



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:18 AM UTC

PDB ID : 8E6R / pdb_00008e6r
EMDB ID : EMD-27923
Title : Human TRPM2 ion channel in 1 mM dADPR
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on : 2022-08-23
Resolution : 5.60 Å(reported)

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

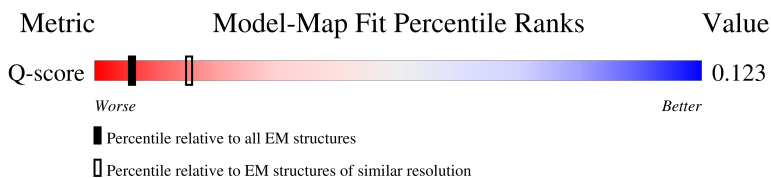
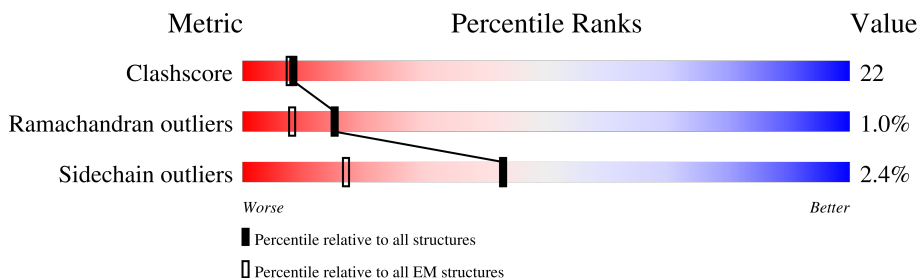
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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	513 (5.10 - 6.10)

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	1503	36% 51% 35% 12%
1	B	1503	37% 51% 35% 12%
1	C	1503	36% 51% 35% 12%
1	D	1503	38% 51% 35% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AR6	A	1602	X	-	-	-
3	AR6	B	1602	X	-	-	-
3	AR6	C	1602	X	-	-	-
3	AR6	D	1602	X	-	-	-

2 Entry composition [i](#)

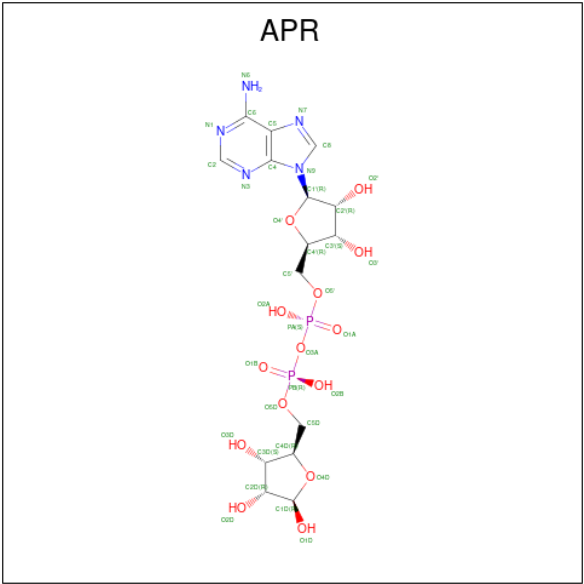
There are 3 unique types of molecules in this entry. The entry contains 42336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	B	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	C	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		
1	D	1323	Total	C	N	O	S	0	0
			10523	6796	1829	1848	50		

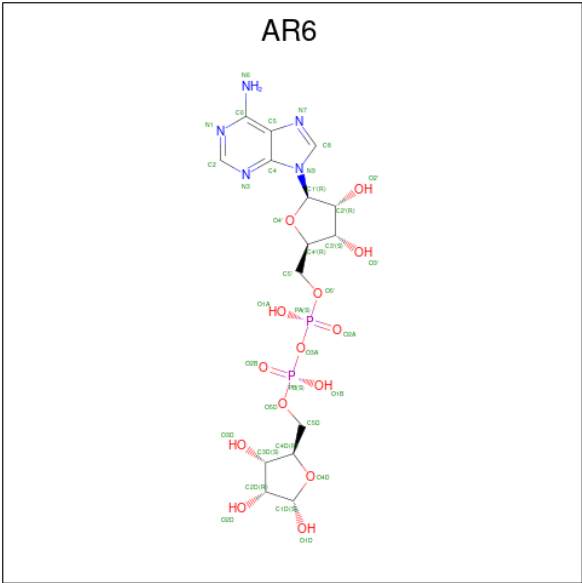
- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	C	1	26	10	5	9	2	0
2	D	1	26	10	5	9	2	0

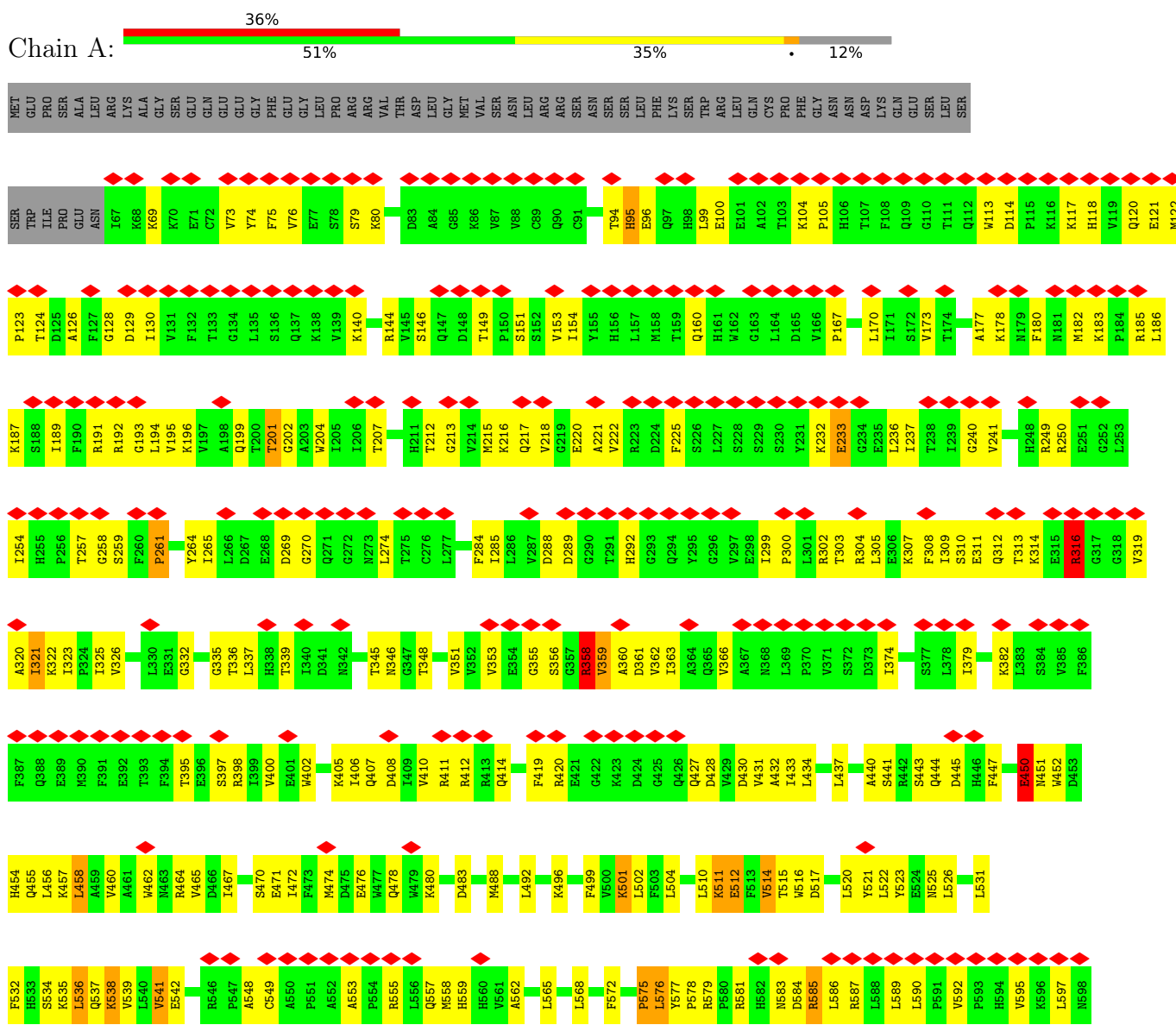
- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL[HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).

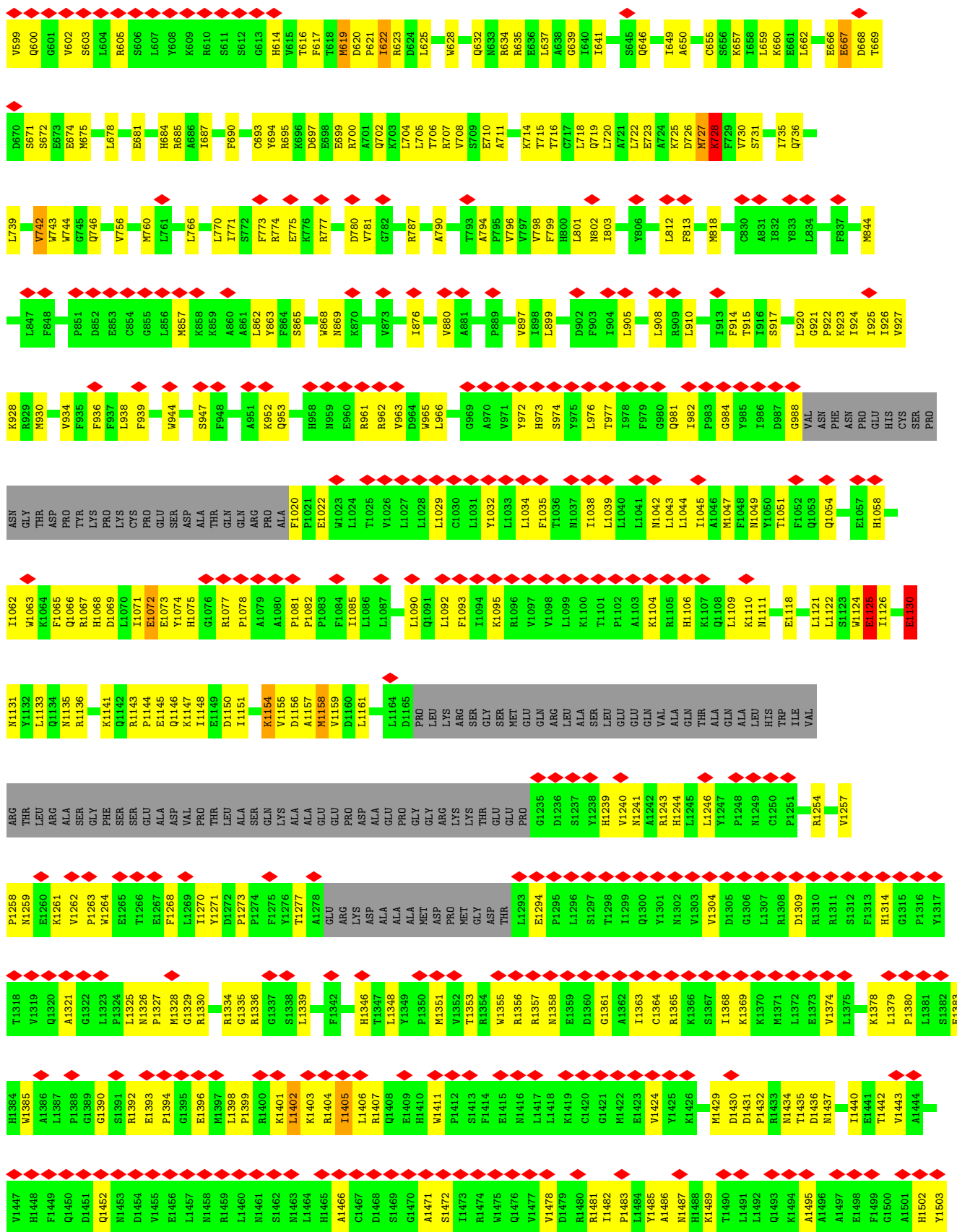


3 Residue-property plots

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: Transient receptor potential cation channel subfamily M member 2



