



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 7RK6 / pdb_00007rk6
EMDB ID : EMD-24493
Title : Aplysia Slo1 with Barium
Authors : Zhu, J.; Srivastava, S.; Cachau, R.; Holmgren, M.
Deposited on : 2021-07-22
Resolution : 2.91 Å(reported)
Based on initial model : 5TJ6

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

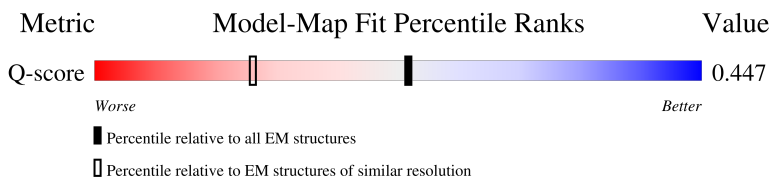
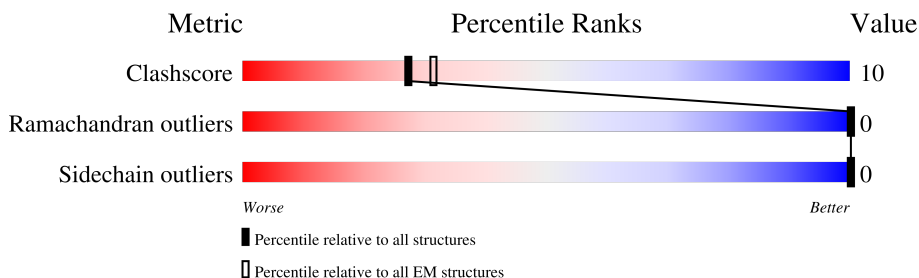
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.91 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	12972 (2.41 - 3.41)

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

Mol	Chain	Length	Quality of chain
1	A	1079	11% 62% 21% 17%
1	B	1079	11% 62% 21% 17%
1	C	1079	11% 61% 21% 17%
1	D	1079	11% 62% 20% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28615 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 BK channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	B	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	C	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	D	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	conflict	UNP Q5QJC5
A	1071	SER	-	expression tag	UNP Q5QJC5
A	1072	ASN	-	expression tag	UNP Q5QJC5
A	1073	PHE	-	expression tag	UNP Q5QJC5
A	1074	LEU	-	expression tag	UNP Q5QJC5
A	1075	GLU	-	expression tag	UNP Q5QJC5
A	1076	VAL	-	expression tag	UNP Q5QJC5
A	1077	LEU	-	expression tag	UNP Q5QJC5
A	1078	PHE	-	expression tag	UNP Q5QJC5
A	1079	GLN	-	expression tag	UNP Q5QJC5
B	2	ALA	THR	conflict	UNP Q5QJC5
B	1071	SER	-	expression tag	UNP Q5QJC5
B	1072	ASN	-	expression tag	UNP Q5QJC5
B	1073	PHE	-	expression tag	UNP Q5QJC5
B	1074	LEU	-	expression tag	UNP Q5QJC5
B	1075	GLU	-	expression tag	UNP Q5QJC5
B	1076	VAL	-	expression tag	UNP Q5QJC5
B	1077	LEU	-	expression tag	UNP Q5QJC5
B	1078	PHE	-	expression tag	UNP Q5QJC5
B	1079	GLN	-	expression tag	UNP Q5QJC5
C	2	ALA	THR	conflict	UNP Q5QJC5
C	1071	SER	-	expression tag	UNP Q5QJC5

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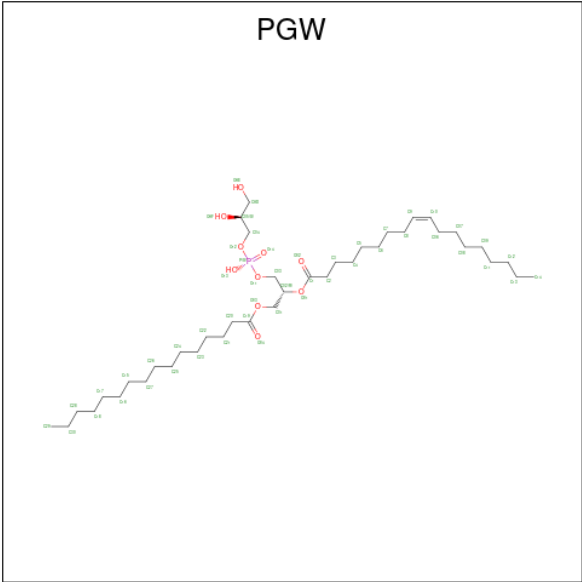
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1072	ASN	-	expression tag	UNP Q5QJC5
C	1073	PHE	-	expression tag	UNP Q5QJC5
C	1074	LEU	-	expression tag	UNP Q5QJC5
C	1075	GLU	-	expression tag	UNP Q5QJC5
C	1076	VAL	-	expression tag	UNP Q5QJC5
C	1077	LEU	-	expression tag	UNP Q5QJC5
C	1078	PHE	-	expression tag	UNP Q5QJC5
C	1079	GLN	-	expression tag	UNP Q5QJC5
D	2	ALA	THR	conflict	UNP Q5QJC5
D	1071	SER	-	expression tag	UNP Q5QJC5
D	1072	ASN	-	expression tag	UNP Q5QJC5
D	1073	PHE	-	expression tag	UNP Q5QJC5
D	1074	LEU	-	expression tag	UNP Q5QJC5
D	1075	GLU	-	expression tag	UNP Q5QJC5
D	1076	VAL	-	expression tag	UNP Q5QJC5
D	1077	LEU	-	expression tag	UNP Q5QJC5
D	1078	PHE	-	expression tag	UNP Q5QJC5
D	1079	GLN	-	expression tag	UNP Q5QJC5

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Ba 2 2	0
2	B	2	Total Ba 2 2	0
2	C	2	Total Ba 2 2	0
2	D	2	Total Ba 2 2	0

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			9	9			
3	A	1	Total	C			0
			9	9			
3	A	1	Total	C			0
			9	9			
3	A	1	Total	C	O	P	0
			19	12	6	1	
3	B	1	Total	C			0
			9	9			
3	B	1	Total	C			0
			9	9			
3	B	1	Total	C			0
			9	9			
3	B	1	Total	C	O	P	0
			19	12	6	1	
3	C	1	Total	C			0
			9	9			
3	C	1	Total	C			0
			9	9			
3	C	1	Total	C			0
			9	9			
3	C	1	Total	C	O	P	0
			19	12	6	1	
3	D	1	Total	C			0
			9	9			
3	D	1	Total	C			0
			9	9			

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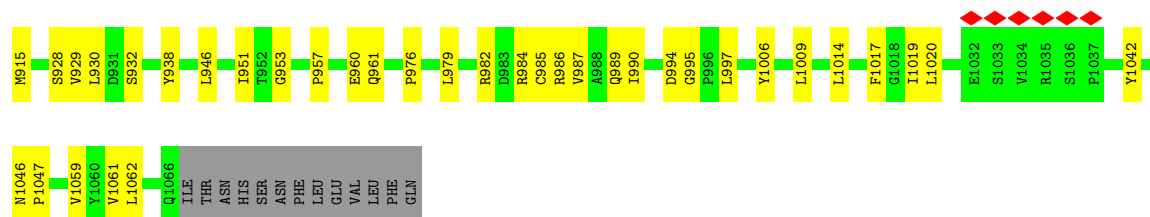
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C			0
			9	9			
3	D	1	Total	C	O	P	0
			19	12	6	1	

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

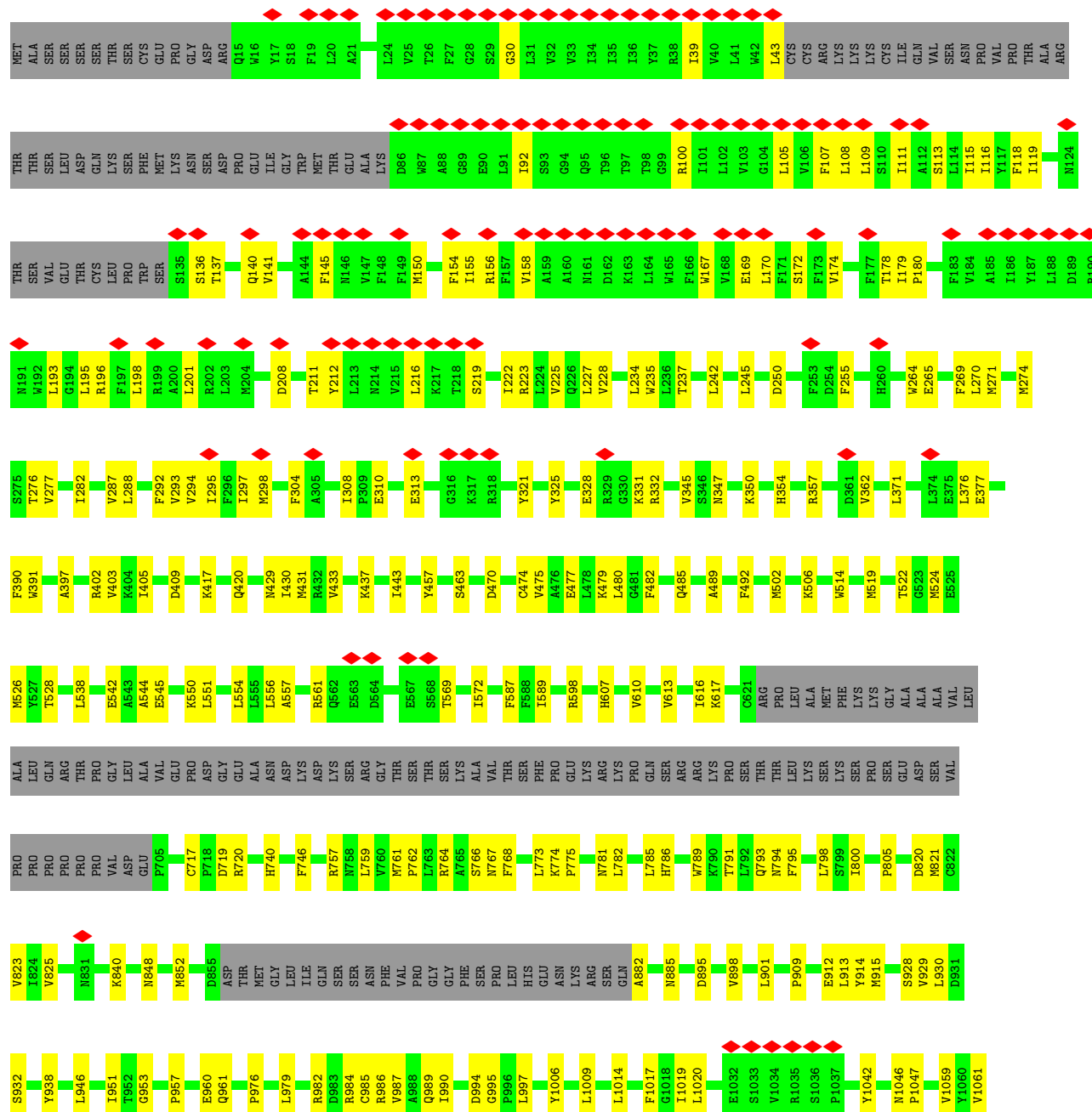
Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	K	0
			3	3	

