



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2025 – 06:27 PM JST

PDB ID : 8WCI / pdb\_00008wci  
EMDB ID : EMD-37440  
Title : Cryo-EM structure of the inhibitor-bound Vo complex from *Enterococcus hirae*  
Authors : Suzuki, K.; Mikuriya, S.; Adachi, N.; Kawasaki, M.; Senda, T.; Moriya, T.;  
Murata, T.  
Deposited on : 2023-09-12  
Resolution : 2.20 Å (reported)  
Based on initial models : ., 2BL2

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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

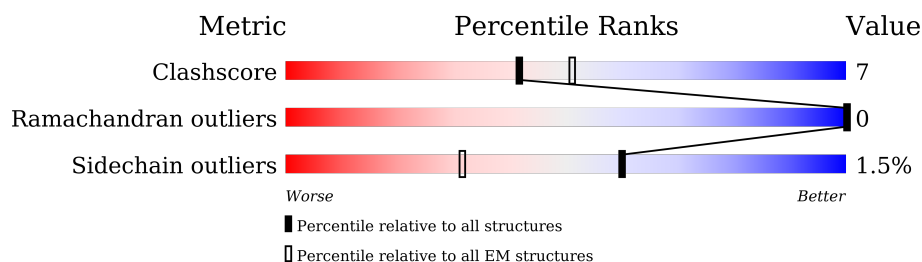
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 Å.

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




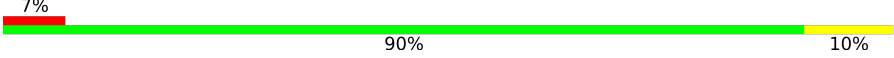
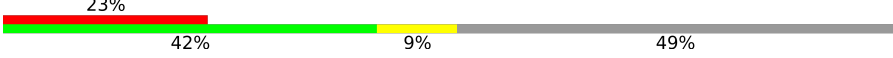
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	156	<div> <div>6%</div> <div>86%</div> <div>14%</div> </div>
1	B	156	<div> <div>6%</div> <div>83%</div> <div>17%</div> </div>
1	C	156	<div> <div>6%</div> <div>78%</div> <div>22%</div> </div>
1	D	156	<div> <div>6%</div> <div>85%</div> <div>15%</div> </div>
1	E	156	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
1	F	156	<div> <div>7%</div> <div>83%</div> <div>17%</div> </div>
1	G	156	<div> <div>7%</div> <div>83%</div> <div>17%</div> </div>
1	H	156	<div> <div>6%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	156	
1	J	156	
2	P	672	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14876 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 V-type sodium ATPase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	156	Total	C	N	O	S	4	0
			1147	760	176	203	8		
1	B	156	Total	C	N	O	S	6	0
			1157	769	177	204	7		
1	C	156	Total	C	N	O	S	4	0
			1149	760	178	204	7		
1	D	156	Total	C	N	O	S	7	0
			1163	773	178	205	7		
1	E	156	Total	C	N	O	S	5	0
			1152	764	177	204	7		
1	F	156	Total	C	N	O	S	5	0
			1152	764	177	204	7		
1	G	156	Total	C	N	O	S	4	0
			1158	764	180	207	7		
1	H	156	Total	C	N	O	S	0	0
			1128	743	176	202	7		
1	I	156	Total	C	N	O	S	5	0
			1167	769	182	209	7		
1	J	156	Total	C	N	O	S	4	0
			1158	764	180	207	7		

- Molecule 2 is a protein called V-type sodium ATPase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	343	Total	C	N	O	S	1	0
			2685	1775	424	472	14		

There are 8 discrepancies between the modelled and reference sequences:

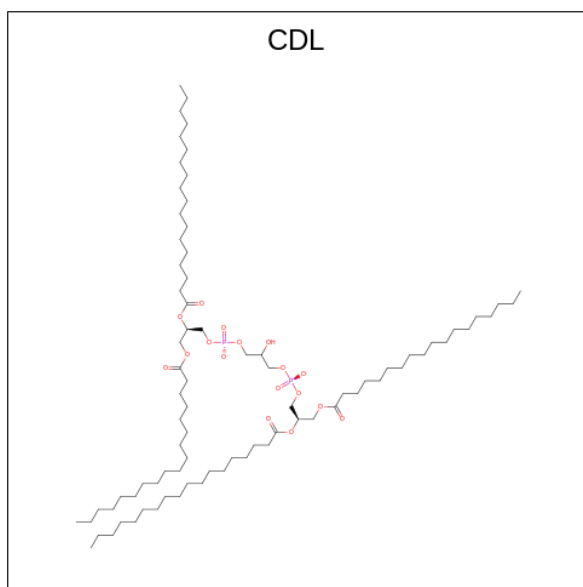
Chain	Residue	Modelled	Actual	Comment	Reference
P	665	GLU	-	expression tag	UNP P43439
P	666	HIS	-	expression tag	UNP P43439
P	667	LEU	-	expression tag	UNP P43439
P	668	TYR	-	expression tag	UNP P43439

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Chain	Residue	Modelled	Actual	Comment	Reference
P	669	PHE	-	expression tag	UNP P43439
P	670	GLN	-	expression tag	UNP P43439
P	671	GLY	-	expression tag	UNP P43439
P	672	GLY	-	expression tag	UNP P43439

- Molecule 3 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			83	64	17	2	
3	D	1	Total	C	O	P	0
			81	62	17	2	
3	F	1	Total	C	O	P	0
			79	60	17	2	
3	H	1	Total	C	O	P	0
			83	64	17	2	
3	I	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

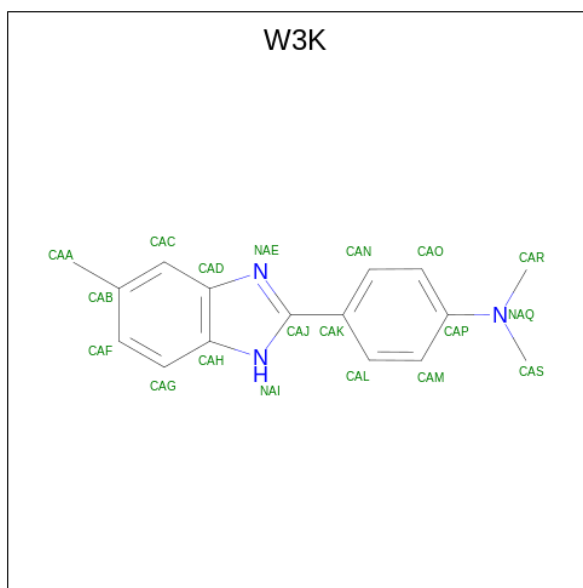
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Na	0
			1	1	
4	B	1	Total	Na	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Na	0
			1	1	
4	E	1	Total	Na	0
			1	1	
4	F	1	Total	Na	0
			1	1	
4	G	1	Total	Na	0
			1	1	
4	H	1	Total	Na	0
			1	1	
4	I	1	Total	Na	0
			1	1	
4	J	1	Total	Na	0
			1	1	

- Molecule 5 is N,N-dimethyl-4-(5-methyl-1H-benzimidazol-2-yl)aniline (CCD ID: W3K) (formula: C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	P	1	Total	C	N	0
			19	16	3	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	21	Total	O	0
			21	21	

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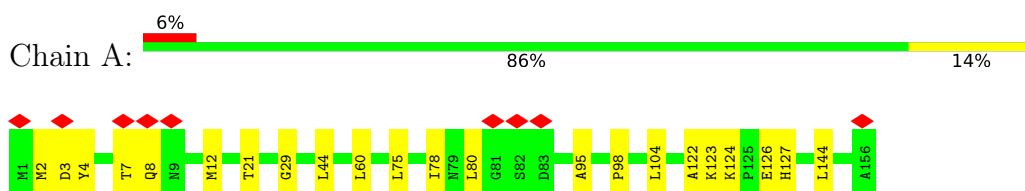
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Mol	Chain	Residues	Atoms		AltConf
6	B	28	Total 28	O 28	0
6	C	18	Total 18	O 18	0
6	D	21	Total 21	O 21	0
6	E	22	Total 22	O 22	0
6	F	16	Total 16	O 16	0
6	G	17	Total 17	O 17	0
6	H	19	Total 19	O 19	0
6	I	24	Total 24	O 24	0
6	J	27	Total 27	O 27	0
6	P	11	Total 11	O 11	0

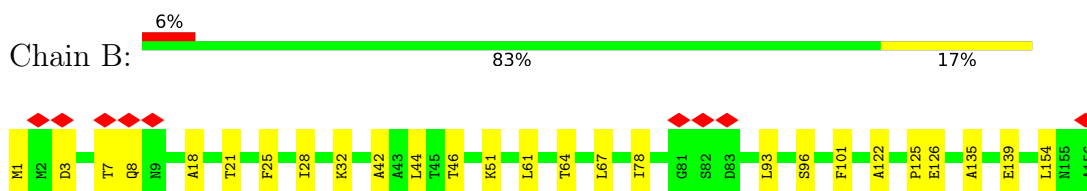
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

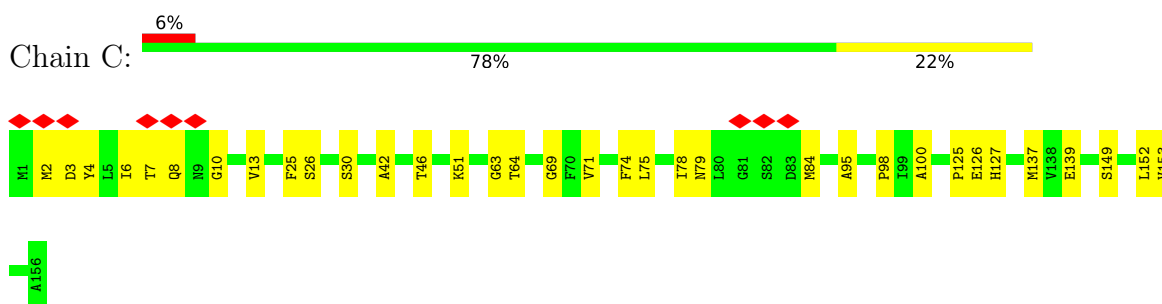
- Molecule 1: V-type sodium ATPase subunit K



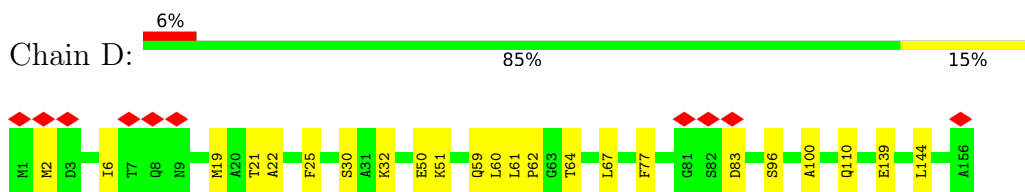
- Molecule 1: V-type sodium ATPase subunit K



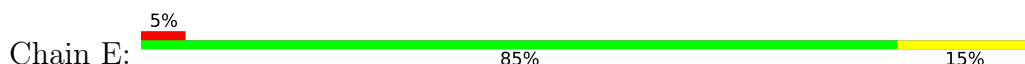
- Molecule 1: V-type sodium ATPase subunit K



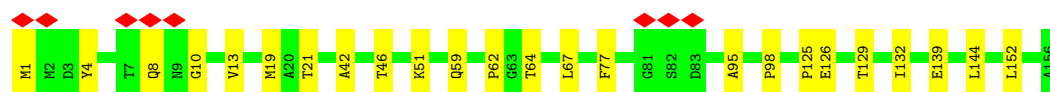
- Molecule 1: V-type sodium ATPase subunit K



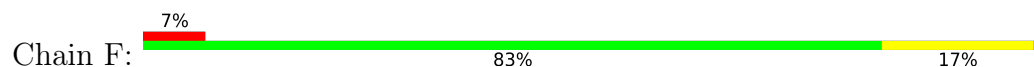
- Molecule 1: V-type sodium ATPase subunit K



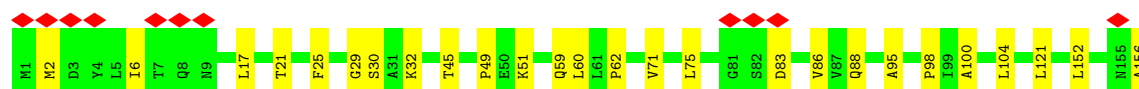
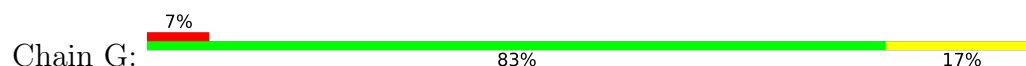




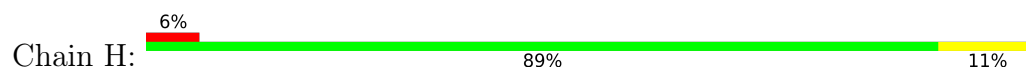
- Molecule 1: V-type sodium ATPase subunit K