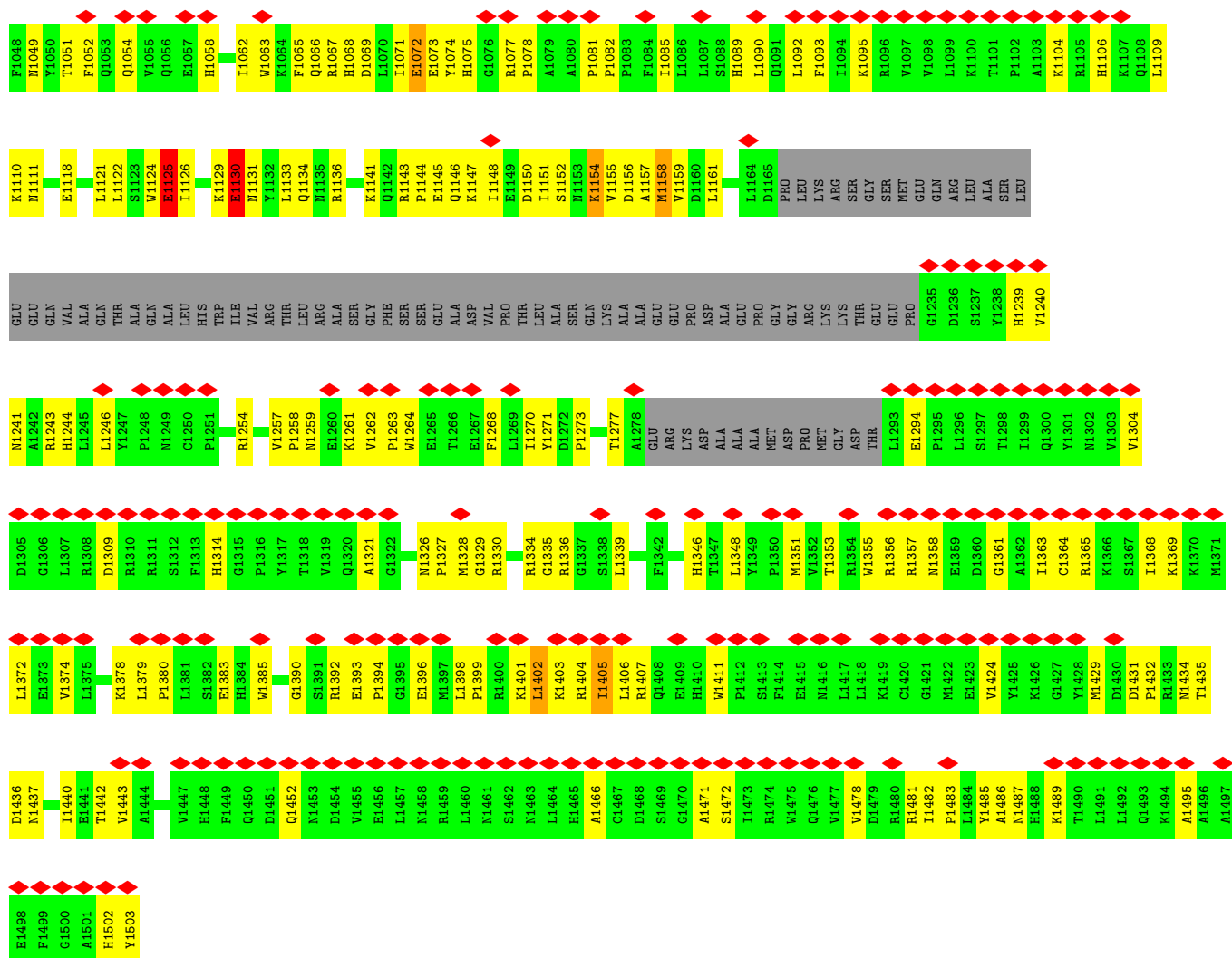


- Molecule 1: Transient receptor potential cation channel subfamily M member 2

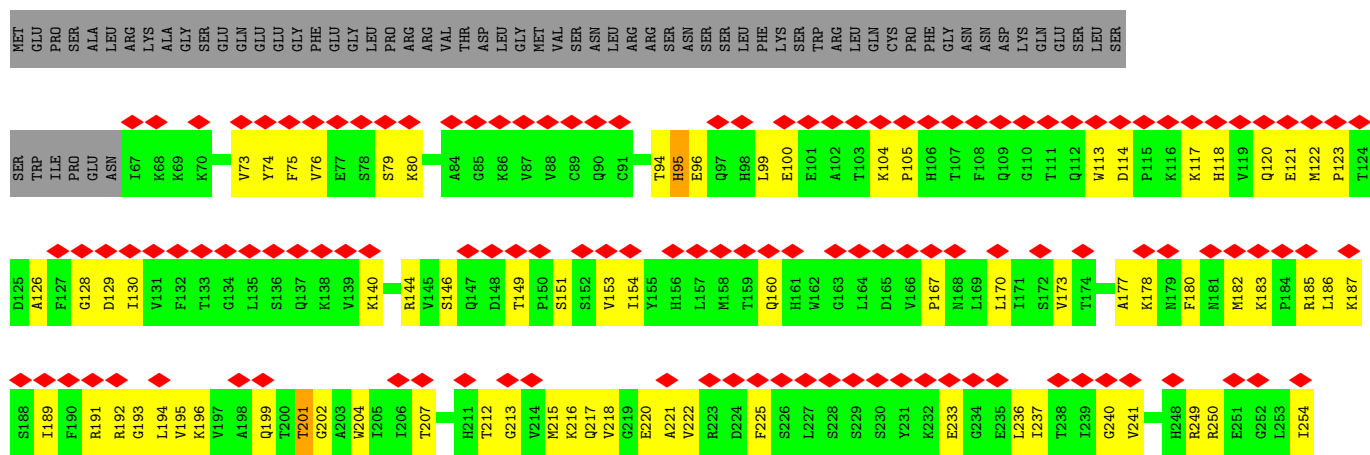


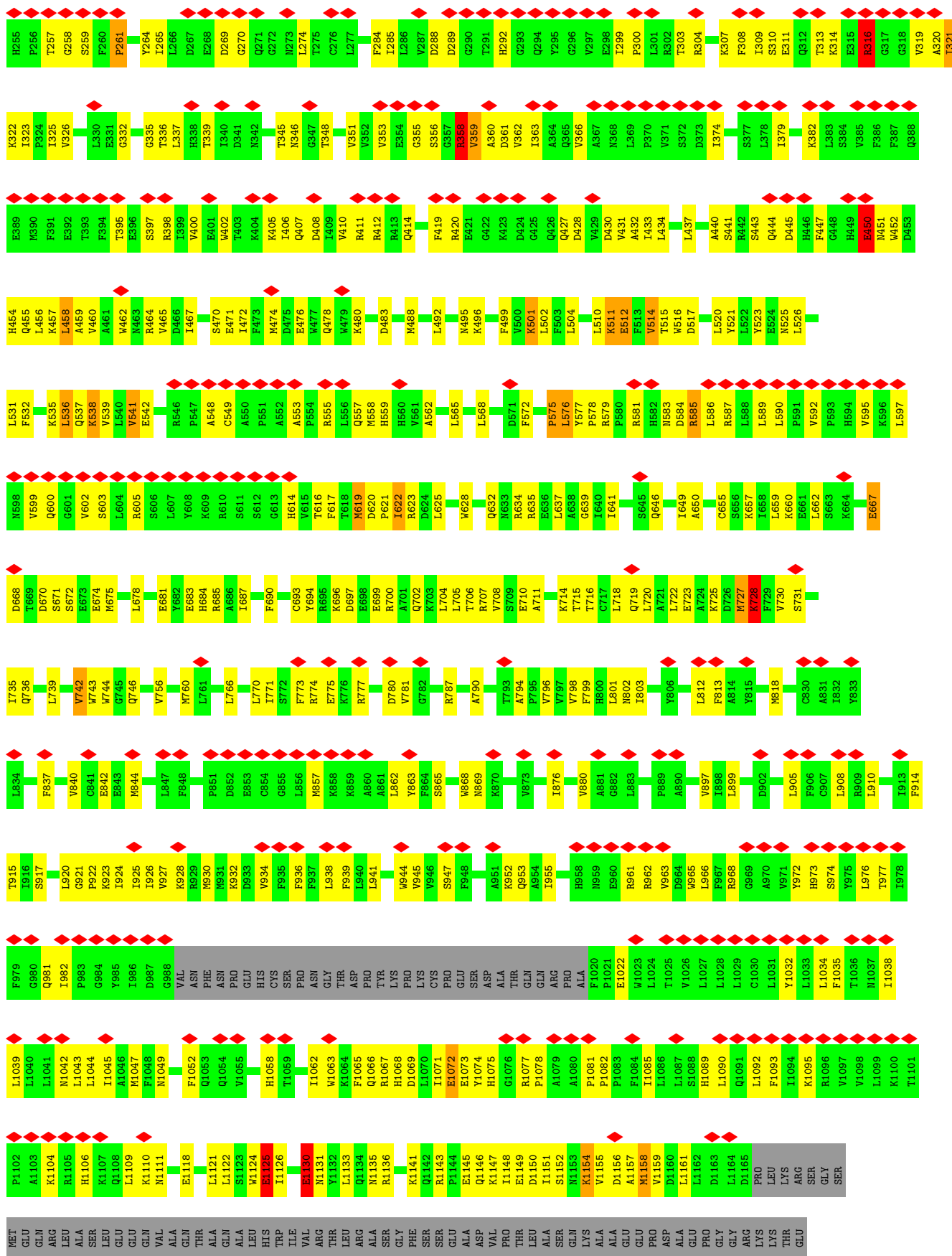


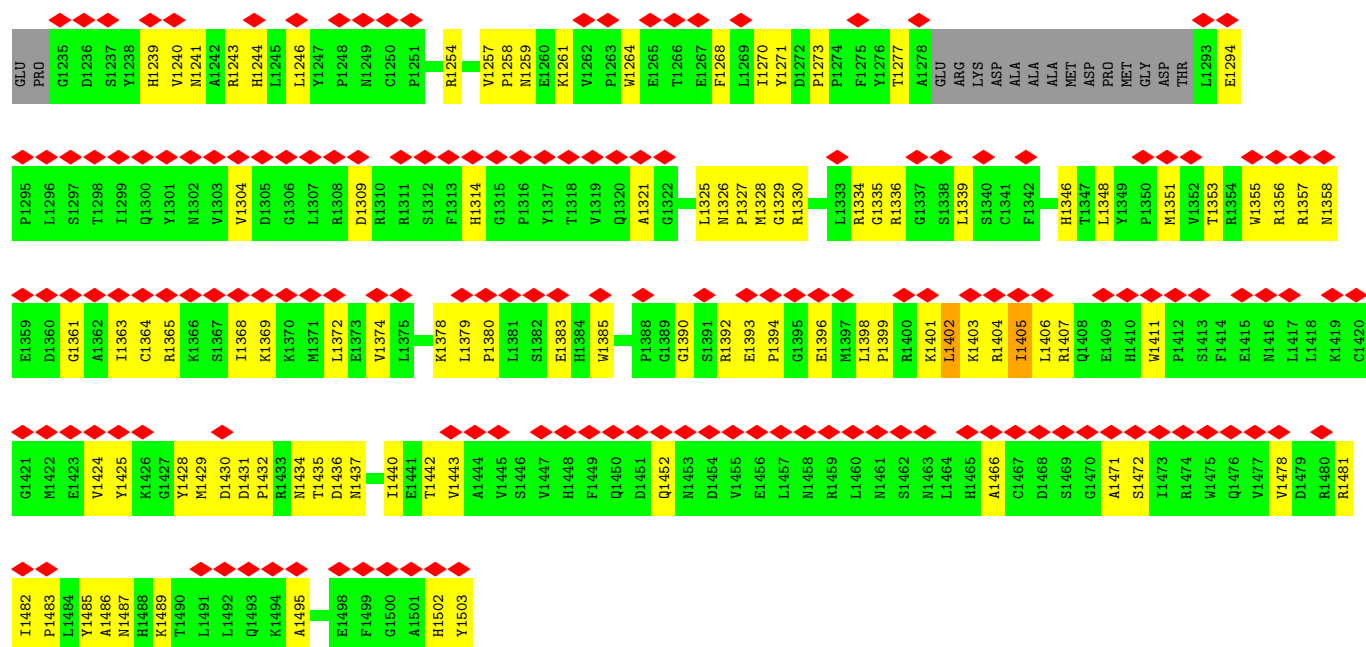
D987	Q988	VAL	ASN	PHE	ASN	ASN	PRQ	GLU	HIS	CYS	SER	PRQ	ASN	GLY	THR	ASP	PRQ	THR	GLN	ARG	PRO	ALA	F1020	V1023	L1024	T1025	V1026	L1027	V1028	L1029	C1030	L1031	Y1032	L1033	L1034	F1035	H973	S974	T1038	L1039	L1040	L1041	N1042	L1043	L1044	T1045	A1046	M1047	I924	I925	I926	I927	K928	R929	M930	M931	K932	K933	D933	S934	SER	F935	F936	F937	L938	F939	F939	L940	L941	A942	V943	W944	V945	V946	SER	S947	F948	G949	V950	A951	K952	Q953	A954	I955	H958	H959	E960	R961	R962	V963	D964	W965	L966	A970	V971	Y972	H973	S974	T975	L976	L977	T978	F979	Q980	Q981	I982	F983	G984	Y985	I986	E843	M844	F848	P851	D852	E853	C854	G855	L856	M857	K858	L859	A860	A861	L862	Y863	F864	S865	W868	K870	V873	I876	V880	A881	L882	L883	P889	A890	V897	I898	L899	D902	F903	I904	L905	F906	C907	L908	R909	L910	F913	F914	S917	L920	G921	F922	K923	Q746	W756	T757	L758	C759	M760	L761	L766	L770	L771	S772	F773	R774	E775	K776	R777	D780	V781	G782	R787	A790	T793	A794	V796	V797	V798	F799	H800	L801	N802	I803	Y806	L812	F813	M818	C828	E829	C830	A831	I832	Y833	L834	F837	V840	C841	E842	E843	M844	F848	P851	D852	E853	C854	G855	L856	M857	K858	L859	A860	A861	L862	Y863	F864	S865	W868	K870	V873	I876	V880	A881	L882	L883	P889	A890	V897	I898	L899	D902	F903	I904	L905	F906	C907	L908	R909	L910	F913	F914	S917	L920	G921	F922	K923	E674	M675	L678	E681	H684	R685	A686	I687	F690	C693	V694	R695	K696	D697	E698	E699	A701	K702	K703	L704	L705	T706	R707	S709	E710	A711	K714	T715	T716	C717	L718	Q719	L722	K725	D726	M727	K728	F729	W730	S731	K735	Q736	L739	V742	W743	W744	G745	G601	V602	S603	L604	R605	S606	L607	V608	R609	S611	S612	G613	H614	F617	T618	M619	D620	P621	T622	L623	D624	L625	W628	Q632	R633	R634	R635	E636	L637	A638	G639	T640	I641	S645	Q646	T649	A650	C655	S656	R657	L658	L659	K660	S661	L662	E666	E667	D668	S671	S672	E673	E674	M675	L678	E681	H684	R685	A686	I687	F690	C693	V694	R695	K696	D697	E698	E699	A701	K702	K703	L704	L705	T706	R707	S709	E710	A711	K714	T715	T716	C717	L718	Q719	L722	K725	D726	M727	K728	F729	W730	S731	K735	Q736	L739	V742	W743	W744	G745	E389	M390	F391	E392	T393	F394	T395	E396	S397	V400	E401	W402	K405	I406	Q407	D408	I409	V410	R411	R412	R413	Q414	F419	R420	E421	G422	K423	D424	G425	Q427	D428	Y429	D430	V431	A432	I433	L434	L437	A440	S441	R442	S443	Q444	D445	H446	F447	E450	N451	W452	D453	H454	Q455	L456	E389	M390	F391	E392	T393	F394	T395	E396	S397	V400	E401	W402	K405	I406	Q407	D408	I409	V410	R411	R412	R413	Q414	F419	R420	E421	G422	K423	D424	G425	Q427	D428	Y429	D430	V431	A432	I433	L434	L437	A440	S441	R442	S443	Q444	D445	H446	F447	E450	N451	W452	D453	H454	Q455	L456	E254	H255	P256	T257	G258	S259	F260	P261	Y264	L265	L266	D267	E268	D269	G270	Q271	G272	N273	L274	T275	C276	L277	F284	I285	L286	V287	D288	D289	G290	T291	H292	G293	Q294	S295	V296	G296	V297	S298	E298	I299	P300	L301	R302	T303	R304	L305	E306	K307	F308	I309	S310	E311	Q312	T313	K314	E315	R316	G317	G318	V319	L254	H255	P256	T257	G258	S259	F260	P261	Y264	L265	L266	D267	E268	D269	G270	Q271	G272	N273	L274	T275	C276	L277	F284	I285	L286	V287	D288	D289	G290	T291	H292	G293	Q294	S295	V296	G296	V297	S298	E298	I299	P300	L301	R302	T303	R304	L305	E306	K307	F308	I309	S310	E311	Q312	T313	K314	E315	R316	G317	G318	V319	K187	S188	I189	F190	R191	G192	G193	L194	V195	