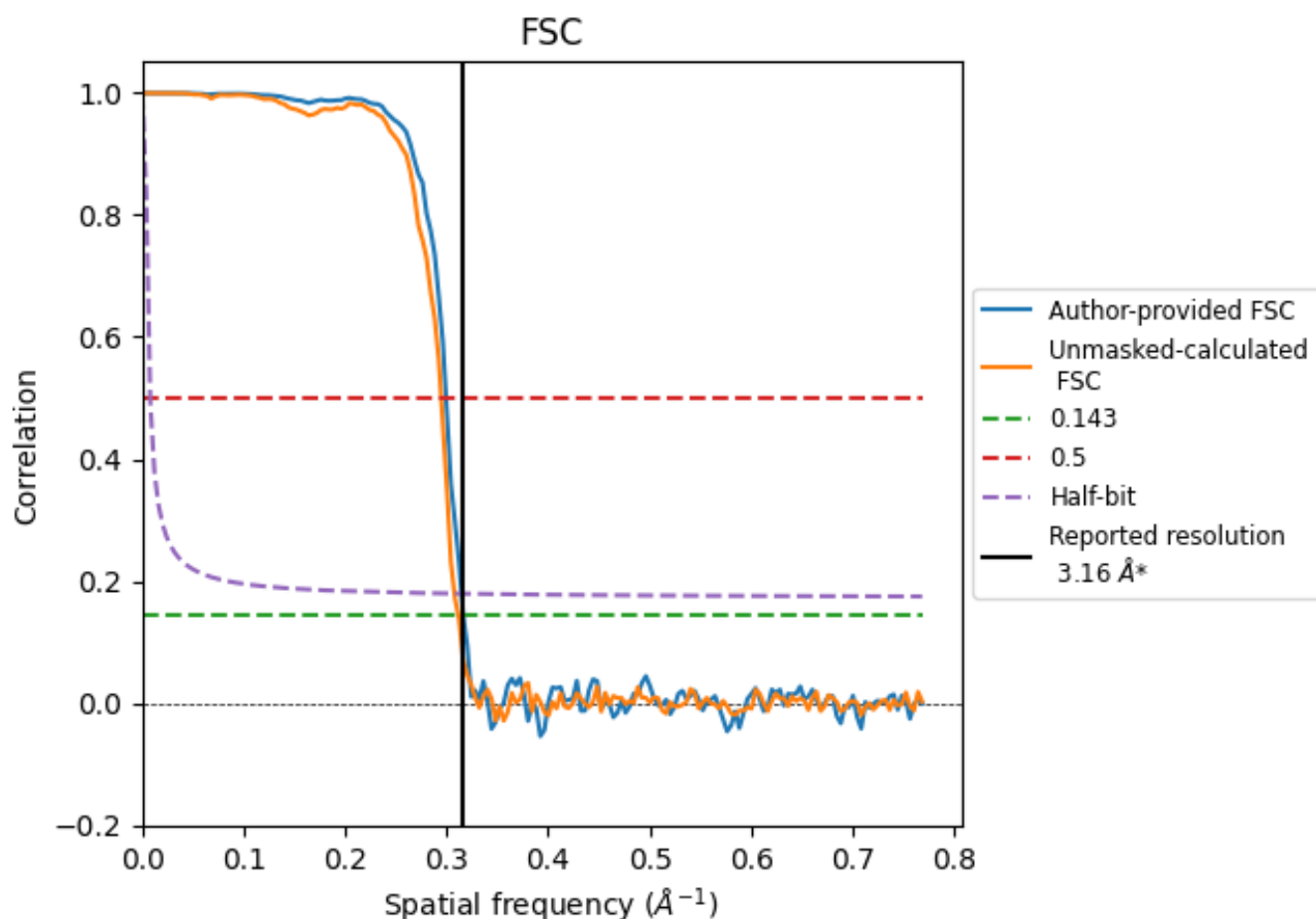


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.316 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

