



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:04 PM UTC

PDB ID : 9NEG / pdb\_00009neg  
EMDB ID : EMD-49308  
Title : AcA-EI-shaker Class C  
Authors : Tan, X.; Swartz, K.J.  
Deposited on : 2025-02-19  
Resolution : 3.17 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](mailto: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:

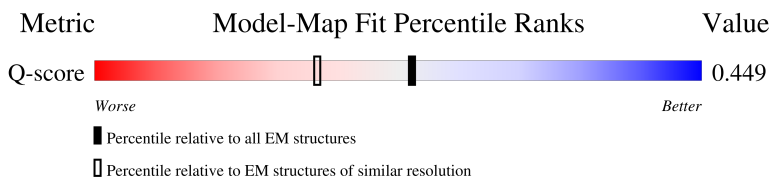
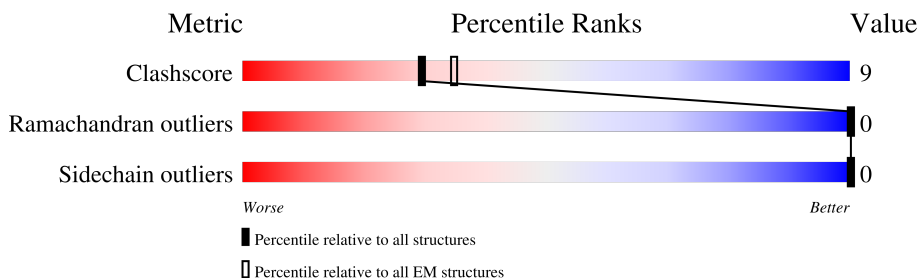
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.17 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.



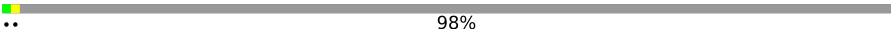
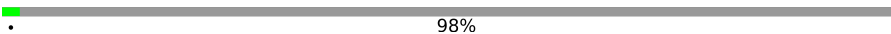
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 ( 2.67 - 3.67 )

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  $\geq 3$ , 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	668	
1	B	668	
1	C	668	
1	D	668	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	I	668	 98%
1	J	668	 98%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10596 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 Potassium voltage-gated channel protein Shaker.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	314	Total	C	N	O	S	0	0
			2530	1680	411	431	8		
1	B	314	Total	C	N	O	S	0	0
			2526	1678	410	430	8		
1	C	314	Total	C	N	O	S	0	0
			2524	1677	408	431	8		
1	D	313	Total	C	N	O	S	0	0
			2525	1677	410	430	8		
1	J	11	Total	C	N	O		0	0
			62	40	10	12			
1	I	12	Total	C	N	O		0	0
			74	49	12	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P08510
A	12	LYS	GLU	engineered mutation	UNP P08510
A	13	LYS	ASP	engineered mutation	UNP P08510
A	513	VAL	-	insertion	UNP P08510
A	657	GLY	-	expression tag	UNP P08510
A	658	SER	-	expression tag	UNP P08510
A	659	GLY	-	expression tag	UNP P08510
A	660	GLY	-	expression tag	UNP P08510
A	661	GLY	-	expression tag	UNP P08510
A	662	SER	-	expression tag	UNP P08510
A	663	GLU	-	expression tag	UNP P08510
A	664	ASN	-	expression tag	UNP P08510
A	665	LEU	-	expression tag	UNP P08510
A	666	TYR	-	expression tag	UNP P08510
A	667	PHE	-	expression tag	UNP P08510
A	668	GLN	-	expression tag	UNP P08510
B	1	ACE	-	acetylation	UNP P08510
B	12	LYS	GLU	engineered mutation	UNP P08510

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LYS	ASP	engineered mutation	UNP P08510
B	513	VAL	-	insertion	UNP P08510
B	657	GLY	-	expression tag	UNP P08510
B	658	SER	-	expression tag	UNP P08510
B	659	GLY	-	expression tag	UNP P08510
B	660	GLY	-	expression tag	UNP P08510
B	661	GLY	-	expression tag	UNP P08510
B	662	SER	-	expression tag	UNP P08510
B	663	GLU	-	expression tag	UNP P08510
B	664	ASN	-	expression tag	UNP P08510
B	665	LEU	-	expression tag	UNP P08510
B	666	TYR	-	expression tag	UNP P08510
B	667	PHE	-	expression tag	UNP P08510
B	668	GLN	-	expression tag	UNP P08510
C	1	ACE	-	acetylation	UNP P08510
C	12	LYS	GLU	engineered mutation	UNP P08510
C	13	LYS	ASP	engineered mutation	UNP P08510
C	513	VAL	-	insertion	UNP P08510
C	657	GLY	-	expression tag	UNP P08510
C	658	SER	-	expression tag	UNP P08510
C	659	GLY	-	expression tag	UNP P08510
C	660	GLY	-	expression tag	UNP P08510
C	661	GLY	-	expression tag	UNP P08510
C	662	SER	-	expression tag	UNP P08510
C	663	GLU	-	expression tag	UNP P08510
C	664	ASN	-	expression tag	UNP P08510
C	665	LEU	-	expression tag	UNP P08510
C	666	TYR	-	expression tag	UNP P08510
C	667	PHE	-	expression tag	UNP P08510
C	668	GLN	-	expression tag	UNP P08510
D	1	ACE	-	acetylation	UNP P08510
D	12	LYS	GLU	engineered mutation	UNP P08510
D	13	LYS	ASP	engineered mutation	UNP P08510
D	513	VAL	-	insertion	UNP P08510
D	657	GLY	-	expression tag	UNP P08510
D	658	SER	-	expression tag	UNP P08510
D	659	GLY	-	expression tag	UNP P08510
D	660	GLY	-	expression tag	UNP P08510
D	661	GLY	-	expression tag	UNP P08510
D	662	SER	-	expression tag	UNP P08510
D	663	GLU	-	expression tag	UNP P08510
D	664	ASN	-	expression tag	UNP P08510

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	665	LEU	-	expression tag	UNP P08510
D	666	TYR	-	expression tag	UNP P08510
D	667	PHE	-	expression tag	UNP P08510
D	668	GLN	-	expression tag	UNP P08510
J	1	ACE	-	acetylation	UNP P08510
J	12	LYS	GLU	engineered mutation	UNP P08510
J	13	LYS	ASP	engineered mutation	UNP P08510
J	513	VAL	-	insertion	UNP P08510
J	657	GLY	-	expression tag	UNP P08510
J	658	SER	-	expression tag	UNP P08510
J	659	GLY	-	expression tag	UNP P08510
J	660	GLY	-	expression tag	UNP P08510
J	661	GLY	-	expression tag	UNP P08510
J	662	SER	-	expression tag	UNP P08510
J	663	GLU	-	expression tag	UNP P08510
J	664	ASN	-	expression tag	UNP P08510
J	665	LEU	-	expression tag	UNP P08510
J	666	TYR	-	expression tag	UNP P08510
J	667	PHE	-	expression tag	UNP P08510
J	668	GLN	-	expression tag	UNP P08510
I	1	ACE	-	acetylation	UNP P08510
I	12	LYS	GLU	engineered mutation	UNP P08510
I	13	LYS	ASP	engineered mutation	UNP P08510
I	513	VAL	-	insertion	UNP P08510
I	657	GLY	-	expression tag	UNP P08510
I	658	SER	-	expression tag	UNP P08510
I	659	GLY	-	expression tag	UNP P08510
I	660	GLY	-	expression tag	UNP P08510
I	661	GLY	-	expression tag	UNP P08510
I	662	SER	-	expression tag	UNP P08510
I	663	GLU	-	expression tag	UNP P08510
I	664	ASN	-	expression tag	UNP P08510
I	665	LEU	-	expression tag	UNP P08510
I	666	TYR	-	expression tag	UNP P08510
I	667	PHE	-	expression tag	UNP P08510
I	668	GLN	-	expression tag	UNP P08510

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			21	17	4	
2	A	1	Total	C		0
			6	6		
2	A	1	Total	C		0
			8	8		
2	A	1	Total	C		0
			12	12		
2	A	1	Total	C	O	0
			13	11	2	
2	A	1	Total	C		0
			10	10		
2	A	1	Total	C		0
			7	7		
2	A	1	Total	C	O	0
			13	11	2	
2	A	1	Total	C	O	0
			11	9	2	
2	B	1	Total	C	O	0
			11	9	2	
2	B	1	Total	C		0
			10	10		
2	B	1	Total	C		0
			7	7		
2	B	1	Total	C	O	0
			21	17	4	
2	B	1	Total	C		0
			6	6		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 8 8	0
2	B	1	Total C 12 12	0
2	B	1	Total C O 11 9 2	0
2	C	1	Total C O 21 17 4	0
2	C	1	Total C 6 6	0
2	C	1	Total C 8 8	0
2	C	1	Total C 12 12	0
2	C	1	Total C O 13 11 2	0
2	C	1	Total C 10 10	0
2	C	1	Total C 7 7	0
2	D	1	Total C 10 10	0
2	D	1	Total C 7 7	0
2	D	1	Total C O 11 9 2	0
2	D	1	Total C O 21 17 4	0
2	D	1	Total C 6 6	0
2	D	1	Total C 8 8	0
2	D	1	Total C 12 12	0
2	D	1	Total C O 13 11 2	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total K 1 1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	K	0
			1	1	

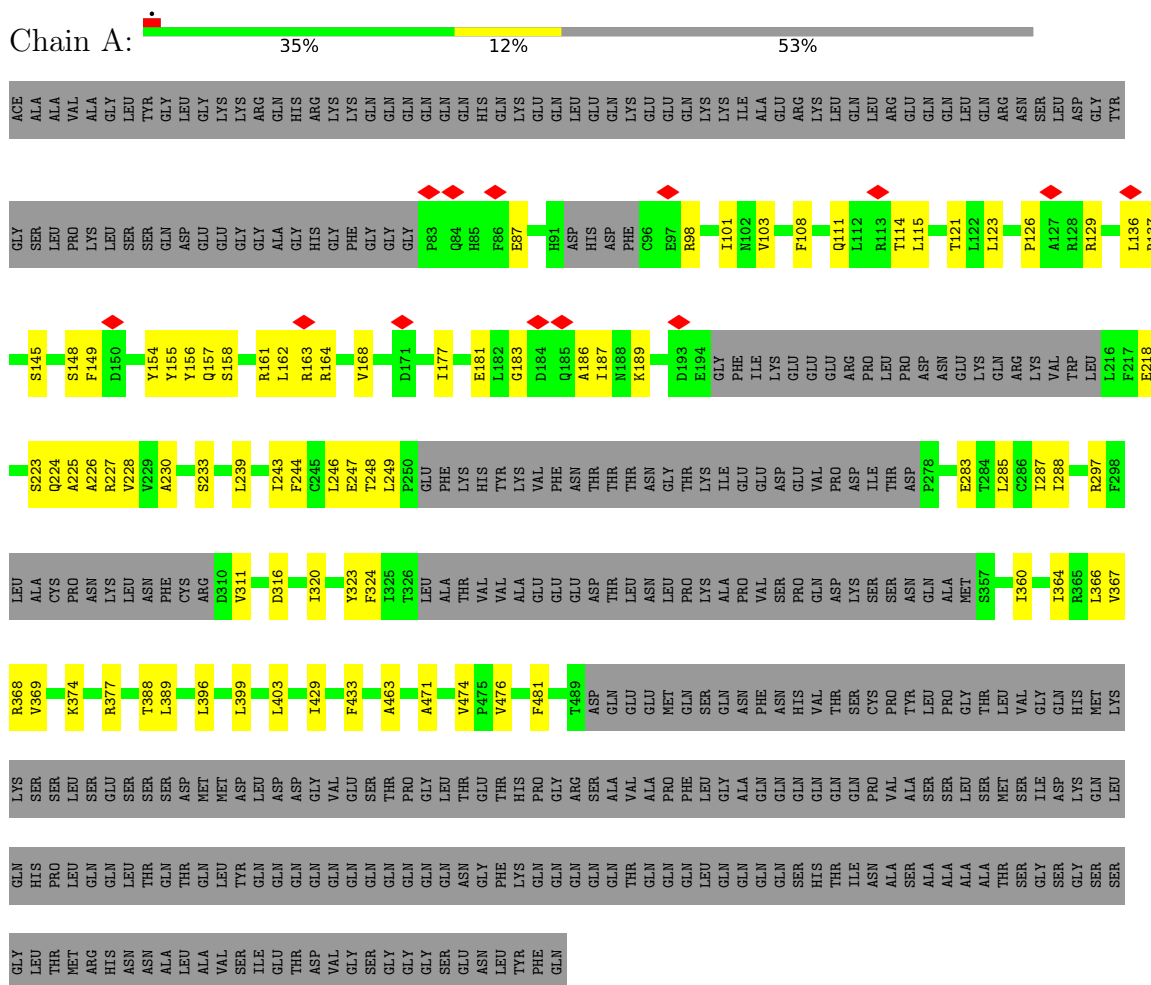
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	O	0
			1	1	

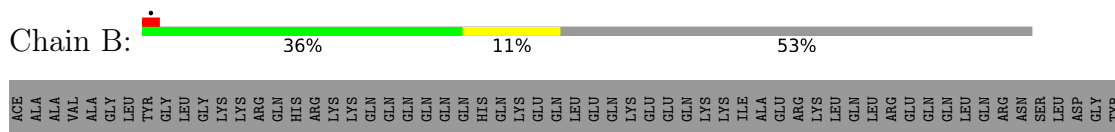
### 3 Residue-property plots

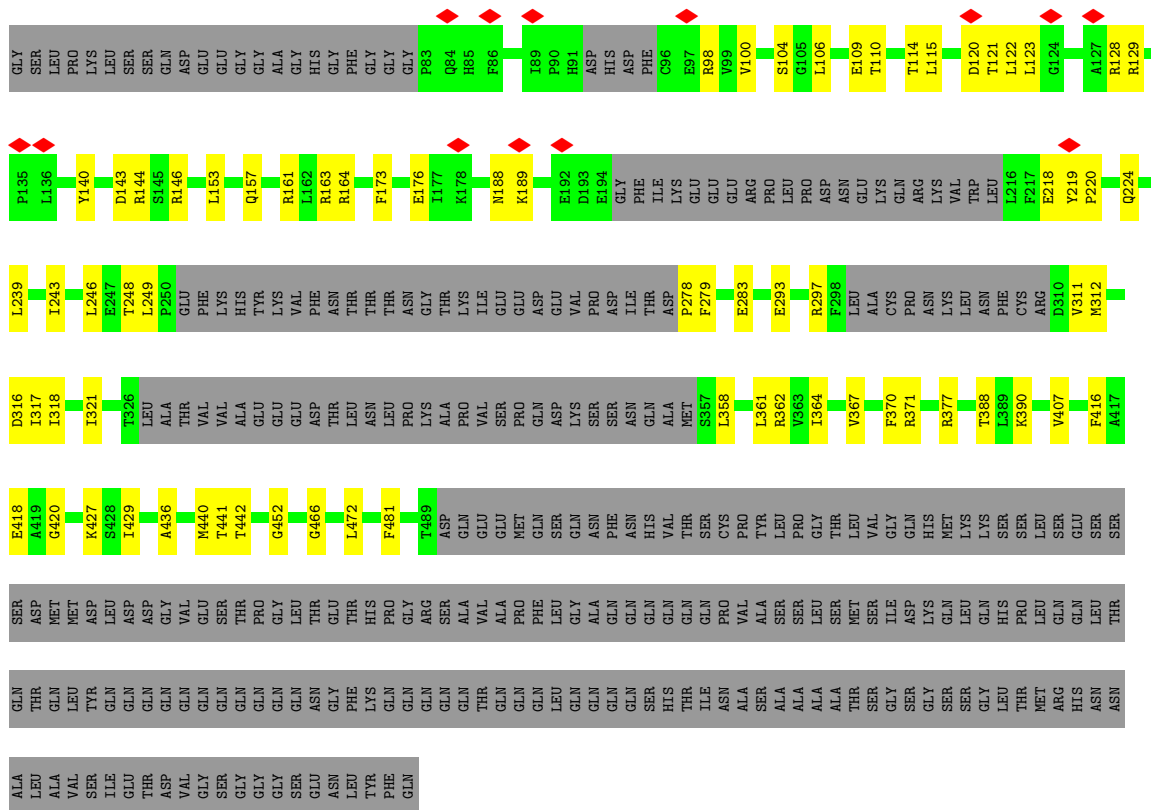
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium voltage-gated channel protein Shaker