K196	V197	L198	Q199	T201	G202	A203	W204	I205	I206	T207	H211	T212	G213	V214	N215	K216	Q217	V218	G219	E220	A221	V222	R223	G224	M225	F225	S226	L227	S228	S229	S230	Y231	K232	E233	G234	E235	L236	I237	T238	I239	G240	V241	H248	R249	R250	E251	G252	L253	P123	T124	D125	A126	F127	G128	D129	I130	V131	F132	T133	G134	L135	S136	Q137	K138	V139	K140	R144	V145	S146	Q147	D148	T149	P150	S151	S152	V153	I154	Y155	H156	L157	M158	T159	Q160	H161	W162	G163	L164	D165	V166	P167	L170	I171	E172	V173	T174	A177	K178	M179	F180	M181	M182	K183	P184	R185	L186
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● Molecule 1: Transient receptor potential cation channel subfamily M member 2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR, AR6

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	0.19	0/10789	0.62	11/14649 (0.1%)
1	B	0.19	0/10789	0.62	11/14649 (0.1%)
1	C	0.19	0/10789	0.62	11/14649 (0.1%)
1	D	0.19	0/10789	0.62	11/14649 (0.1%)
All	All	0.19	0/43156	0.62	44/58596 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ARG	CA-CB-CG	7.37	128.84	114.10
1	B	316	ARG	CA-CB-CG	7.36	128.82	114.10
1	A	316	ARG	CA-CB-CG	7.35	128.80	114.10
1	D	316	ARG	CA-CB-CG	7.33	128.77	114.10
1	A	728	LYS	CB-CG-CD	6.43	126.10	111.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLN	Peptide
1	A	358	ARG	Peptide
1	B	160	GLN	Peptide
1	B	358	ARG	Peptide
1	C	160	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10523	0	10458	475	0
1	B	10523	0	10458	467	0
1	C	10523	0	10458	467	0
1	D	10523	0	10458	468	0
2	A	26	0	10	1	0
2	B	26	0	10	1	0
2	C	26	0	10	1	0
2	D	26	0	10	1	0
3	A	35	0	19	1	0
3	B	35	0	19	1	0
3	C	35	0	19	0	0
3	D	35	0	19	0	0
All	All	42336	0	41948	1817	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 22.

The worst 5 of 1817 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:727:MET:H	1:B:727:MET:HE2	1.20	1.06
1:A:727:MET:H	1:A:727:MET:HE2	1.20	1.06
1:C:727:MET:H	1:C:727:MET:HE2	1.20	1.05
1:D:727:MET:HE2	1:D:727:MET:H	1.20	1.02
1:A:1429:MET:HB3	1:A:1487:ASN:HD21	1.37	0.89

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	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	12	48
1	B	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	12	48
1	C	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	12	48
1	D	1313/1503 (87%)	1140 (87%)	160 (12%)	13 (1%)	12	48
All	All	5252/6012 (87%)	4560 (87%)	640 (12%)	52 (1%)	15	48

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	261	PRO
1	A	1294	GLU
1	A	1321	ALA
1	B	95	HIS

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	1116/1318 (85%)	1089 (98%)	27 (2%)	43	63
1	B	1116/1318 (85%)	1089 (98%)	27 (2%)	43	63
1	C	1116/1318 (85%)	1088 (98%)	28 (2%)	42	62
1	D	1116/1318 (85%)	1089 (98%)	27 (2%)	43	63
All	All	4464/5272 (85%)	4355 (98%)	109 (2%)	43	63

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	458	LEU
1	C	812	LEU
1	D	812	LEU
1	C	511	LYS
1	C	557	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	118	HIS
1	D	1135	ASN
1	D	248	HIS
1	D	478	GLN
1	B	346	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APR	B	1601	-	27,28,39	0.84	1 (3%)	41,43,60	0.75	1 (2%)
3	AR6	C	1602	-	38,38,39	0.53	0	54,58,60	0.63	0
2	APR	C	1601	-	27,28,39	0.85	1 (3%)	41,43,60	0.75	1 (2%)
2	APR	A	1601	-	27,28,39	0.84	1 (3%)	41,43,60	0.75	1 (2%)
3	AR6	A	1602	-	38,38,39	0.52	0	54,58,60	0.63	1 (1%)
3	AR6	D	1602	-	38,38,39	0.53	0	54,58,60	0.63	1 (1%)
3	AR6	B	1602	-	38,38,39	0.53	0	54,58,60	0.63	1 (1%)
2	APR	D	1601	-	27,28,39	0.85	1 (3%)	41,43,60	0.75	1 (2%)