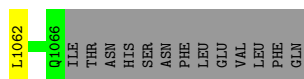
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	O	0
			1	1	
5	B	1	Total	O	0
			1	1	
5	C	1	Total	O	0
			1	1	
5	D	1	Total	O	0
			1	1	

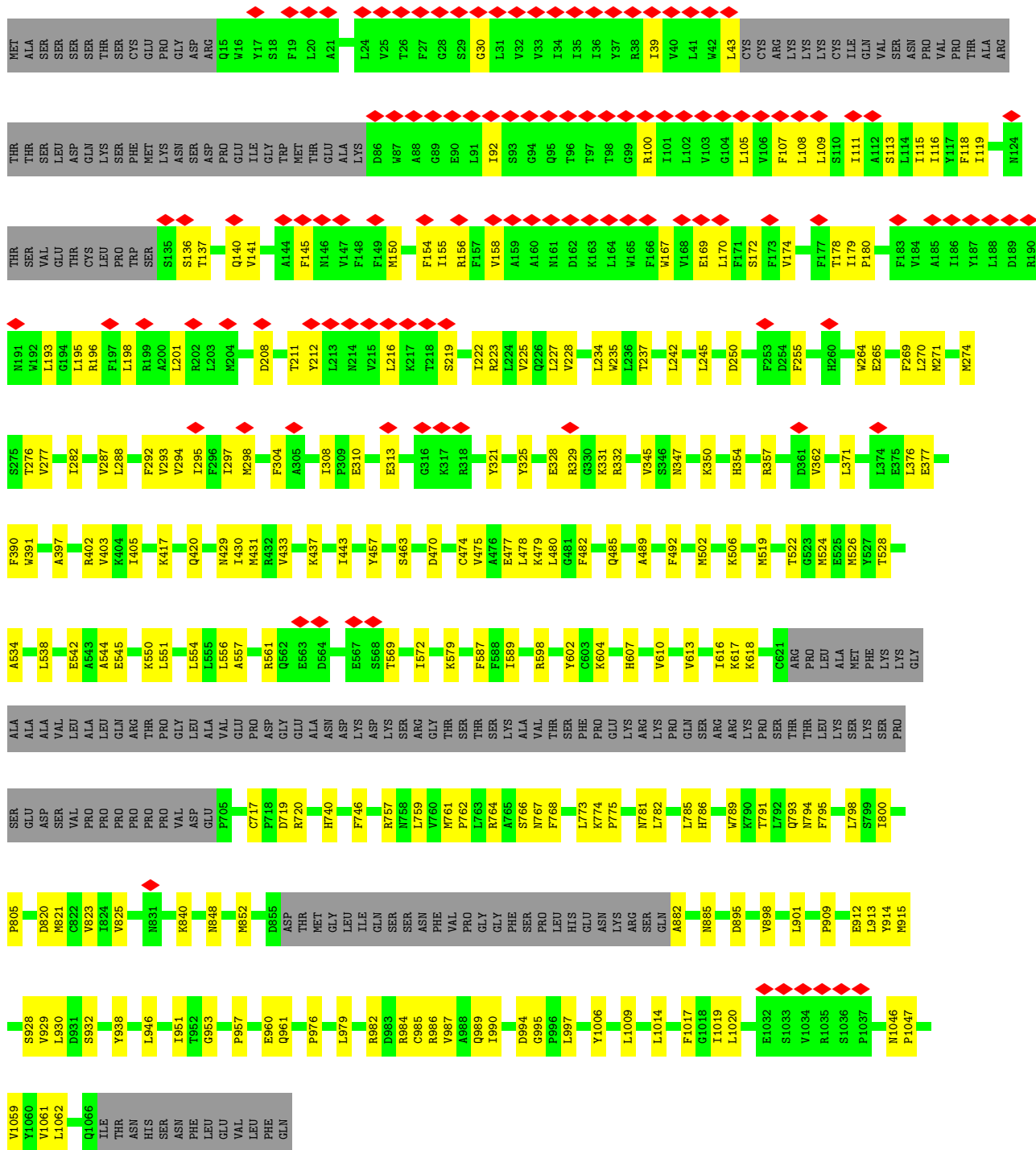


• Molecule 1: BK channel





• Molecule 1: BK channel



• Molecule 1: BK channel



MET	ALA	SER	SER	SER	SER	THR	SER	CYS	GLU	PRO	GLY	ASP	ARG	Q15	W16	Y17	S18	F19	L20	A21	L24	V25	T26	F27	G28	S29	G30	L31	V32	V33	I34	I35	I36	Y37	R38	I39	W40	L41	W42	L43	CYS	CYS	ARG	LYS	LYS	LYS	CYS	ILE	GLN	VAL	SER	ASN	PRO	VAL	PRO	THR	ALA	ARG
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THR	THR	SER	LEU	GLU	ASP	GLN	LYS	SER	PHE	MET	LYS	ASN	SER	ASP	PRO	GLU	ILE	GLY	TRP	MET	THR	ALA	ALA	D86	W87	A88	G89	E90	L91	I92	S93	G94	Q95	T96	T97	T98	G99	R100	I101	L102	V103	G104	L105	V106	F107	L108	L109	S110	I111	A112	S113	L114	I115	I116	Y117	F118	I119	W124
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THR	SER	VAL	GLU	THR	CYS	THR	LEU	PRO	TRP	SER	S135	S136	T137	Q140	V141	A144	F145	N146	V147	F148	F149	M150	F154	I155	F156	F157	V158	A159	A160	N161	D162	K163	L164	W165	F166	W167	V168	E169	L170	F171	S172	F173	V174	F177	T178	I179	P180	F183	V184	A185	I186	Y187	L188	D189	R190
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N191	W192	L193	G194	L195	R196	L197	L198	R199	V293	A200	L201	R202	L203	M204	D208	T211	Y212	L213	N214	V215	L216	K217	T218	S219	I222	R223	L224	V225	Q226	L227	V228	L234	W235	L236	T237	L242	L245	D250	F253	D254	F255	H260	W264	E265	F269	L270	M271	M274
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S275	T276	V277	I282	V287	L288	F292	V293	V294	I296	I297	M298	F304	A305	I308	P309	E310	E313	G316	K317	R318	Y321	Y325	L326	E328	R329	G330	K331	R332	V345	S346	N347	K350	H354	R357	D361	V362	L371	L374	E375	E377
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F390	W391	A397	R402	V403	L405	K417	Q420	M429	I430	M432	R433	K437	I443	Y457	S463	C474	V475	A476	E477	L478	K479	L480	G481	F482	Q485	A489	F492	M502	K506	M519	T522	G523	M524	E525	M526	Y527	T528	L538
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E542	A543	A544	E545	K550	L551	L554	L555	A557	R561	Q562	E563	D564	E567	S568	T569	I572	F587	F588	I589	R598	Y602	H607	V610	V613	I616	K617	C621	ARG	PRO	LEU	ALA	MET	PHE	LYS	LYS	GLY	ALA	ALA	ALA	VAL	LEU	ALA	GLN	ARG
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THR	PRO	GLY	ALA	VAL	GLU	ASP	PRO	GLU	ASP	LYS	LYS	LYS	ARG	GLY	THR	THR	THR	SER	LYS	ALA	VAL	THR	SER	PHE	PRO	GLU	LYS	ARG	ARG	LYS	PRO	SER	THR	THR	THR	LEU	LYS	SER	LYS	SER	PRO	SER	GLU	ASP	SER	VAL	PRO	PRO	PRO
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PRO	PRO	VAL	ASP	GLU	P705	C717	F718	D719	R720	H740	F746	R757	W758	L759	W760	W761	P762	L763	R764	W765	S766	W767	F768	L773	K774	P775	W781	L782	L785	H786	W789	Q793	N794	F795	L798	W799	I800	P805	D820	V823	I824	W825	N831	K840
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N848	M852	D855	ASP	THR	MET	GLY	LEU	ILE	GLN	SER	ASN	R984	C985	R986	V987	A988	Q989	I990	D994	G995	P996	L997	Y1006	L1009	L1014	F1017	G1018	I1019	L1020	E1032	S1033	V1034	R1035	S1036	P1037	N1046	P1047	V1059	Y1060	V1061	L1062	Q1066	ILE	THR	ASN	HIS	SER	ASN
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PHE	LEU	GLU	VAL	LEU	PHE	GLN	T952	G953	P957	E960	Q961	P976	L979	R982	D983	C984	R985	R986	V987	A988	Q989	I990	D994	G995	P996	L997	Y1006	L1009	L1014	F1017	G1018	I1019	L1020	E1032	S1033	V1034	R1035	S1036	P1037	N1046	P1047	V1059	Y1060	V1061	L1062	Q1066	ILE	THR	ASN	HIS	SER	ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	973760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	44.569	Depositor
Minimum map value	-20.460	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	340.48, 340.48, 340.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.33, 1.33, 1.33	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: PGW, K, BA

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	0.12	0/7272	0.29	0/9869
1	B	0.12	0/7272	0.29	0/9869
1	C	0.12	0/7272	0.29	0/9869
1	D	0.12	0/7272	0.29	0/9869
All	All	0.12	0/29088	0.29	0/39476

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	7104	0	7064	143	0
1	B	7104	0	7064	141	0
1	C	7104	0	7064	145	0
1	D	7104	0	7064	140	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	46	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	57	4	0
3	C	46	0	57	4	0
3	D	46	0	57	4	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	28615	0	28484	557	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 10.