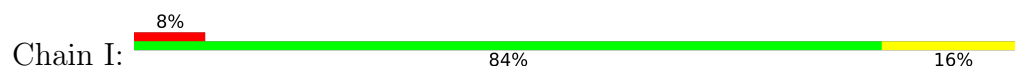
- Molecule 1: V-type sodium ATPase subunit K



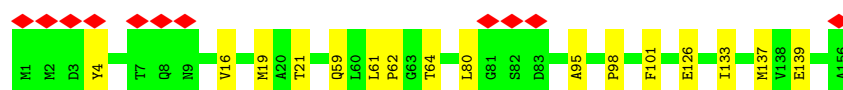
- Molecule 1: V-type sodium ATPase subunit K



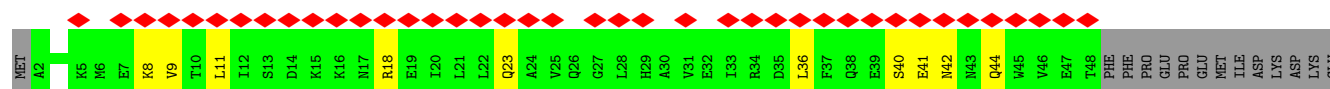
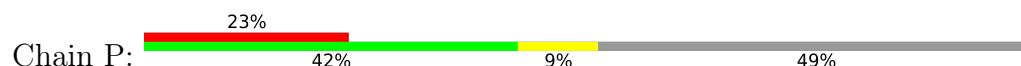
- Molecule 1: V-type sodium ATPase subunit K



- Molecule 1: V-type sodium ATPase subunit K



- Molecule 2: V-type sodium ATPase subunit I



LEU	TYR	ASN	LEU	TYR	ASN	GLY	K400	E302	LEU	ILE	LYS	LEU
PHE	LEU	LEU	L401	E303	GLU	PHE	L401	E303	GLN	ASN	GLU	ALA
GLN	TYR	TYR	V402	K304	TRP	ALA	V402	K304	ILE	ALA	GLU	TRP
GLY	GLY	GLY	V403	Q305	GLN	GLN	V403	Q305	LYS	TYR	LEU	TYR
	LEU	LEU	L404	E306	GLY	ASP	L404	E306	ASP	LEU	GLN	LYS
	T562		P405	L307	ILE	GLN	P405	L307	GLN	GLU	VAL	LEU
	G563		R406	I308	LEU	LYS	R406	I308	ILE	ASP	GLU	ASP
	Y564		G407	H309	GLY	GLY	G407	H309	ASN	GLU	ASP	THR
	I565		M408	M310	ILE	LEU	M408	M310	SER	ARG	ARG	ILE
			Q409	L311	ILE	GLU	Q409	L311	SER	GLN	GLN	THR
			R410	Q312	LEU	LEU	R410	Q312	PRO	GLN	GLN	THR
			F411	N313	ILE	ALA	F411	N313	THR	THR	GLU	ALA
			K413	I314	LEU	GLY	K413	I314	ALA	THR	ASP	ILE
			F414	I315	GLY	ALA	F414	I315	CYS	PHE	GLU	ILE
			P415		THR		P415		SER	ALA	ASN	GLU
					MET				GLY	TYR	TRP	HIS
					ILE		I420		TYR	ILE	LEU	HIS
					LEU		P421		GLU	VAL	LEU	GLY
					LYS				ILE	VAL	LEU	GLY
					ASN		A436		LYS	LEU	ASN	GLU
					ALA		L437		ASP	LEU	ASP	LYS
					PHE		P438		PHE	ALA	GLN	SER
					VAL		K439		GLU	ASP	ASN	GLN
					TYR		GLU		TRP	GLU	LEU	LYS
					LEU		ILE		THR	SER	ASP	LYS
					GLY		PHE		E270	ARG	LEU	GLN
					ALA		ILE		E271	MET	ALA	HIS
					ALA		ILE		I272	GLU	PRO	LEU
					LEU		HIS		F273	GLU	LYS	LYS
					ALA		L446		L274	ALA	ALA	ARG
					VAL		P447		A275	SER	PHE	ARG
					LEU		F448		A276	GLN	ASP	GLU
					SER				R276	TYR	SER	LEU
					ALA		D455		S277	GLY	MET	LEU
					VAL		D456		E278	PHE	THR	ASP
					CYS		ILE		R279	VAL	LYS	THR
					ILE		I460		E280	LYS	LEU	LEU
					LEU		L461		A281	GLU	VAL	GLU
					ILE		I462		I282	ASP	ILE	LYS
					PRO				K283	TYR	GLY	ASN
					VAL				D284	LEU	THR	TYR
					PHE		F477		R285	GLY	VAL	SER
					GLN		I478		I286	THR	ASN	GLY
					SER		A479		ILE	ALA	LYS	ALA
					SER		A480		PRO	GLN	ALA	SER
					LYS		K481		GLN	GLN	GLU	LYS
					ALA		E482		LEU	LEU	SER	LEU
					LYS		H483		VAL	VAL	PHE	LEU
					GLY		ILE		ALA	ALA	LYS	GLU
					ALA		ARG		ILE	ALA	GLU	VAL
					LYS		LYS		L294	LYS	VAL	LEU
					GLY		GLY		I295	GLN	GLU	LEU
					ALA		ALA		Q296	GLN	ALA	LE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	225359	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 ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: W3K, CDL, NA

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	0.39	0/1178	0.54	0/1593
1	B	0.39	0/1194	0.50	0/1616
1	C	0.37	0/1180	0.52	0/1596
1	D	0.39	0/1203	0.52	0/1628
1	E	0.38	0/1186	0.51	0/1605
1	F	0.38	0/1186	0.50	0/1605
1	G	0.39	0/1177	0.53	0/1593
1	H	0.39	0/1147	0.51	0/1551
1	I	0.38	0/1186	0.52	0/1605
1	J	0.38	0/1177	0.50	0/1593
2	P	0.35	0/2744	0.49	0/3721
All	All	0.38	0/14558	0.51	0/19706

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	1147	0	1219	14	0
1	B	1157	0	1238	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1149	0	1218	21	0
1	D	1163	0	1246	18	0
1	E	1152	0	1227	17	0
1	F	1152	0	1227	21	0
1	G	1158	0	1215	17	0
1	H	1128	0	1181	16	0
1	I	1167	0	1222	17	0
1	J	1158	0	1215	12	0
2	P	2685	0	2694	35	0
3	A	83	0	116	8	0
3	D	81	0	109	4	0
3	F	79	0	102	4	0
3	H	83	0	116	5	0
3	I	82	0	114	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	P	19	0	0	0	0
6	A	21	0	0	0	0
6	B	28	0	0	0	0
6	C	18	0	0	1	0
6	D	21	0	0	0	0
6	E	22	0	0	0	0
6	F	16	0	0	1	0
6	G	17	0	0	1	0
6	H	19	0	0	0	0
6	I	24	0	0	0	0
6	J	27	0	0	0	0
6	P	11	0	0	1	0
All	All	14876	0	15459	198	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 7.