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	APR	B	1601	-	-	5/16/28/54	0/3/3/4
3	AR6	C	1602	-	1/1/9/10	6/22/50/54	0/4/4/4
2	APR	A	1601	-	-	5/16/28/54	0/3/3/4
2	APR	C	1601	-	-	5/16/28/54	0/3/3/4
3	AR6	D	1602	-	1/1/9/10	6/22/50/54	0/4/4/4
3	AR6	A	1602	-	1/1/9/10	6/22/50/54	0/4/4/4
3	AR6	B	1602	-	1/1/9/10	6/22/50/54	0/4/4/4
2	APR	D	1601	-	-	5/16/28/54	0/3/3/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1601	APR	PB-O1B	3.34	1.60	1.50
2	B	1601	APR	PB-O1B	3.32	1.60	1.50
2	A	1601	APR	PB-O1B	3.32	1.60	1.50
2	D	1601	APR	PB-O1B	3.32	1.60	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1601	APR	O5D-PB-O2B	2.78	118.22	107.80
2	D	1601	APR	O5D-PB-O2B	2.77	118.19	107.80
2	B	1601	APR	O5D-PB-O2B	2.77	118.18	107.80
2	A	1601	APR	O5D-PB-O2B	2.76	118.17	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1602	AR6	O4D-C1D-C2D	-2.02	101.88	104.67

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1602	AR6	C1'
3	B	1602	AR6	C1'
3	C	1602	AR6	C1'
3	D	1602	AR6	C1'

5 of 44 torsion outliers are listed below:

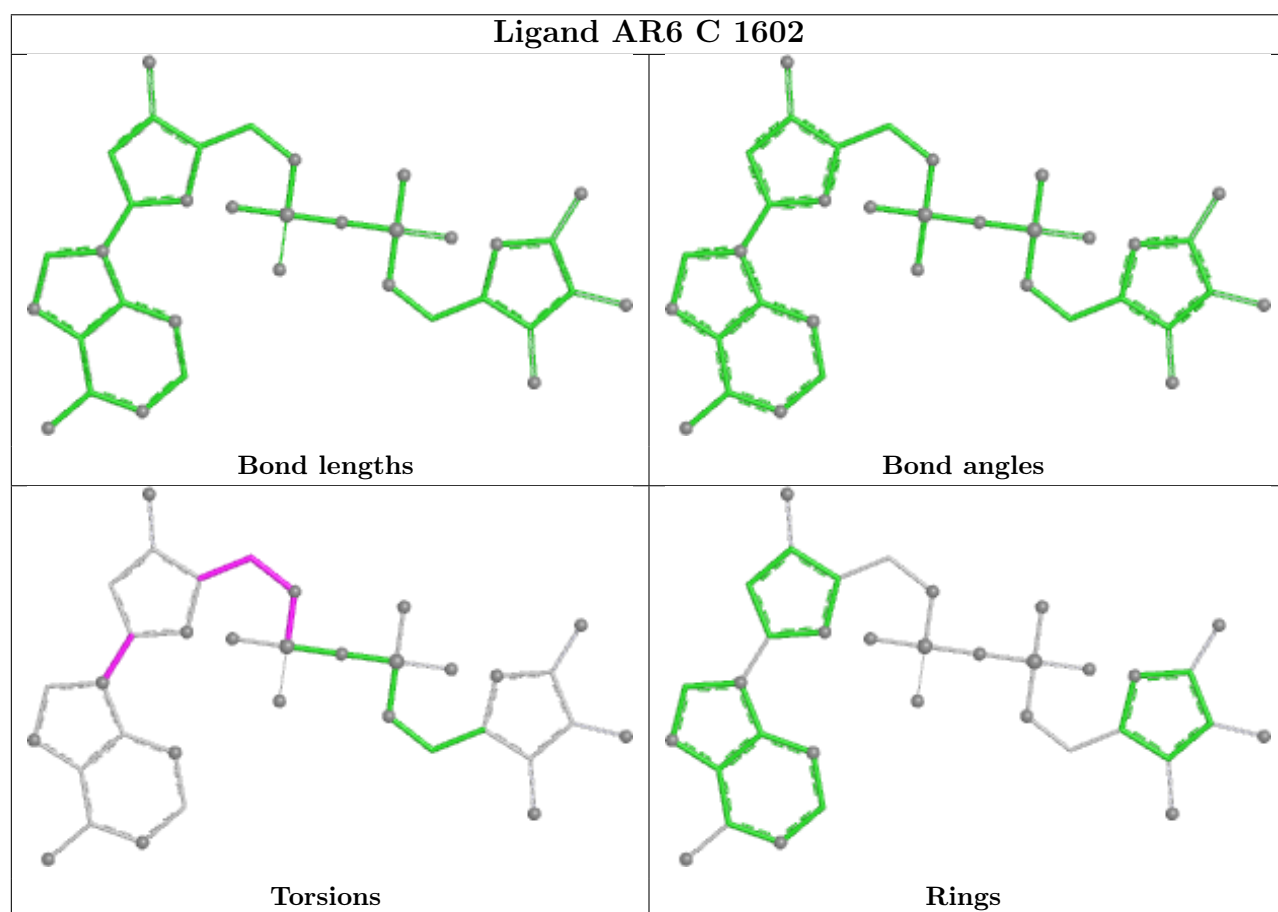
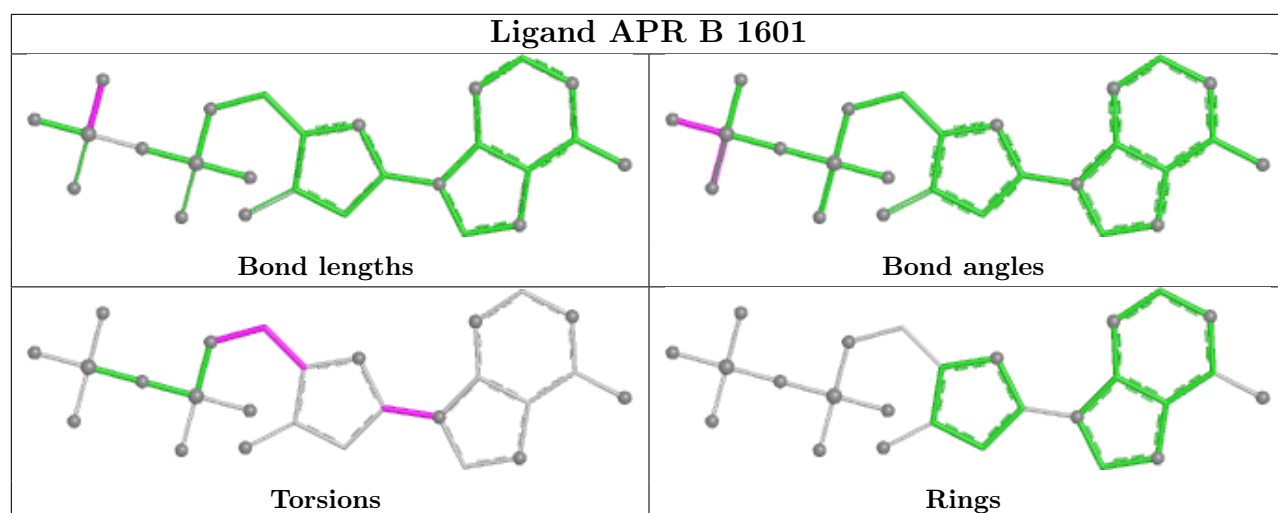
Mol	Chain	Res	Type	Atoms
3	A	1602	AR6	C5'-O5'-PA-O3A
3	A	1602	AR6	C3'-C4'-C5'-O5'
3	A	1602	AR6	O4'-C4'-C5'-O5'
3	B	1602	AR6	C5'-O5'-PA-O3A
3	B	1602	AR6	C3'-C4'-C5'-O5'

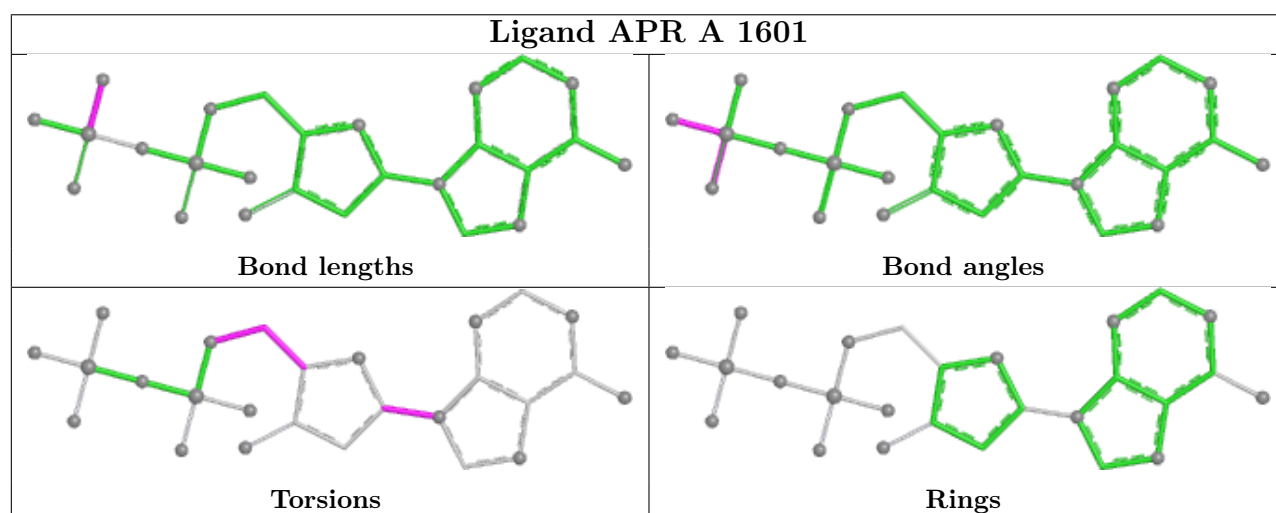
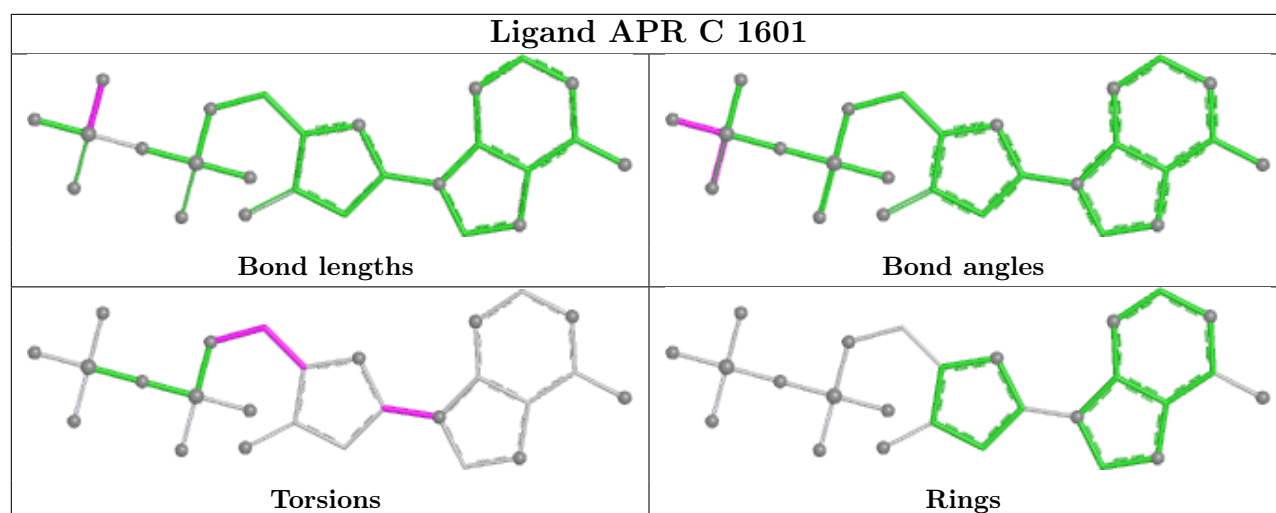
There are no ring outliers.