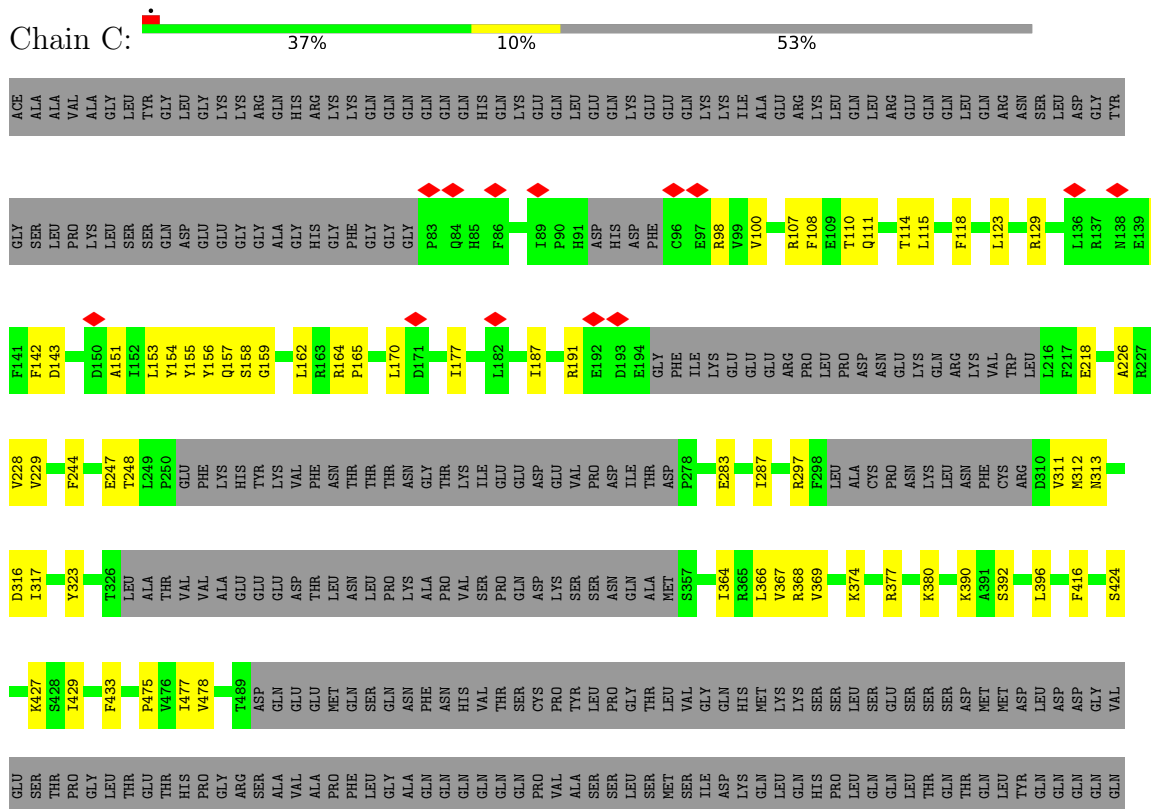


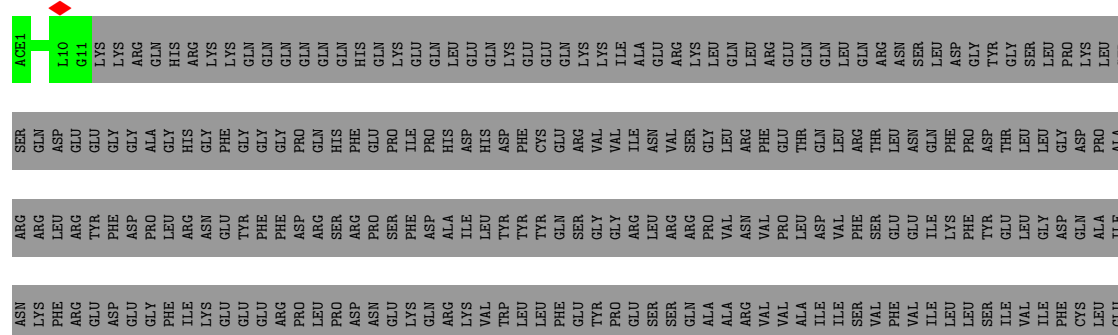
#### • Molecule 1: Potassium voltage-gated channel protein Shaker





- Molecule 1: Potassium voltage-gated channel protein Shaker





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

- Molecule 1: Potassium voltage-gated channel protein Shaker

Chain I:  ..

98%

[illegible]

ASN  
LEU  
TYR  
PHE  
GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.585	Depositor
Minimum map value	-0.293	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: K, POV, ACE

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	0.22	0/2595	0.36	0/3523
1	B	0.21	0/2591	0.35	0/3518
1	C	0.18	0/2589	0.33	0/3516
1	D	0.18	0/2590	0.35	0/3516
1	I	0.92	0/72	0.86	0/96
1	J	0.14	0/60	0.31	0/81
All	All	0.21	0/10497	0.35	0/14250

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	2530	0	2548	53	0
1	B	2526	0	2542	50	0
1	C	2524	0	2537	56	0
1	D	2525	0	2546	54	0
1	I	74	0	80	5	0
1	J	62	0	58	0	0
2	A	101	0	133	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	86	0	113	2	0
2	C	77	0	105	4	0
2	D	88	0	117	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
All	All	10596	0	10779	197	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 9.

All (197) 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:C:297:ARG:NE	1:C:377:ARG:HH12	1.45	1.14
1:C:297:ARG:CZ	1:C:377:ARG:HH12	1.65	1.08
1:C:297:ARG:CZ	1:C:377:ARG:NH1	2.34	0.90
1:C:297:ARG:NE	1:C:377:ARG:NH1	2.20	0.89
1:D:218:GLU:HB2	1:D:224:GLN:HE21	1.49	0.76
1:A:218:GLU:HB2	1:A:224:GLN:HE21	1.50	0.75
1:B:104:SER:O	1:B:146:ARG:NH2	2.22	0.73
1:A:164:ARG:NH2	1:A:168:VAL:O	2.22	0.72
1:B:316:ASP:OD2	1:B:377:ARG:NH2	2.25	0.70
1:A:98:ARG:HA	1:A:111:GLN:HA	1.75	0.68
1:C:297:ARG:NH2	1:C:377:ARG:NH2	2.44	0.66
1:B:110:THR:HG21	1:B:153:LEU:HD11	1.76	0.66
1:A:177:ILE:HD12	1:A:187:ILE:HD12	1.78	0.65
1:C:164:ARG:HH12	1:C:170:LEU:HB3	1.62	0.64
1:C:312:MET:HE3	1:C:377:ARG:HE	1.62	0.64
1:C:475:PRO:HA	1:C:478:VAL:HG12	1.78	0.64
1:C:477:ILE:HG22	1:D:472:LEU:HD21	1.78	0.64
1:D:177:ILE:HD12	1:D:187:ILE:HD12	1.80	0.64
1:C:311:VAL:HG21	2:C:701:POV:H32	1.80	0.64
1:C:100:VAL:HG21	1:C:107:ARG:HH21	1.63	0.64
1:B:100:VAL:HG12	1:B:109:GLU:HG2	1.79	0.63
1:C:297:ARG:CZ	1:C:377:ARG:HH22	2.10	0.63
1:C:154:TYR:HA	1:C:157:GLN:HB2	1.81	0.63
1:D:185:GLN:O	1:D:189:LYS:NZ	2.32	0.62
1:B:420:GLY:HA3	1:D:362:ARG:NH2	2.14	0.62
1:B:420:GLY:CA	1:D:362:ARG:NH2	2.62	0.62
1:A:248:THR:HG21	1:C:429:ILE:HD12	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:HA	1:B:367:VAL:HG12	1.83	0.60
1:D:418:GLU:OE2	1:D:452:GLY:N	2.25	0.60
1:C:248:THR:HG21	1:D:429:ILE:HB	1.84	0.59
1:A:283:GLU:OE2	1:A:368:ARG:NH1	2.36	0.59
1:A:123:LEU:O	1:A:129:ARG:NH1	2.35	0.59
1:C:297:ARG:NH2	1:C:377:ARG:CZ	2.65	0.59
1:D:123:LEU:O	1:D:129:ARG:NH1	2.36	0.58
1:A:157:GLN:NE2	1:B:143:ASP:OD1	2.35	0.58
1:C:364:ILE:HA	1:C:367:VAL:HG12	1.84	0.58
1:C:187:ILE:O	1:C:191:ARG:HG3	2.03	0.58
1:D:154:TYR:HA	1:D:157:GLN:HB2	1.86	0.57
1:C:129:ARG:NH1	1:C:140:TYR:OH	2.37	0.57
1:A:316:ASP:OD1	1:A:374:LYS:NZ	2.32	0.57
1:A:471:ALA:HA	1:I:4:VAL:HG12	1.87	0.57
1:B:407:VAL:HG23	1:B:436:ALA:HB3	1.85	0.57
1:B:429:ILE:HD12	1:D:248:THR:HG21	1.86	0.57
1:B:120:ASP:OD1	1:B:128:ARG:NH2	2.37	0.57
1:C:114:THR:HG22	1:C:156:TYR:HB3	1.87	0.57
1:C:297:ARG:CZ	1:C:377:ARG:NH2	2.68	0.56
1:A:246:LEU:HD13	1:A:249:LEU:HD12	1.86	0.56
1:D:283:GLU:OE2	1:D:368:ARG:NH1	2.37	0.56
1:A:463:ALA:HB1	1:B:441:THR:HG21	1.88	0.56
1:B:106:LEU:HB2	1:B:146:ARG:NH1	2.21	0.56
1:C:98:ARG:HA	1:C:111:GLN:HA	1.86	0.56
1:D:219:TYR:CE2	1:D:296:VAL:HG11	2.42	0.55
1:A:364:ILE:HA	1:A:367:VAL:HG12	1.89	0.54
1:B:164:ARG:HG3	1:B:173:PHE:CG	2.43	0.54
1:B:472:LEU:HD21	1:D:477:ILE:HG22	1.88	0.54
1:C:283:GLU:OE1	1:C:368:ARG:NH1	2.40	0.54
1:D:291:THR:O	1:D:295:THR:HG23	2.07	0.54
1:C:297:ARG:NH2	1:C:377:ARG:NH1	2.55	0.54
1:I:8:TYR:CD2	1:I:9:GLY:N	2.75	0.54
1:B:420:GLY:HA3	1:D:362:ARG:CZ	2.37	0.54
1:D:364:ILE:HA	1:D:367:VAL:HG12	1.90	0.53
1:B:390:LYS:HB2	2:B:705:POV:H33	1.89	0.53
1:C:110:THR:HG21	1:C:153:LEU:HD11	1.90	0.53
1:C:297:ARG:CZ	1:C:377:ARG:CZ	2.87	0.53
1:B:297:ARG:HH11	1:B:297:ARG:HB3	1.74	0.53
1:I:7:LEU:H	1:I:7:LEU:HD23	1.74	0.53
1:A:429:ILE:HD12	1:B:248:THR:HG21	1.91	0.52
1:C:297:ARG:NH1	1:C:377:ARG:HH22	2.06	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:OD1	1:D:157:GLN:NE2	2.41	0.52
1:D:114:THR:HG22	1:D:156:TYR:HB3	1.92	0.51
1:I:8:TYR:CG	1:I:9:GLY:N	2.78	0.51
1:D:136:LEU:HD12	1:D:137:ARG:HG3	1.93	0.51
1:A:161:ARG:HD2	1:A:163:ARG:HH11	1.76	0.50
1:B:297:ARG:HB3	1:B:297:ARG:NH1	2.27	0.50
1:A:287:ILE:HG21	1:A:323:TYR:CD2	2.47	0.50
1:B:293:GLU:O	1:B:297:ARG:HG3	2.11	0.50
1:A:433:PHE:HB3	2:A:705:POV:H26A	1.94	0.50
1:C:247:GLU:OE2	1:C:368:ARG:NH2	2.32	0.49
1:C:433:PHE:HB3	2:C:705:POV:H26A	1.94	0.49
1:B:98:ARG:HH21	1:D:137:ARG:HH21	1.59	0.49
1:D:239:LEU:O	1:D:243:ILE:HG12	2.13	0.49
1:C:478:VAL:HG21	1:D:475:PRO:HG2	1.93	0.49
1:D:178:LYS:HZ1	1:D:187:ILE:HG21	1.77	0.49
1:B:239:LEU:O	1:B:243:ILE:HG12	2.13	0.49
1:B:420:GLY:HA2	1:D:362:ARG:NH2	2.28	0.49
1:D:188:ASN:OD1	1:D:189:LYS:N	2.46	0.49
1:C:287:ILE:HG21	1:C:323:TYR:CD2	2.48	0.49
1:B:416:PHE:HE2	1:D:244:PHE:HZ	1.62	0.48
1:B:218:GLU:HB2	1:B:224:GLN:NE2	2.29	0.48
1:D:182:LEU:HB2	1:D:187:ILE:HD11	1.96	0.48
1:C:478:VAL:HG11	1:I:7:LEU:HD21	1.95	0.48
1:D:126:PRO:HA	1:D:129:ARG:HG2	1.96	0.48
1:B:311:VAL:HG11	2:B:705:POV:H3A	1.95	0.48
1:C:108:PHE:HD2	1:C:153:LEU:HD22	1.77	0.48
1:D:220:PRO:HB3	1:D:297:ARG:HH12	1.79	0.48
1:B:312:MET:HB3	1:B:377:ARG:NH2	2.28	0.48
1:D:365:ARG:HH11	1:D:365:ARG:HG3	1.78	0.48
1:B:317:ILE:O	1:B:321:ILE:HG12	2.13	0.47
1:C:313:ASN:O	1:C:317:ILE:HG12	2.14	0.47
1:D:164:ARG:HB3	1:D:173:PHE:CD2	2.48	0.47
1:A:186:ALA:HA	1:A:189:LYS:NZ	2.29	0.47
1:C:155:TYR:CD1	1:C:162:LEU:HB2	2.50	0.47
1:A:114:THR:HG22	1:A:156:TYR:HB3	1.96	0.47
1:B:188:ASN:OD1	1:B:189:LYS:N	2.48	0.47
1:A:154:TYR:HA	1:A:157:GLN:HB2	1.96	0.47
1:D:100:VAL:HG12	1:D:109:GLU:HG2	1.97	0.47
1:D:155:TYR:CD1	1:D:162:LEU:HB2	2.50	0.47
1:A:239:LEU:O	1:A:243:ILE:HG12	2.15	0.47
1:C:390:LYS:HB2	2:C:701:POV:H33	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HG21	2:A:701:POV:H3A	1.97	0.46
1:D:171:ASP:OD1	1:D:172:VAL:N	2.49	0.46
1:A:225:ALA:O	1:A:228:VAL:HG12	2.16	0.46
1:C:244:PHE:HZ	1:D:416:PHE:HE2	1.62	0.46
1:A:297:ARG:HH12	1:A:377:ARG:CZ	2.28	0.46
1:A:297:ARG:HH12	1:A:377:ARG:NE	2.13	0.46
1:B:361:LEU:HD13	1:B:364:ILE:HD11	1.98	0.46
1:D:169:PRO:HB2	1:D:171:ASP:OD1	2.16	0.46
1:A:115:LEU:HD23	1:A:123:LEU:HB3	1.96	0.46
1:C:123:LEU:HA	1:C:129:ARG:HD3	1.98	0.46
1:D:287:ILE:HG21	1:D:323:TYR:CD2	2.50	0.46
1:A:320:ILE:HD12	1:A:324:PHE:HE2	1.80	0.45
1:C:424:SER:O	1:C:427:LYS:NZ	2.38	0.45
1:A:225:ALA:C	1:A:227:ARG:H	2.23	0.45
1:C:154:TYR:CE1	1:C:158:SER:HB3	2.52	0.45
1:C:316:ASP:OD1	1:C:374:LYS:NZ	2.50	0.45
1:A:244:PHE:HZ	1:C:416:PHE:HE2	1.64	0.45
1:D:186:ALA:HA	1:D:189:LYS:HZ3	1.81	0.45
1:A:126:PRO:HA	1:A:129:ARG:HG2	1.98	0.45
1:A:145:SER:OG	1:A:148:SER:OG	2.30	0.45
1:B:388:THR:HG21	1:B:481:PHE:HB2	1.99	0.45
1:A:223:SER:O	1:A:226:ALA:N	2.41	0.45
1:B:246:LEU:O	1:B:249:LEU:HB2	2.17	0.45
1:B:120:ASP:CG	1:B:121:THR:H	2.25	0.45
1:A:158:SER:HB2	1:A:161:ARG:HB3	1.98	0.44
1:D:487:ARG:HG2	1:D:487:ARG:HH11	1.81	0.44
1:C:115:LEU:HA	1:C:156:TYR:HD2	1.82	0.44
1:B:161:ARG:HH22	1:B:163:ARG:HH21	1.65	0.44
1:D:146:ARG:N	1:D:147:PRO:HD2	2.32	0.44
1:D:246:LEU:O	1:D:249:LEU:HB2	2.18	0.44
1:D:384:ILE:HG23	1:D:484:PHE:HB3	2.00	0.44
1:A:155:TYR:CG	1:A:162:LEU:HD12	2.53	0.44
1:A:360:ILE:O	1:A:364:ILE:HG12	2.17	0.44
1:C:392:SER:O	1:C:396:LEU:HD13	2.18	0.44
1:A:136:LEU:HD12	1:A:137:ARG:HG3	1.99	0.44
1:B:114:THR:HG21	1:B:157:GLN:HE21	1.83	0.44
1:C:118:PHE:HE2	1:C:159:GLY:HA2	1.82	0.44
1:C:226:ALA:O	1:C:229:VAL:N	2.49	0.44
1:D:487:ARG:HG2	1:D:487:ARG:NH1	2.33	0.44
1:B:278:PRO:HB2	1:B:279:PHE:H	1.66	0.43
1:C:177:ILE:HD12	1:C:187:ILE:HD12	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG21	1:A:481:PHE:HB2	2.00	0.43
1:A:87:GLU:OE2	1:B:144:ARG:NH1	2.52	0.43
1:A:161:ARG:HG3	1:A:163:ARG:HG2	2.01	0.43
1:B:219:TYR:N	1:B:220:PRO:HD2	2.33	0.43
1:B:418:GLU:OE2	1:B:452:GLY:N	2.35	0.43
1:C:366:LEU:O	1:C:369:VAL:HG12	2.19	0.43
1:A:163:ARG:HA	1:A:163:ARG:HD2	1.80	0.43
1:B:441:THR:O	1:B:442:THR:OG1	2.36	0.43
1:B:122:LEU:O	1:B:129:ARG:HG3	2.18	0.42
1:A:101:ILE:HB	1:A:108:PHE:HB2	2.00	0.42
1:D:427:LYS:N	1:D:427:LYS:HD2	2.33	0.42
1:D:366:LEU:O	1:D:369:VAL:HG12	2.19	0.42
1:A:225:ALA:C	1:A:227:ARG:N	2.77	0.42
1:A:230:ALA:O	1:A:233:SER:N	2.52	0.42
1:B:318:ILE:HG21	1:B:370:PHE:HD2	1.85	0.42
1:B:440:MET:HE2	1:B:466:GLY:HA2	2.01	0.42
1:C:140:TYR:HB3	1:C:142:PHE:HE1	1.84	0.42
1:C:297:ARG:NH2	1:C:377:ARG:HH22	2.13	0.42
1:D:218:GLU:H	1:D:218:GLU:HG3	1.67	0.41
1:A:389:LEU:HD22	1:A:396:LEU:HD11	2.02	0.41
1:B:115:LEU:HD22	1:B:123:LEU:HB3	2.03	0.41
2:C:705:POV:H23	1:D:453:VAL:HG23	2.01	0.41
1:A:121:THR:HA	1:A:181:GLU:HG2	2.01	0.41
1:A:366:LEU:O	1:A:369:VAL:HG12	2.20	0.41
1:A:103:VAL:HG21	1:A:149:PHE:CG	2.56	0.41
1:A:474:VAL:C	1:A:476:VAL:H	2.29	0.41
1:D:278:PRO:HB2	1:D:279:PHE:H	1.76	0.41
1:D:365:ARG:HG3	1:D:365:ARG:NH1	2.36	0.41
1:B:283:GLU:OE2	1:B:371:ARG:NH2	2.53	0.41
1:B:129:ARG:HB3	1:B:140:TYR:HE2	1.86	0.41
1:C:218:GLU:H	1:C:218:GLU:HG3	1.68	0.41
1:A:244:PHE:O	1:A:247:GLU:HG2	2.21	0.41
1:B:427:LYS:HD3	1:B:427:LYS:HA	1.75	0.41
1:D:88:PRO:HG3	1:D:117:GLN:NE2	2.36	0.40
1:D:440:MET:HE2	1:D:466:GLY:HA2	2.02	0.40
1:B:144:ARG:HE	1:B:176:GLU:CD	2.30	0.40
1:C:380:LYS:HE2	1:C:380:LYS:HB2	1.88	0.40
1:A:183:GLY:O	1:A:187:ILE:HG12	2.21	0.40
1:B:358:LEU:O	1:B:362:ARG:HG3	2.20	0.40
1:C:151:ALA:HB2	1:C:165:PRO:HD3	2.04	0.40
1:D:218:GLU:CB	1:D:224:GLN:HE21	2.27	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HA	1:A:288:ILE:HG22	2.04	0.40
1:A:320:ILE:HD12	1:A:324:PHE:CE2	2.57	0.40
1:A:399:LEU:O	1:A:403:LEU:HD23	2.21	0.40
1:C:155:TYR:CE1	1:C:162:LEU:HB2	2.56	0.40
1:C:226:ALA:C	1:C:228:VAL:N	2.80	0.40
1:D:399:LEU:HD13	1:D:473:PRO:HG2	2.03	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	302/668 (45%)	288 (95%)	14 (5%)	0	100	100
1	B	302/668 (45%)	290 (96%)	12 (4%)	0	100	100
1	C	302/668 (45%)	286 (95%)	16 (5%)	0	100	100
1	D	301/668 (45%)	290 (96%)	11 (4%)	0	100	100
1	I	10/668 (2%)	4 (40%)	6 (60%)	0	100	100
1	J	9/668 (1%)	7 (78%)	2 (22%)	0	100	100
All	All	1226/4008 (31%)	1165 (95%)	61 (5%)	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	274/585 (47%)	274 (100%)	0	100	100
1	B	273/585 (47%)	273 (100%)	0	100	100
1	C	273/585 (47%)	273 (100%)	0	100	100
1	D	274/585 (47%)	274 (100%)	0	100	100
1	I	5/585 (1%)	5 (100%)	0	100	100
1	J	3/585 (0%)	3 (100%)	0	100	100
All	All	1102/3510 (31%)	1102 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
1	B	157	GLN
1	B	313	ASN
1	B	480	ASN
1	C	480	ASN
1	D	117	GLN
1	D	313	ASN
1	D	480	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.