All (198) 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)
2:P:270:GLU:O	2:P:274:LEU:HB2	1.89	0.73
3:A:201:CDL:HA21	1:B:32:LYS:NZ	2.07	0.69
1:G:2:MET:HG3	1:H:1:MET:HB2	1.77	0.67
2:P:387:TYR:O	2:P:391:MET:HG3	1.94	0.67
1:F:127:HIS:HB3	1:F:130:LYS:HD2	1.77	0.67
1:I:152:LEU:HD13	1:J:16:VAL:HG13	1.77	0.67
1:E:4:TYR:CE1	1:E:8:GLN:HG3	2.30	0.67
2:P:36:LEU:HD21	2:P:296:GLN:HG3	1.79	0.65
1:B:154:LEU:HD11	2:P:594:PHE:HZ	1.62	0.65
1:F:3:ASP:O	1:F:7:THR:HG23	1.99	0.62
1:I:2:MET:O	1:I:6:ILE:HG13	2.00	0.62
1:D:67[B]:LEU:HD22	2:P:562:THR:HG22	1.83	0.60
3:I:201:CDL:H511	3:I:201:CDL:HB62	1.84	0.60
1:B:126:GLU:H	1:B:126:GLU:CD	2.04	0.60
3:A:201:CDL:HA21	1:B:32:LYS:HZ1	1.67	0.60
1:B:154:LEU:HD11	2:P:594:PHE:CZ	2.36	0.59
3:F:202:CDL:H511	3:F:202:CDL:H722	1.84	0.59
1:D:6:ILE:HD12	1:E:4:TYR:CG	2.37	0.59
3:H:201:CDL:H511	3:H:201:CDL:HB62	1.84	0.58
1:H:126:GLU:H	1:H:126:GLU:CD	2.06	0.58
1:I:126:GLU:HG2	1:I:127:HIS:CD2	2.38	0.58
1:H:61:LEU:HD11	1:H:132:ILE:HG23	1.85	0.58
2:P:275:ALA:HB2	2:P:652:THR:HG23	1.84	0.58
1:C:51:LYS:HE2	1:C:125:PRO:HB3	1.85	0.58
1:I:43:ALA:O	1:I:46:THR:OG1	2.20	0.58
1:A:126:GLU:H	1:A:126:GLU:CD	2.08	0.57
1:C:126:GLU:CD	1:C:126:GLU:H	2.08	0.57
1:E:126:GLU:H	1:E:126:GLU:CD	2.06	0.57
1:C:126:GLU:HG2	1:C:127:HIS:CD2	2.39	0.57
1:C:4:TYR:CE1	1:C:8:GLN:HG3	2.39	0.57
1:F:64:THR:OG1	1:F:139:GLU:OE2	2.23	0.56
1:F:4:TYR:CE1	1:F:8:GLN:HG3	2.41	0.56
1:F:137:MET:SD	1:G:60:LEU:HD21	2.47	0.55
1:F:35:GLY:O	1:F:39:GLU:HG3	2.07	0.55
1:F:126:GLU:H	1:F:126:GLU:CD	2.10	0.55
1:A:124:LYS:HB3	1:A:127:HIS:HD2	1.72	0.54
1:G:88:GLN:NE2	1:G:156:ALA:O	2.40	0.54
3:I:201:CDL:H232	1:J:21[B]:THR:HG22	1.88	0.54
1:G:32:LYS:NZ	6:G:302:HOH:O	2.40	0.54
1:J:59:GLN:O	1:J:62:PRO:HD2	2.08	0.54
1:D:22:ALA:HB2	1:D:96:SER:HB2	1.89	0.54
1:H:101:PHE:CE2	3:H:201:CDL:H352	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:CE2	1:A:8:GLN:HG3	2.43	0.54
1:H:126:GLU:HG2	1:H:127:HIS:CD2	2.43	0.53
1:I:6:ILE:HD13	1:J:4:TYR:CG	2.44	0.53
2:P:348:PRO:HG3	2:P:413:LYS:HD2	1.92	0.52
1:E:64:THR:OG1	1:E:139:GLU:OE2	2.27	0.52
1:C:2:MET:O	1:C:6:ILE:HG13	2.09	0.52
1:B:3:ASP:O	1:B:7:THR:HG23	2.10	0.51
1:A:144:LEU:HD11	1:B:67:LEU:HD23	1.91	0.51
1:G:25:PHE:HB2	1:G:100:ALA:HB1	1.91	0.51
1:D:67[B]:LEU:HD11	2:P:565:ILE:HD12	1.93	0.51
2:P:601:PHE:HA	2:P:605:ILE:HG12	1.92	0.51
1:F:10:GLY:O	1:F:13[B]:VAL:HG12	2.12	0.50
2:P:11:LEU:HB2	2:P:295:ILE:HB	1.93	0.50
2:P:42:ASN:ND2	2:P:331:GLU:OE2	2.41	0.50
1:E:51:LYS:HE2	1:E:125:PRO:HB3	1.93	0.49
2:P:338:THR:N	2:P:645:ARG:O	2.40	0.49
1:B:21[A]:THR:HB	1:B:96:SER:HG	1.76	0.49
1:G:51:LYS:HB3	1:G:121:LEU:HD11	1.95	0.49
1:C:152:LEU:HD21	1:D:19:MET:SD	2.52	0.49
1:H:19:MET:CE	1:H:77:PHE:HB2	2.42	0.49
2:P:387:TYR:CG	2:P:616:MET:HG3	2.47	0.49
1:C:75:LEU:O	1:C:79:ASN:ND2	2.42	0.48
6:C:205:HOH:O	2:P:629:ARG:NH1	2.46	0.48
2:P:298:TRP:CH2	2:P:327:PRO:HB3	2.48	0.48
1:J:133:ILE:O	1:J:137:MET:HG2	2.13	0.48
1:A:29:GLY:HA3	1:A:104:LEU:HA	1.95	0.48
1:C:71:VAL:HG11	2:P:575:MET:HE1	1.95	0.48
1:G:71:VAL:O	1:G:75[B]:LEU:HG	2.13	0.48
1:F:126:GLU:HG2	1:F:127:HIS:ND1	2.29	0.48
1:D:2:MET:O	1:D:6:ILE:HG12	2.13	0.48
1:E:19:MET:HE3	1:E:77:PHE:HB2	1.96	0.48
1:A:12:MET:SD	1:A:80:LEU:HD13	2.53	0.47
1:G:152:LEU:HD21	1:H:19:MET:SD	2.53	0.47
2:P:8:LYS:NZ	2:P:331:GLU:OE2	2.27	0.47
1:J:19:MET:CE	1:J:80:LEU:HD11	2.44	0.47
1:B:42:ALA:O	1:B:46:THR:HG23	2.15	0.47
1:I:17[B]:LEU:O	1:I:21[B]:THR:HG23	2.15	0.47
1:B:64:THR:OG1	1:B:139:GLU:OE2	2.33	0.47
3:A:201:CDL:H221	1:B:25:PHE:HE1	1.80	0.47
3:I:201:CDL:HB62	3:I:201:CDL:H712	1.67	0.47
1:D:83:ASP:OD1	1:D:83:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:VAL:HG23	1:I:4:TYR:CE1	2.50	0.46
3:F:202:CDL:H511	3:F:202:CDL:HB62	1.98	0.46
2:P:9:VAL:HG22	2:P:324:PHE:CD1	2.50	0.46
1:B:101:PHE:CD2	3:D:202:CDL:H771	2.50	0.46
1:H:18:ALA:HB2	1:H:93:LEU:HA	1.98	0.46
1:E:59:GLN:O	1:E:62:PRO:HD2	2.16	0.46
1:I:22:ALA:HB2	1:I:96:SER:HB2	1.97	0.46
1:F:19:MET:HE3	1:F:77:PHE:HB2	1.98	0.46
1:F:74:PHE:O	1:F:78:ILE:HG23	2.15	0.46
1:C:30:SER:OG	1:C:63:GLY:HA2	2.16	0.46
1:E:21[B]:THR:HG22	3:F:202:CDL:H821	1.98	0.46
1:H:6:ILE:HD13	1:H:6:ILE:HA	1.69	0.46
2:P:23:GLN:OE1	2:P:279:ARG:NH1	2.49	0.45
1:C:84:MET:HE3	1:C:84:MET:HB2	1.60	0.45
1:G:17[B]:LEU:HG	3:H:201:CDL:H832	1.98	0.45
1:I:152:LEU:HD21	1:J:19:MET:CE	2.47	0.45
1:F:1:MET:HE3	1:F:1:MET:HA	1.99	0.45
1:H:19:MET:HE3	1:H:77:PHE:HB2	1.97	0.45
1:A:75[B]:LEU:HD23	1:A:78:ILE:HD11	1.98	0.45
1:C:10:GLY:O	1:C:13[B]:VAL:HG12	2.17	0.45
3:F:202:CDL:HB62	3:F:202:CDL:H712	1.67	0.45
1:I:9:ASN:HD22	1:I:83:ASP:HB3	1.81	0.45
2:P:420:ILE:HB	2:P:421:PRO:HD3	1.99	0.45
3:A:201:CDL:H151	1:B:25:PHE:HE2	1.82	0.45
2:P:578:GLY:HA3	6:P:808:HOH:O	2.16	0.45
1:D:21[B]:THR:HG22	3:D:202:CDL:H222	1.98	0.45
1:F:59:GLN:O	1:F:62:PRO:HD2	2.16	0.45
1:H:45:THR:HG23	1:H:49:PRO:HA	1.98	0.45
1:C:3:ASP:O	1:C:7:THR:HG23	2.17	0.44
1:H:6:ILE:HD12	1:I:4:TYR:CG	2.52	0.44
1:J:64:THR:OG1	1:J:139:GLU:OE2	2.36	0.44
1:I:24:ILE:HG21	3:I:201:CDL:H781	1.99	0.44
1:I:75[B]:LEU:O	1:I:79:ASN:ND2	2.43	0.44
1:A:124:LYS:HB3	1:A:127:HIS:CD2	2.50	0.44
3:H:201:CDL:HB62	3:H:201:CDL:H711	1.32	0.44
3:I:201:CDL:H132	3:I:201:CDL:H341	1.99	0.44
1:C:64:THR:HG21	1:C:139:GLU:CD	2.38	0.44
1:I:3:ASP:O	1:I:7:THR:HG23	2.17	0.44
1:C:74:PHE:O	1:C:78:ILE:HG23	2.18	0.44
2:P:311:LEU:HD13	2:P:322:LEU:HD11	1.99	0.44
1:C:95:ALA:O	1:C:98:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLU:OE2	2:P:573:ARG:NH2	2.50	0.43
1:H:101:PHE:CD1	3:I:201:CDL:H792	2.52	0.43
1:I:44:LEU:HD13	1:I:122:ALA:HB2	2.00	0.43
1:B:154:LEU:HD21	2:P:594:PHE:HE2	1.82	0.43
1:E:42:ALA:O	1:E:46:THR:HG23	2.17	0.43
1:G:95:ALA:O	1:G:98:PRO:HD2	2.18	0.43
1:J:126:GLU:H	1:J:126:GLU:CD	2.22	0.43
1:C:137:MET:SD	1:D:60:LEU:HD21	2.59	0.43
1:F:126:GLU:HG2	1:F:127:HIS:CE1	2.54	0.43
1:B:18:ALA:HB2	1:B:93:LEU:HA	1.99	0.43
1:B:28:ILE:O	1:B:32:LYS:HG3	2.18	0.43
1:E:144:LEU:HD11	1:F:67:LEU:HD23	1.99	0.43
1:D:144:LEU:HD11	1:E:67:LEU:HD23	1.99	0.43
1:D:64:THR:OG1	1:D:139:GLU:OE2	2.37	0.43
2:P:327:PRO:HG2	2:P:332:ILE:HD11	2.01	0.43
1:A:3:ASP:O	1:A:7:THR:HG22	2.18	0.43
1:I:88:GLN:NE2	1:I:156:ALA:O	2.48	0.43
1:B:61:LEU:HD23	1:B:135:ALA:HB3	2.01	0.43
1:G:6:ILE:HG13	1:G:86:VAL:HG21	2.00	0.42
1:A:44:LEU:HD13	1:A:122:ALA:HB2	2.01	0.42
1:F:19:MET:HE1	1:F:77:PHE:HD1	1.84	0.42
1:J:95:ALA:O	1:J:98:PRO:HD2	2.19	0.42
2:P:309:HIS:O	2:P:312:GLN:HG3	2.19	0.42
1:I:25:PHE:HB2	1:I:100:ALA:HB1	2.01	0.42
1:E:129:THR:HA	1:E:132:ILE:HD12	2.01	0.42
1:G:17[B]:LEU:O	1:G:21[B]:THR:HG23	2.19	0.42
1:B:51:LYS:HE2	1:B:125:PRO:HB3	2.00	0.42
2:P:404:LEU:HD22	2:P:408:MET:HB3	2.00	0.42
1:E:19:MET:HE1	1:E:77:PHE:CD1	2.55	0.42
2:P:446:LEU:HB2	2:P:448:PHE:CD1	2.55	0.42
3:D:202:CDL:H711	3:D:202:CDL:HB62	1.93	0.42
1:G:59:GLN:O	1:G:62:PRO:HD2	2.20	0.42
1:A:95:ALA:O	1:A:98:PRO:HD2	2.19	0.42
2:P:592:VAL:HG21	2:P:608:ILE:HD13	2.01	0.42
3:A:201:CDL:HA21	1:B:32:LYS:HZ3	1.84	0.42
1:C:149:SER:O	1:C:153:VAL:HG23	2.19	0.42
1:F:117:GLY:O	6:F:301:HOH:O	2.21	0.42
3:A:201:CDL:H171	3:A:201:CDL:H142	1.79	0.42
1:D:110:GLN:HE22	1:D:139:GLU:HB2	1.85	0.42
1:D:61:LEU:HB2	1:D:62:PRO:HD3	2.02	0.41
1:D:19:MET:CE	1:D:77:PHE:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:LEU:HD13	1:H:16:VAL:HG13	2.02	0.41
2:P:648:LYS:HB2	2:P:648:LYS:HE2	1.86	0.41
1:D:59:GLN:O	1:D:62:PRO:HD2	2.19	0.41
2:P:40:SER:O	2:P:44:GLN:HG2	2.20	0.41
3:A:201:CDL:H781	1:J:101:PHE:CG	2.55	0.41
1:D:50:GLU:HG2	1:D:51:LYS:HG3	2.02	0.41
1:E:152:LEU:HD13	1:F:16:VAL:HG13	2.03	0.41
1:G:45:THR:HG23	1:G:49:PRO:HA	2.02	0.41
1:E:95:ALA:O	1:E:98:PRO:HD2	2.20	0.41
1:G:29:GLY:HA3	1:G:104:LEU:HA	2.02	0.41
1:E:10:GLY:O	1:E:13[B]:VAL:HG22	2.21	0.41
1:G:83:ASP:OD2	1:G:83:ASP:N	2.52	0.41
2:P:460:ILE:HG22	2:P:575:MET:HG3	2.01	0.41
1:C:42:ALA:O	1:C:46:THR:HG23	2.20	0.41
1:F:99:ILE:HD12	1:F:99:ILE:HA	1.89	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.87	0.41
3:A:201:CDL:H221	1:B:25:PHE:CE1	2.55	0.41
1:C:25:PHE:HB2	1:C:100:ALA:HB1	2.03	0.41
2:P:309:HIS:CE1	2:P:312:GLN:HE21	2.39	0.41
2:P:336:VAL:N	2:P:645:ARG:HH21	2.18	0.41
1:H:101:PHE:HE2	3:H:201:CDL:H352	1.84	0.40
1:B:44:LEU:HD13	1:B:122:ALA:HB2	2.03	0.40
1:C:26:SER:OG	1:C:69:GLY:HA3	2.21	0.40
1:J:61:LEU:HD23	1:J:61:LEU:HA	1.91	0.40
1:D:25:PHE:HB2	1:D:100:ALA:HB1	2.03	0.40
1:D:32:LYS:NZ	3:D:202:CDL:OA2	2.54	0.40
1:F:44:LEU:HD13	1:F:122:ALA:HB2	2.03	0.40
1:A:75[A]:LEU:HD12	1:A:78:ILE:HD11	2.02	0.40
1:F:19:MET:HE1	1:F:77:PHE:CD1	2.56	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	158/156 (101%)	156 (99%)	2 (1%)	0	100	100
1	B	160/156 (103%)	158 (99%)	2 (1%)	0	100	100
1	C	158/156 (101%)	154 (98%)	4 (2%)	0	100	100
1	D	161/156 (103%)	161 (100%)	0	0	100	100
1	E	159/156 (102%)	158 (99%)	1 (1%)	0	100	100
1	F	159/156 (102%)	157 (99%)	2 (1%)	0	100	100
1	G	158/156 (101%)	157 (99%)	1 (1%)	0	100	100
1	H	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
1	I	159/156 (102%)	155 (98%)	4 (2%)	0	100	100
1	J	158/156 (101%)	157 (99%)	1 (1%)	0	100	100
2	P	332/672 (49%)	319 (96%)	13 (4%)	0	100	100
All	All	1916/2232 (86%)	1882 (98%)	34 (2%)	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	117/113 (104%)	115 (98%)	2 (2%)	56	71
1	B	119/113 (105%)	117 (98%)	2 (2%)	56	71
1	C	117/113 (104%)	117 (100%)	0	100	100
1	D	120/113 (106%)	119 (99%)	1 (1%)	79	88
1	E	118/113 (104%)	117 (99%)	1 (1%)	79	88
1	F	118/113 (104%)	117 (99%)	1 (1%)	79	88
1	G	117/113 (104%)	116 (99%)	1 (1%)	75	86
1	H	113/113 (100%)	111 (98%)	2 (2%)	54	69
1	I	118/113 (104%)	118 (100%)	0	100	100
1	J	117/113 (104%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	281/579 (48%)	270 (96%)	11 (4%)	27	37
All	All	1455/1709 (85%)	1434 (99%)	21 (1%)	60	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	123	LYS
1	B	1	MET
1	B	8	GLN
1	D	30	SER
1	E	1	MET
1	F	1	MET
1	G	30	SER
1	H	83	ASP
1	H	123	LYS
2	P	18	ARG
2	P	41	GLU
2	P	299	VAL
2	P	313	ASN
2	P	334	GLU
2	P	371	MET
2	P	406	ARG
2	P	409	GLN
2	P	411	PHE
2	P	446	LEU
2	P	629	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
3	CDL	H	201	-	82,82,99	0.30	0	88,94,111	0.82	4 (4%)
3	CDL	I	201	-	81,81,99	0.31	0	87,93,111	0.90	4 (4%)
5	W3K	P	701	-	21,21,21	2.49	7 (33%)	25,30,30	1.09	2 (8%)
3	CDL	D	202	-	80,80,99	0.32	0	86,92,111	0.45	0
3	CDL	F	202	-	78,78,99	0.32	0	84,90,111	0.89	5 (5%)
3	CDL	A	201	-	82,82,99	0.30	0	88,94,111	0.43	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	CDL	H	201	-	-	26/93/93/110	-
3	CDL	I	201	-	-	28/92/92/110	-
5	W3K	P	701	-	-	0/8/8/8	0/3/3/3
3	CDL	D	202	-	-	27/91/91/110	-
3	CDL	F	202	-	-	22/89/89/110	-
3	CDL	A	201	-	-	22/93/93/110	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	701	W3K	CAK-CAJ	-5.71	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	701	W3K	CAC-CAD	-5.58	1.33	1.41
5	P	701	W3K	CAG-CAH	-4.62	1.33	1.41
5	P	701	W3K	CAA-CAB	-3.33	1.39	1.51
5	P	701	W3K	CAJ-NAE	-2.89	1.32	1.35
5	P	701	W3K	CAH-CAD	-2.66	1.33	1.42
5	P	701	W3K	CAJ-NAI	-2.59	1.32	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	201	CDL	OB6-CB5-C51	5.88	124.17	111.50
3	F	202	CDL	OB6-CB5-C51	5.51	123.37	111.50
3	H	201	CDL	OB6-CB5-C51	5.00	122.27	111.50
5	P	701	W3K	CAK-CAJ-NAI	2.96	127.45	123.55
3	I	201	CDL	OB6-CB5-OB7	-2.61	117.39	123.70
3	F	202	CDL	OB6-CB5-OB7	-2.53	117.58	123.70
3	F	202	CDL	OB6-CB4-CB6	2.51	117.50	108.40
3	H	201	CDL	OB6-CB4-CB6	2.38	117.01	108.40
3	H	201	CDL	OB6-CB5-OB7	-2.33	118.08	123.70
3	I	201	CDL	CB4-OB6-CB5	2.28	123.39	117.79
3	F	202	CDL	OA6-CA4-CA3	2.16	116.22	108.40
3	F	202	CDL	CB4-OB6-CB5	2.09	122.93	117.79
3	H	201	CDL	CB4-OB6-CB5	2.07	122.89	117.79
3	I	201	CDL	OB6-CB4-CB6	2.03	115.75	108.40
5	P	701	W3K	CAG-CAF-CAB	-2.01	118.00	121.64