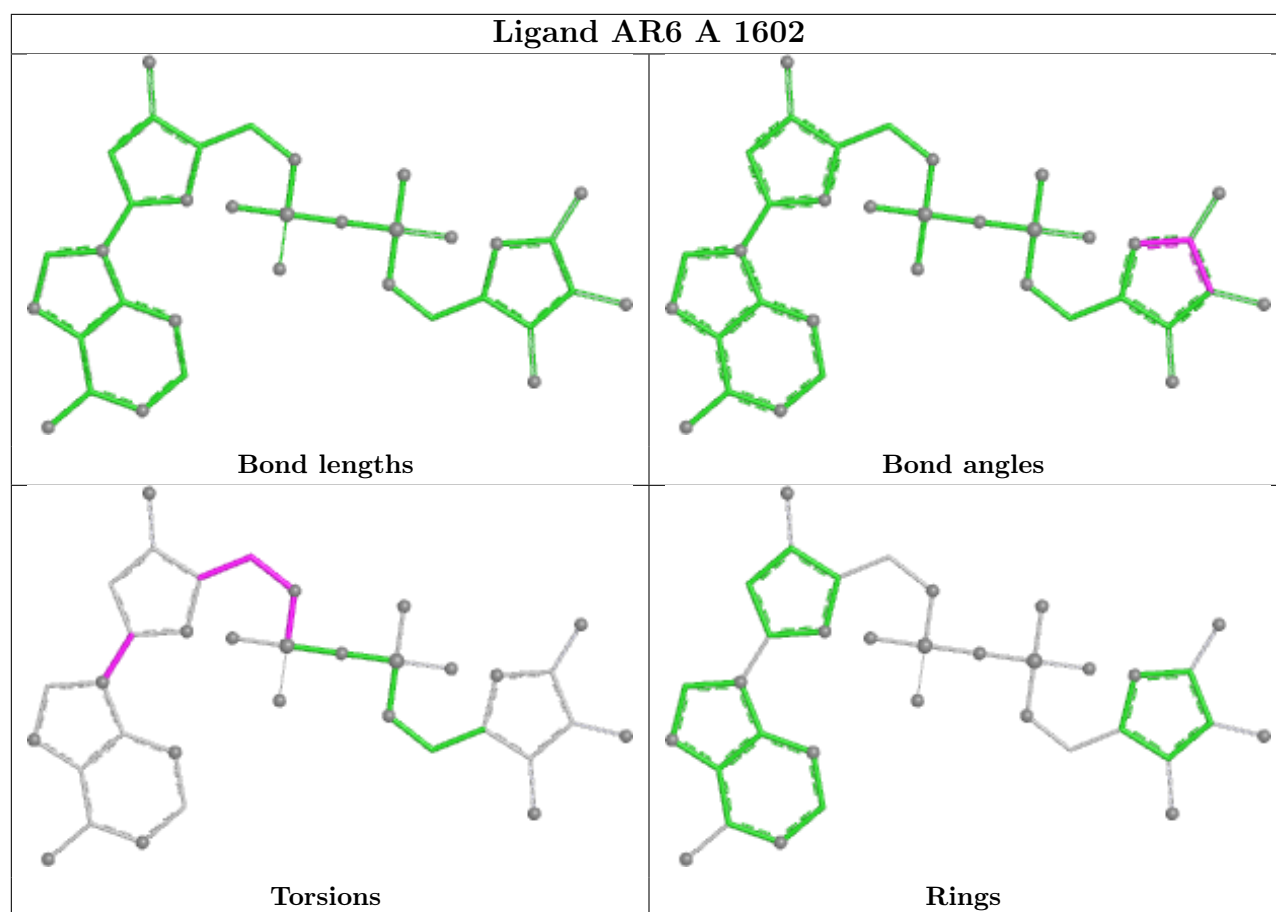
6 monomers are involved in 6 short contacts:

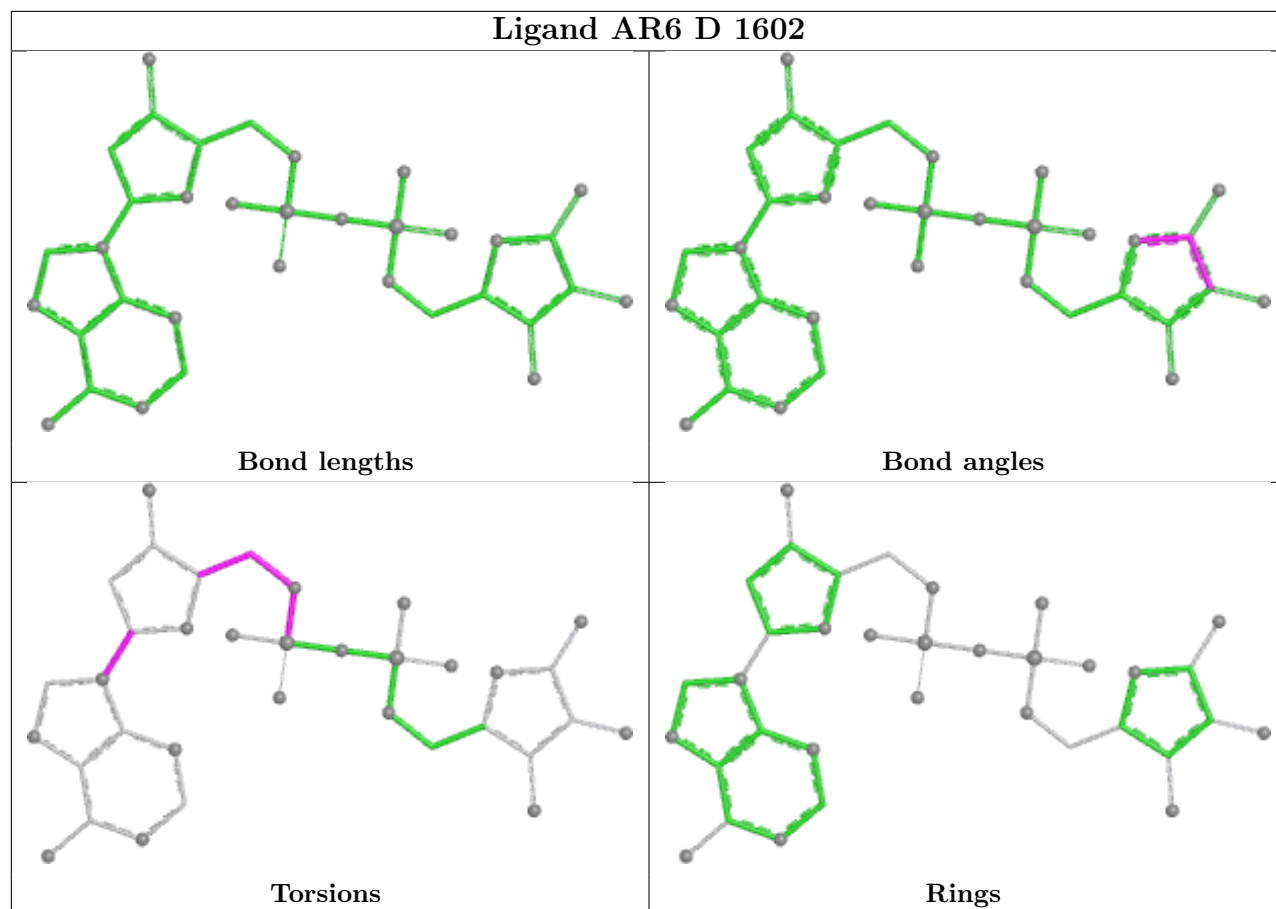
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	APR	1	0
2	C	1601	APR	1	0
2	A	1601	APR	1	0
3	A	1602	AR6	1	0
3	B	1602	AR6	1	0
2	D	1601	APR	1	0

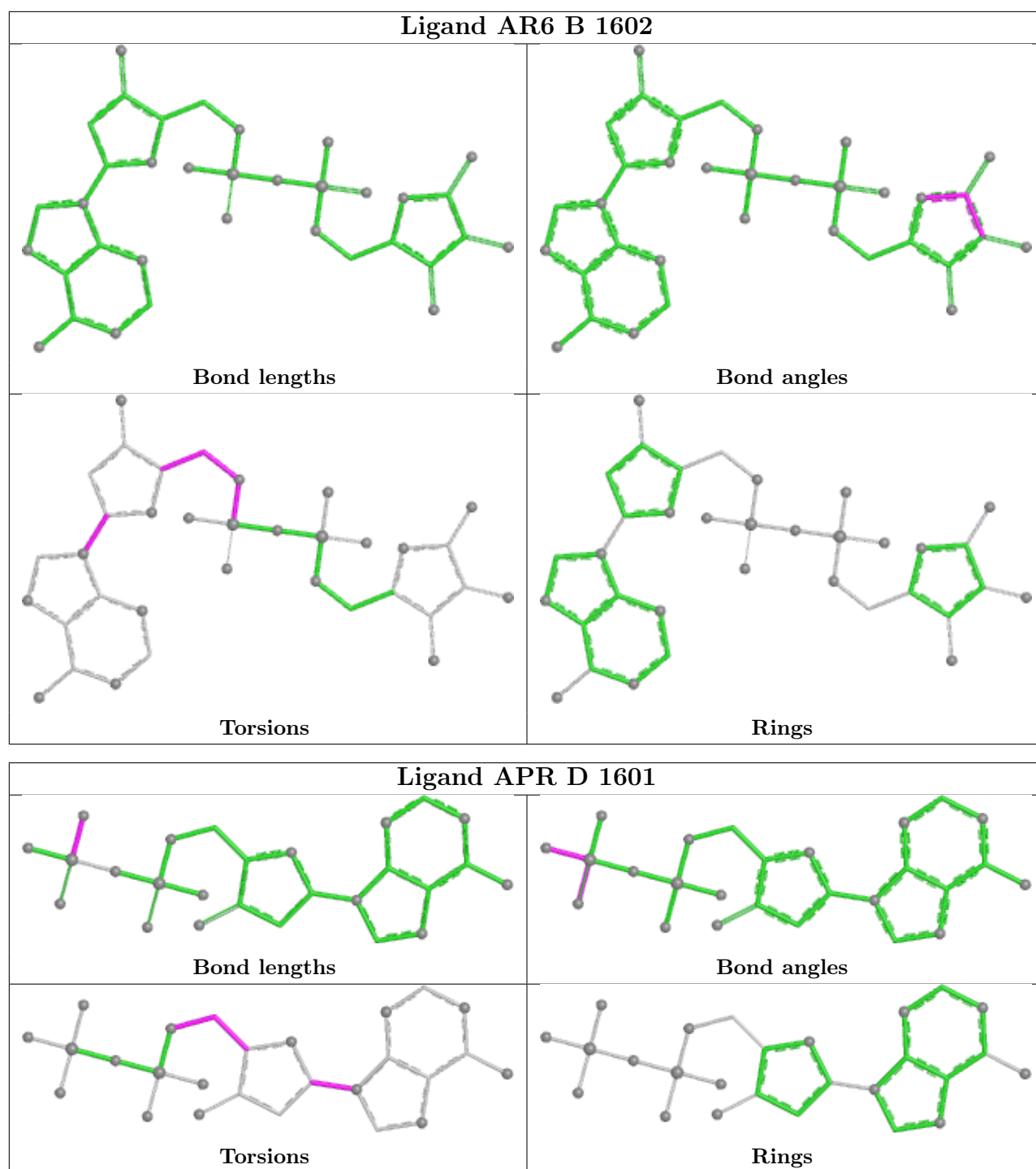
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	462:TRP	C	463:ASN	N	3.00
1	B	462:TRP	C	463:ASN	N	3.00
1	C	462:TRP	C	463:ASN	N	3.00
1	D	462:TRP	C	463:ASN	N	3.00