The worst 5 of 557 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:B:506:LYS:H	1:B:519:MET:HE2	1.51	0.76
1:A:506:LYS:H	1:A:519:MET:HE2	1.51	0.76
1:C:506:LYS:H	1:C:519:MET:HE2	1.51	0.75
1:D:506:LYS:H	1:D:519:MET:HE2	1.51	0.75
1:A:357:ARG:HG2	1:A:502:MET:HE2	1.70	0.73

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	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
1	B	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
1	C	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
All	All	3524/4316 (82%)	3372 (96%)	152 (4%)	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	777/945 (82%)	777 (100%)	0	100	100
1	B	777/945 (82%)	777 (100%)	0	100	100
1	C	777/945 (82%)	777 (100%)	0	100	100
1	D	777/945 (82%)	777 (100%)	0	100	100
All	All	3108/3780 (82%)	3108 (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. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	615	GLN
1	D	454	ASN
1	C	406	GLN
1	D	383	HIS
1	B	758	ASN

5.3.3 RNA ⓘ

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 27 ligands modelled in this entry, 11 are monoatomic - leaving 16 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	PGW	C	1104	-	8,8,50	0.75	0	7,7,56	0.41	0
3	PGW	D	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	C	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)
3	PGW	D	1104	-	8,8,50	0.76	0	7,7,56	0.41	0
3	PGW	B	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	A	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)
3	PGW	B	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.49	1 (4%)
3	PGW	B	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	B	1104	-	8,8,50	0.75	0	7,7,56	0.42	0
3	PGW	C	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.90	0
3	PGW	D	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	D	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)
3	PGW	A	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	A	1104	-	8,8,50	0.76	0	7,7,56	0.41	0
3	PGW	A	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	C	1103	-	8,8,50	0.76	0	7,7,56	0.42	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	PGW	C	1104	-	-	6/6/6/55	-
3	PGW	D	1103	-	-	6/6/6/55	-
3	PGW	C	1106	-	-	10/17/17/55	-
3	PGW	D	1104	-	-	6/6/6/55	-
3	PGW	B	1103	-	-	6/6/6/55	-
3	PGW	A	1106	-	-	10/17/17/55	-
3	PGW	B	1106	-	-	10/17/17/55	-
3	PGW	B	1105	-	-	2/6/6/55	-
3	PGW	B	1104	-	-	6/6/6/55	-
3	PGW	C	1105	-	-	2/6/6/55	-
3	PGW	D	1105	-	-	2/6/6/55	-
3	PGW	D	1106	-	-	10/17/17/55	-
3	PGW	A	1103	-	-	6/6/6/55	-
3	PGW	A	1104	-	-	6/6/6/55	-
3	PGW	A	1105	-	-	2/6/6/55	-
3	PGW	C	1103	-	-	6/6/6/55	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1106	PGW	P-O14	7.40	1.73	1.50
3	A	1106	PGW	P-O14	7.39	1.73	1.50
3	C	1106	PGW	P-O14	7.39	1.73	1.50
3	D	1106	PGW	P-O14	7.39	1.73	1.50
3	A	1106	PGW	P-O11	4.52	1.74	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1106	PGW	O13-P-O12	5.12	127.01	107.80
3	A	1106	PGW	O13-P-O12	5.11	126.96	107.80
3	C	1106	PGW	O13-P-O12	5.11	126.96	107.80
3	D	1106	PGW	O13-P-O12	5.11	126.96	107.80

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

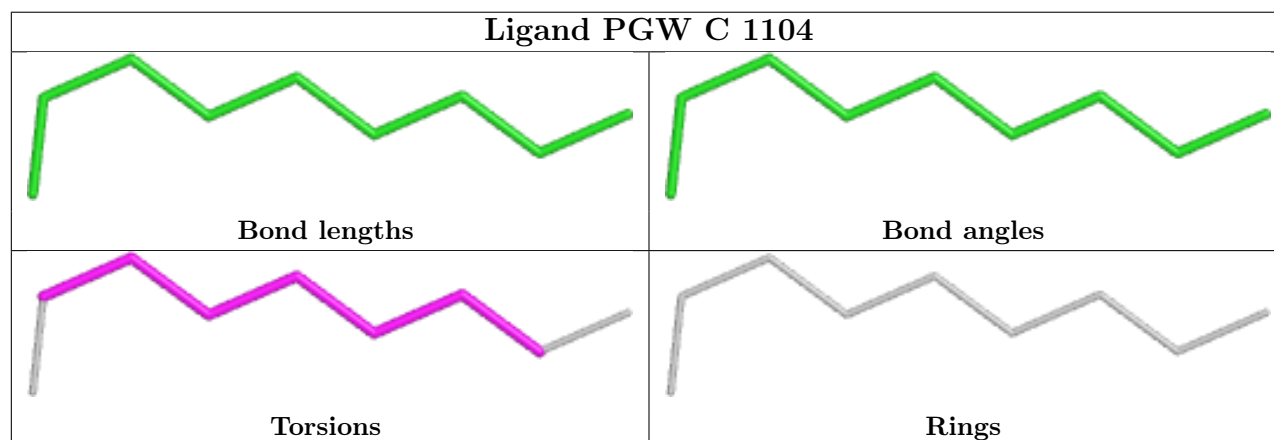
Mol	Chain	Res	Type	Atoms
3	A	1106	PGW	C03-O11-P-O13
3	A	1106	PGW	C02-C03-O11-P
3	B	1106	PGW	C03-O11-P-O13
3	B	1106	PGW	C02-C03-O11-P
3	C	1106	PGW	C03-O11-P-O13

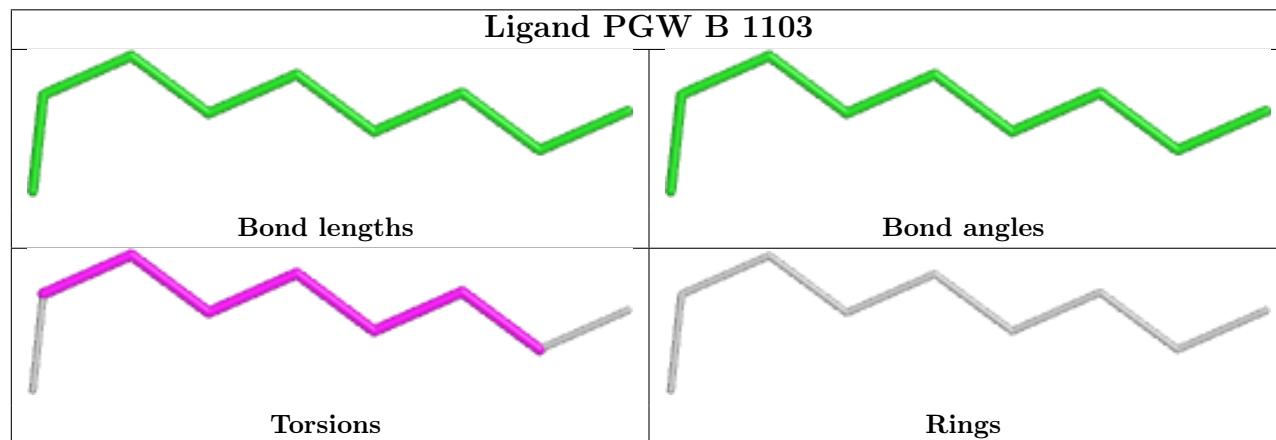
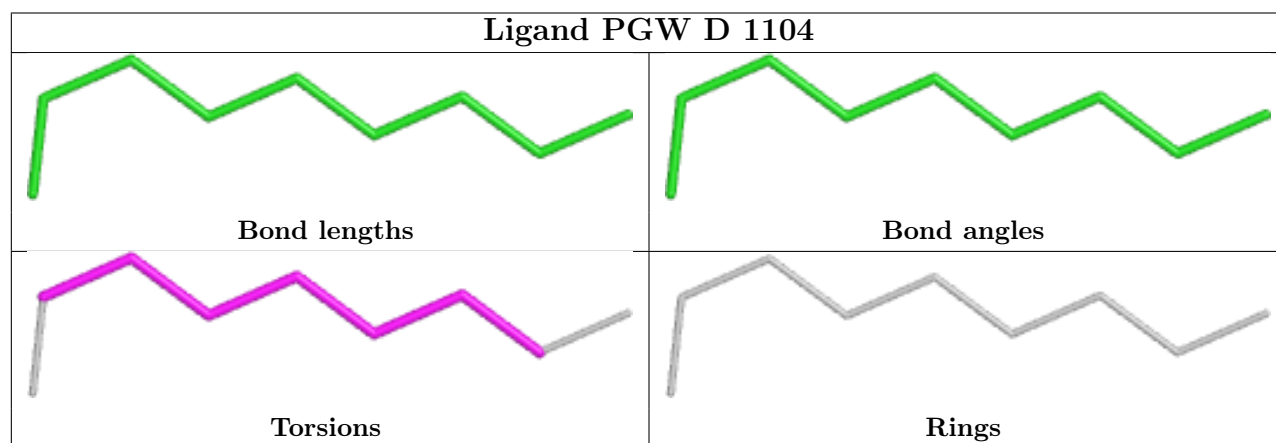
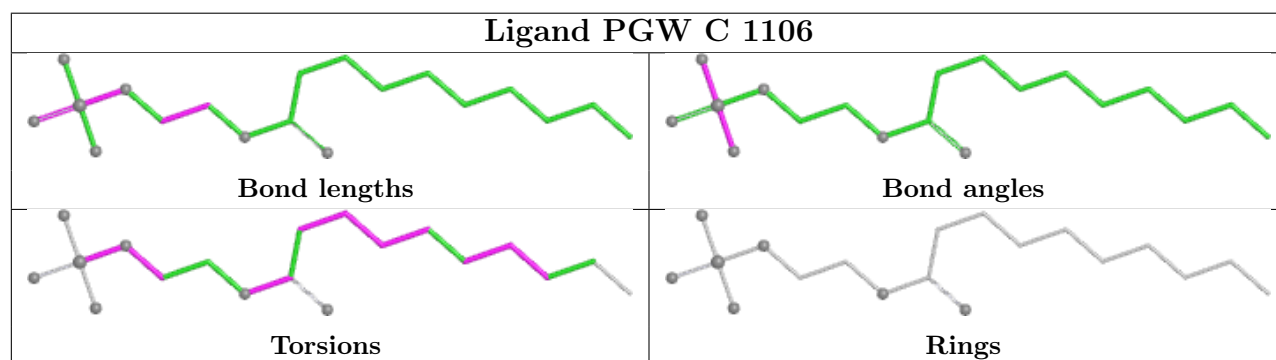
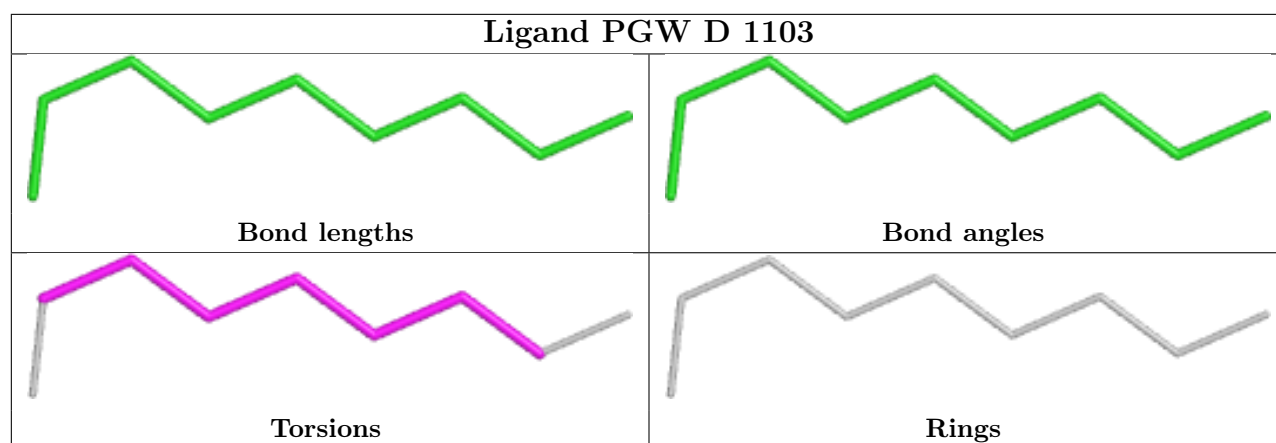
There are no ring outliers.