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	CDL	OA9-CA7-OA8-CA6
3	A	201	CDL	C31-CA7-OA8-CA6
3	A	201	CDL	OB9-CB7-OB8-CB6
3	A	201	CDL	C71-CB7-OB8-CB6
3	D	202	CDL	CA3-OA5-PA1-OA4
3	D	202	CDL	CA4-CA3-OA5-PA1
3	D	202	CDL	CB3-OB5-PB2-OB3
3	D	202	CDL	OB9-CB7-OB8-CB6
3	D	202	CDL	C71-CB7-OB8-CB6
3	F	202	CDL	CA4-CA3-OA5-PA1
3	F	202	CDL	OA9-CA7-OA8-CA6
3	F	202	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
3	F	202	CDL	OB7-CB5-OB6-CB4
3	F	202	CDL	C51-CB5-OB6-CB4
3	F	202	CDL	OB9-CB7-OB8-CB6
3	F	202	CDL	C71-CB7-OB8-CB6
3	H	201	CDL	OA9-CA7-OA8-CA6
3	H	201	CDL	C31-CA7-OA8-CA6
3	H	201	CDL	OB7-CB5-OB6-CB4
3	H	201	CDL	C51-CB5-OB6-CB4
3	H	201	CDL	OB9-CB7-OB8-CB6
3	H	201	CDL	C71-CB7-OB8-CB6
3	I	201	CDL	OA9-CA7-OA8-CA6
3	I	201	CDL	C31-CA7-OA8-CA6
3	I	201	CDL	C1-CB2-OB2-PB2
3	I	201	CDL	OB7-CB5-OB6-CB4
3	I	201	CDL	C51-CB5-OB6-CB4
3	I	201	CDL	OB9-CB7-OB8-CB6
3	I	201	CDL	C71-CB7-OB8-CB6
3	D	202	CDL	OA6-CA4-CA6-OA8
3	D	202	CDL	CB5-C51-C52-C53
3	F	202	CDL	CA5-C11-C12-C13
3	F	202	CDL	CB5-C51-C52-C53
3	I	201	CDL	C76-C77-C78-C79
3	D	202	CDL	CA3-OA5-PA1-OA2
3	D	202	CDL	CB3-OB5-PB2-OB2
3	F	202	CDL	C74-C75-C76-C77
3	I	201	CDL	C11-C12-C13-C14
3	I	201	CDL	C51-C52-C53-C54
3	H	201	CDL	C34-C35-C36-C37
3	I	201	CDL	C14-C15-C16-C17
3	A	201	CDL	C81-C82-C83-C84
3	I	201	CDL	C73-C74-C75-C76
3	H	201	CDL	CB5-C51-C52-C53
3	H	201	CDL	C54-C55-C56-C57
3	H	201	CDL	C81-C82-C83-C84
3	H	201	CDL	C21-C22-C23-C24
3	A	201	CDL	C75-C76-C77-C78
3	H	201	CDL	C18-C19-C20-C21
3	I	201	CDL	C31-C32-C33-C34
3	F	202	CDL	C14-C15-C16-C17
3	H	201	CDL	OB5-CB3-CB4-CB6
3	D	202	CDL	CA3-CA4-CA6-OA8
3	D	202	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
3	H	201	CDL	CB3-CB4-CB6-OB8
3	I	201	CDL	C21-C22-C23-C24
3	F	202	CDL	C75-C76-C77-C78
3	A	201	CDL	C17-C18-C19-C20
3	I	201	CDL	OB5-CB3-CB4-CB6
3	D	202	CDL	C81-C82-C83-C84
3	A	201	CDL	C12-C13-C14-C15
3	A	201	CDL	CB3-CB4-CB6-OB8
3	I	201	CDL	CB3-CB4-CB6-OB8
3	I	201	CDL	C55-C56-C57-C58
3	D	202	CDL	OB6-CB4-CB6-OB8
3	F	202	CDL	C20-C21-C22-C23
3	F	202	CDL	OB5-CB3-CB4-CB6
3	I	201	CDL	OA5-CA3-CA4-CA6
3	A	201	CDL	C13-C14-C15-C16
3	A	201	CDL	CA3-CA4-CA6-OA8
3	A	201	CDL	OA6-CA4-CA6-OA8
3	A	201	CDL	OB6-CB4-CB6-OB8
3	H	201	CDL	OA6-CA4-CA6-OA8
3	D	202	CDL	C53-C54-C55-C56
3	I	201	CDL	CA2-OA2-PA1-OA5
3	H	201	CDL	C76-C77-C78-C79
3	A	201	CDL	O1-C1-CA2-OA2
3	A	201	CDL	C11-C12-C13-C14
3	D	202	CDL	CB3-OB5-PB2-OB4
3	D	202	CDL	OB5-CB3-CB4-CB6
3	H	201	CDL	CA3-CA4-CA6-OA8
3	F	202	CDL	OA6-CA4-CA6-OA8
3	I	201	CDL	OA6-CA4-CA6-OA8
3	F	202	CDL	CB7-C71-C72-C73
3	H	201	CDL	CA5-C11-C12-C13
3	D	202	CDL	C80-C81-C82-C83
3	I	201	CDL	CA6-CA4-OA6-CA5
3	D	202	CDL	C75-C76-C77-C78
3	D	202	CDL	CB2-OB2-PB2-OB5
3	F	202	CDL	CA2-OA2-PA1-OA5
3	H	201	CDL	CA2-OA2-PA1-OA5
3	A	201	CDL	C24-C25-C26-C27
3	I	201	CDL	C15-C16-C17-C18
3	I	201	CDL	CA5-C11-C12-C13
3	D	202	CDL	OB5-CB3-CB4-OB6
3	H	201	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
3	I	201	CDL	C79-C80-C81-C82
3	D	202	CDL	C55-C56-C57-C58
3	A	201	CDL	CA3-CA4-OA6-CA5
3	F	202	CDL	CA3-CA4-OA6-CA5
3	A	201	CDL	C74-C75-C76-C77
3	F	202	CDL	OA5-CA3-CA4-CA6
3	H	201	CDL	C14-C15-C16-C17
3	H	201	CDL	C72-C73-C74-C75
3	H	201	CDL	CB2-C1-CA2-OA2
3	I	201	CDL	CA3-CA4-CA6-OA8
3	H	201	CDL	C74-C75-C76-C77
3	I	201	CDL	C75-C76-C77-C78
3	A	201	CDL	C80-C81-C82-C83
3	A	201	CDL	C14-C15-C16-C17
3	D	202	CDL	CB6-CB4-OB6-CB5
3	D	202	CDL	OA5-CA3-CA4-OA6
3	A	201	CDL	C78-C79-C80-C81
3	F	202	CDL	C72-C71-CB7-OB8
3	H	201	CDL	C53-C54-C55-C56
3	H	201	CDL	C24-C25-C26-C27
3	F	202	CDL	C72-C71-CB7-OB9
3	D	202	CDL	CB2-OB2-PB2-OB3
3	F	202	CDL	CA3-OA5-PA1-OA3
3	I	201	CDL	C74-C75-C76-C77
3	I	201	CDL	CB6-CB4-OB6-CB5
3	D	202	CDL	C12-C11-CA5-OA6
3	D	202	CDL	C32-C31-CA7-OA8
3	D	202	CDL	C12-C11-CA5-OA7
3	A	201	CDL	C52-C51-CB5-OB6

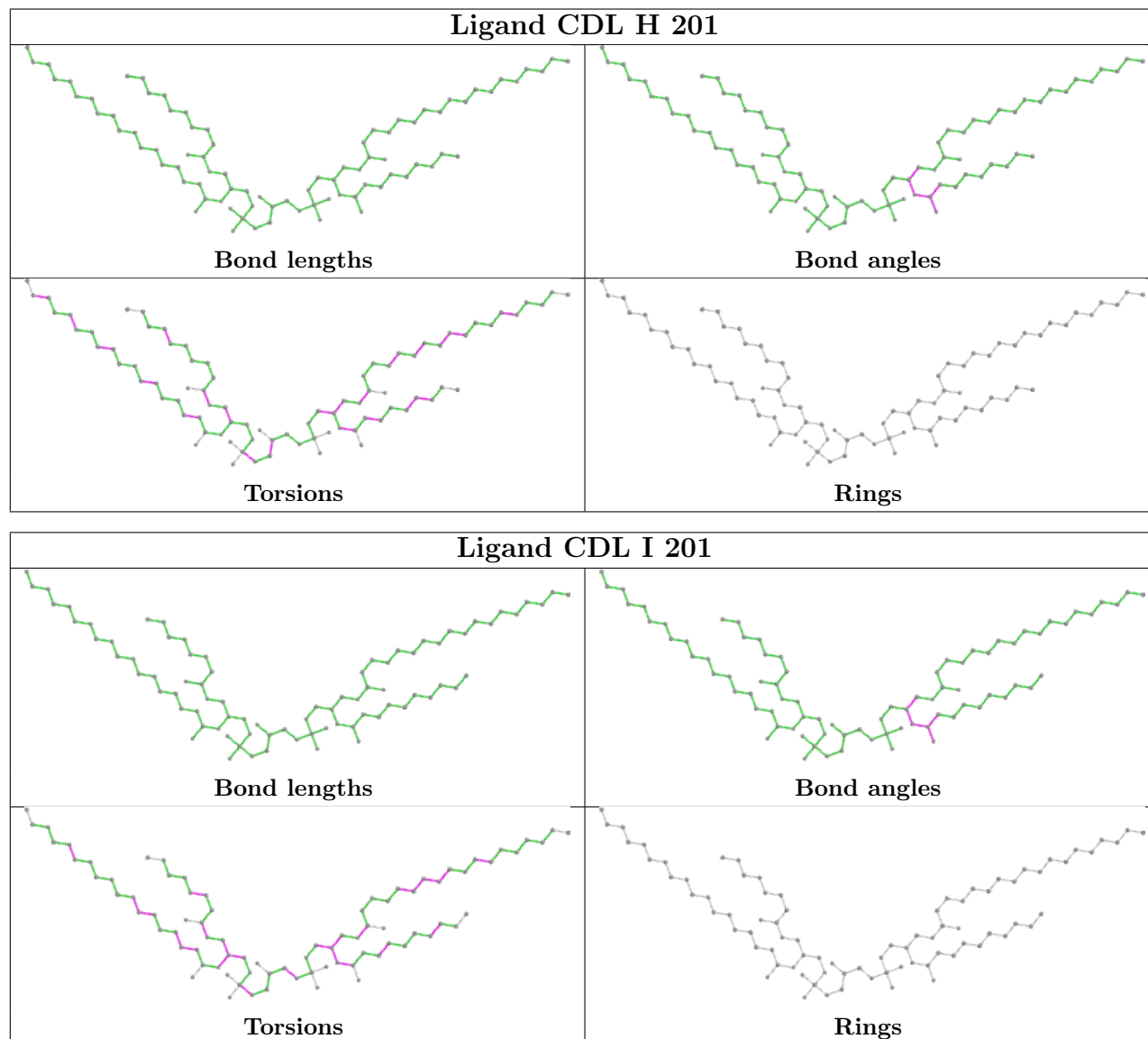
There are no ring outliers.