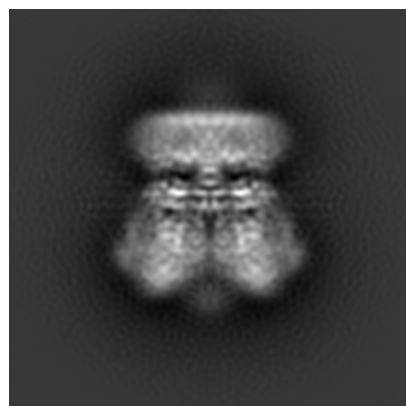
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27923. These allow visual inspection of the internal detail of the map and identification of artifacts.

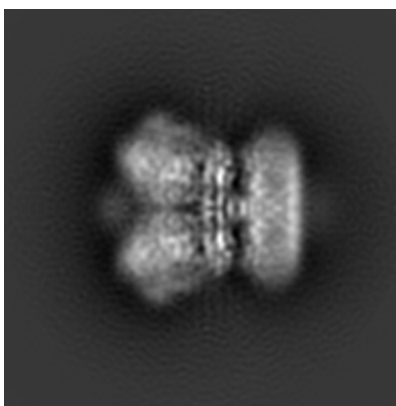
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

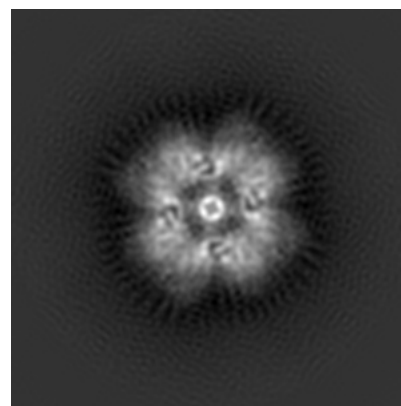
6.1.1 Primary map



X

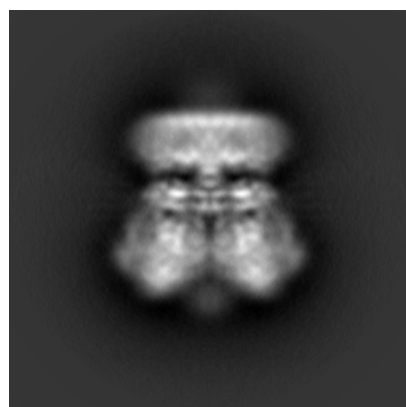


Y

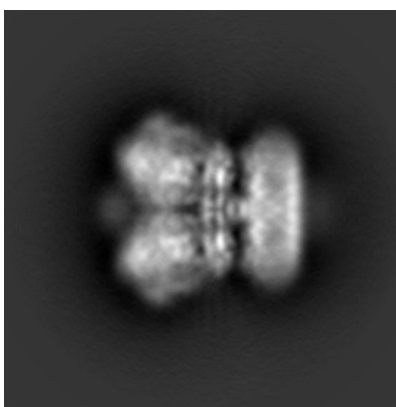


Z

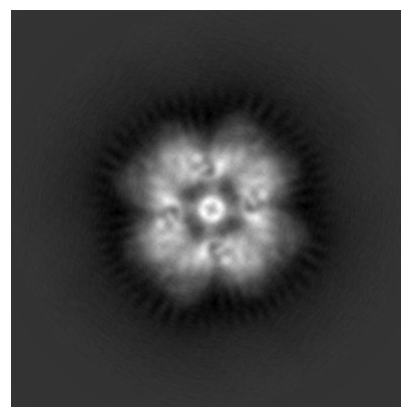
6.1.2 Raw map



X



Y



Z

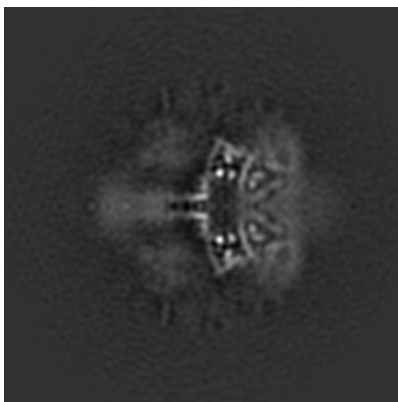
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

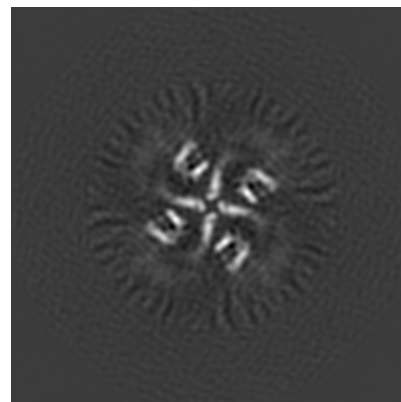
6.2.1 Primary map



X Index: 150

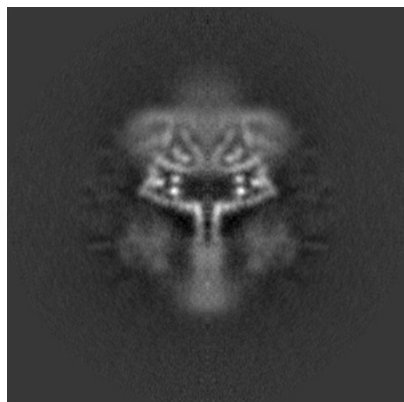


Y Index: 150

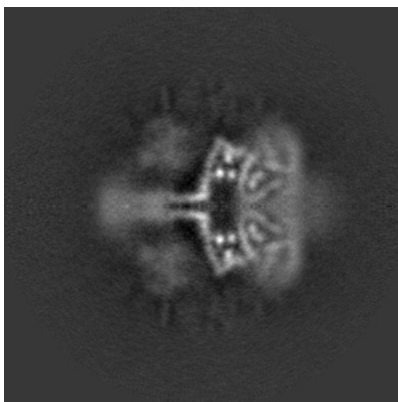


Z Index: 150

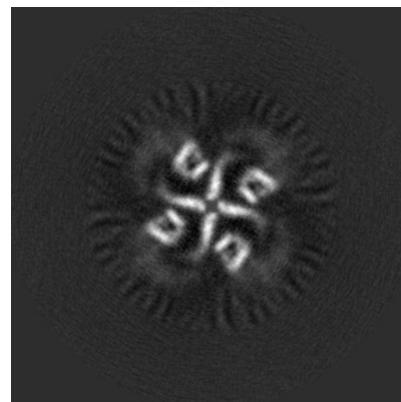
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

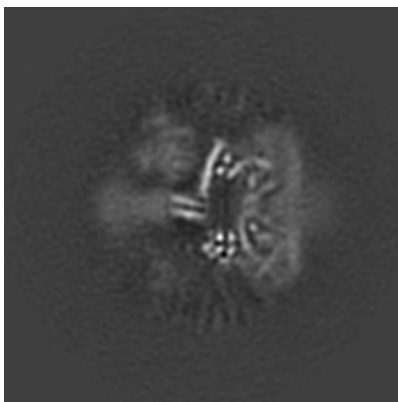
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

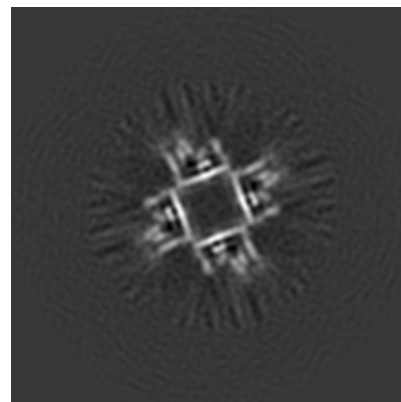
6.3.1 Primary map



X Index: 154

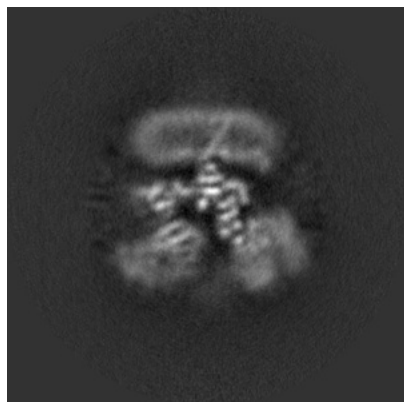


Y Index: 146

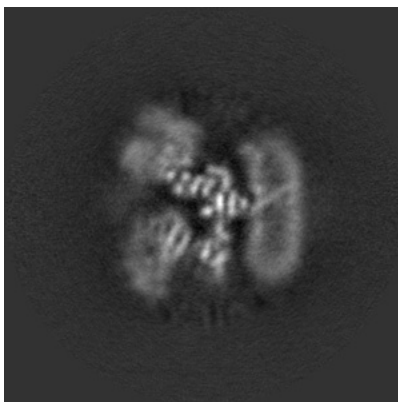


Z Index: 161

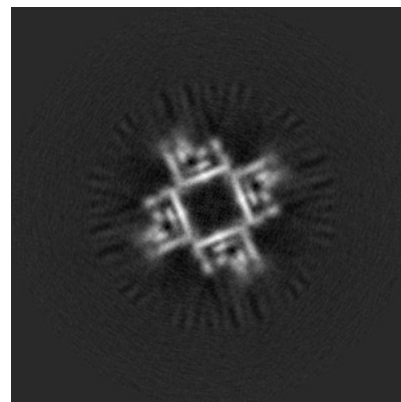
6.3.2 Raw map



X Index: 174



Y Index: 126

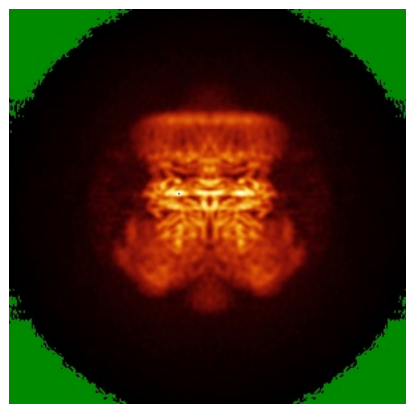


Z Index: 162

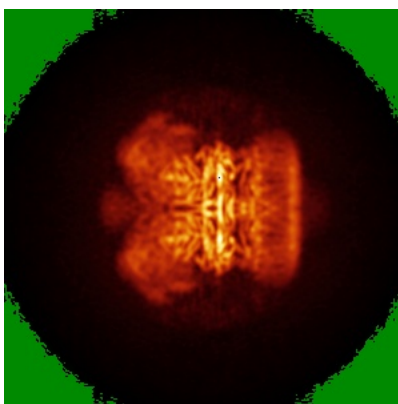
The images above show the largest variance slices of the map in three orthogonal directions.