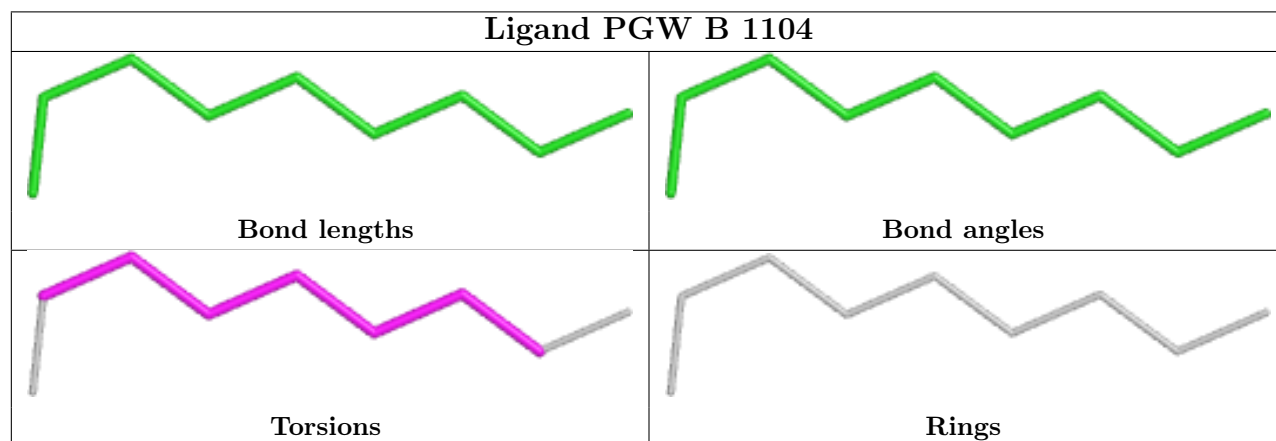
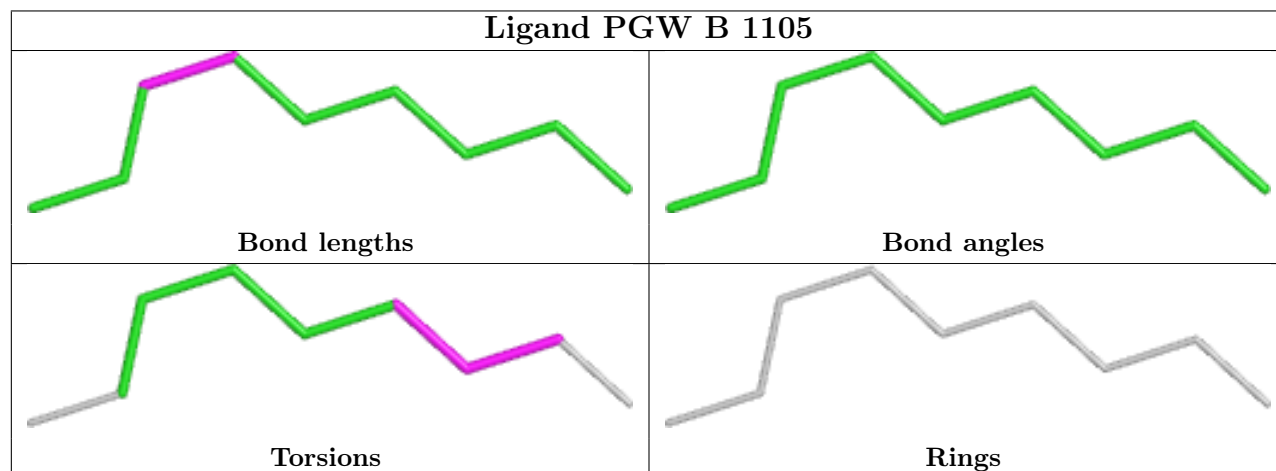
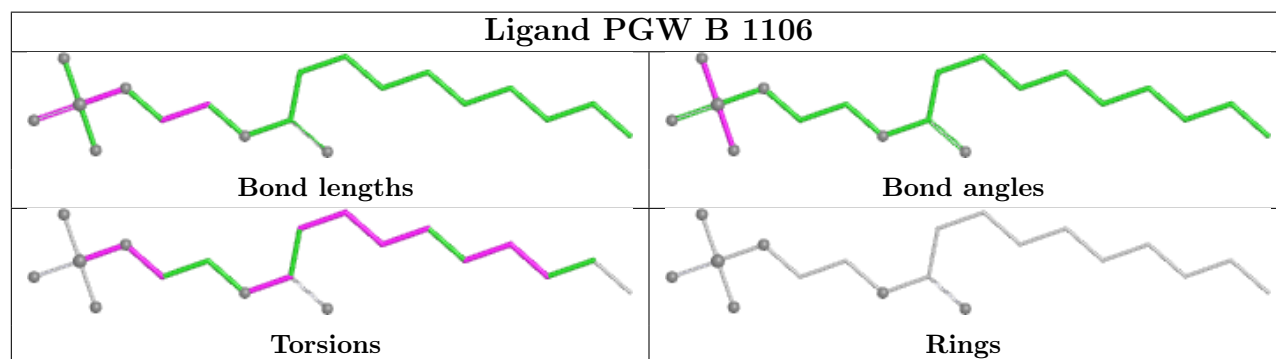
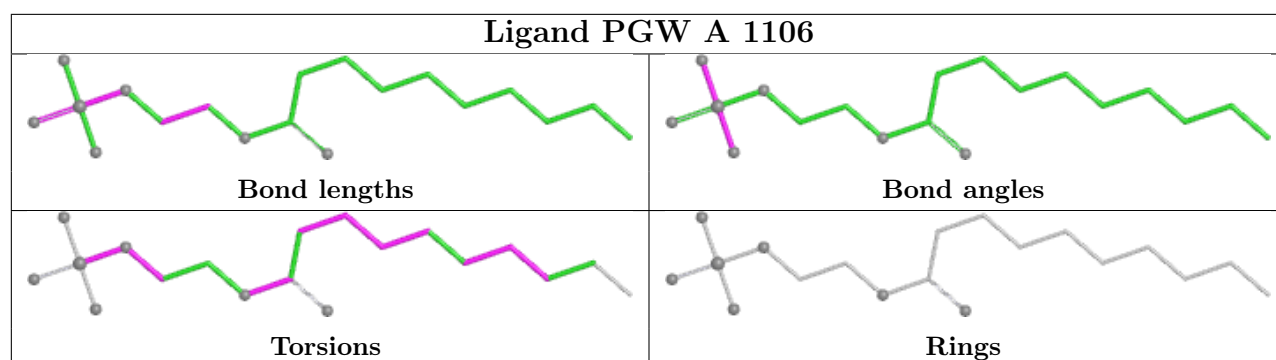
8 monomers are involved in 15 short contacts:

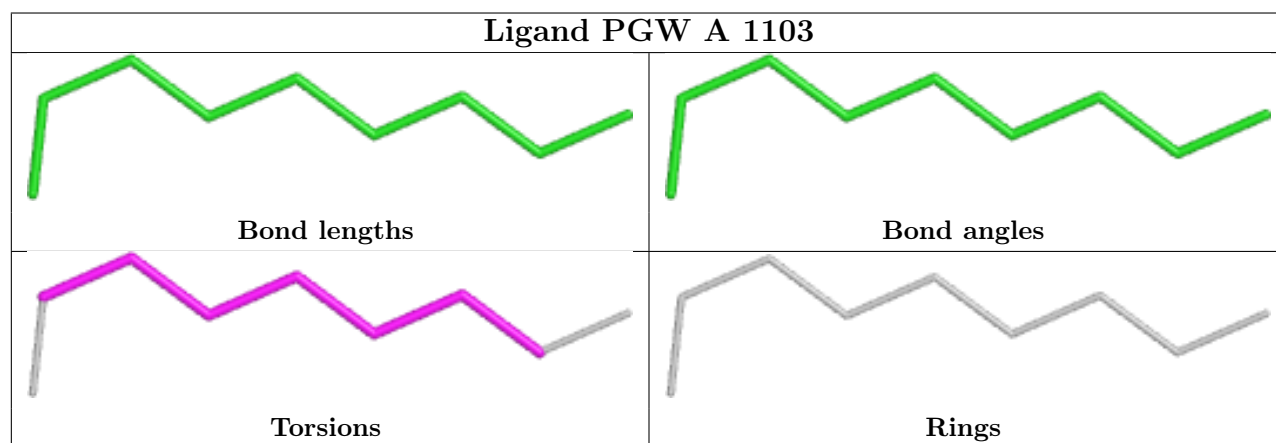
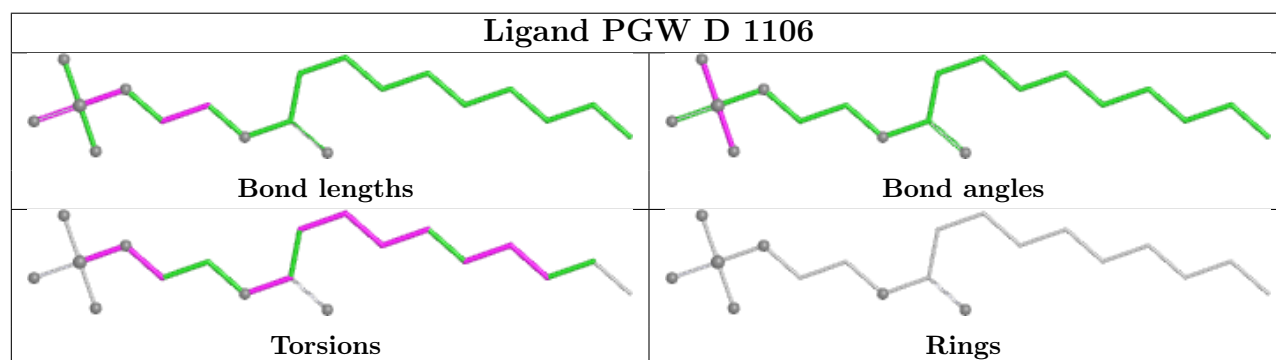
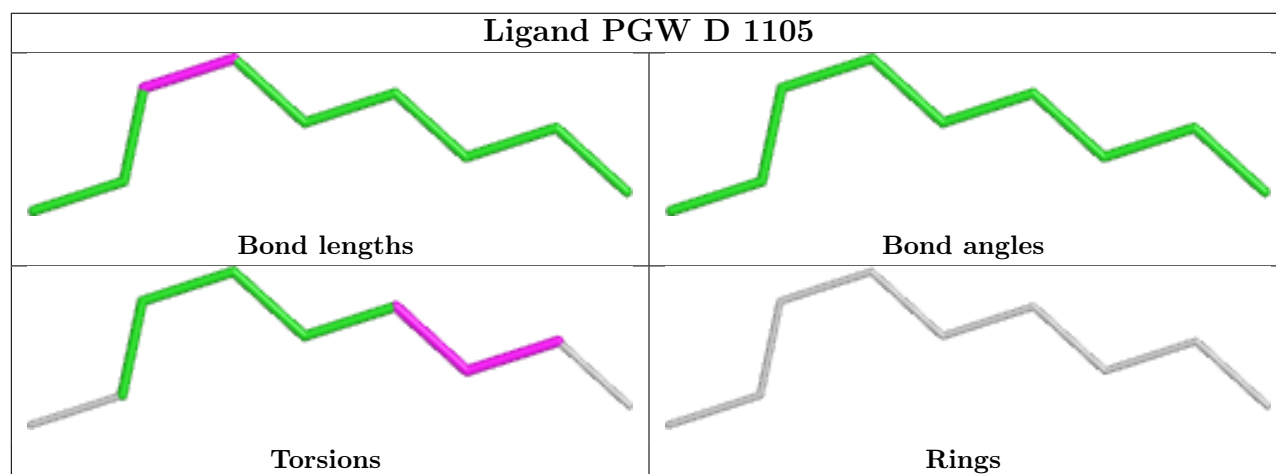
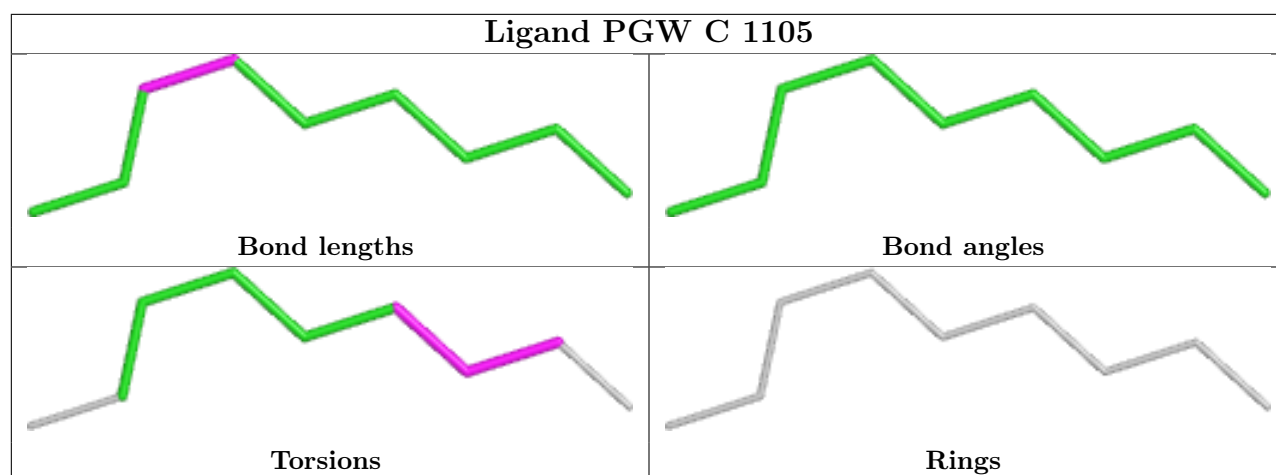
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1103	PGW	1	0
3	C	1106	PGW	3	0
3	B	1103	PGW	1	0
3	A	1106	PGW	2	0
3	B	1106	PGW	3	0
3	D	1106	PGW	3	0
3	A	1103	PGW	1	0
3	C	1103	PGW	1	0

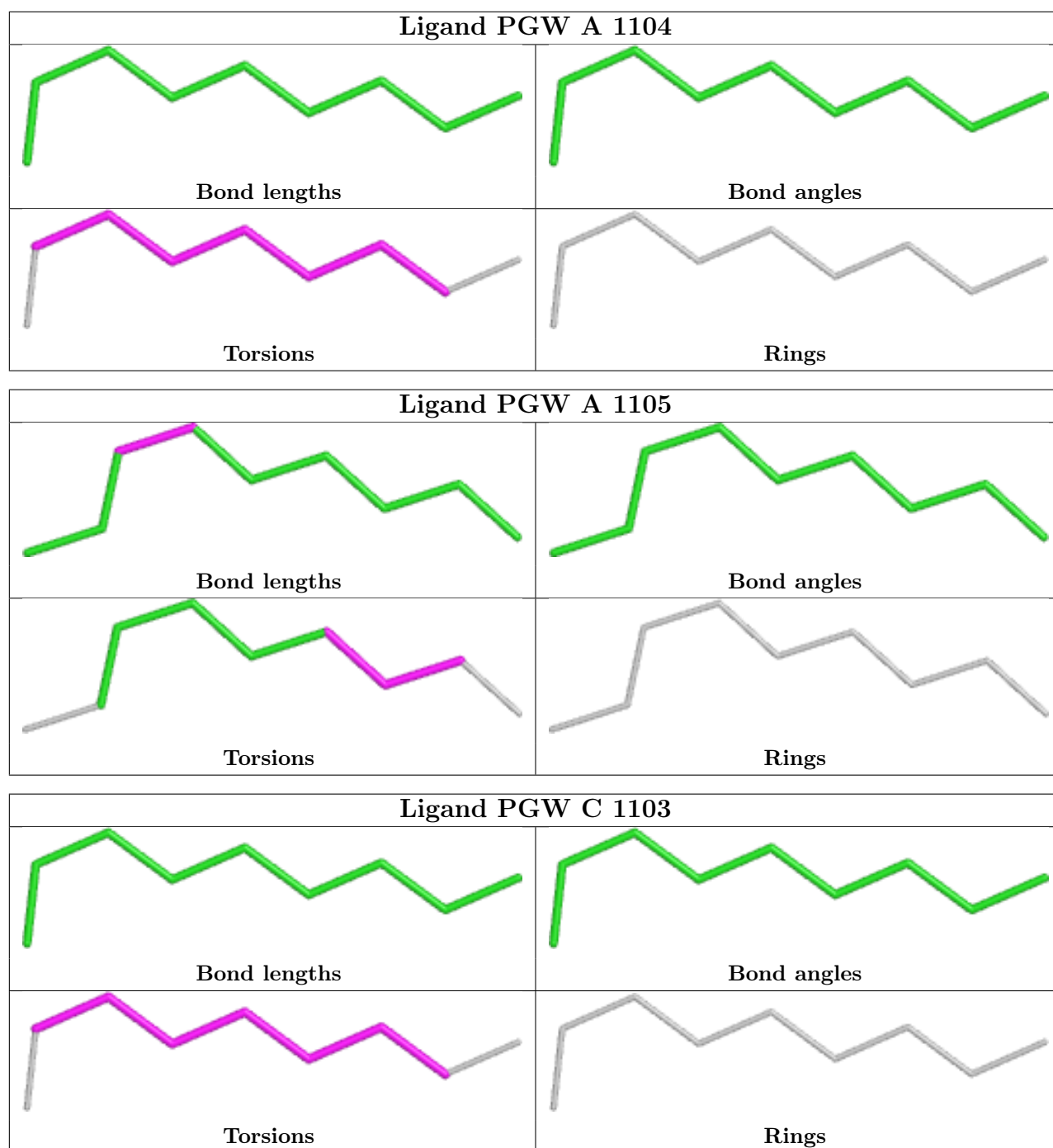
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

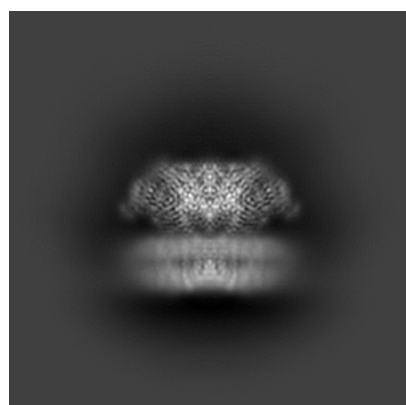
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24493. These allow visual inspection of the internal detail of the map and identification of artifacts.