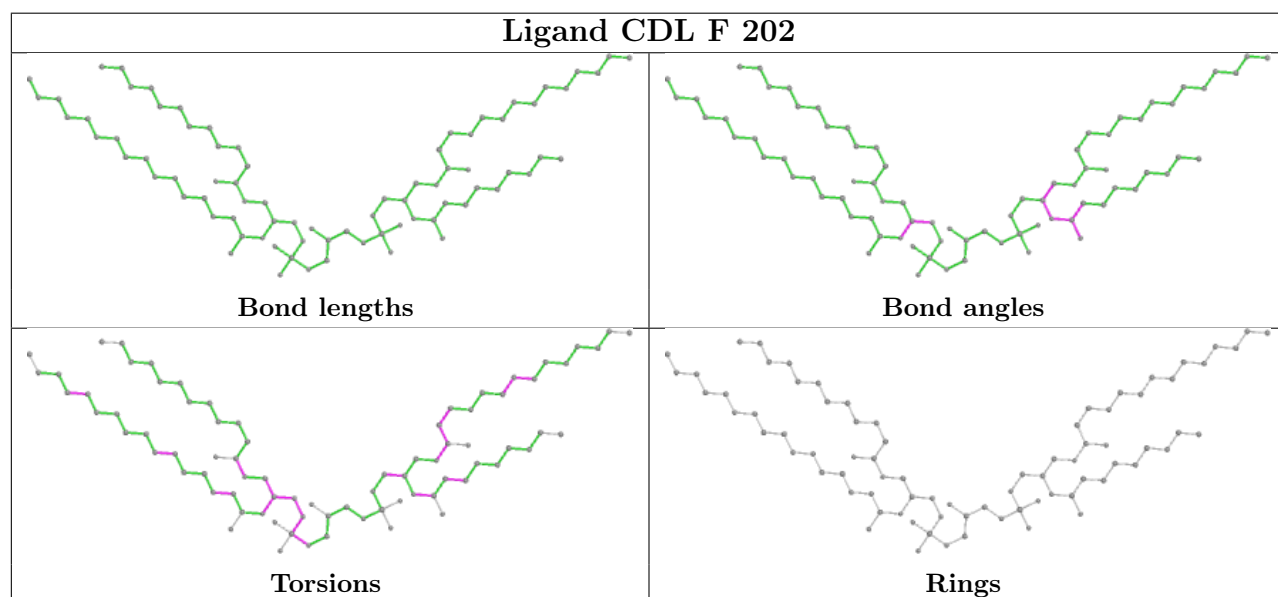
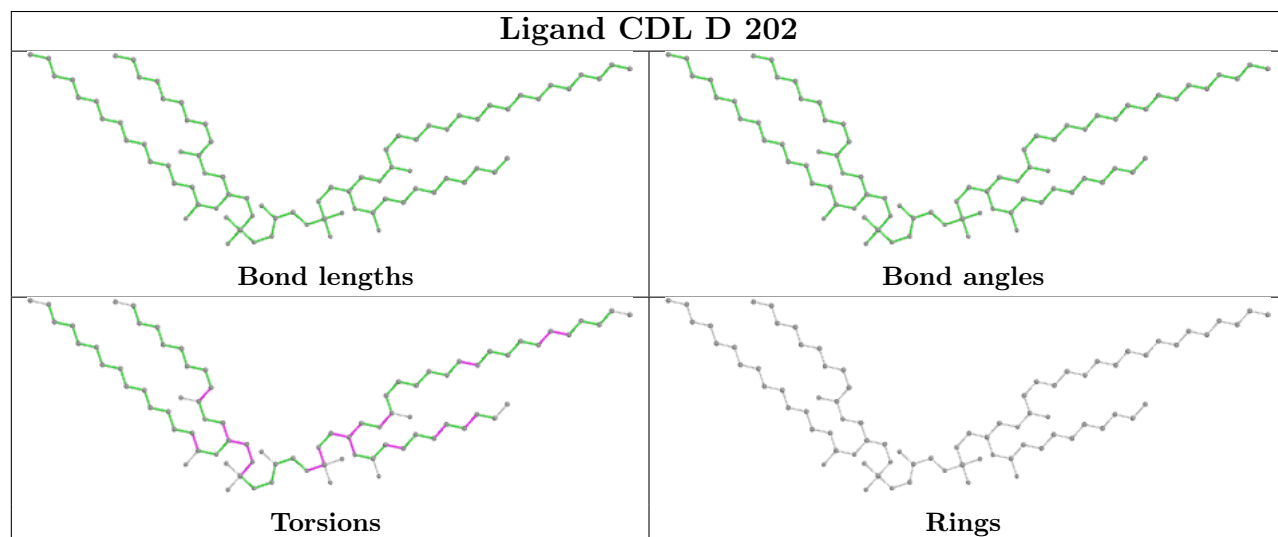
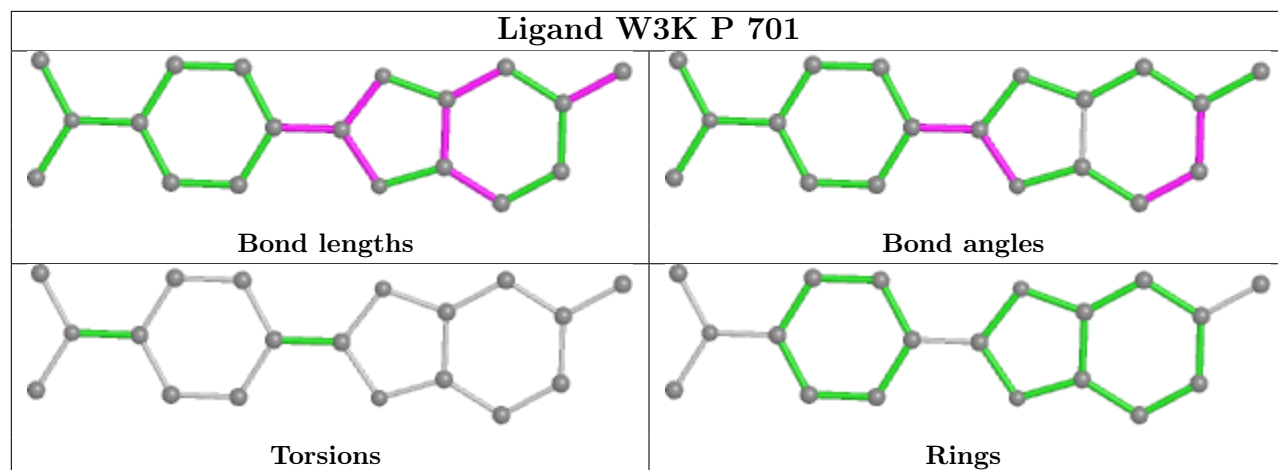
5 monomers are involved in 27 short contacts:

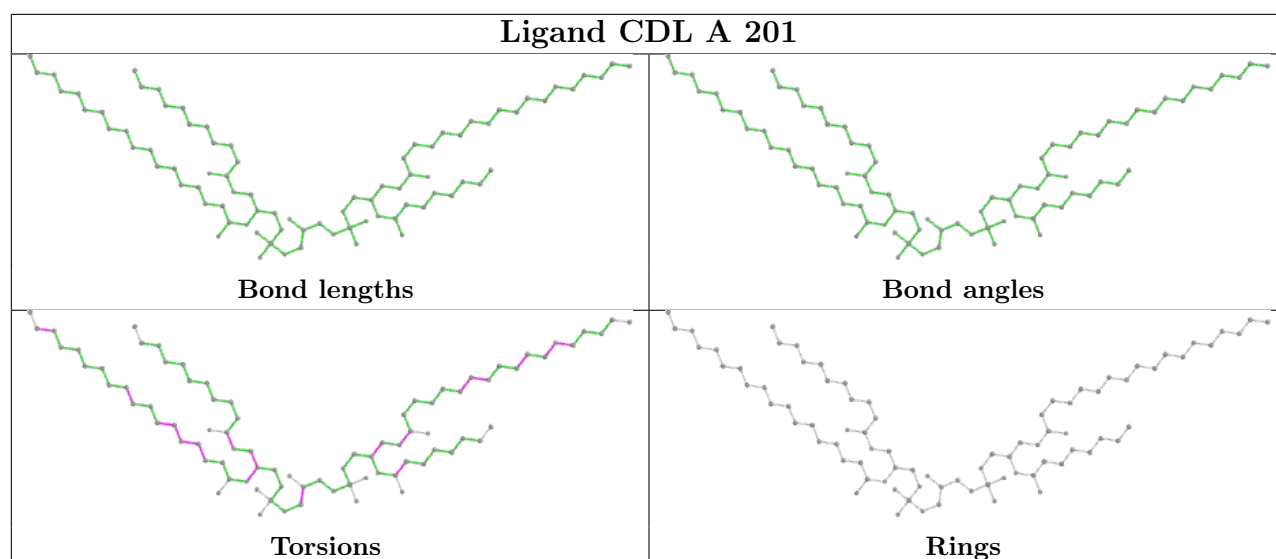
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	201	CDL	5	0
3	I	201	CDL	6	0
3	D	202	CDL	4	0
3	F	202	CDL	4	0
3	A	201	CDL	8	0

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.

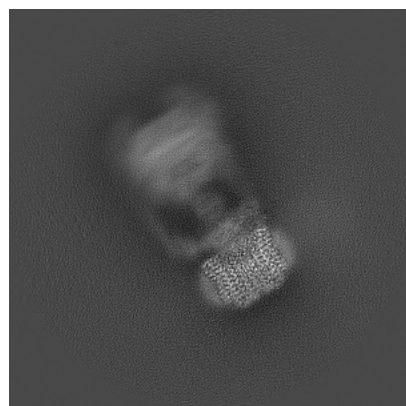
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37440. These allow visual inspection of the internal detail of the map and identification of artifacts.

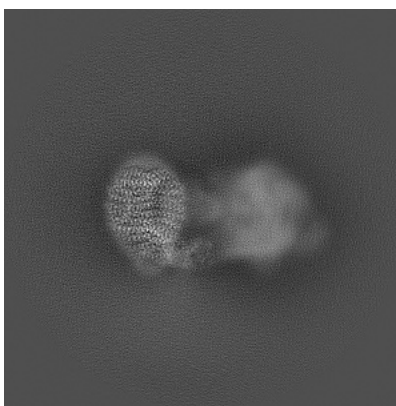
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

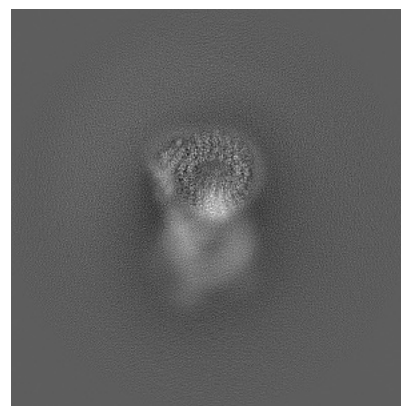
#### 6.1.1 Primary map



X

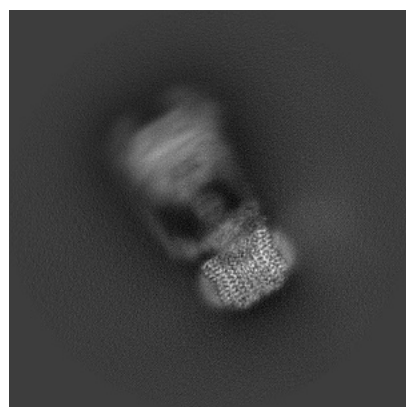


Y

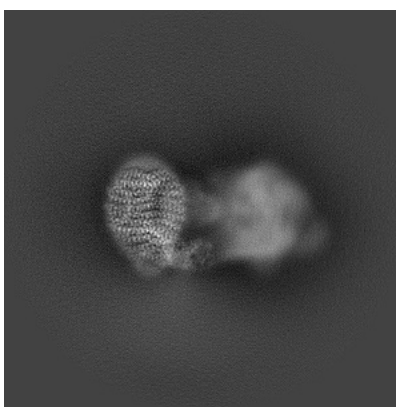


Z

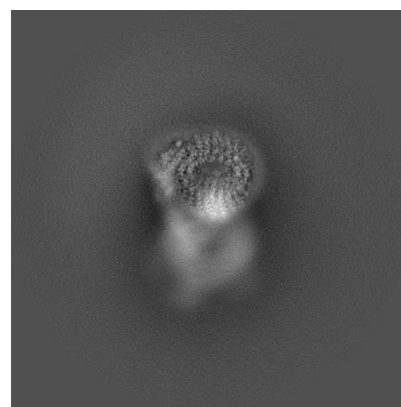
#### 6.1.2 Raw map



X



Y

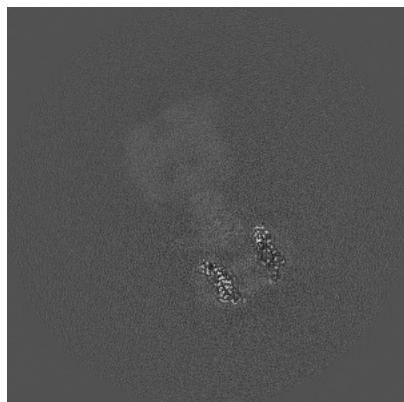


Z

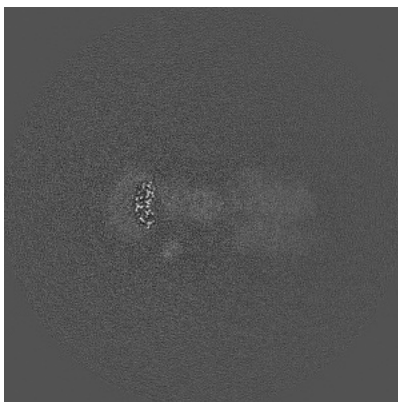
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