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

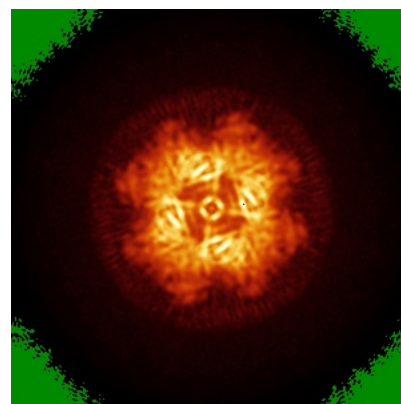
6.4.1 Primary map



X

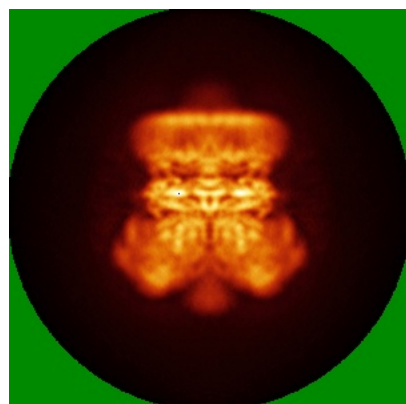


Y

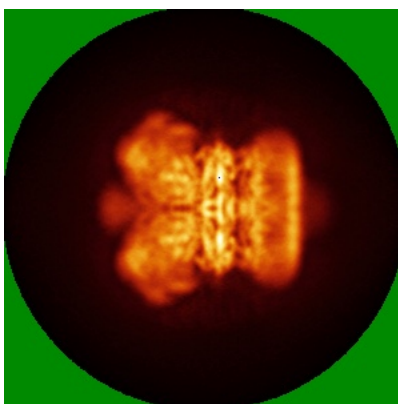


Z

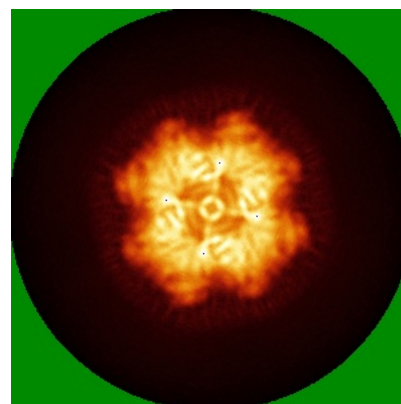
6.4.2 Raw map



X



Y

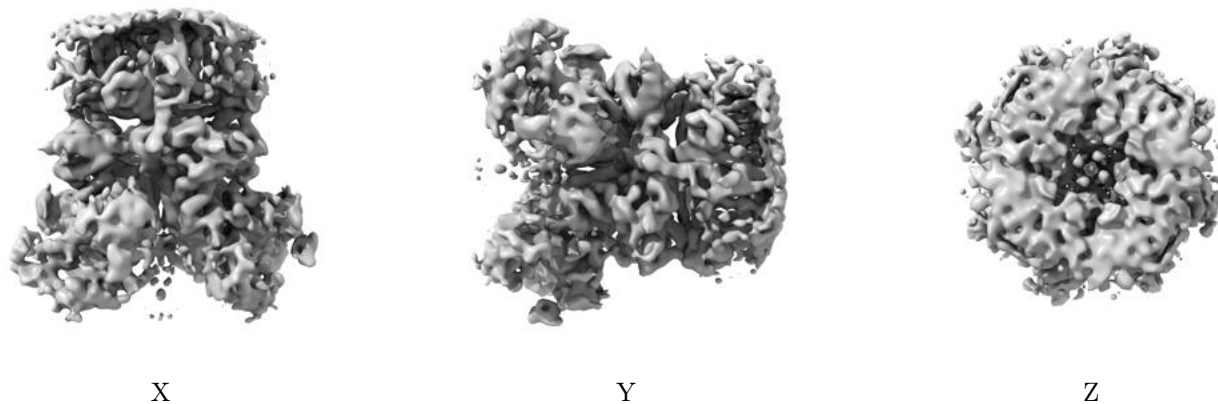


Z

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.

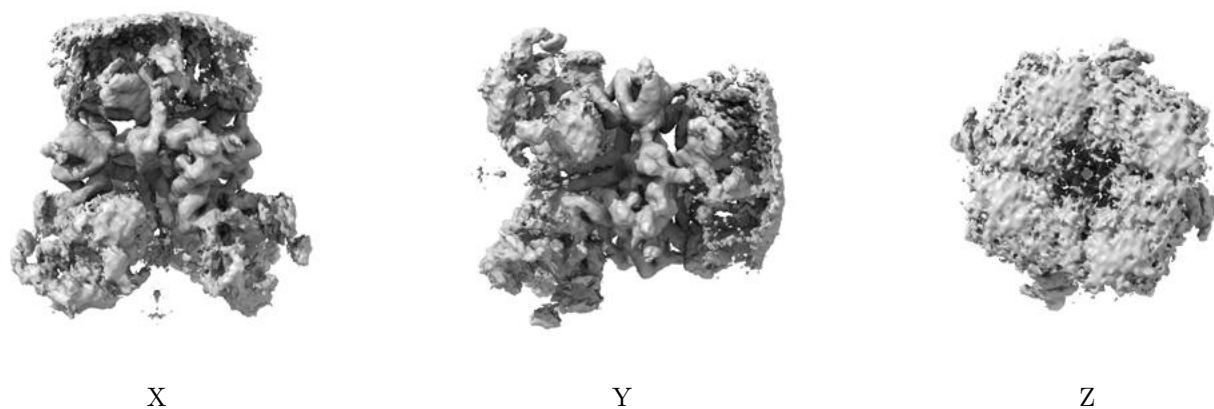
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0118. 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.

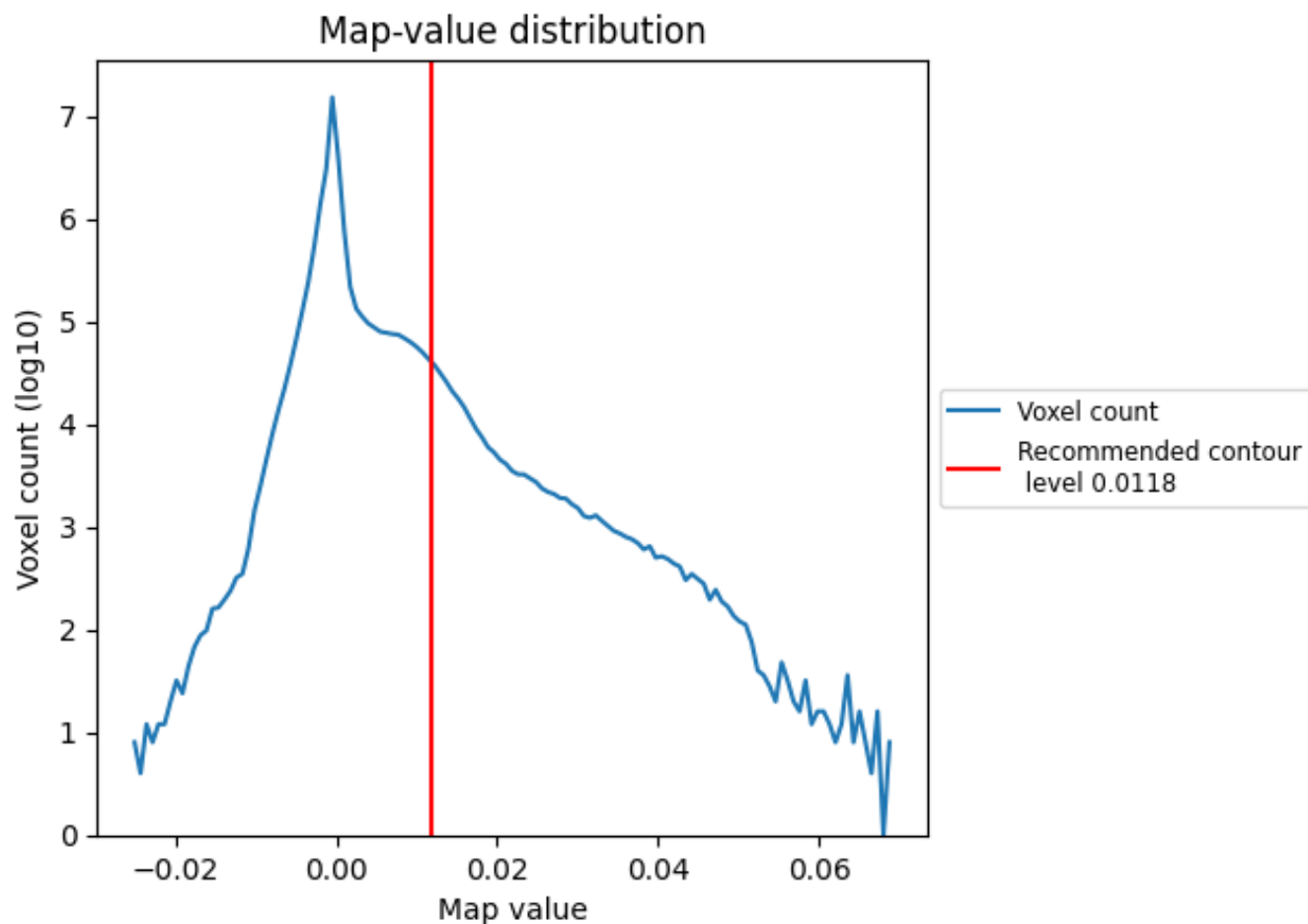
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