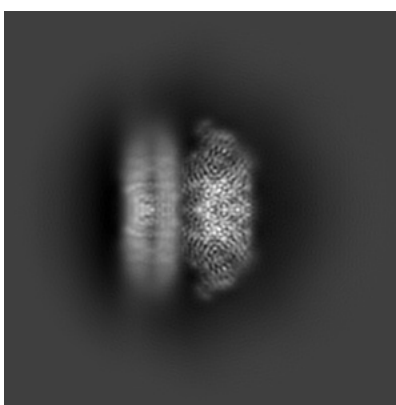
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

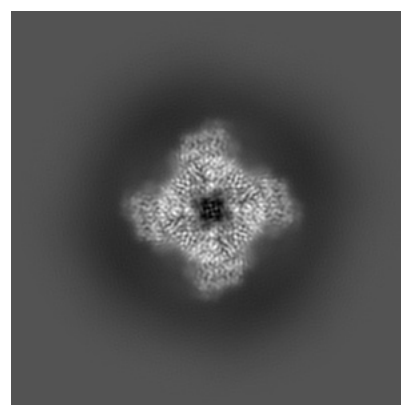
6.1.1 Primary map



X



Y

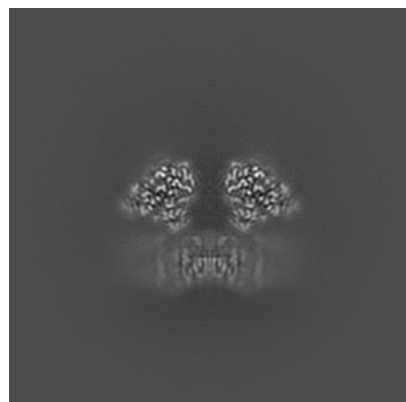


Z

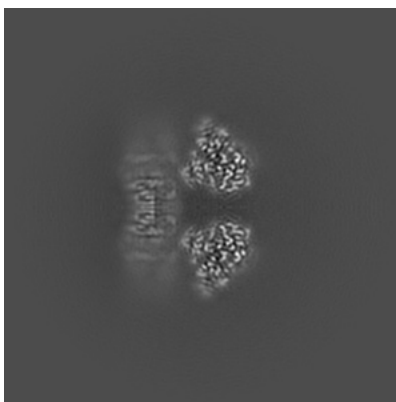
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

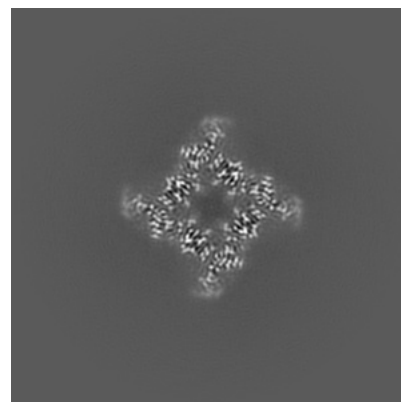
6.2.1 Primary map



X Index: 128



Y Index: 128

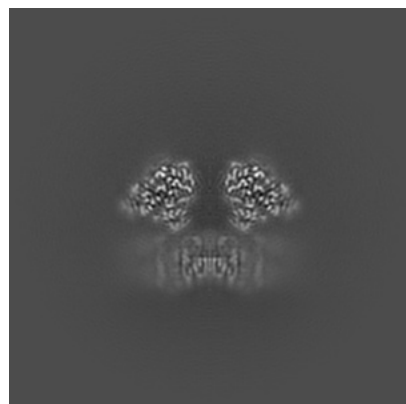


Z Index: 128

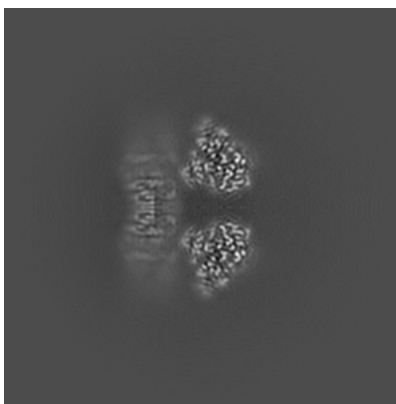
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

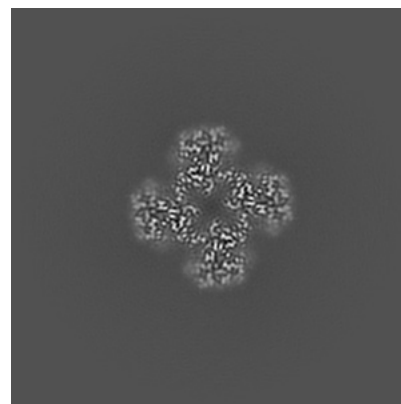
6.3.1 Primary map



X Index: 128



Y Index: 128

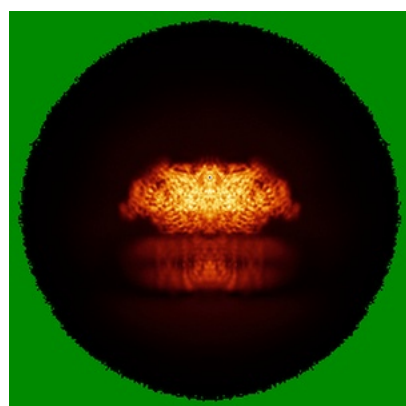


Z Index: 140

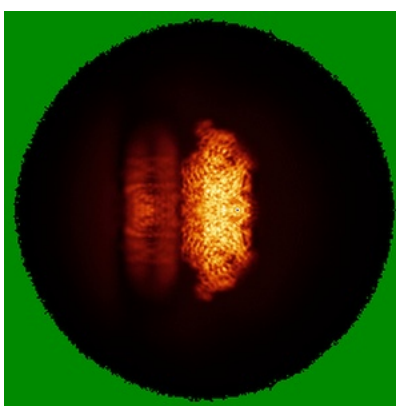
The images above show the largest variance slices of the map in three orthogonal directions.

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

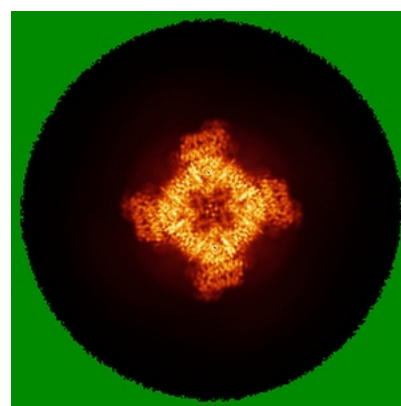
6.4.1 Primary map



X



Y



Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

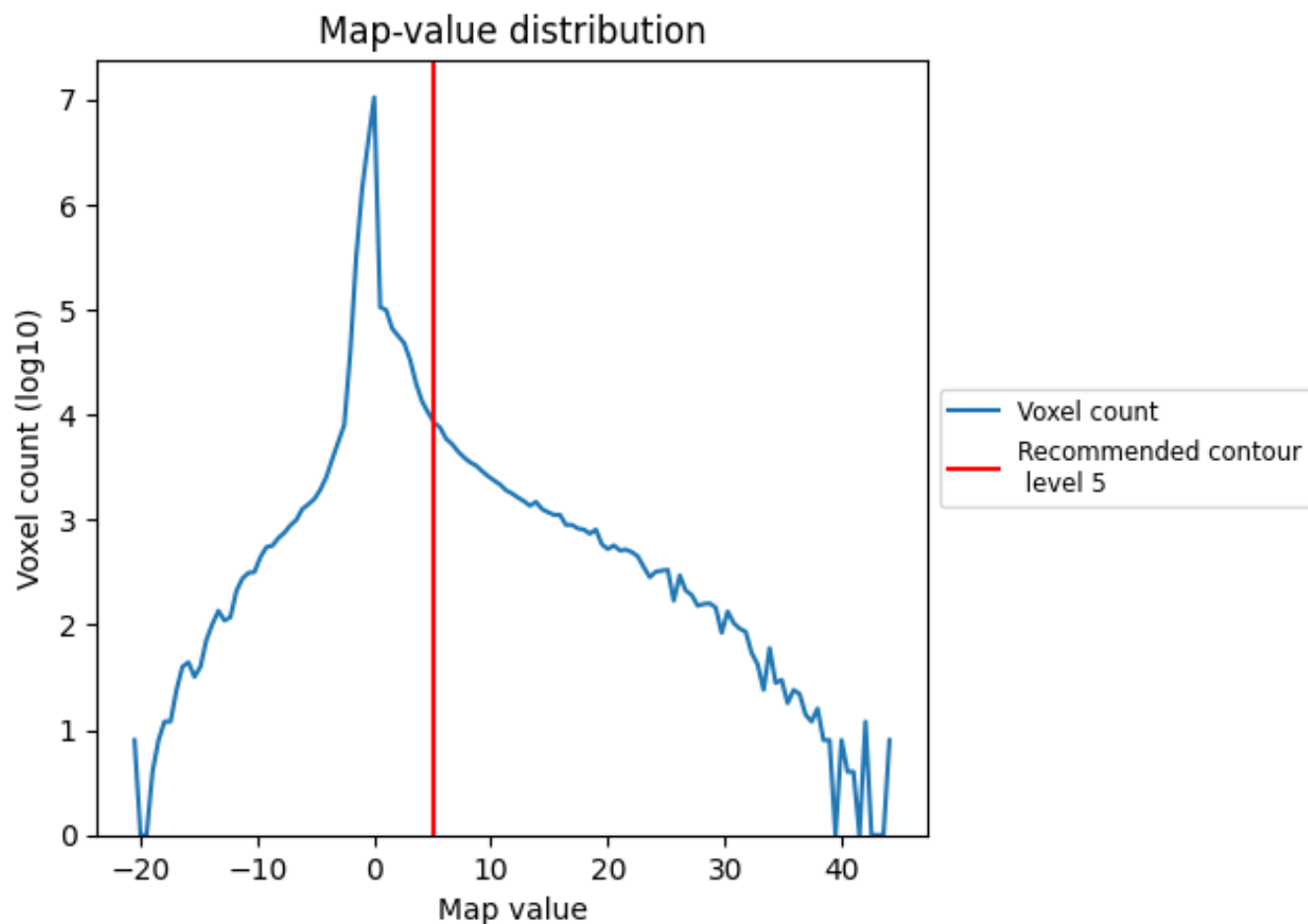
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