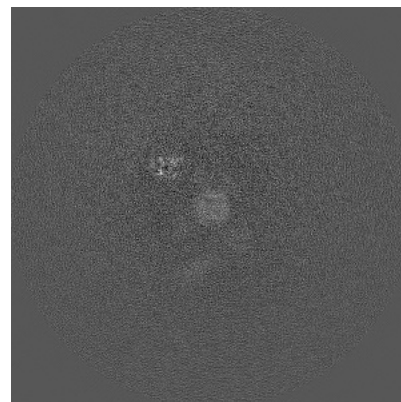
### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

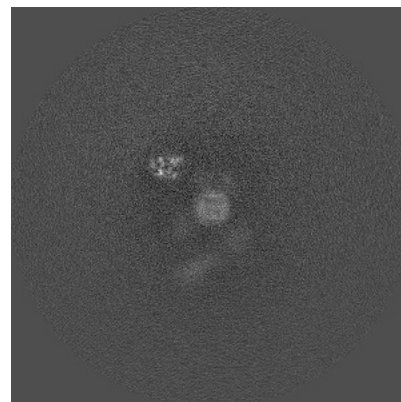
### 6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

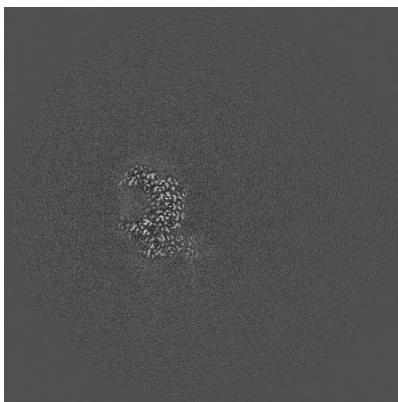


## 6.3 Largest variance slices [i](#)

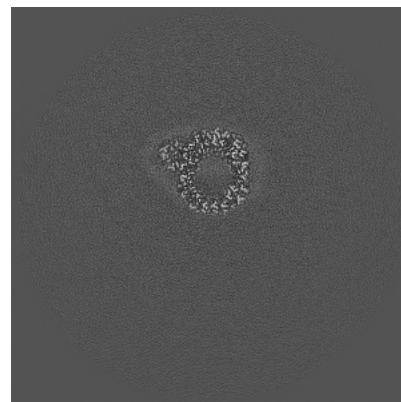
### 6.3.1 Primary map



X Index: 230



Y Index: 322

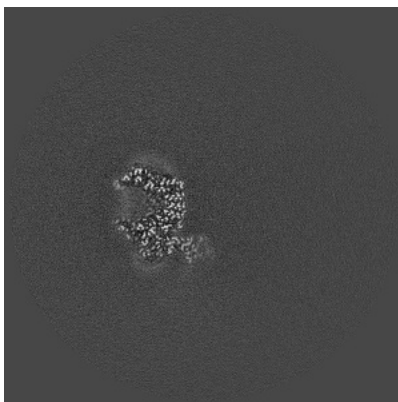


Z Index: 184

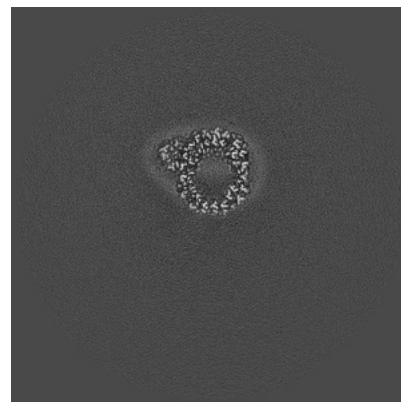
### 6.3.2 Raw map



X Index: 230



Y Index: 320

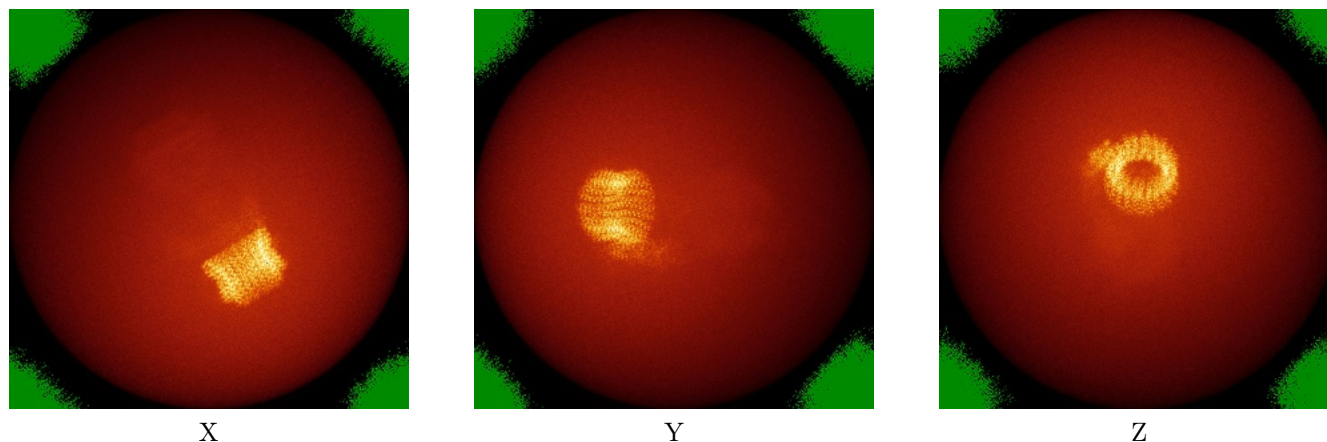


Z Index: 184

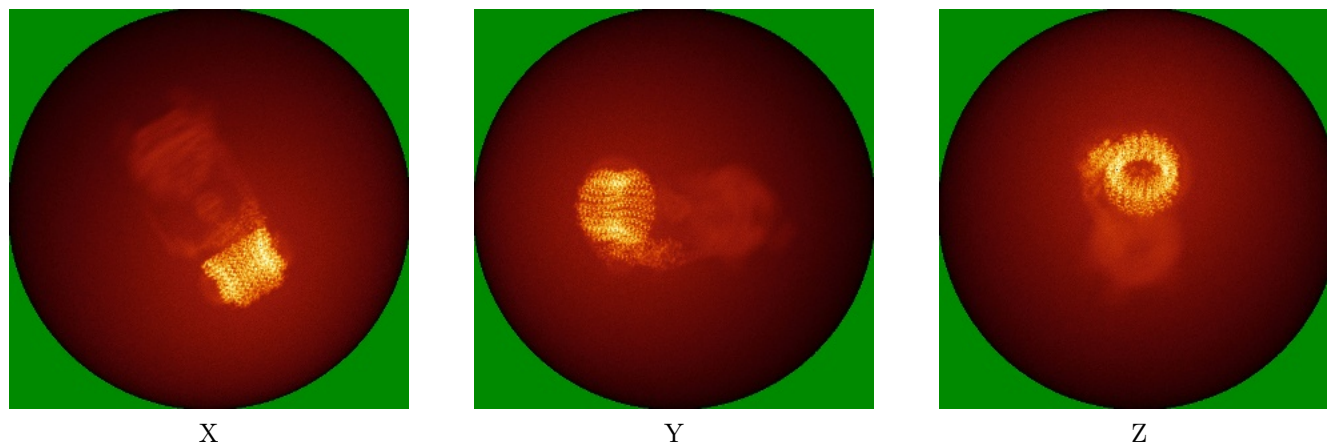
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

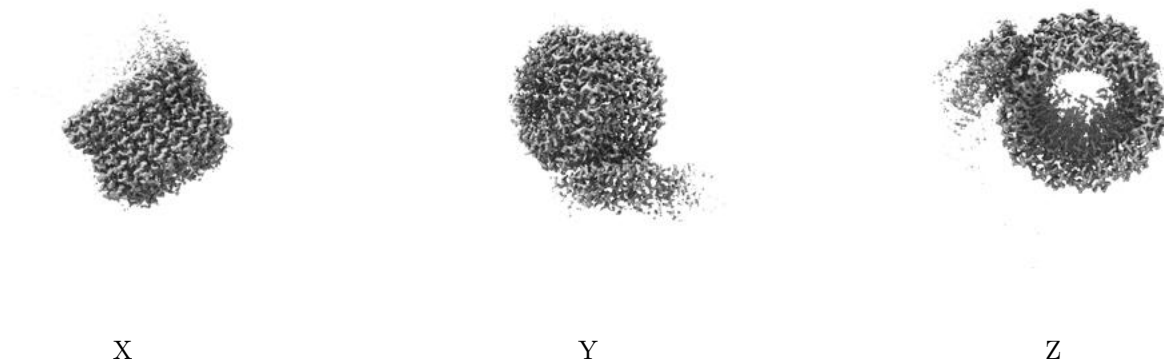


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



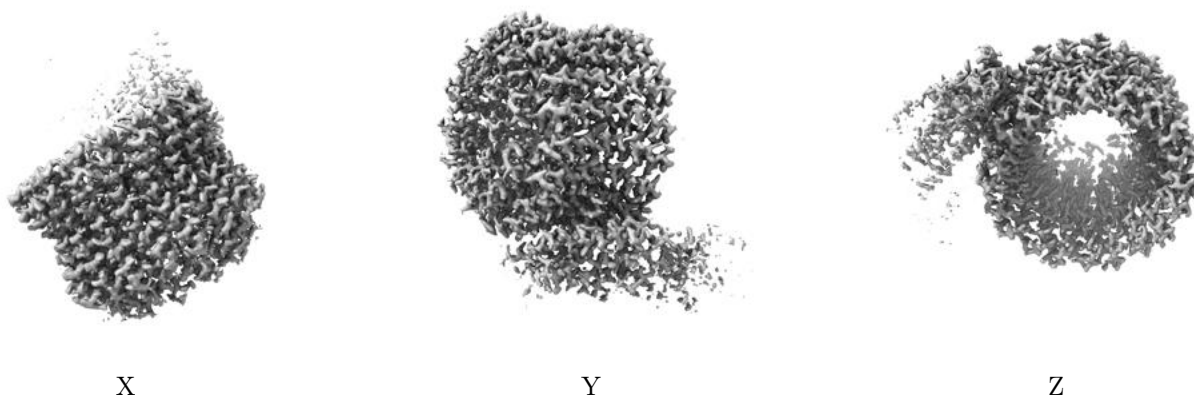
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.034. 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.