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	$\# Z  > 2$
2	POV	A	704	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	A	706	-	9,9,51	0.78	0	8,8,59	0.81	0
2	POV	C	701	-	20,20,51	1.51	3 (15%)	22,22,59	1.38	2 (9%)
2	POV	D	703	-	10,10,51	1.51	1 (10%)	10,10,59	1.10	1 (10%)
2	POV	A	705	-	12,12,51	1.44	2 (16%)	12,12,59	1.20	0
2	POV	A	707	-	6,6,51	0.73	0	5,5,59	0.72	0
2	POV	C	703	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	A	702	-	5,5,51	0.65	0	4,4,59	0.62	0
2	POV	D	704	-	20,20,51	1.51	3 (15%)	22,22,59	1.39	2 (9%)
2	POV	B	703	-	9,9,51	0.78	0	8,8,59	0.82	0
2	POV	D	706	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	C	706	-	9,9,51	0.78	0	8,8,59	0.81	0
2	POV	D	707	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	A	710	-	10,10,51	1.50	1 (10%)	10,10,59	1.10	1 (10%)
2	POV	C	707	-	6,6,51	0.73	0	5,5,59	0.71	0
2	POV	D	702	-	6,6,51	0.73	0	5,5,59	0.73	0
2	POV	D	708	-	12,12,51	1.44	2 (16%)	12,12,59	1.20	0
2	POV	C	705	-	12,12,51	1.43	2 (16%)	12,12,59	1.20	0
2	POV	B	701	-	10,10,51	1.50	1 (10%)	10,10,59	1.08	1 (10%)
2	POV	D	701	-	9,9,51	0.78	0	8,8,59	0.81	0
2	POV	D	705	-	5,5,51	0.66	0	4,4,59	0.62	0
2	POV	B	705	-	20,20,51	1.50	3 (15%)	22,22,59	1.40	2 (9%)
2	POV	A	709	-	12,12,51	1.44	2 (16%)	12,12,59	1.20	0
2	POV	B	708	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	B	706	-	5,5,51	0.65	0	4,4,59	0.62	0
2	POV	C	704	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	B	704	-	6,6,51	0.73	0	5,5,59	0.69	0
2	POV	A	703	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	C	702	-	5,5,51	0.66	0	4,4,59	0.62	0
2	POV	B	709	-	10,10,51	1.50	1 (10%)	10,10,59	1.09	0
2	POV	A	701	-	20,20,51	1.52	3 (15%)	22,22,59	1.39	2 (9%)
2	POV	B	707	-	7,7,51	0.81	0	6,6,59	0.75	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
2	POV	A	704	-	-	4/9/9/55	-
2	POV	A	706	-	-	2/7/7/55	-
2	POV	C	701	-	-	14/21/21/55	-
2	POV	D	703	-	-	8/9/9/55	-
2	POV	A	705	-	-	7/10/10/55	-
2	POV	A	707	-	-	2/4/4/55	-
2	POV	C	703	-	-	2/5/5/55	-
2	POV	A	702	-	-	3/3/3/55	-
2	POV	D	704	-	-	12/21/21/55	-
2	POV	B	703	-	-	2/7/7/55	-
2	POV	D	706	-	-	2/5/5/55	-
2	POV	C	706	-	-	2/7/7/55	-
2	POV	D	707	-	-	4/9/9/55	-
2	POV	A	710	-	-	8/9/9/55	-
2	POV	C	707	-	-	3/4/4/55	-
2	POV	D	702	-	-	3/4/4/55	-
2	POV	D	708	-	-	5/10/10/55	-
2	POV	C	705	-	-	5/10/10/55	-
2	POV	B	701	-	-	5/9/9/55	-
2	POV	D	701	-	-	3/7/7/55	-
2	POV	D	705	-	-	3/3/3/55	-
2	POV	B	705	-	-	12/21/21/55	-
2	POV	A	709	-	-	7/10/10/55	-
2	POV	B	708	-	-	5/9/9/55	-
2	POV	B	706	-	-	3/3/3/55	-
2	POV	C	704	-	-	4/9/9/55	-
2	POV	B	704	-	-	3/4/4/55	-
2	POV	A	703	-	-	2/5/5/55	-
2	POV	C	702	-	-	3/3/3/55	-
2	POV	B	709	-	-	5/9/9/55	-
2	POV	A	701	-	-	14/21/21/55	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	707	-	-	2/5/5/55	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	POV	O31-C31	3.89	1.44	1.33
2	C	701	POV	O31-C31	3.88	1.44	1.33
2	D	704	POV	O31-C31	3.85	1.44	1.33
2	B	705	POV	O31-C31	3.84	1.44	1.33
2	D	703	POV	O31-C31	3.73	1.44	1.33
2	A	710	POV	O31-C31	3.71	1.44	1.33
2	B	709	POV	O31-C31	3.70	1.44	1.33
2	B	701	POV	O31-C31	3.70	1.44	1.33
2	D	708	POV	O21-C21	3.38	1.42	1.30
2	A	709	POV	O21-C21	3.38	1.42	1.30
2	A	705	POV	O21-C21	3.36	1.41	1.30
2	C	705	POV	O21-C21	3.34	1.41	1.30
2	D	704	POV	O21-C21	2.85	1.42	1.34
2	C	701	POV	O21-C21	2.85	1.42	1.34
2	A	701	POV	O21-C21	2.84	1.42	1.34
2	B	705	POV	O21-C21	2.80	1.42	1.34
2	A	705	POV	C22-C21	2.61	1.56	1.50
2	C	705	POV	C22-C21	2.60	1.56	1.50
2	D	708	POV	C22-C21	2.60	1.56	1.50
2	A	709	POV	C22-C21	2.58	1.56	1.50
2	A	701	POV	O21-C2	-2.30	1.43	1.47
2	B	705	POV	O21-C2	-2.28	1.43	1.47
2	D	704	POV	O21-C2	-2.27	1.43	1.47
2	C	701	POV	O21-C2	-2.27	1.43	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	705	POV	O21-C21-C22	3.83	119.78	111.48
2	A	701	POV	O21-C21-C22	3.79	119.69	111.48
2	D	704	POV	O21-C21-C22	3.77	119.63	111.48
2	C	701	POV	O21-C21-C22	3.74	119.57	111.48
2	D	704	POV	O31-C31-C32	2.78	120.32	111.83
2	A	701	POV	O31-C31-C32	2.73	120.14	111.83
2	C	701	POV	O31-C31-C32	2.72	120.14	111.83
2	B	705	POV	O31-C31-C32	2.70	120.06	111.83
2	D	703	POV	O31-C31-C32	2.11	120.10	112.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	710	POV	O31-C31-C32	2.10	120.07	112.14
2	B	701	POV	O31-C31-C32	2.02	119.76	112.14

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	POV	C1-C2-O21-C21
2	B	705	POV	C1-C2-O21-C21
2	C	701	POV	C1-C2-O21-C21
2	D	704	POV	C1-C2-O21-C21
2	A	701	POV	O32-C31-O31-C3
2	B	705	POV	O32-C31-O31-C3
2	C	701	POV	O32-C31-O31-C3
2	D	704	POV	O32-C31-O31-C3
2	A	701	POV	C32-C31-O31-C3
2	B	705	POV	C32-C31-O31-C3
2	C	701	POV	C32-C31-O31-C3
2	D	704	POV	C32-C31-O31-C3
2	B	709	POV	C32-C31-O31-C3
2	B	709	POV	O32-C31-O31-C3
2	B	705	POV	C22-C21-O21-C2
2	A	710	POV	C32-C31-O31-C3
2	B	701	POV	C32-C31-O31-C3
2	D	703	POV	C32-C31-O31-C3
2	B	705	POV	O22-C21-O21-C2
2	A	701	POV	C22-C21-O21-C2
2	C	701	POV	C21-C22-C23-C24
2	A	701	POV	C31-C32-C33-C34
2	B	701	POV	O32-C31-O31-C3
2	A	701	POV	C21-C22-C23-C24
2	B	705	POV	C21-C22-C23-C24
2	D	704	POV	C21-C22-C23-C24
2	A	701	POV	O22-C21-O21-C2
2	A	710	POV	O32-C31-O31-C3
2	D	703	POV	O32-C31-O31-C3
2	D	704	POV	C22-C21-O21-C2
2	C	701	POV	O22-C21-O21-C2
2	D	704	POV	O22-C21-O21-C2
2	C	701	POV	C22-C21-O21-C2
2	B	705	POV	C31-C32-C33-C34
2	D	707	POV	C35-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	704	POV	C32-C33-C34-C35
2	B	701	POV	C33-C34-C35-C36
2	C	707	POV	C33-C34-C35-C36
2	A	709	POV	C23-C24-C25-C26
2	D	702	POV	C33-C34-C35-C36
2	A	705	POV	C23-C24-C25-C26
2	B	704	POV	C32-C33-C34-C35
2	C	704	POV	C32-C33-C34-C35
2	D	707	POV	C32-C33-C34-C35
2	C	705	POV	C23-C24-C25-C26
2	A	704	POV	C35-C36-C37-C38
2	A	707	POV	C33-C34-C35-C36
2	C	704	POV	C35-C36-C37-C38
2	D	706	POV	C33-C34-C35-C36
2	A	710	POV	C33-C34-C35-C36
2	B	708	POV	C33-C34-C35-C36
2	B	708	POV	C35-C36-C37-C38
2	A	703	POV	C33-C34-C35-C36
2	B	704	POV	C33-C34-C35-C36
2	D	703	POV	C33-C34-C35-C36
2	B	708	POV	C32-C33-C34-C35
2	C	704	POV	C33-C34-C35-C36
2	B	707	POV	C33-C34-C35-C36
2	B	709	POV	C33-C34-C35-C36
2	A	706	POV	C35-C36-C37-C38
2	B	701	POV	C32-C33-C34-C35
2	C	706	POV	C35-C36-C37-C38
2	D	701	POV	C35-C36-C37-C38
2	A	704	POV	C33-C34-C35-C36
2	D	708	POV	C23-C24-C25-C26
2	C	703	POV	C33-C34-C35-C36
2	D	707	POV	C33-C34-C35-C36
2	C	701	POV	C26-C27-C28-C29
2	C	705	POV	C21-C22-C23-C24
2	A	701	POV	C26-C27-C28-C29
2	B	705	POV	C26-C27-C28-C29
2	D	704	POV	C26-C27-C28-C29
2	B	703	POV	C35-C36-C37-C38
2	D	708	POV	C26-C27-C28-C29
2	D	704	POV	C31-C32-C33-C34
2	B	705	POV	C24-C25-C26-C27
2	D	703	POV	C31-C32-C33-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	705	POV	C26-C27-C28-C29
2	A	709	POV	C21-C22-C23-C24
2	A	709	POV	C24-C25-C26-C27
2	A	705	POV	C26-C27-C28-C29
2	C	705	POV	C24-C25-C26-C27
2	C	706	POV	C33-C34-C35-C36
2	A	705	POV	C24-C25-C26-C27
2	B	703	POV	C33-C34-C35-C36
2	D	701	POV	C33-C34-C35-C36
2	A	706	POV	C33-C34-C35-C36
2	D	704	POV	C24-C25-C26-C27
2	D	708	POV	C24-C25-C26-C27
2	A	710	POV	C32-C33-C34-C35
2	A	709	POV	C26-C27-C28-C29
2	D	703	POV	C32-C33-C34-C35
2	B	706	POV	C33-C34-C35-C36
2	C	707	POV	C32-C33-C34-C35
2	C	702	POV	C33-C34-C35-C36
2	D	705	POV	C33-C34-C35-C36
2	C	703	POV	C35-C36-C37-C38
2	A	710	POV	C31-C32-C33-C34
2	A	703	POV	C35-C36-C37-C38
2	A	702	POV	C32-C33-C34-C35
2	A	702	POV	C33-C34-C35-C36
2	D	705	POV	C32-C33-C34-C35
2	C	702	POV	C32-C33-C34-C35
2	A	701	POV	C32-C33-C34-C35
2	C	701	POV	C25-C26-C27-C28
2	C	701	POV	C31-C32-C33-C34
2	A	701	POV	C24-C25-C26-C27
2	B	707	POV	C35-C36-C37-C38
2	C	701	POV	C24-C25-C26-C27
2	B	706	POV	C32-C33-C34-C35
2	D	706	POV	C35-C36-C37-C38
2	A	701	POV	C25-C26-C27-C28
2	C	701	POV	C32-C33-C34-C35
2	B	705	POV	C32-C33-C34-C35
2	D	702	POV	C31-C32-C33-C34
2	A	701	POV	C3-C2-O21-C21
2	B	705	POV	C3-C2-O21-C21
2	C	701	POV	C3-C2-O21-C21
2	D	704	POV	C3-C2-O21-C21