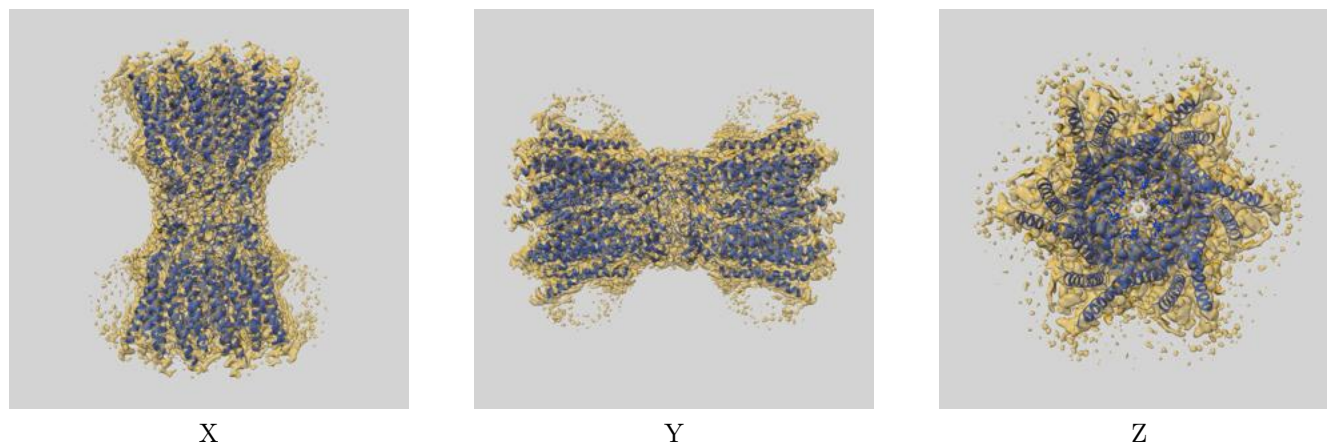
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.34	3.18
Unmasked-calculated*	3.21	3.40	3.25

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

9 Map-model fit [i](#)

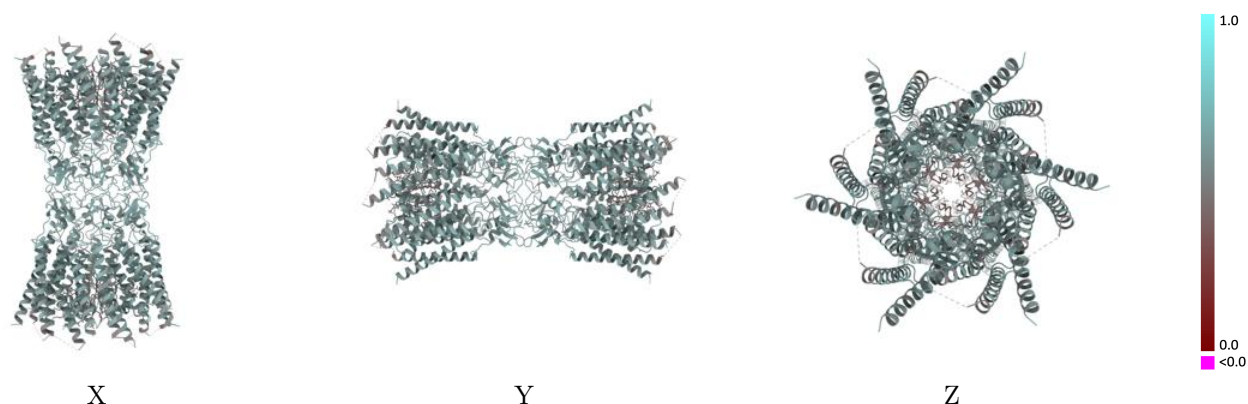
This section contains information regarding the fit between EMDB map EMD-53245 and PDB model 9QNF. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



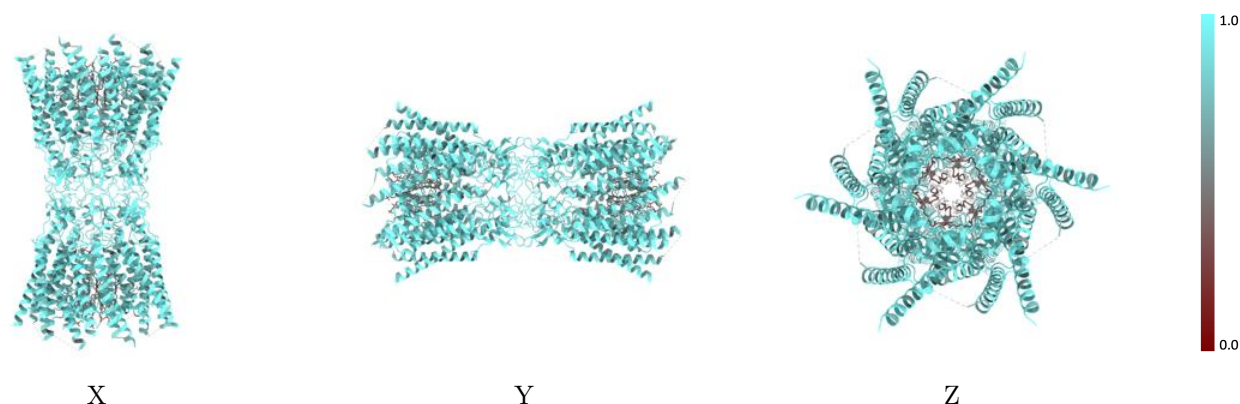
The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