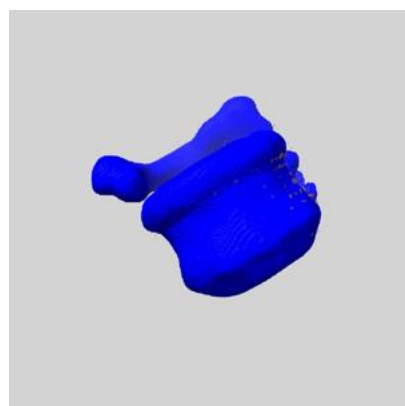
## 6.6 Mask visualisation [i](#)

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

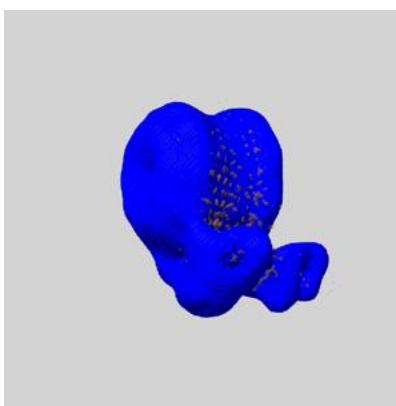
A mask typically either:

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

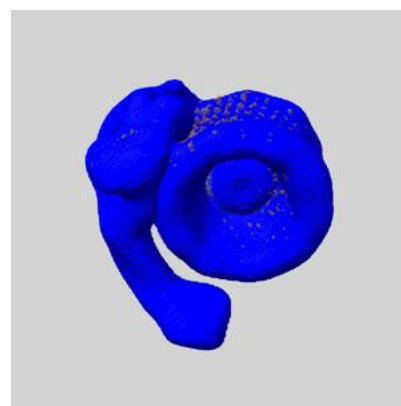
### 6.6.1 emd\_37440\_msk\_1.map [i](#)



X



Y

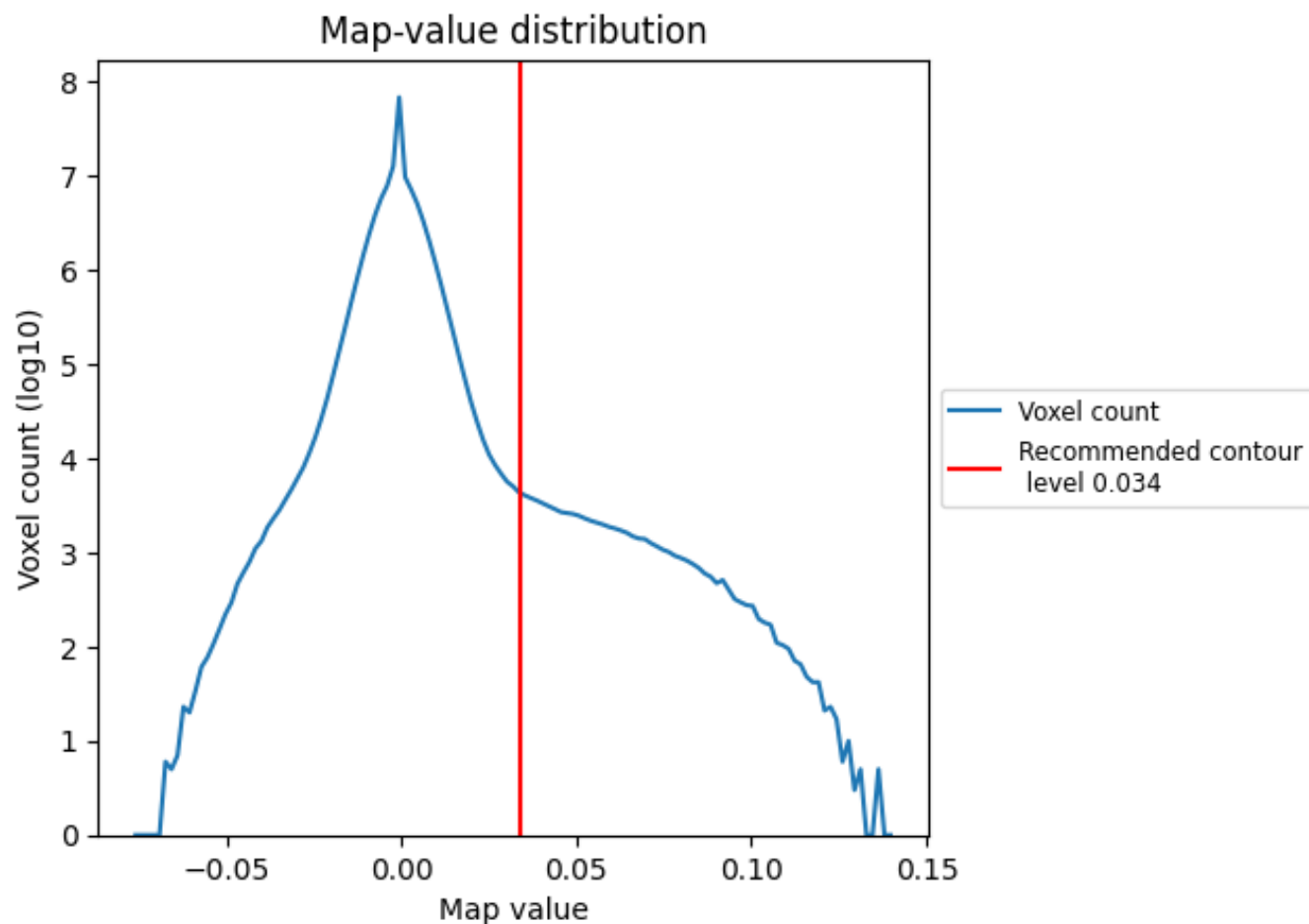


Z

## 7 Map analysis [i](#)

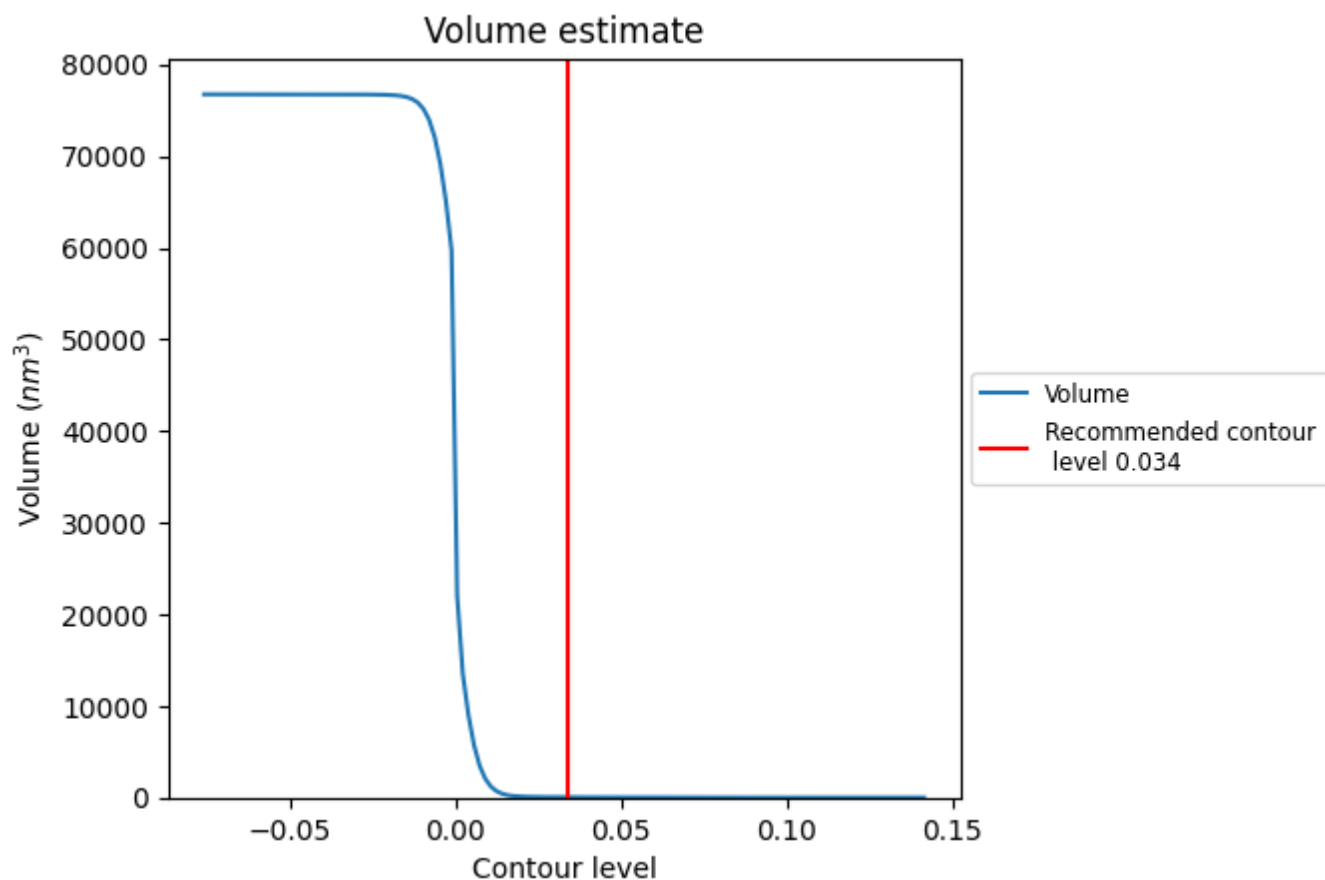
This section contains the results of statistical analysis of the map.

### 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.

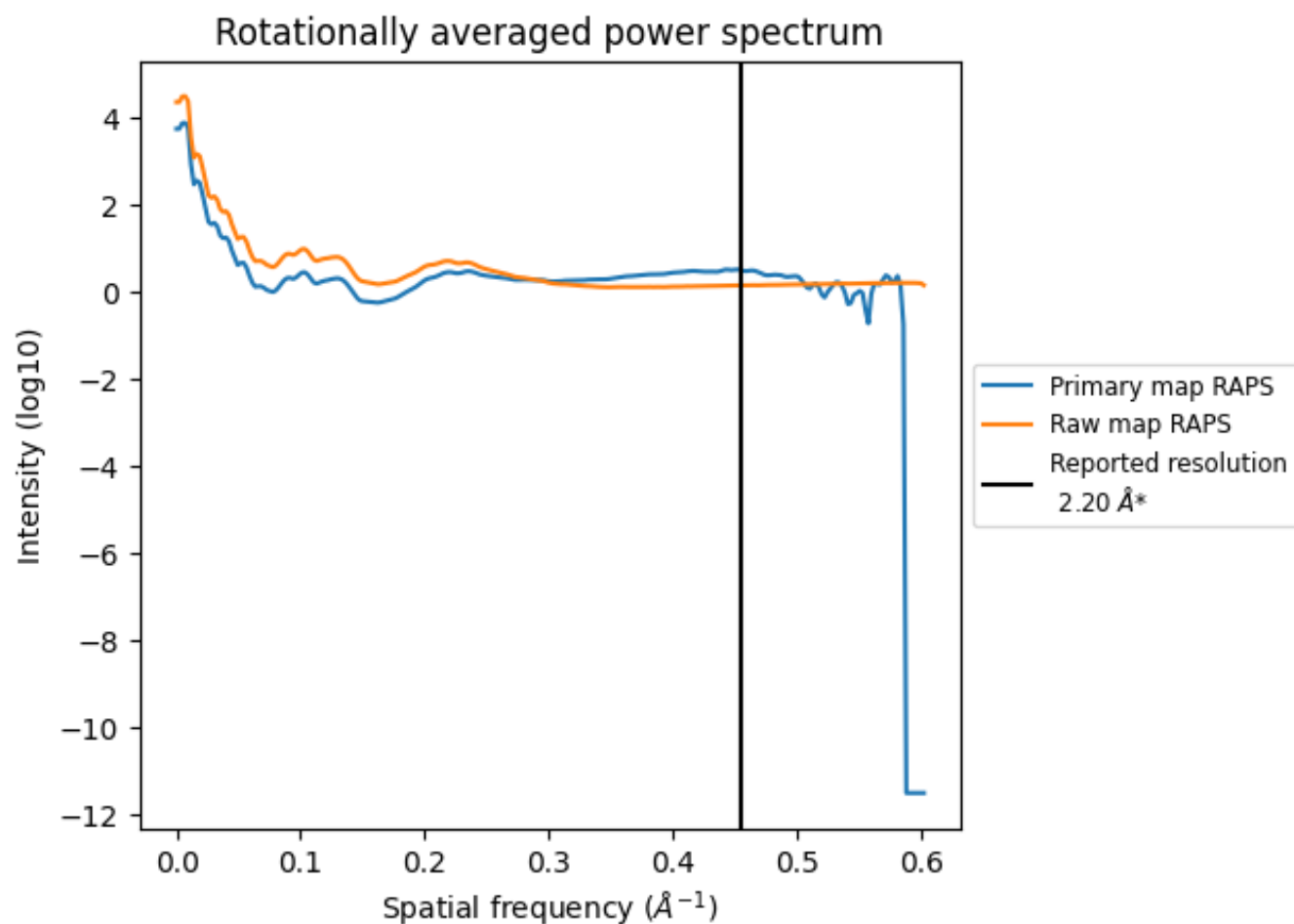
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; this corresponds to an approximate mass of 35 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 ⓘ