*Continued on next page...*

*Continued from previous page...*

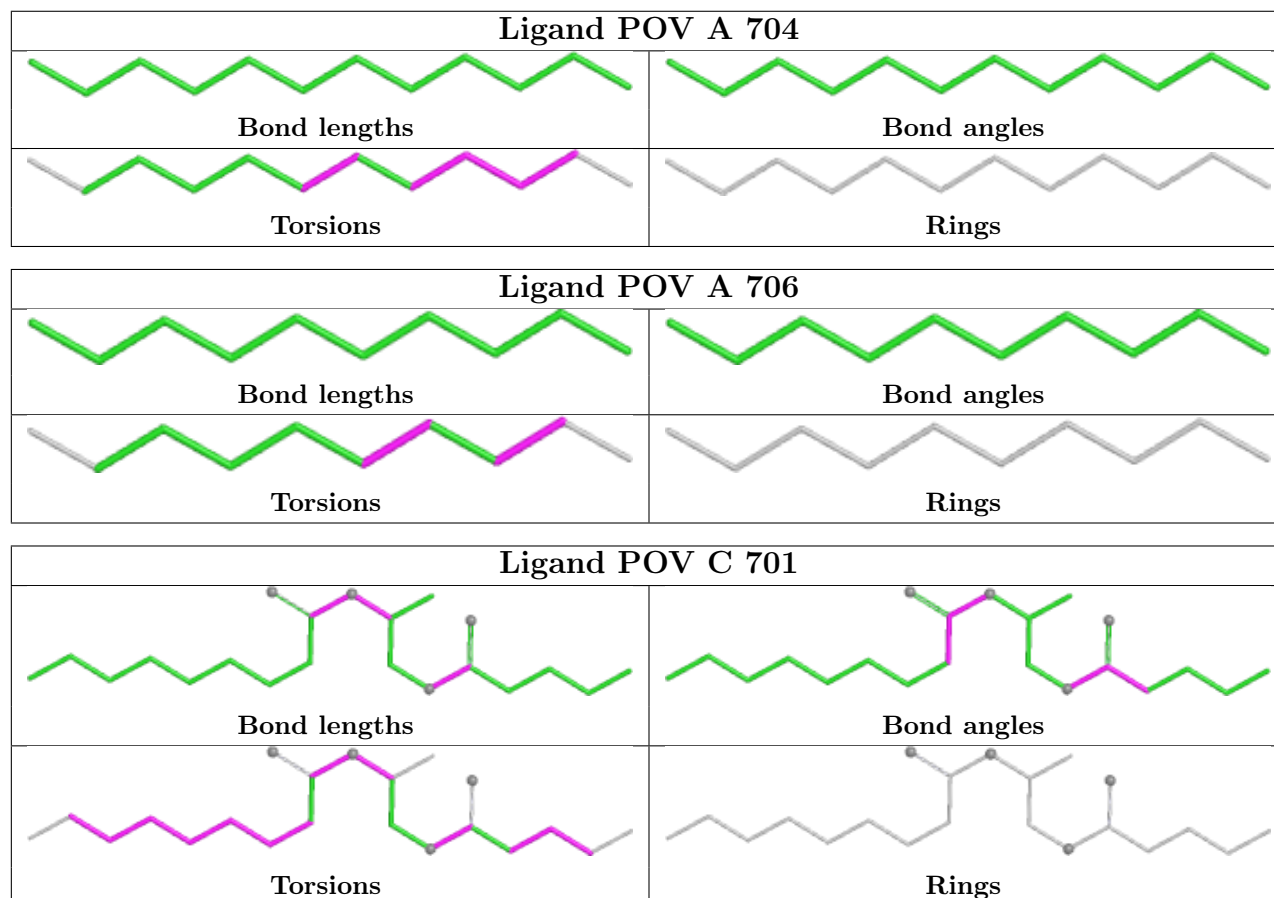
Mol	Chain	Res	Type	Atoms
2	D	701	POV	C37-C38-C39-C310
2	B	705	POV	C25-C26-C27-C28
2	A	701	POV	C23-C24-C25-C26
2	D	704	POV	C25-C26-C27-C28
2	B	701	POV	C35-C36-C37-C38
2	B	709	POV	C35-C36-C37-C38
2	B	709	POV	O31-C31-C32-C33
2	B	706	POV	C31-C32-C33-C34
2	A	707	POV	C31-C32-C33-C34
2	C	707	POV	C31-C32-C33-C34
2	D	705	POV	C31-C32-C33-C34
2	C	701	POV	C23-C24-C25-C26
2	C	702	POV	C31-C32-C33-C34
2	B	704	POV	C31-C32-C33-C34
2	D	704	POV	C32-C33-C34-C35
2	A	704	POV	C31-C32-C33-C34
2	A	710	POV	C35-C36-C37-C38
2	B	708	POV	C31-C32-C33-C34
2	B	708	POV	C34-C35-C36-C37
2	A	702	POV	C31-C32-C33-C34
2	A	705	POV	C27-C28-C29-C210
2	C	705	POV	C27-C28-C29-C210
2	A	709	POV	C27-C28-C29-C210
2	A	705	POV	C22-C23-C24-C25
2	C	701	POV	C22-C23-C24-C25
2	D	703	POV	C35-C36-C37-C38
2	C	704	POV	C31-C32-C33-C34
2	A	701	POV	C22-C23-C24-C25
2	D	702	POV	C32-C33-C34-C35
2	D	707	POV	C31-C32-C33-C34
2	D	703	POV	O31-C31-C32-C33
2	A	710	POV	O31-C31-C32-C33
2	D	708	POV	C21-C22-C23-C24
2	A	709	POV	O21-C21-C22-C23
2	D	703	POV	O32-C31-C32-C33
2	A	705	POV	O21-C21-C22-C23
2	A	710	POV	O32-C31-C32-C33
2	A	705	POV	O22-C21-C22-C23
2	A	709	POV	O22-C21-C22-C23
2	D	708	POV	O21-C21-C22-C23

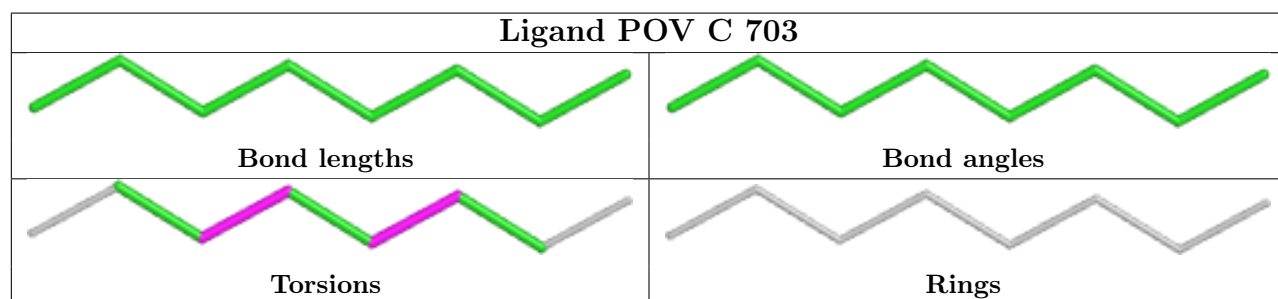
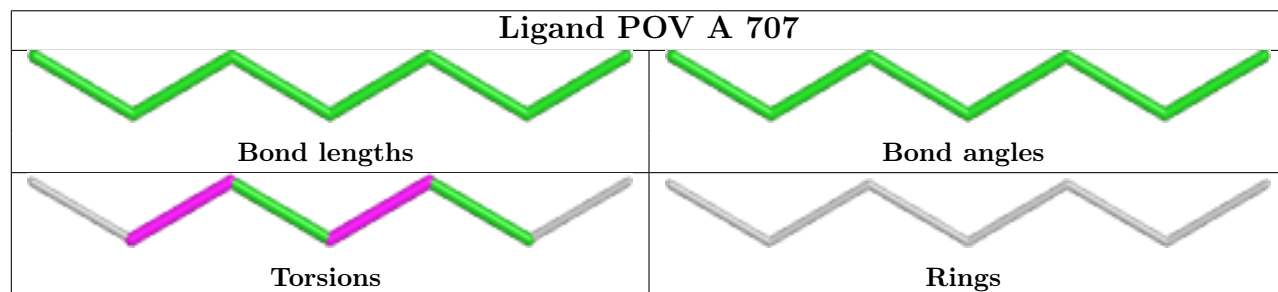
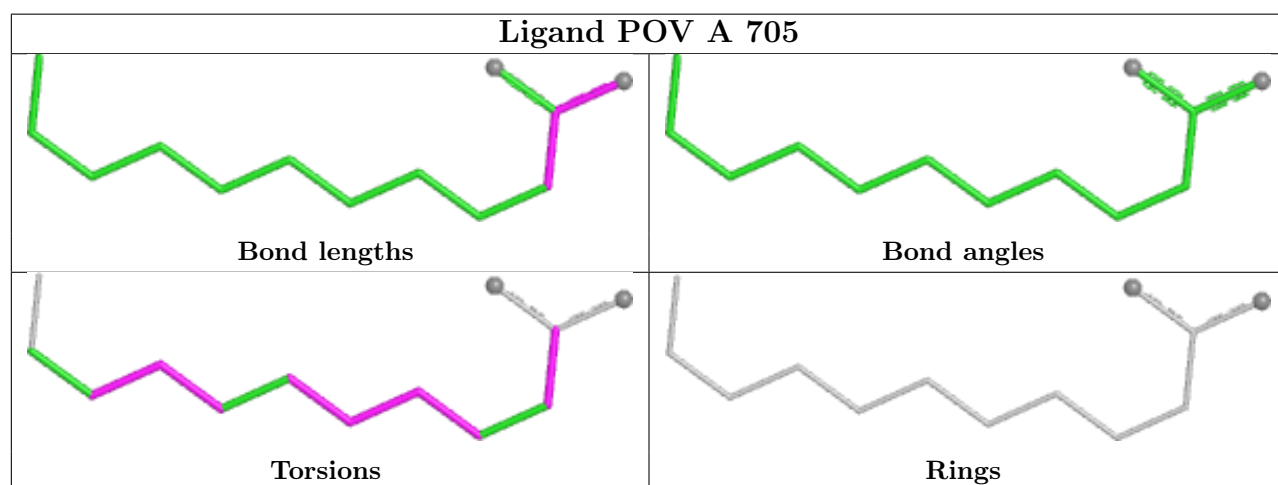
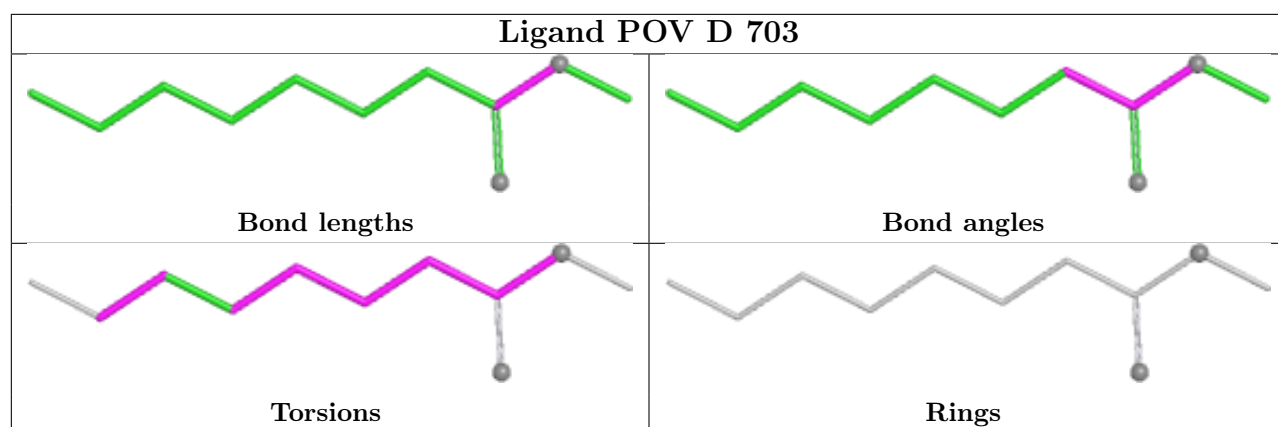
There are no ring outliers.

5 monomers are involved in 8 short contacts:

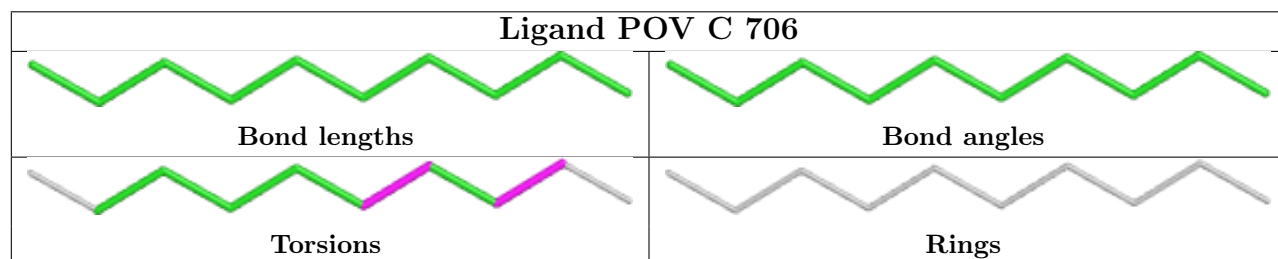
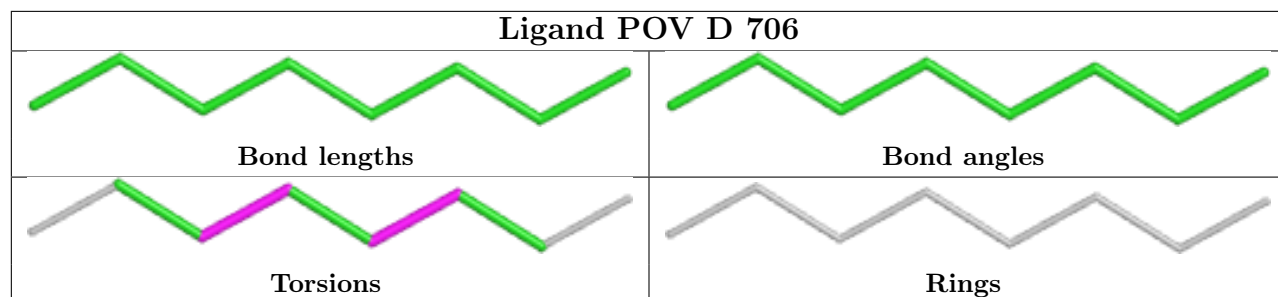
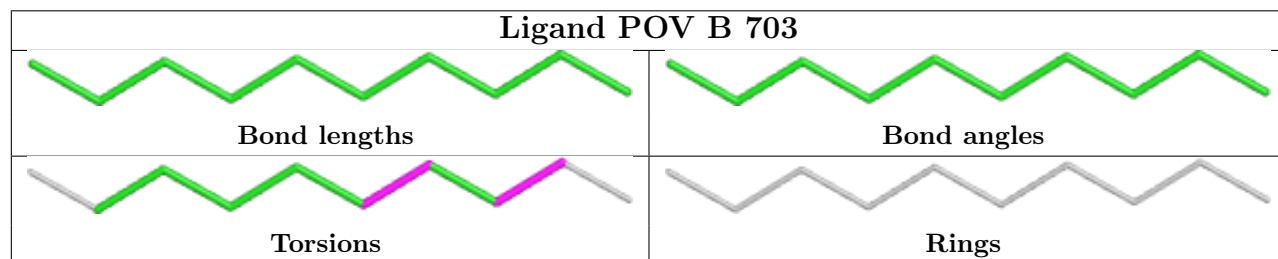
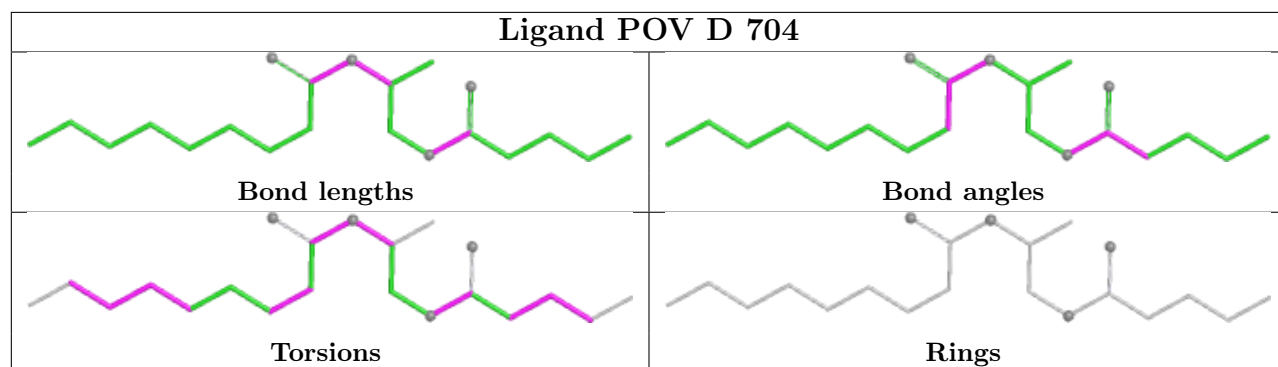
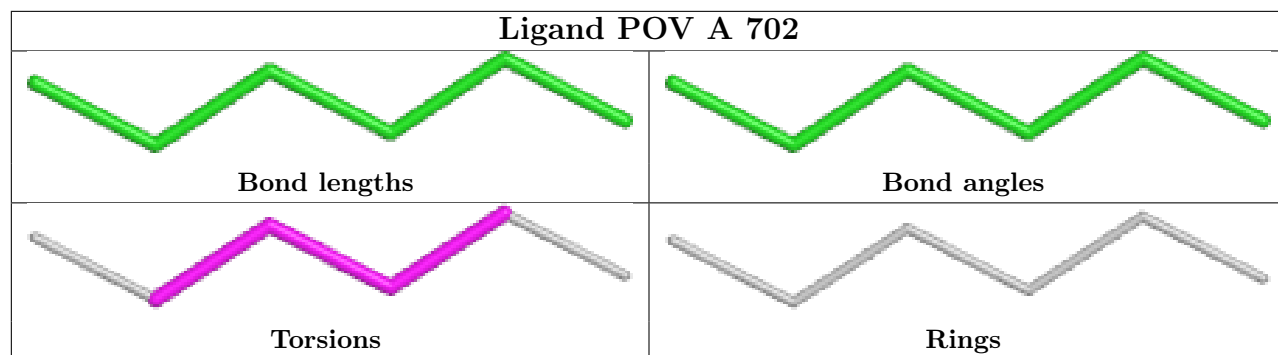
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	POV	2	0
2	A	705	POV	1	0
2	C	705	POV	2	0
2	B	705	POV	2	0
2	A	701	POV	1	0