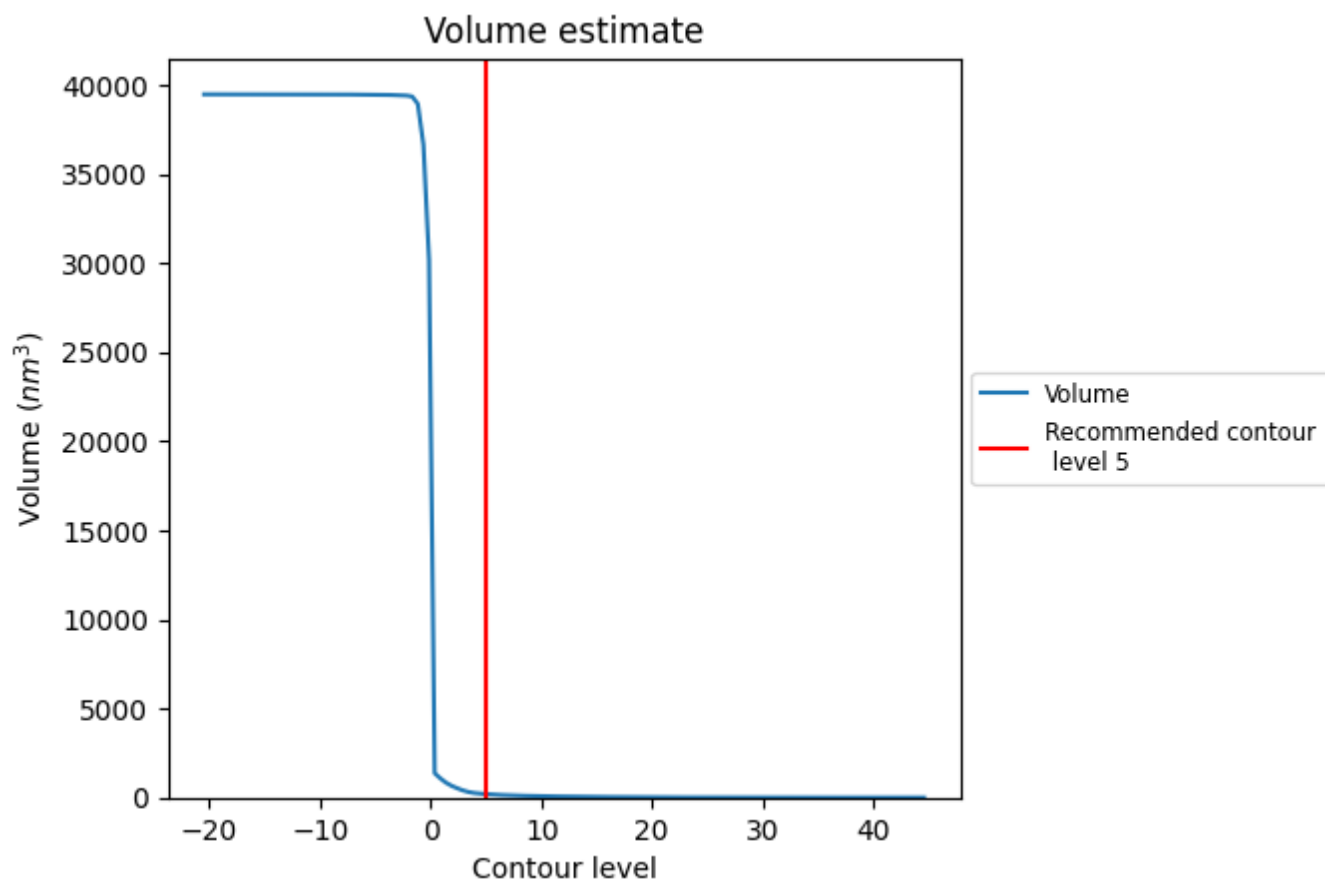
This section contains the results of statistical analysis of the map.

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.

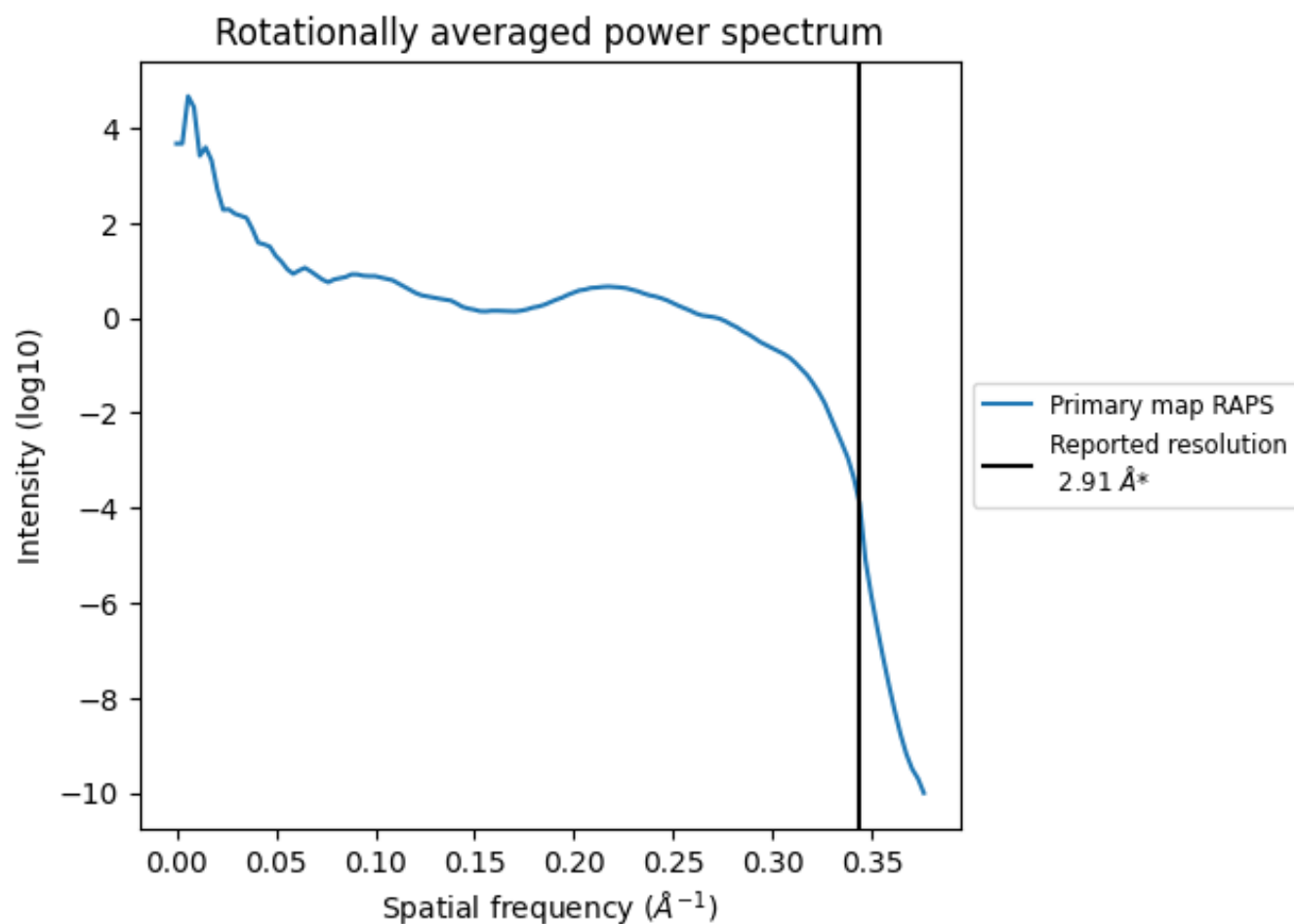
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm^3 ; this corresponds to an approximate mass of 175 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 ⓘ