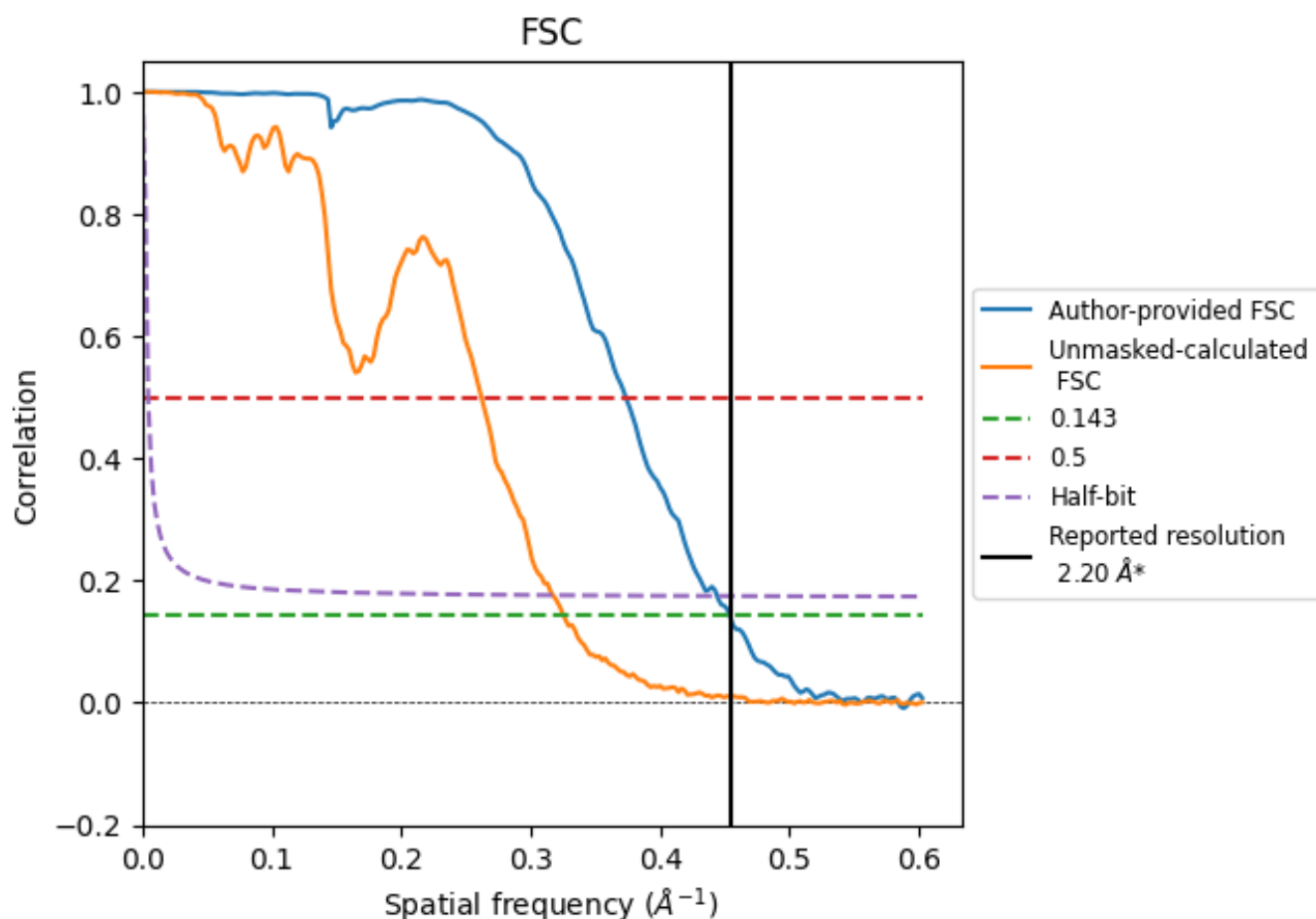


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

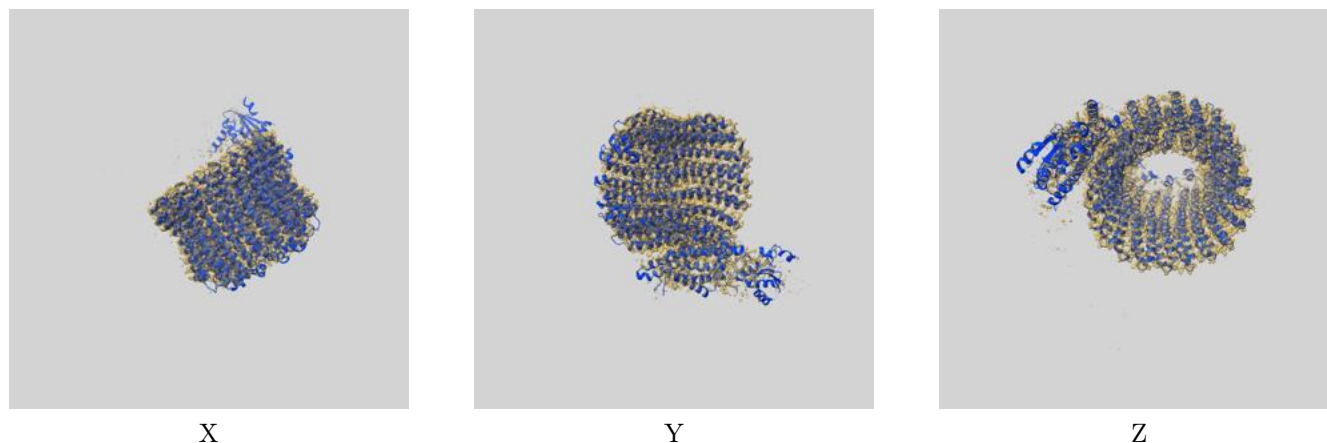
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.68	2.25
Unmasked-calculated*	3.07	3.82	3.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-37440 and PDB model 8WCI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

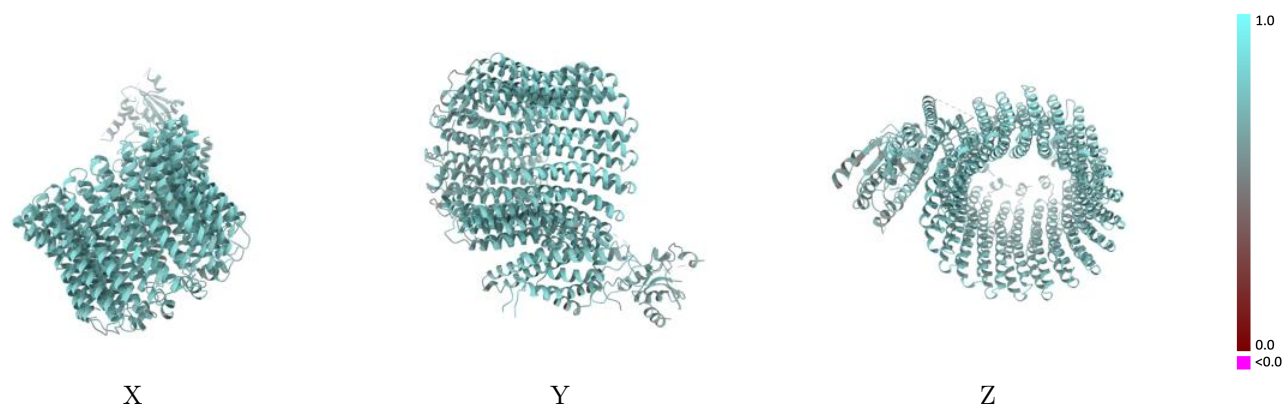
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.034 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.

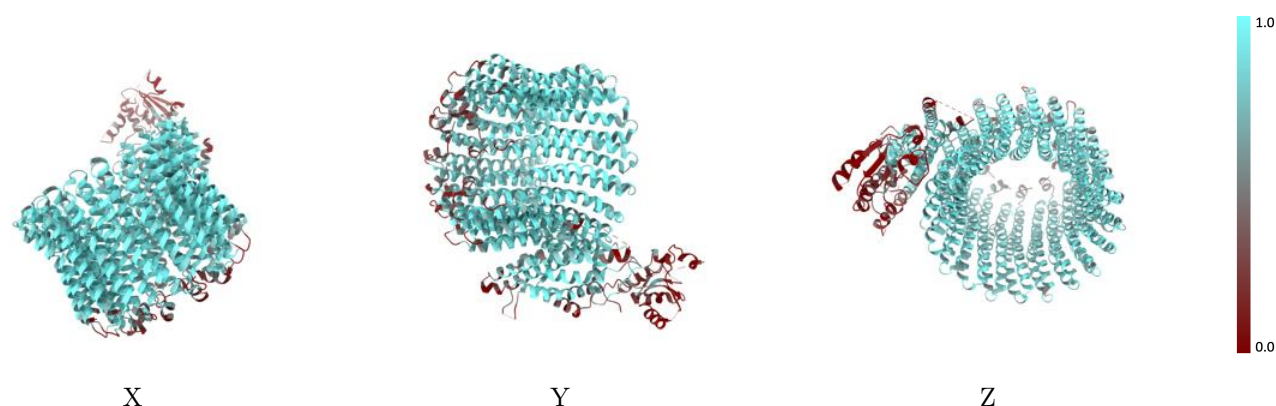


## 9.2 Q-score mapped to coordinate model [i](#)



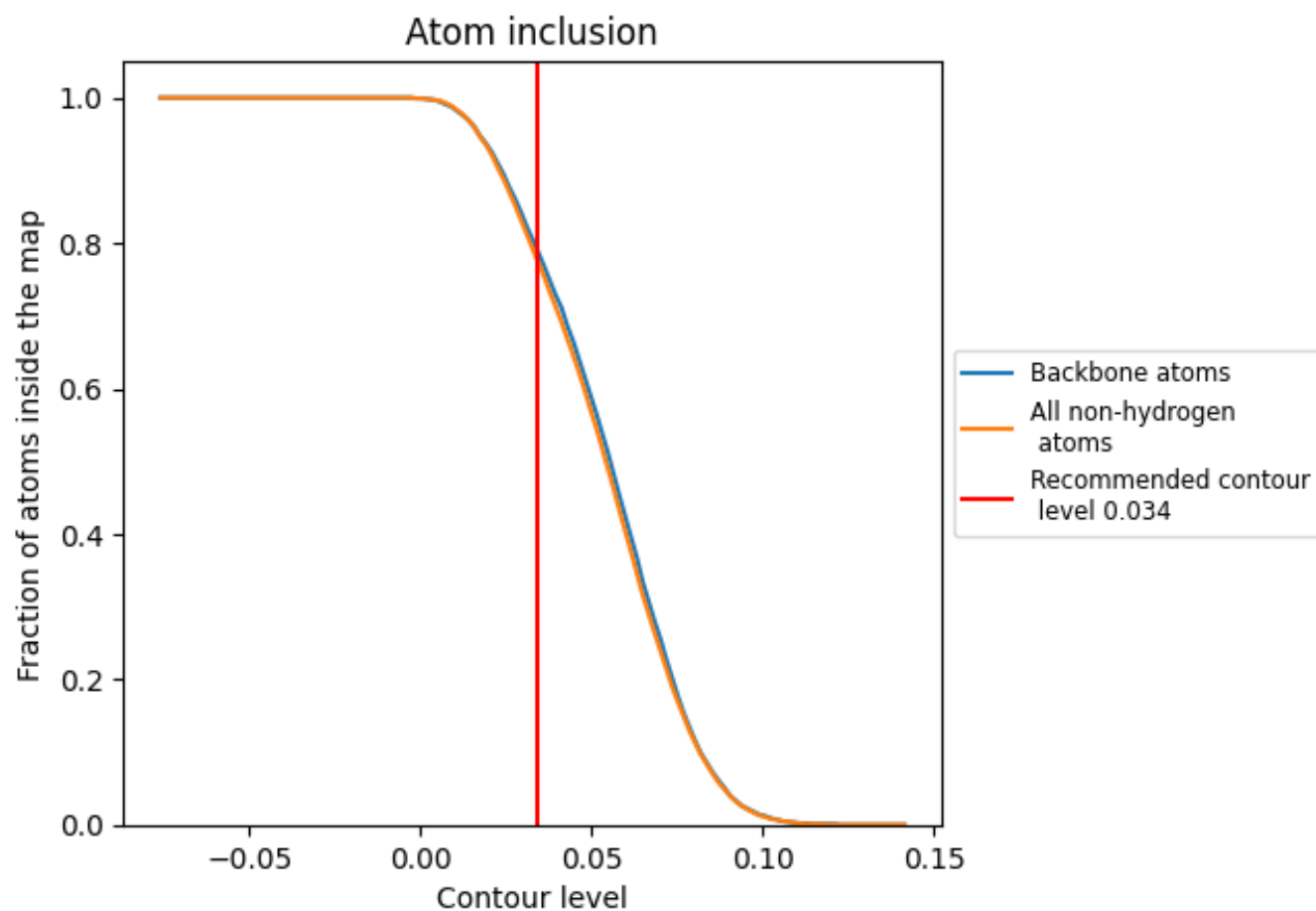
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.7250
A	<div></div> 0.8270	<div></div> 0.7310
B	<div></div> 0.8890	<div></div> 0.7470
C	<div></div> 0.8880	<div></div> 0.7540
D	<div></div> 0.8230	<div></div> 0.7350
E	<div></div> 0.8690	<div></div> 0.7440
F	<div></div> 0.8140	<div></div> 0.7340
G	<div></div> 0.8630	<div></div> 0.7440
H	<div></div> 0.8160	<div></div> 0.7300
I	<div></div> 0.7980	<div></div> 0.7260
J	<div></div> 0.8540	<div></div> 0.7360
P	<div></div> 0.4970	<div></div> 0.6700

1.0

0.0

<0.0