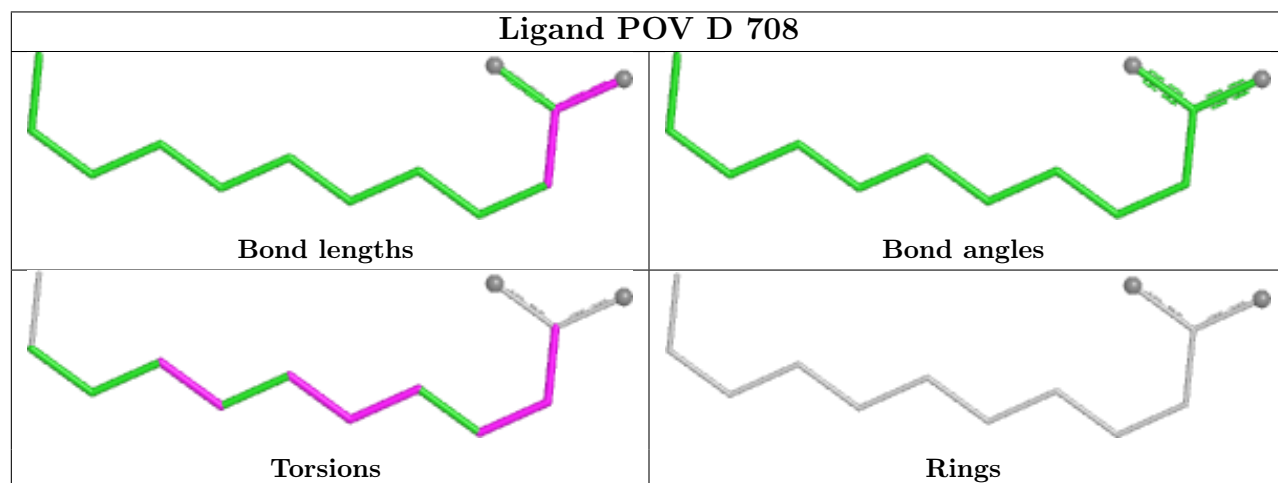
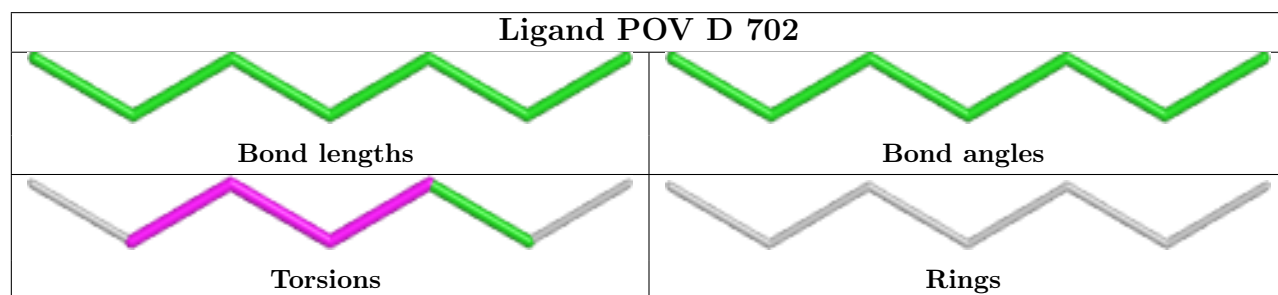
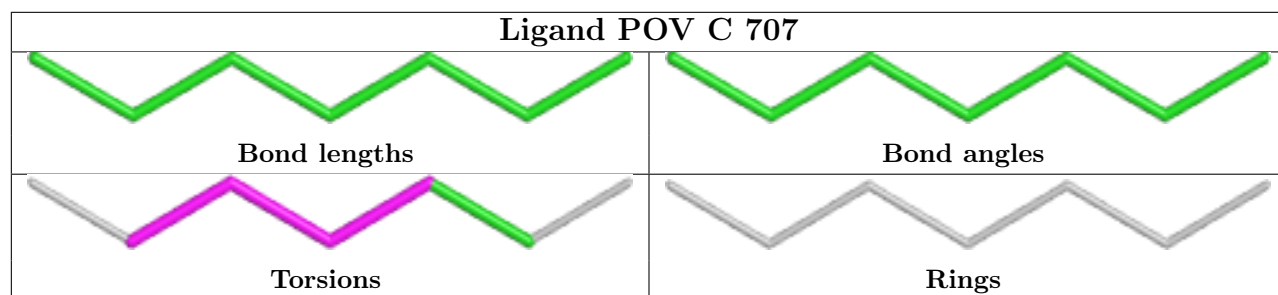
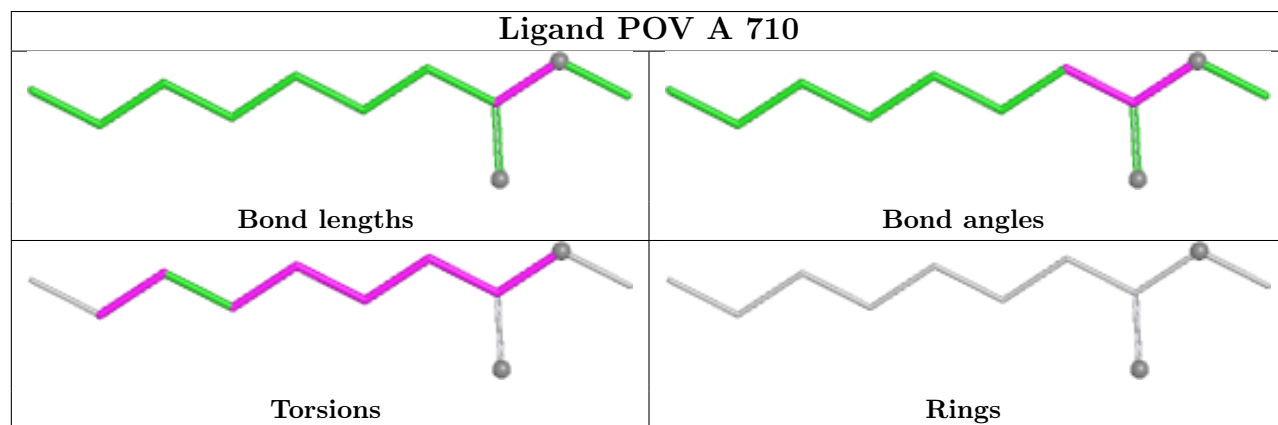
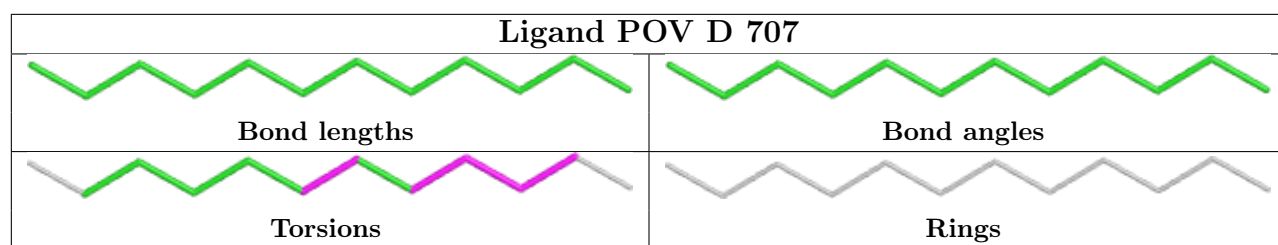
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

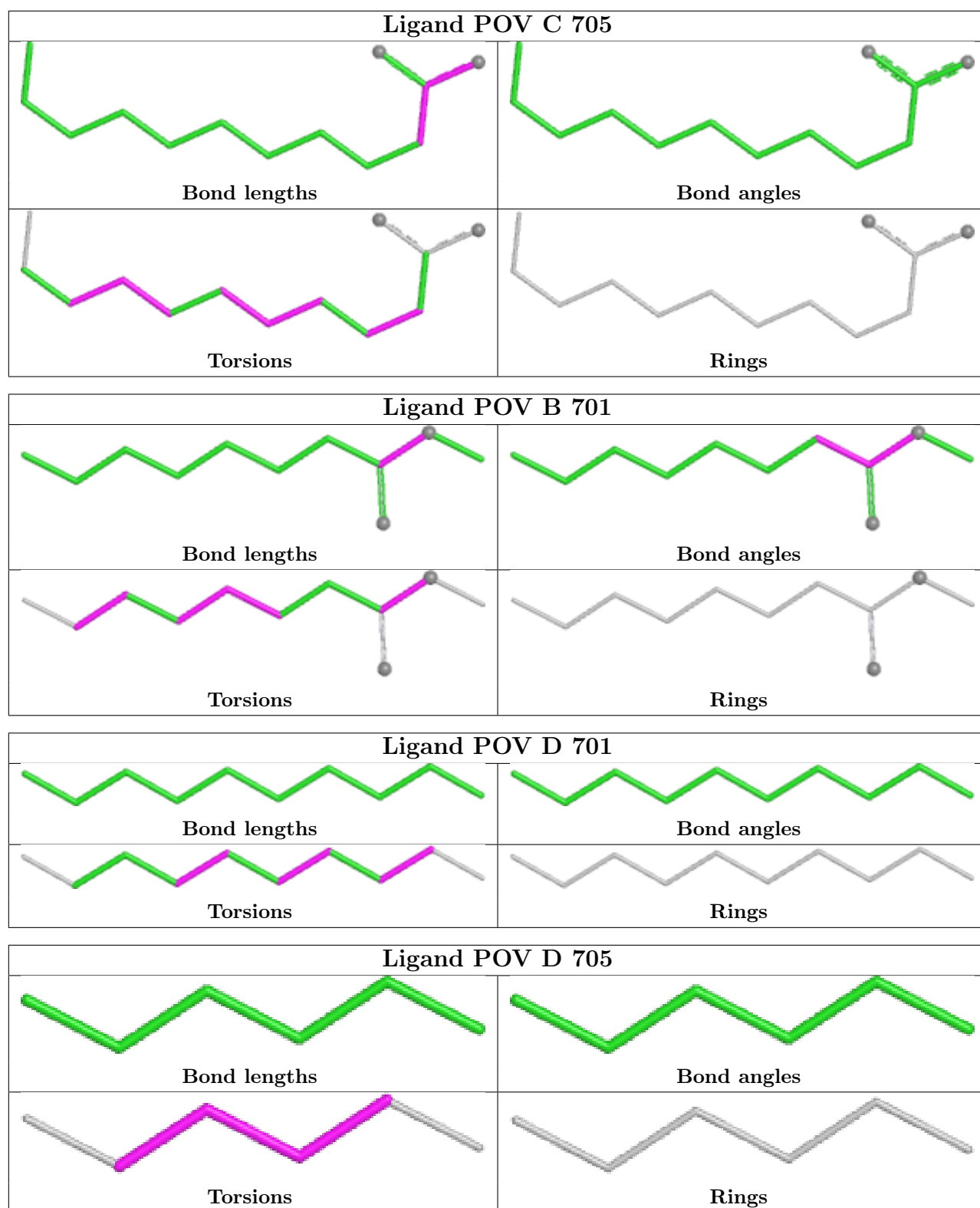


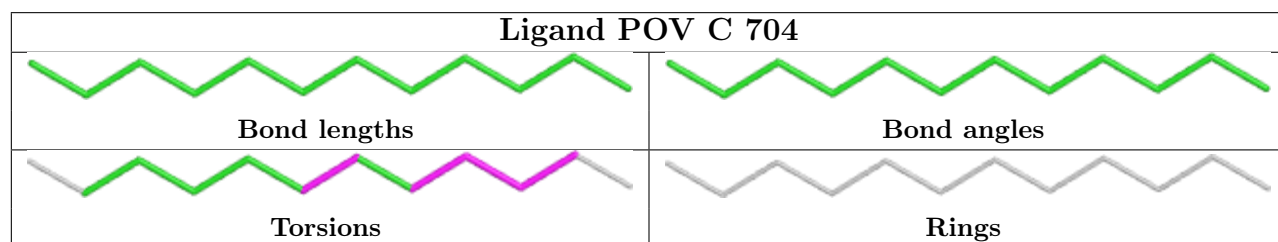
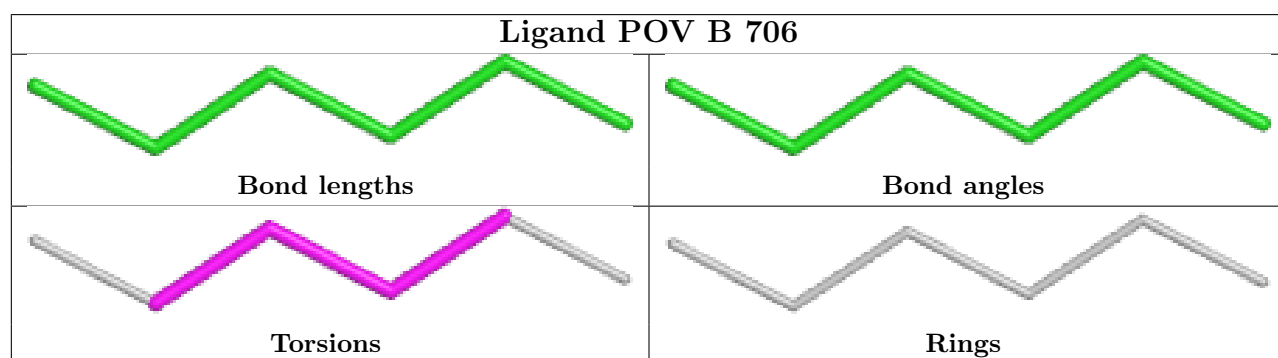
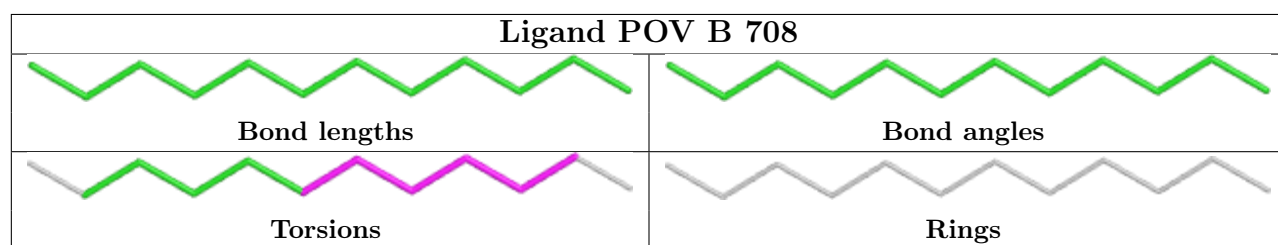
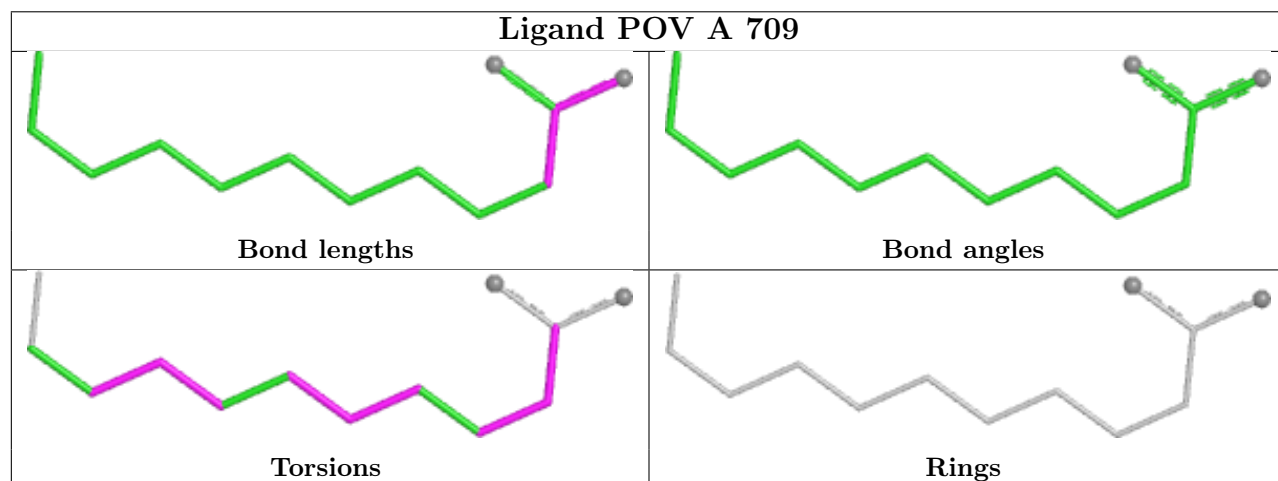
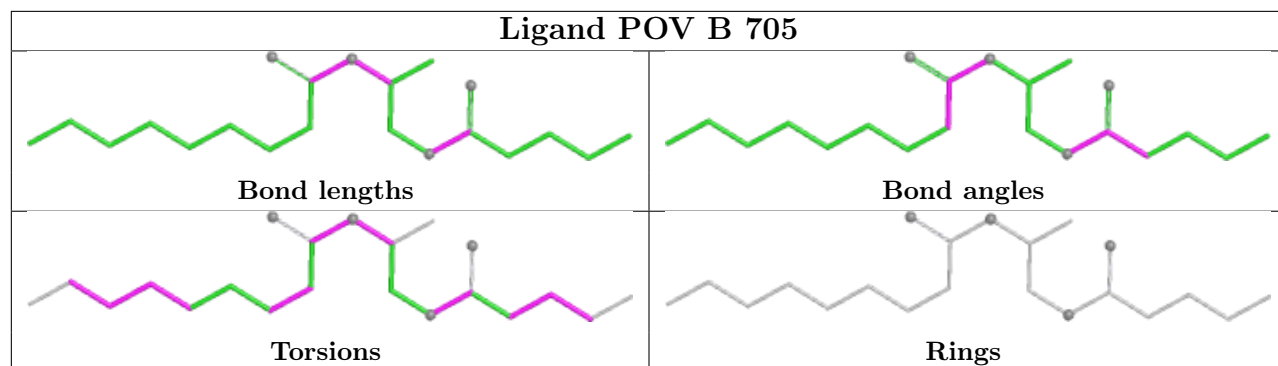