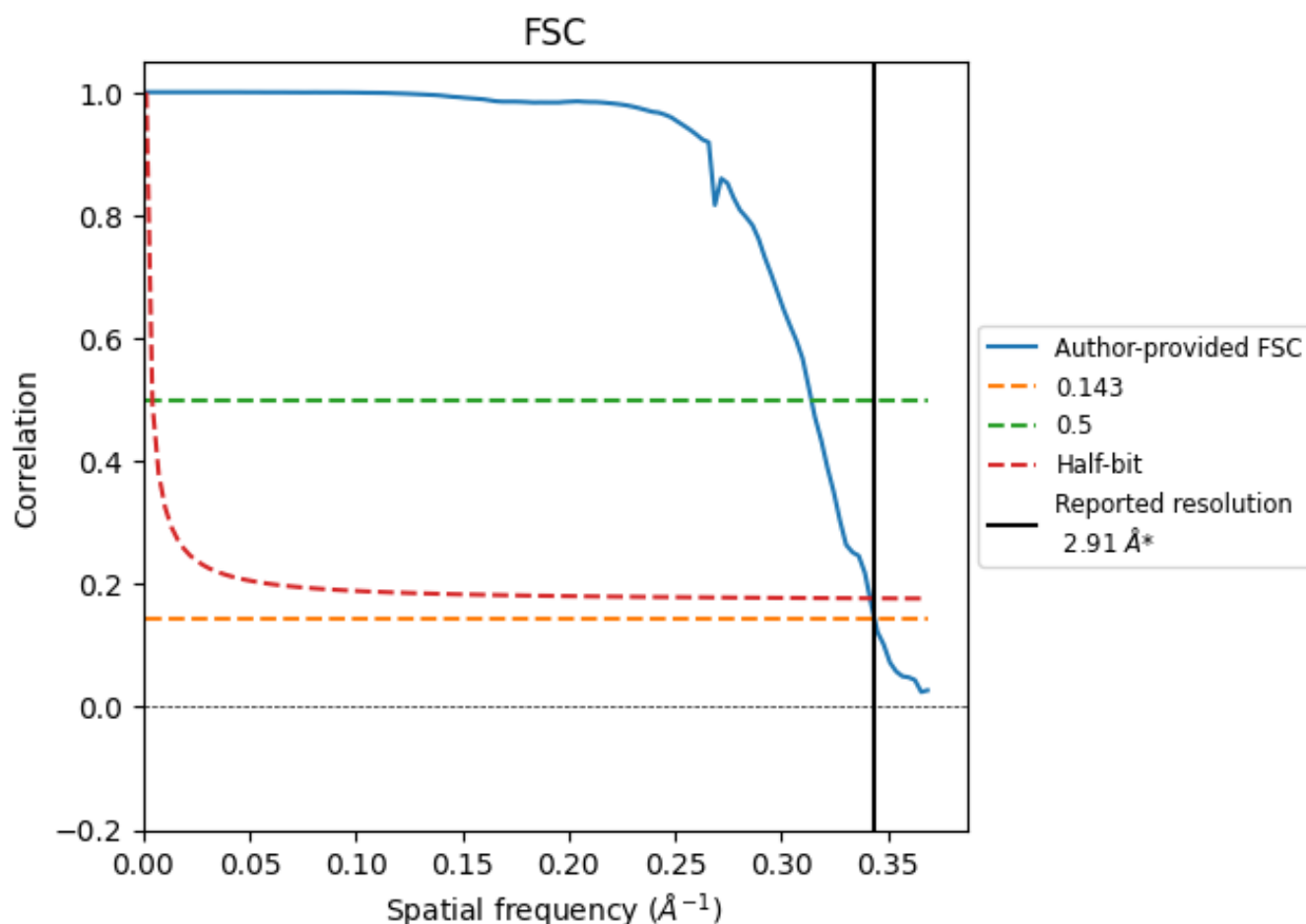


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

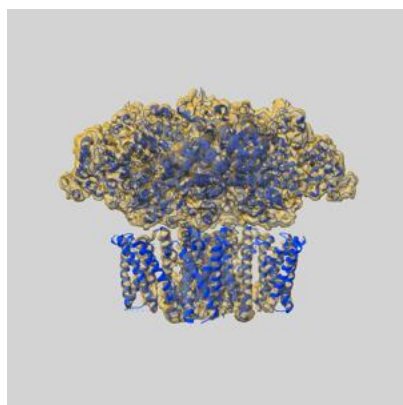
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.18	2.93
Unmasked-calculated*	-	-	-

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

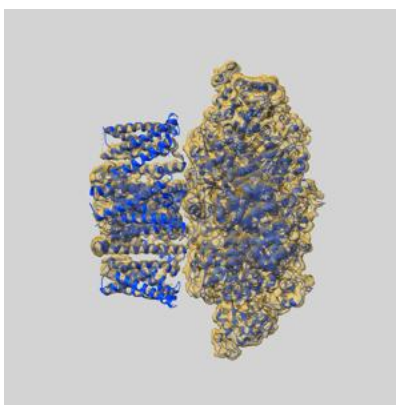
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24493 and PDB model 7RK6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

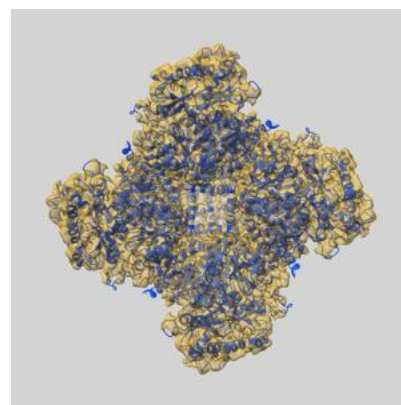
9.1 Map-model overlay [i](#)



X



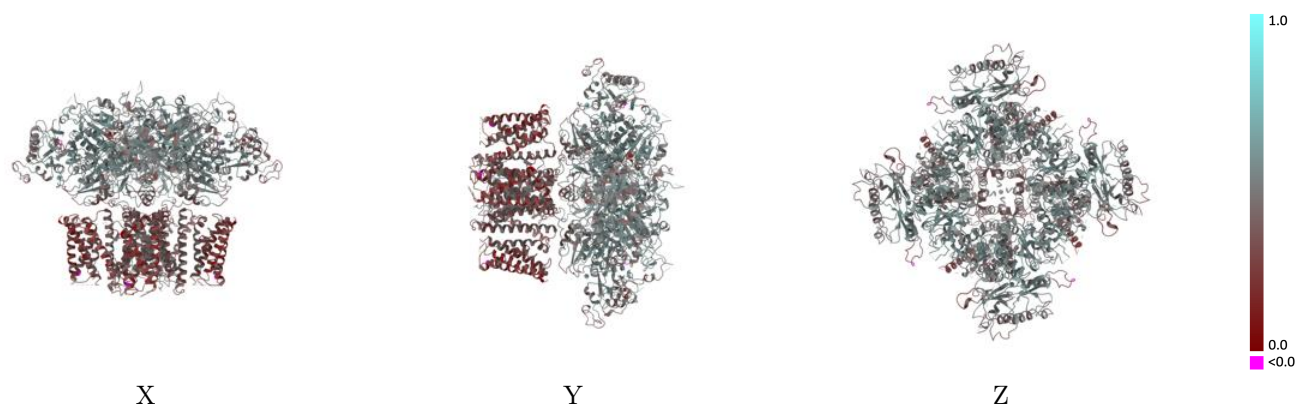
Y



Z

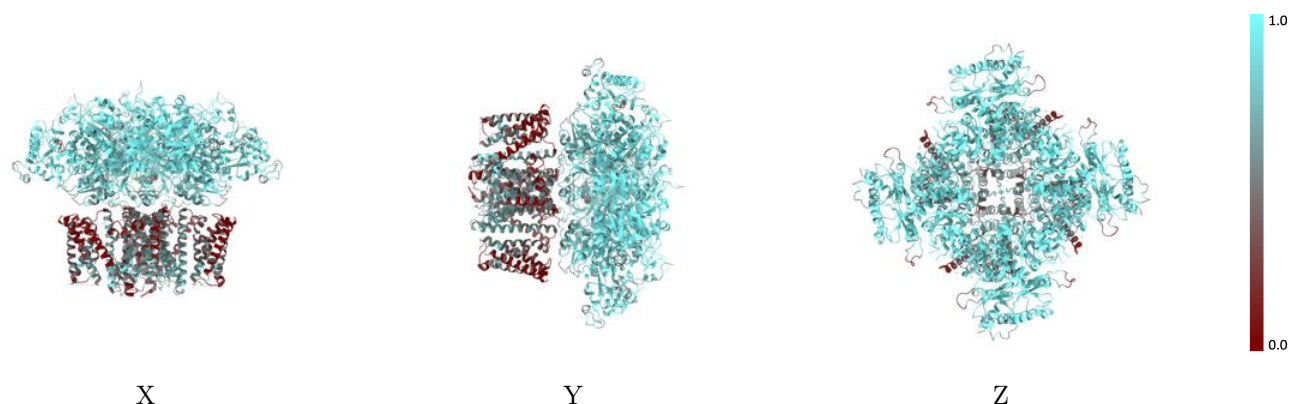
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



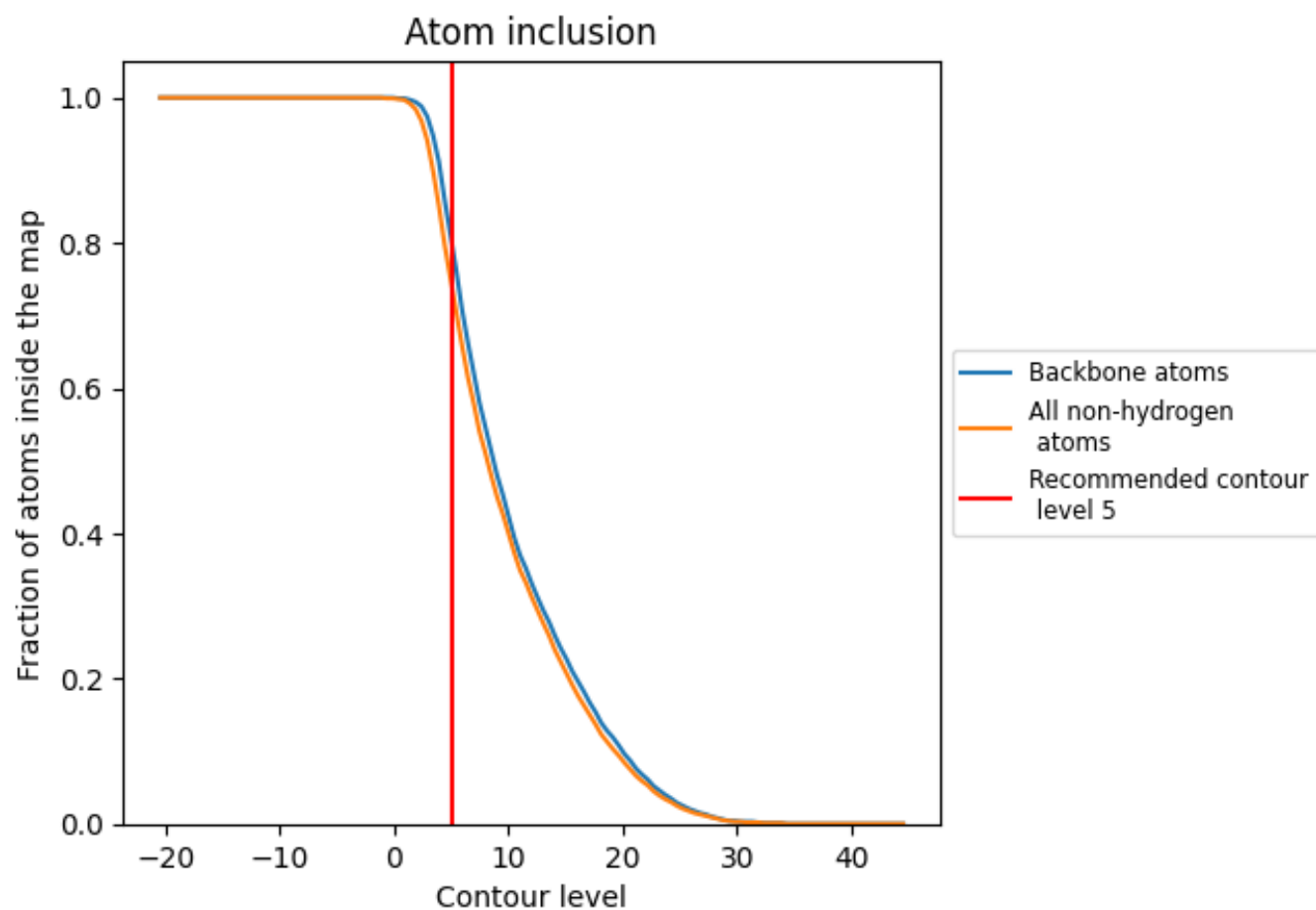
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.4470
A	0.7510	0.4470
B	0.7510	0.4470
C	0.7510	0.4470
D	0.7510	0.4470