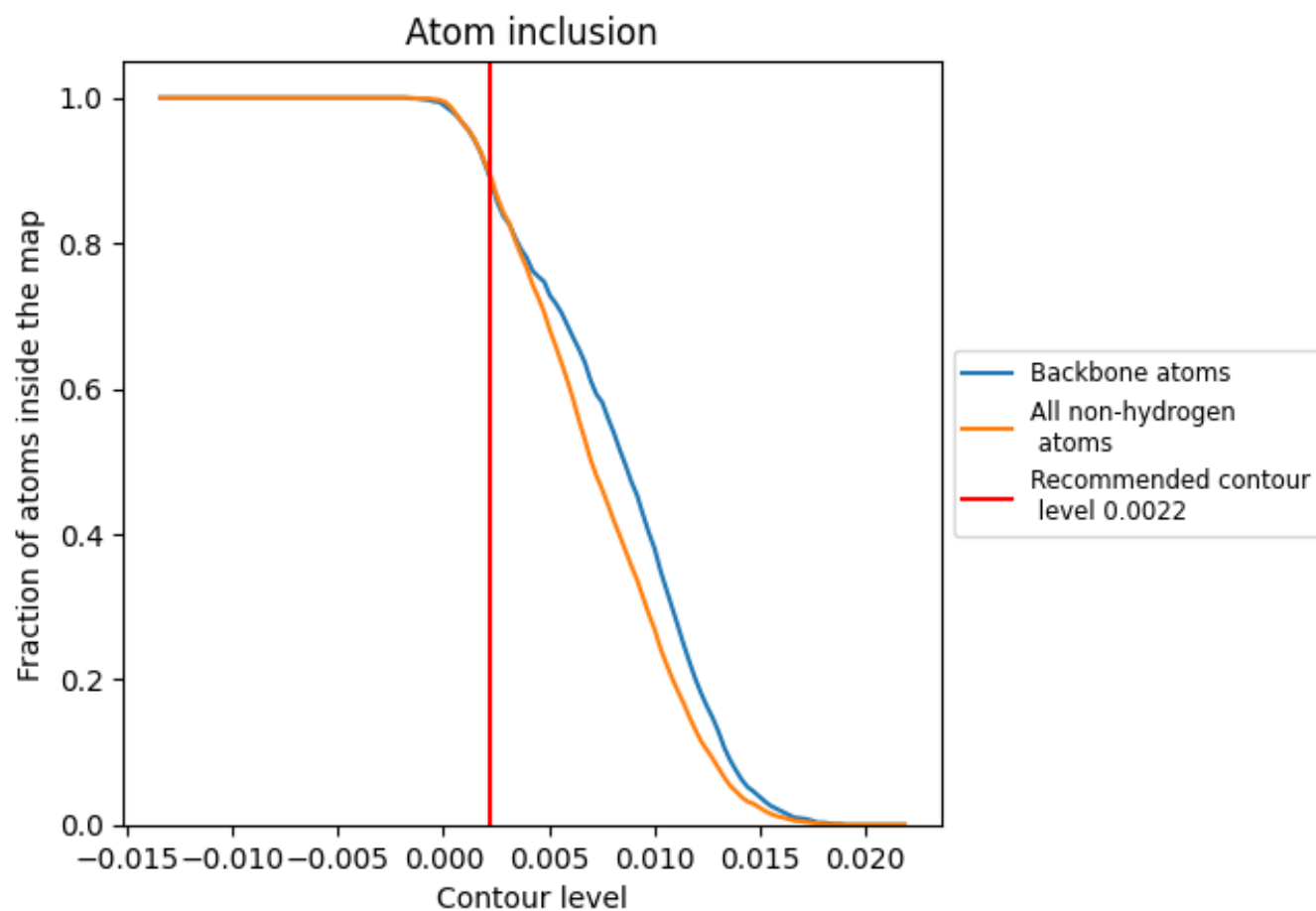
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5670
A	0.8780	0.5620
B	0.8940	0.5680
C	0.8970	0.5660
D	0.8940	0.5660
E	0.8950	0.5650
F	0.9120	0.5730
G	0.8930	0.5650
H	0.8790	0.5620
I	0.8970	0.5660
J	0.8960	0.5660
K	0.8940	0.5660
L	0.9140	0.5730

1.0

0.0

<0.0