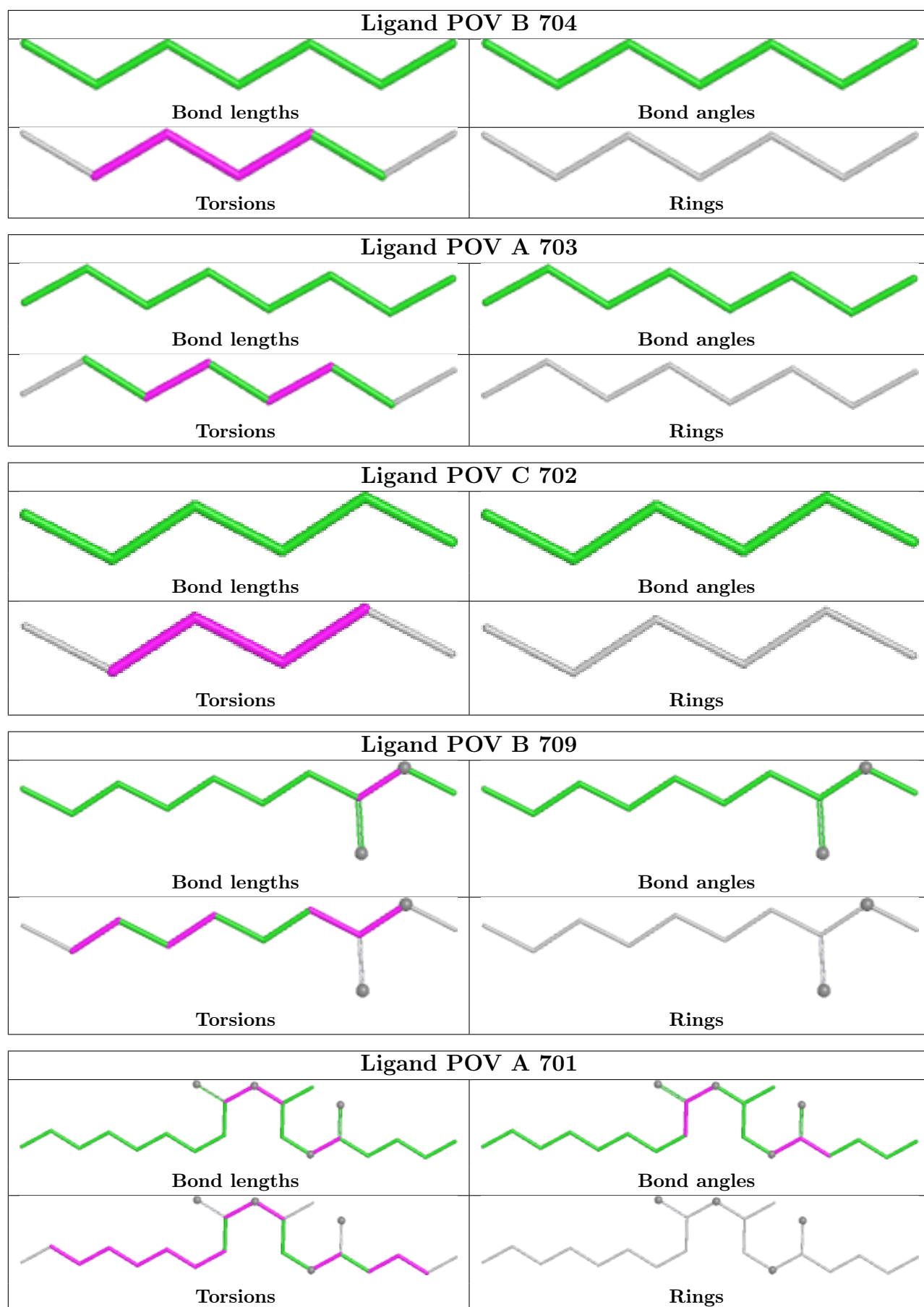


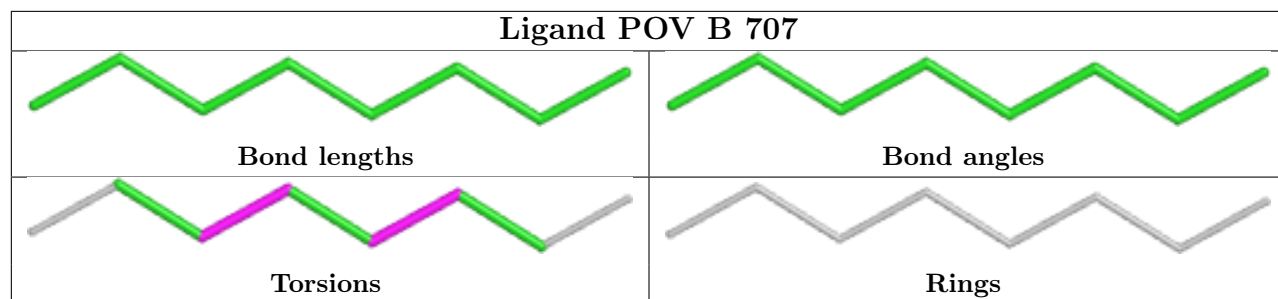












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

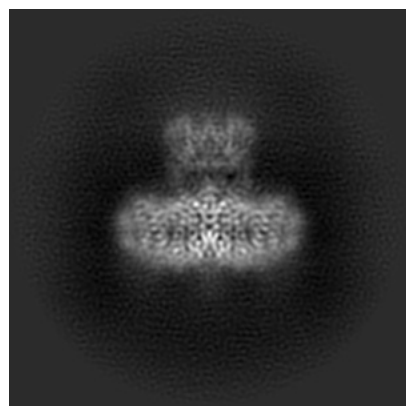
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49308. These allow visual inspection of the internal detail of the map and identification of artifacts.

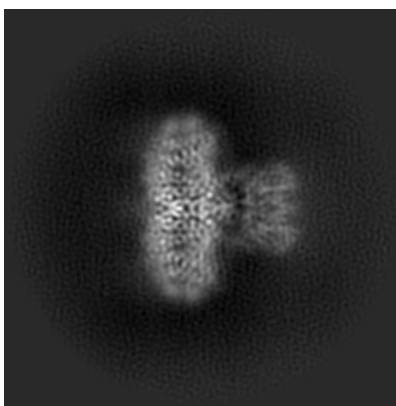
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

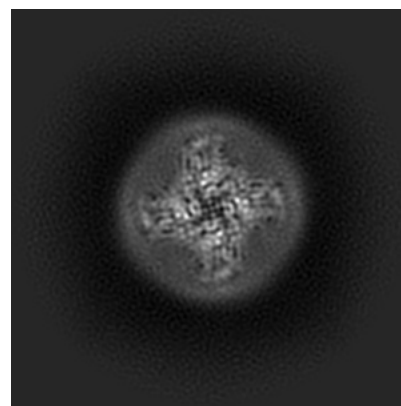
#### 6.1.1 Primary map



X

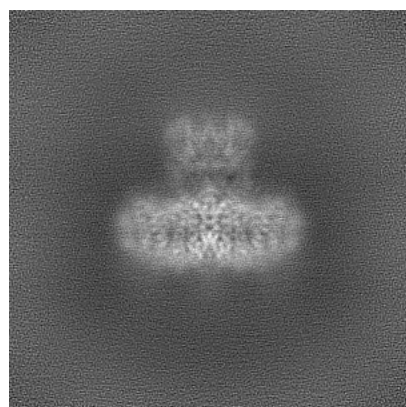


Y

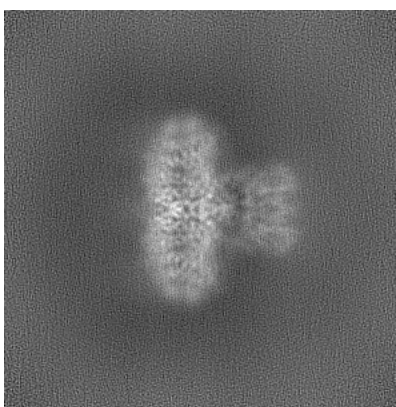


Z

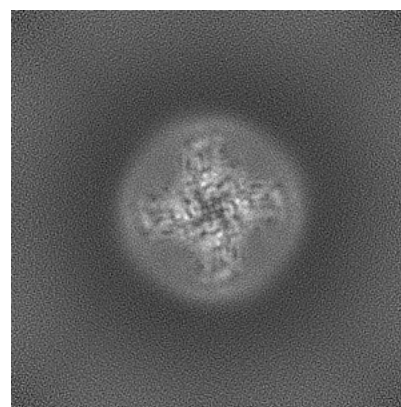
#### 6.1.2 Raw map



X



Y



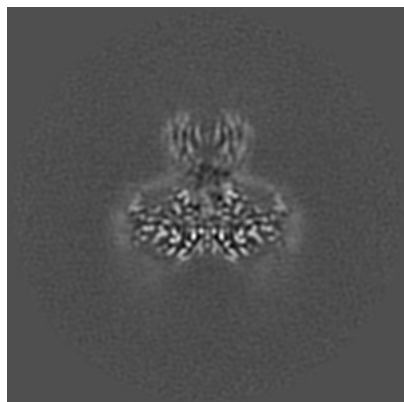
Z

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

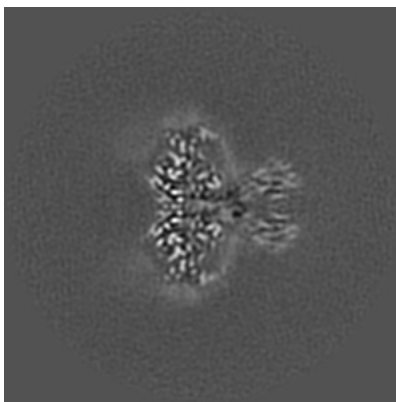


## 6.2 Central slices [i](#)

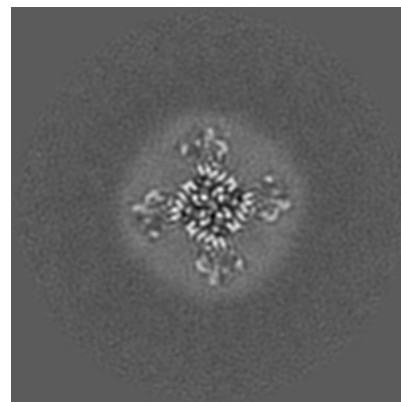
### 6.2.1 Primary map



X Index: 150

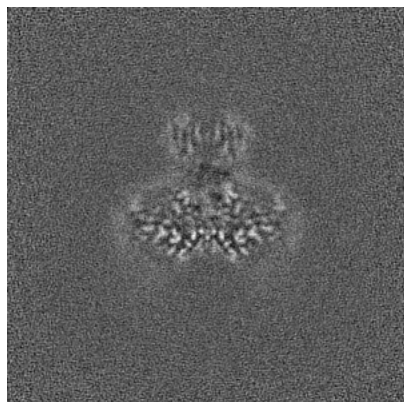


Y Index: 150

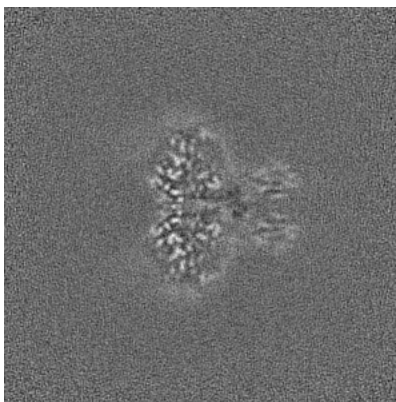


Z Index: 150

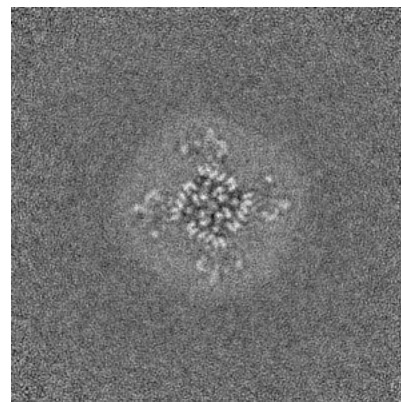
### 6.2.2 Raw map



X Index: 150



Y Index: 150



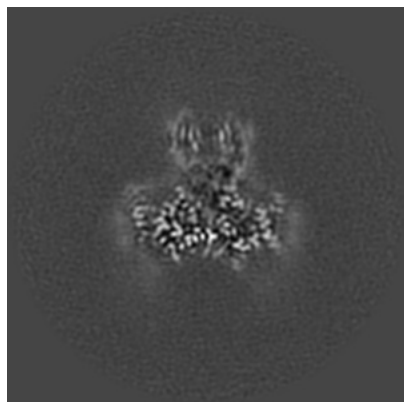
Z Index: 150

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

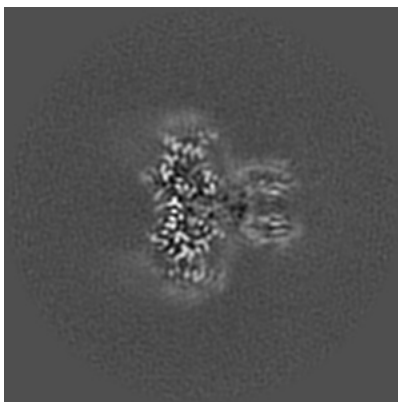


## 6.3 Largest variance slices [i](#)

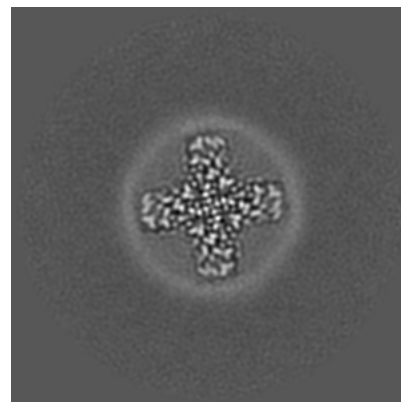
### 6.3.1 Primary map



X Index: 154

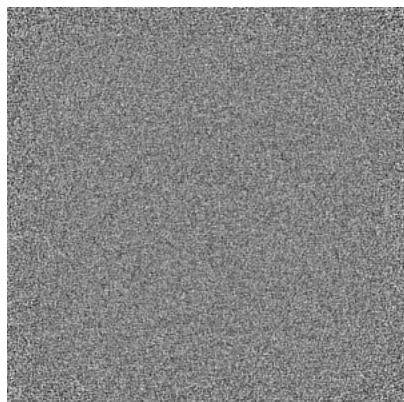


Y Index: 146

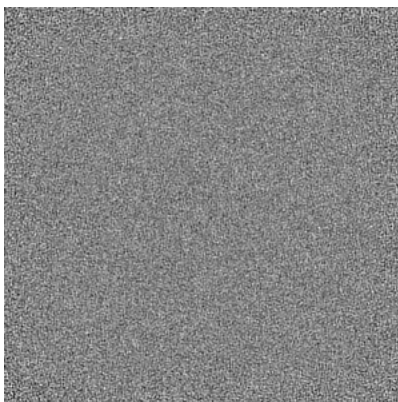


Z Index: 125

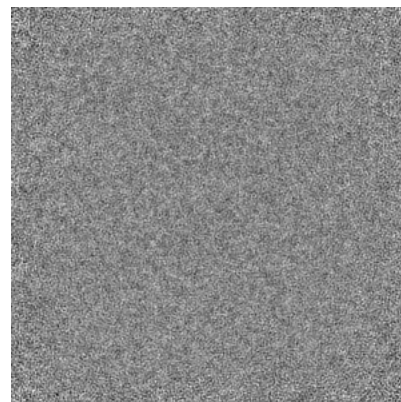
### 6.3.2 Raw map



X Index: 0



Y Index: 0

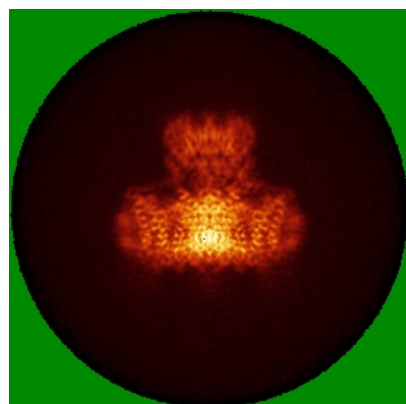


Z Index: 299

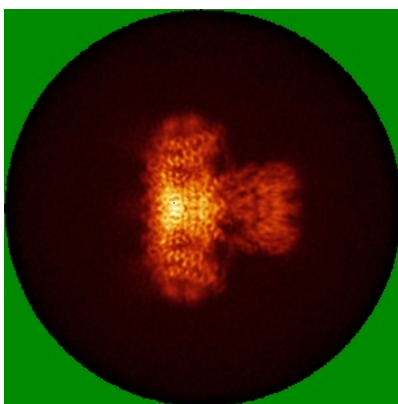
The images above show the largest variance slices of the map in three orthogonal directions.

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

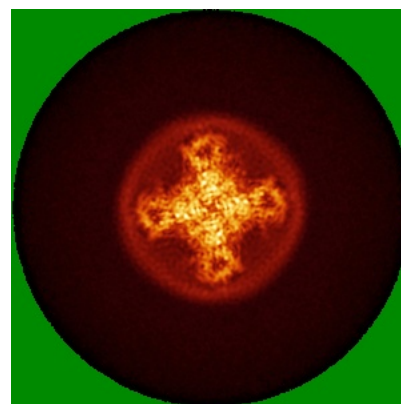
### 6.4.1 Primary map



X

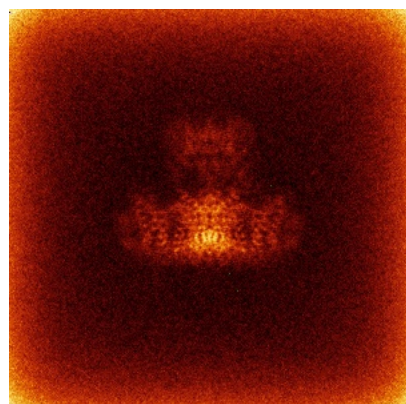


Y

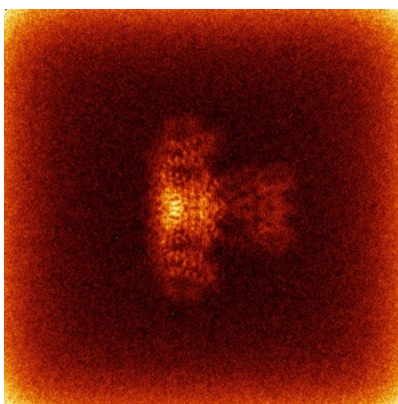


Z

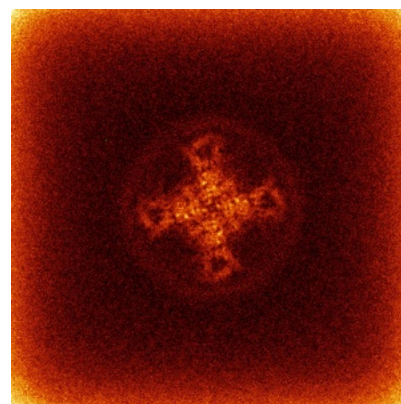
### 6.4.2 Raw map



X



Y

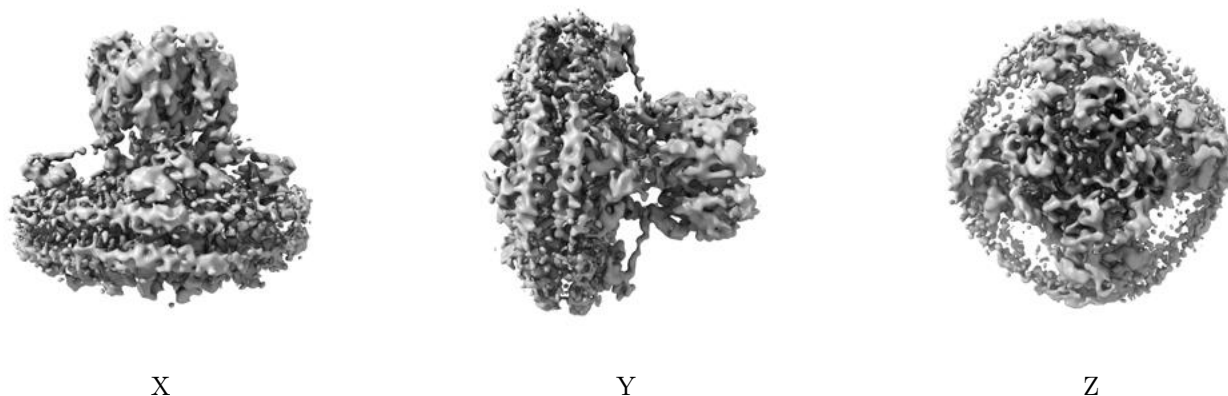


Z

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.

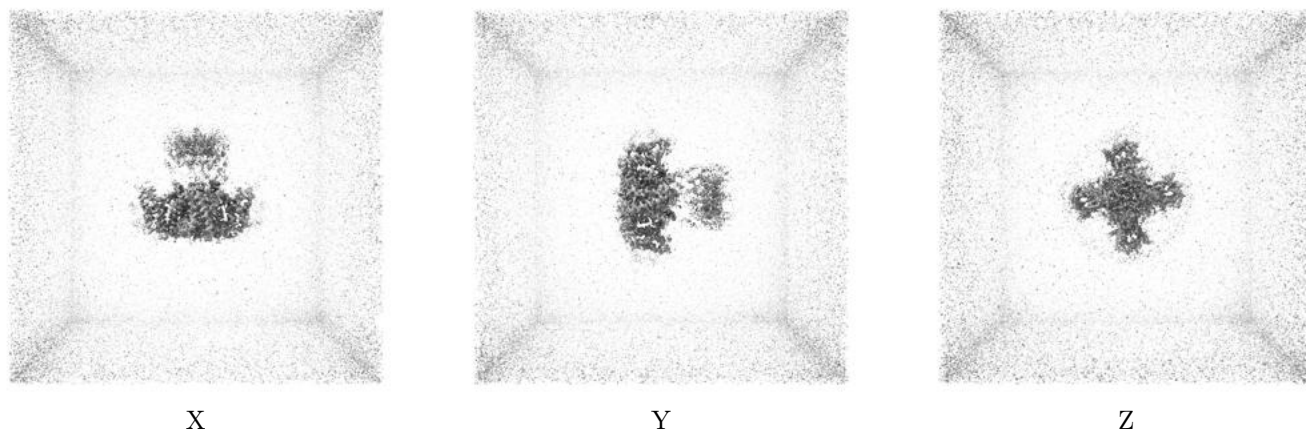
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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.

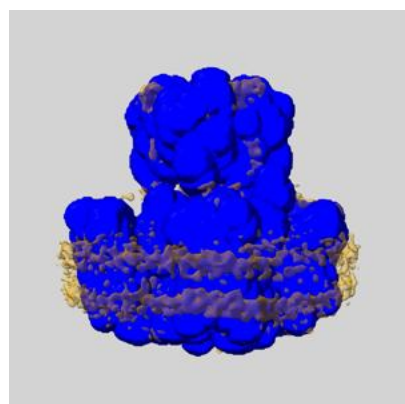
## 6.6 Mask visualisation [i](#)

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

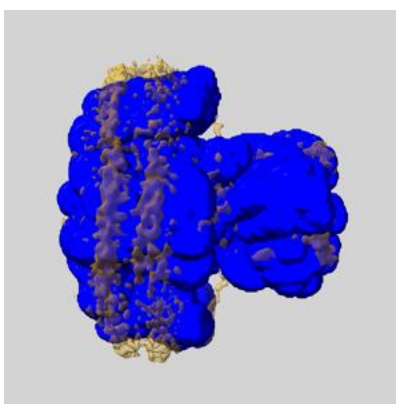
A mask typically either:

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

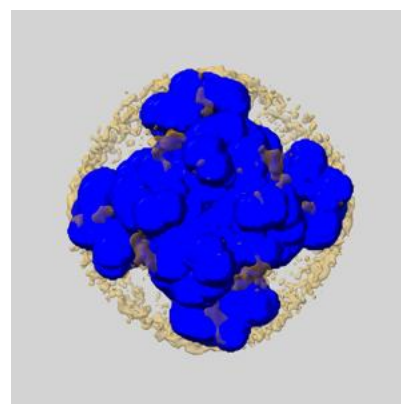
### 6.6.1 emd\_49308\_msk\_1.map [i](#)



X



Y

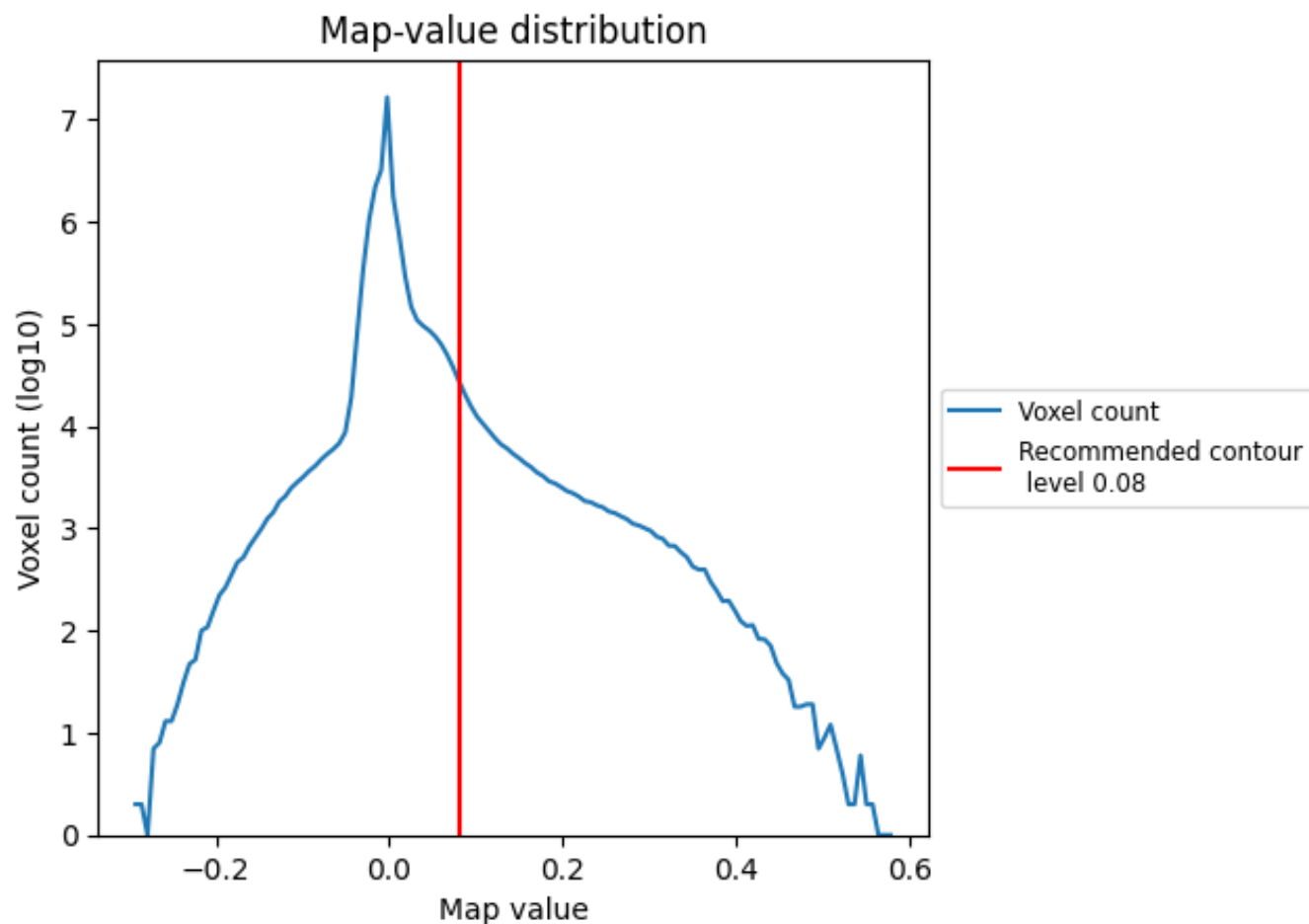


Z

## 7 Map analysis [i](#)

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

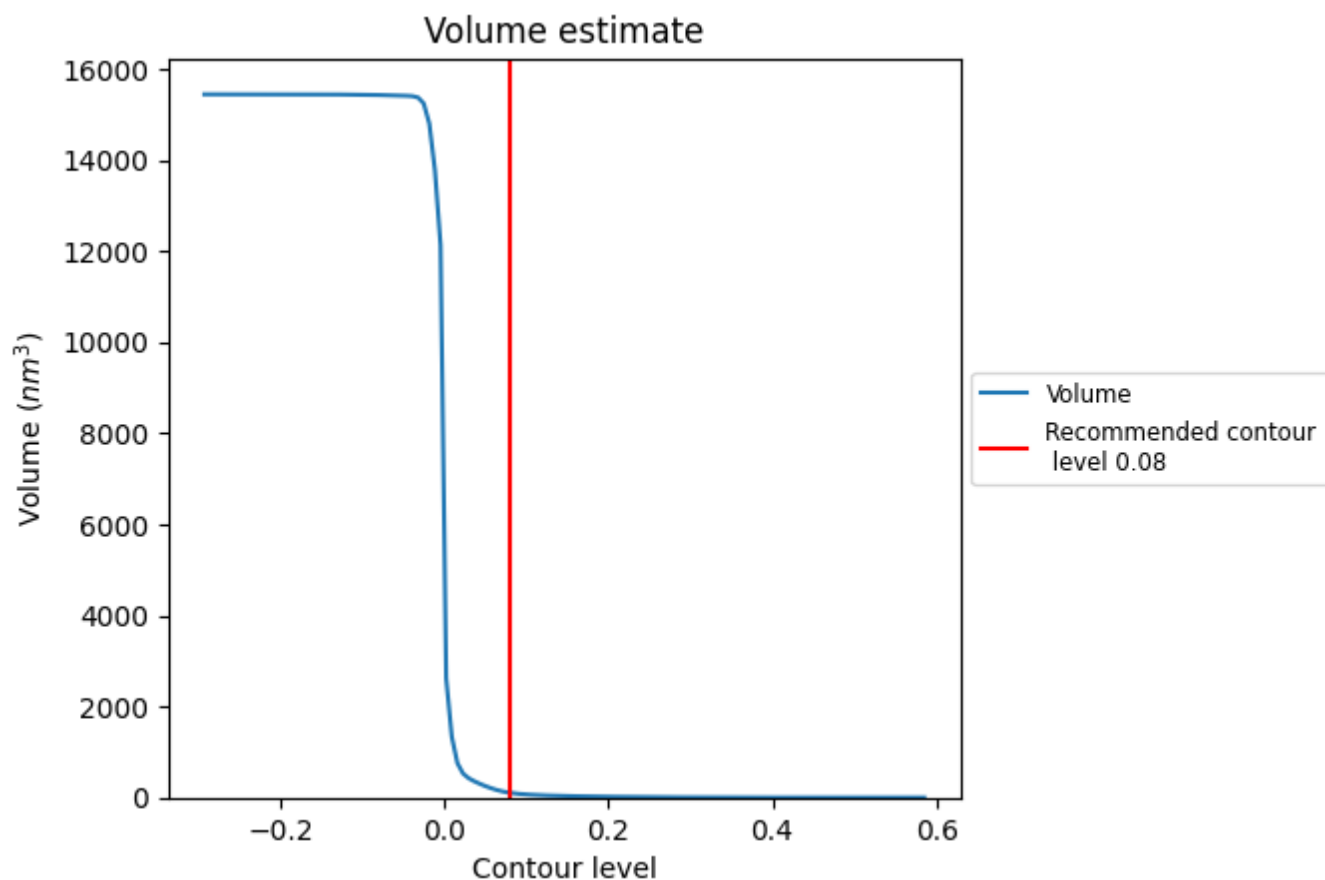
### 7.1 Map-value distribution [i](#)



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.



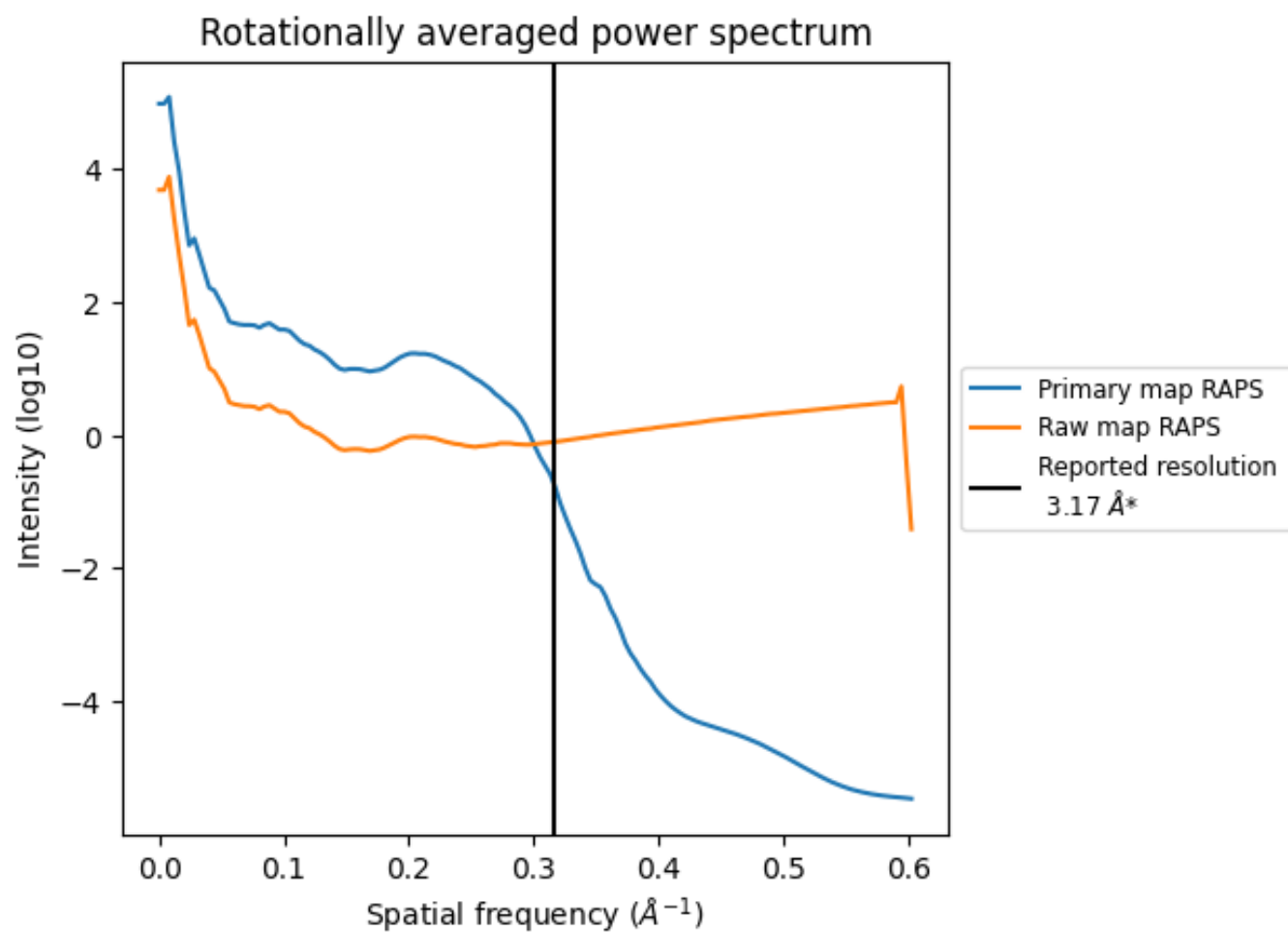
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm<sup>3</sup>; this corresponds to an approximate mass of 94 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 ⓘ

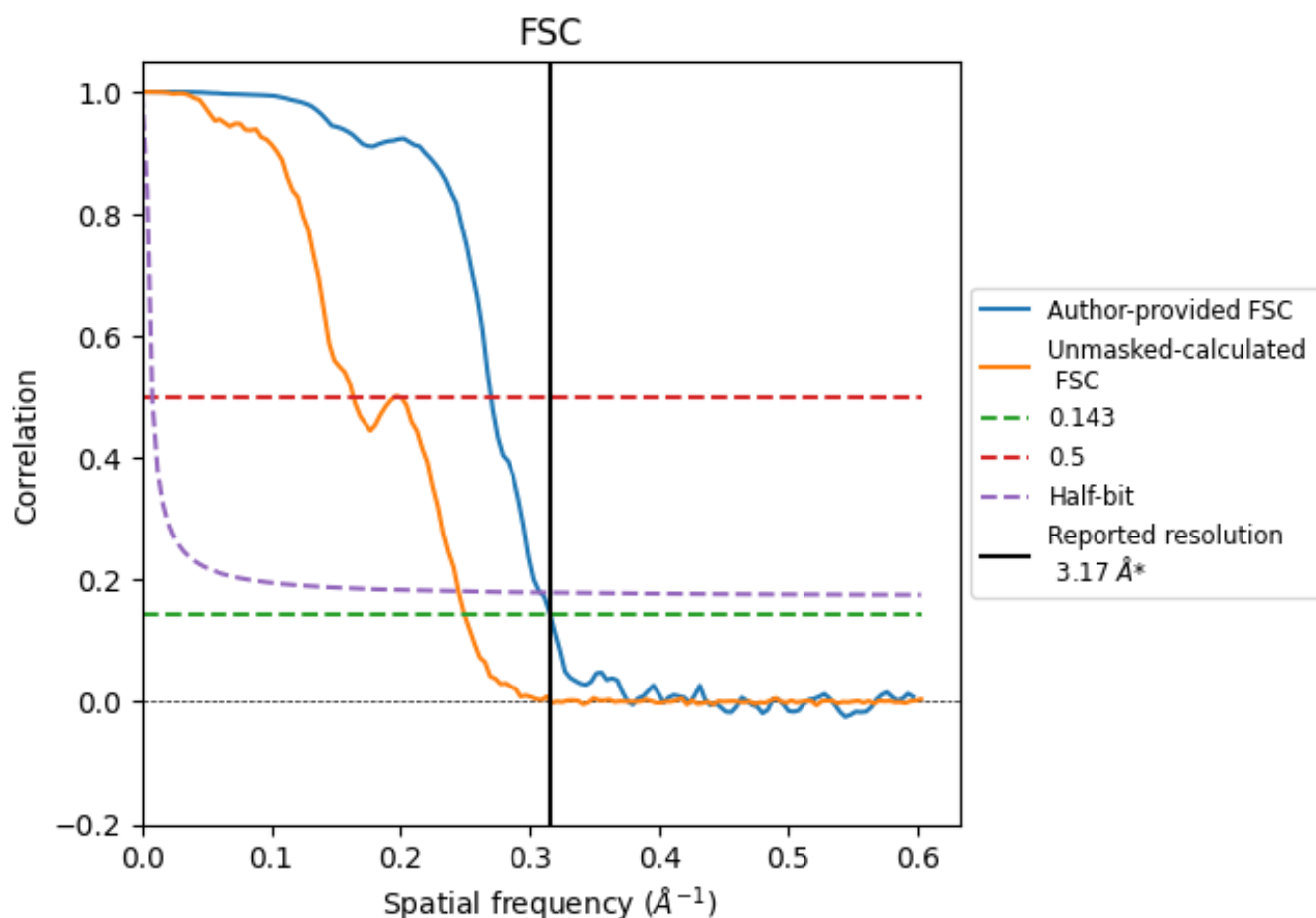


\*Reported resolution corresponds to spatial frequency of  $0.315 \text{ \AA}^{-1}$

## 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 0.315  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

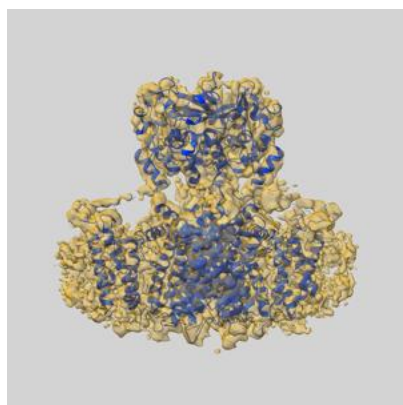
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.71	3.24
Unmasked-calculated*	4.01	6.12	4.09

\*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 4.01 differs from the reported value 3.17 by more than 10 %

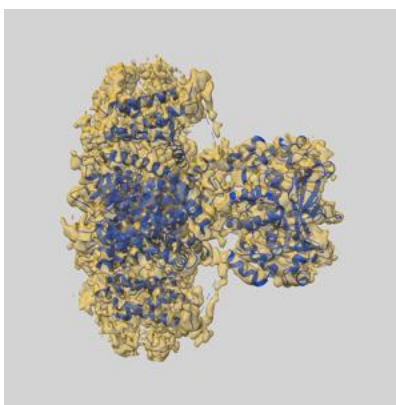
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49308 and PDB model 9NEG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

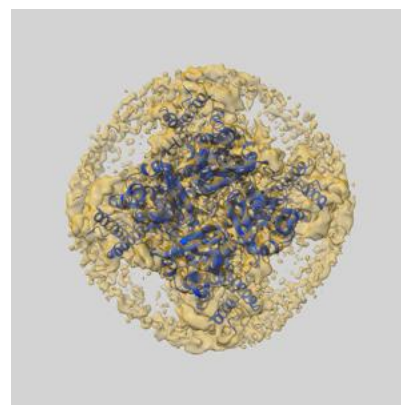
### 9.1 Map-model overlay [i](#)



X



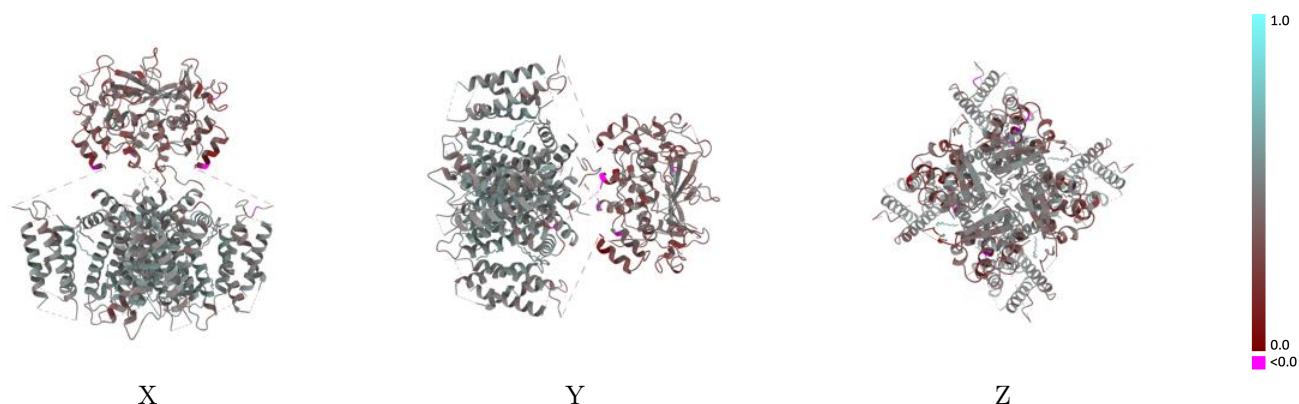
Y



Z

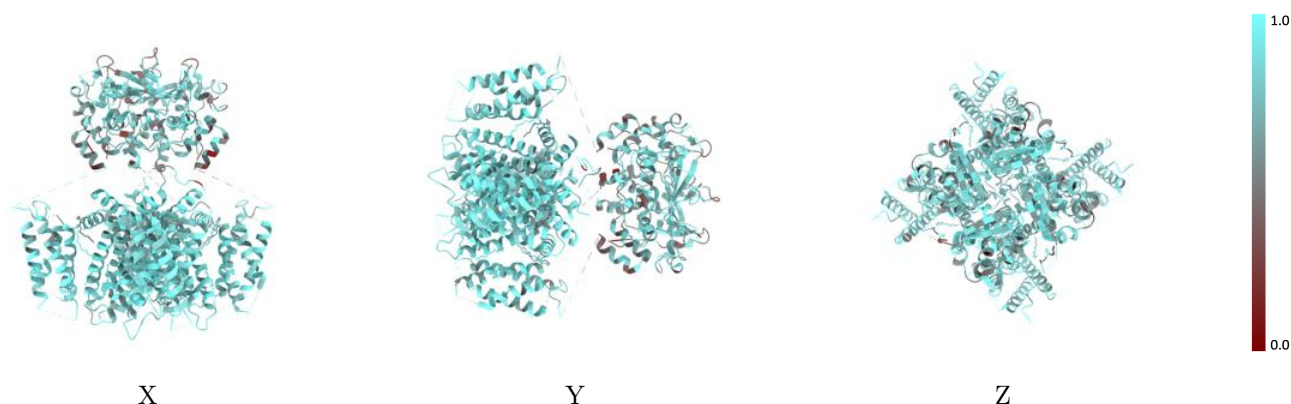
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



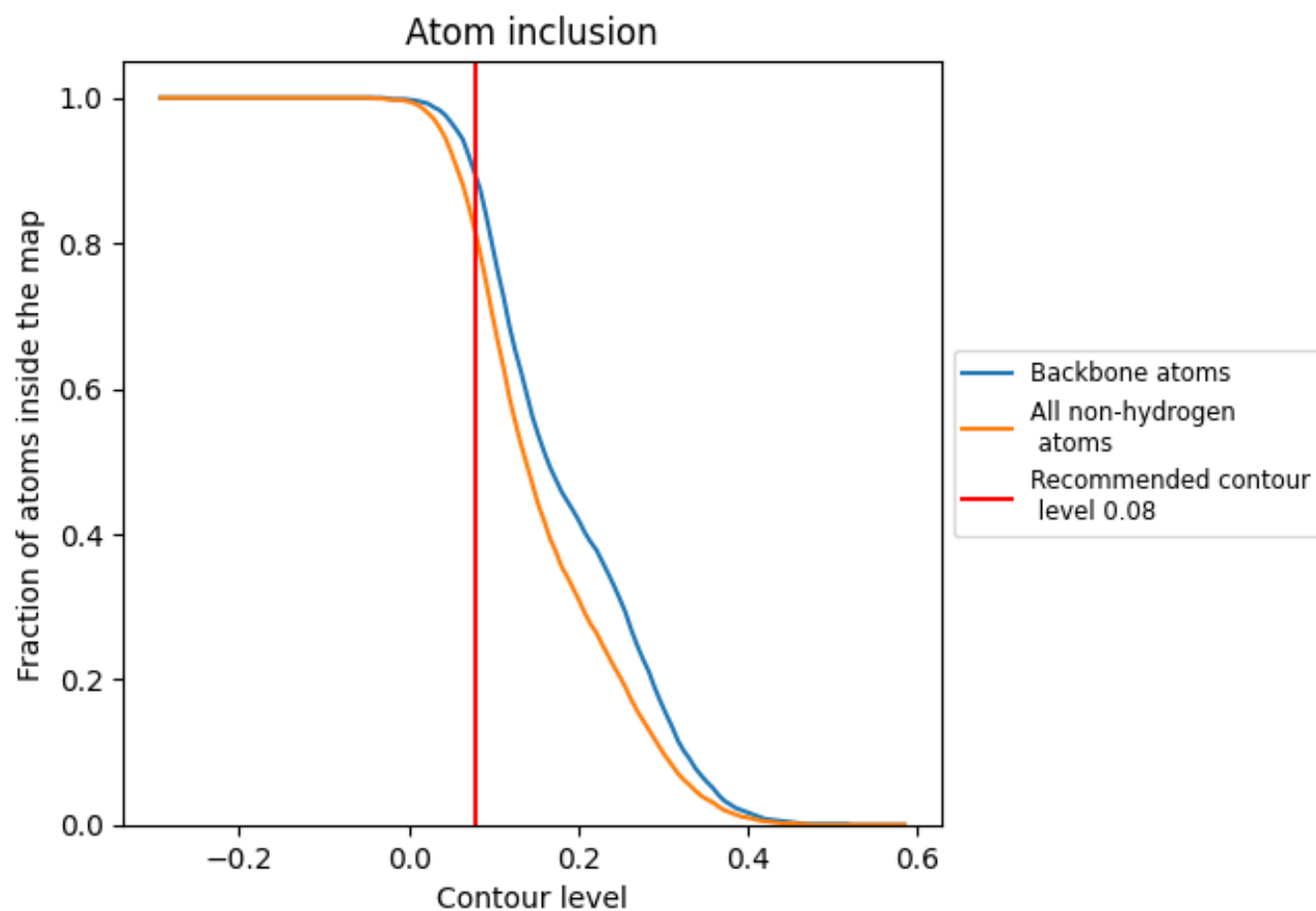
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8090</div>	<div><div></div>0.4490</div>
A	<div><div></div>0.8080</div>	<div><div></div>0.4490</div>
B	<div><div></div>0.8150</div>	<div><div></div>0.4490</div>
C	<div><div></div>0.8140</div>	<div><div></div>0.4460</div>
D	<div><div></div>0.8120</div>	<div><div></div>0.4540</div>
I	<div><div></div>0.8610</div>	<div><div></div>0.4440</div>
J	<div><div></div>0.7830</div>	<div><div></div>0.4150</div>

1.0

0.0

<0.0