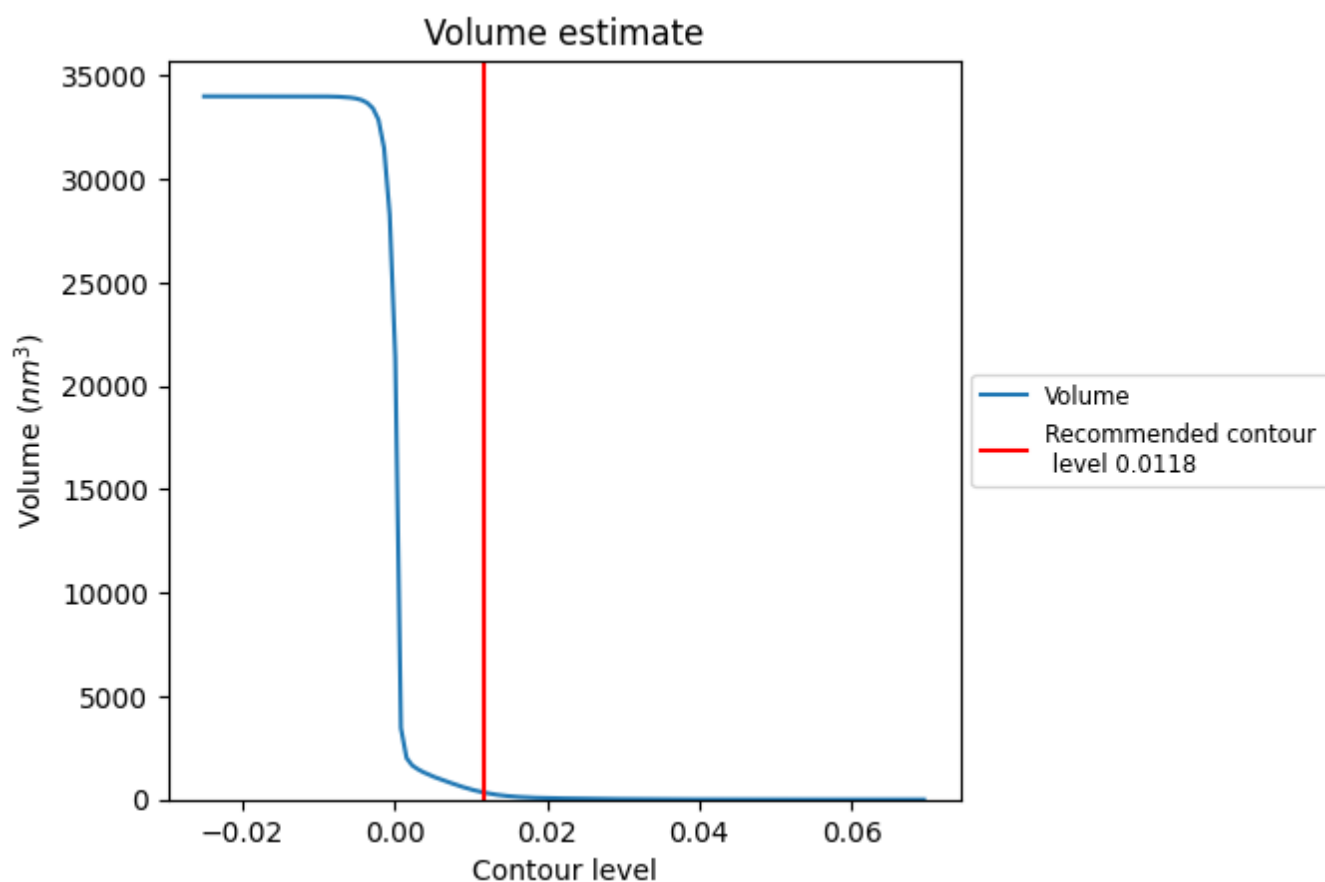
This section contains the results of statistical analysis of the map.

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.

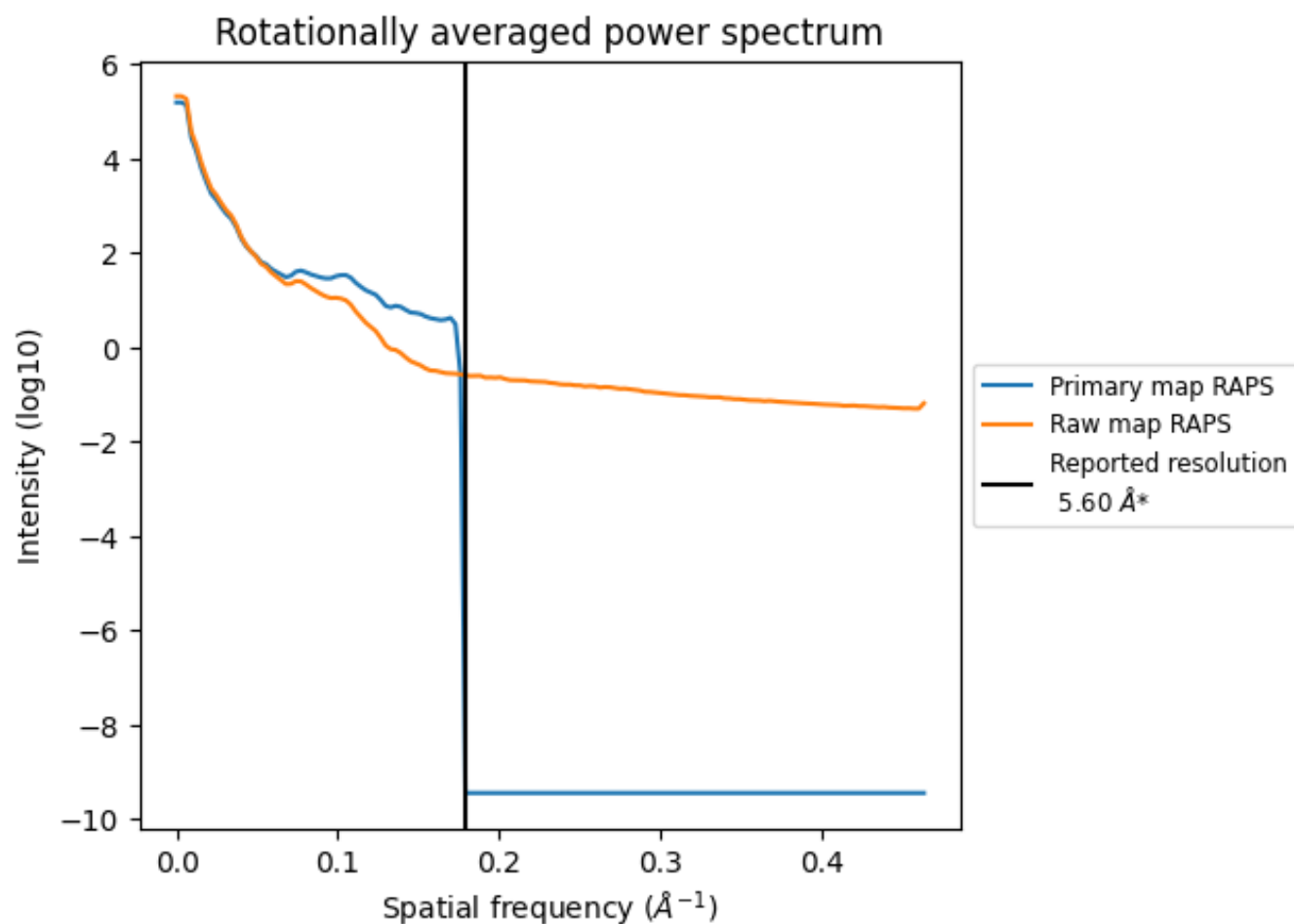
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334 nm³; this corresponds to an approximate mass of 302 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 ⓘ

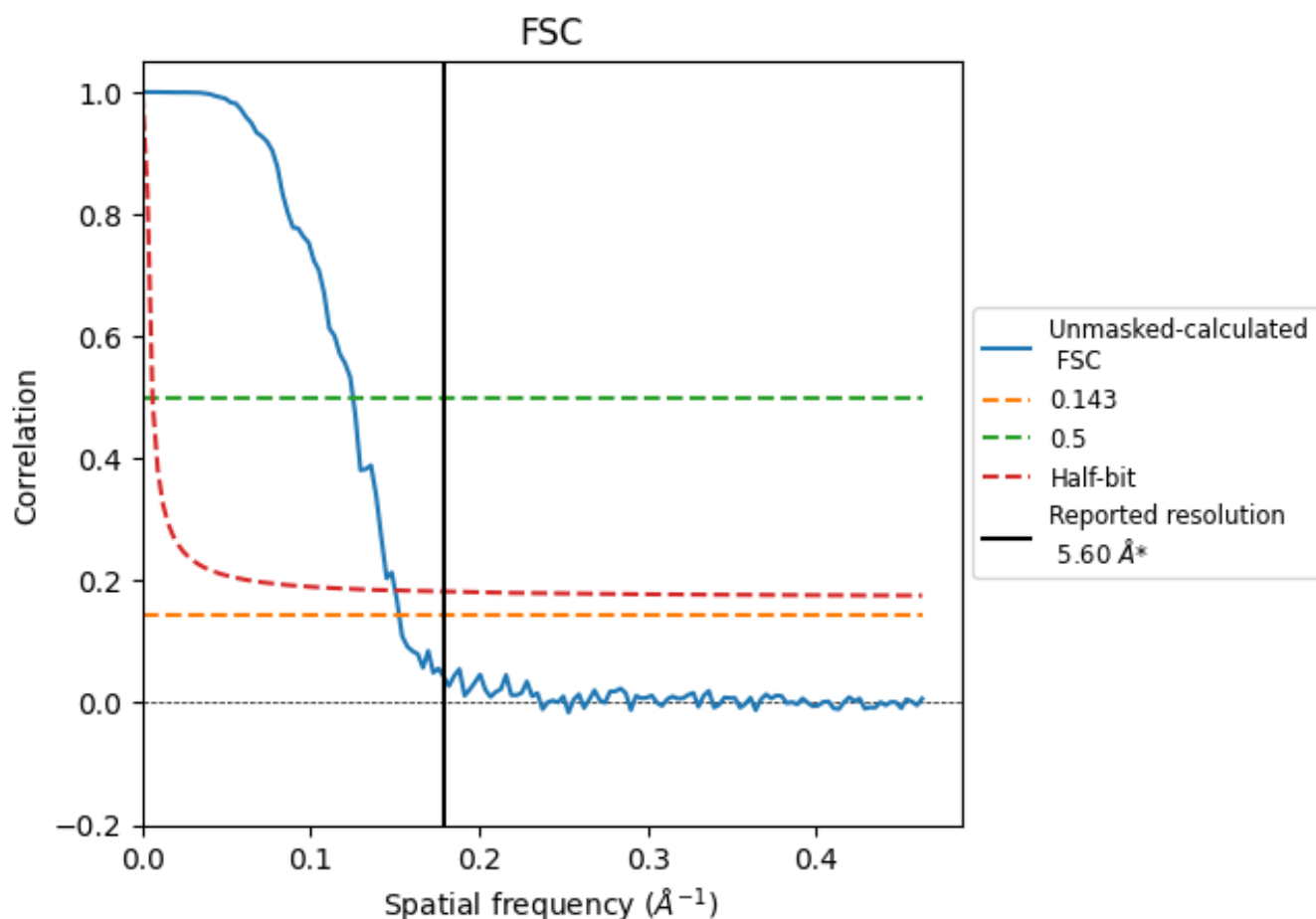


*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

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 0.179 Å⁻¹

8.2 Resolution estimates [i](#)

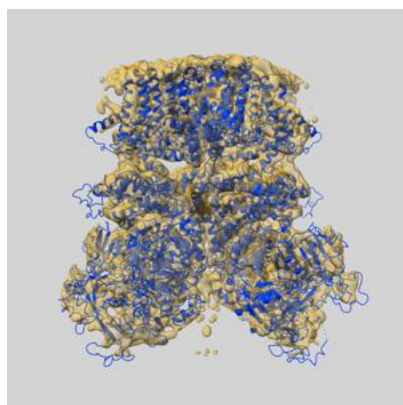
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.55	7.99	6.66

*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 6.55 differs from the reported value 5.6 by more than 10 %

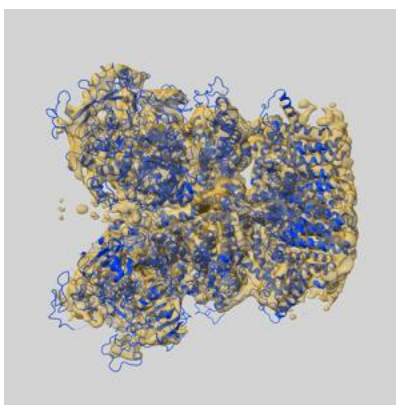
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27923 and PDB model 8E6R. Per-residue inclusion information can be found in section [3](#) on page [6](#).

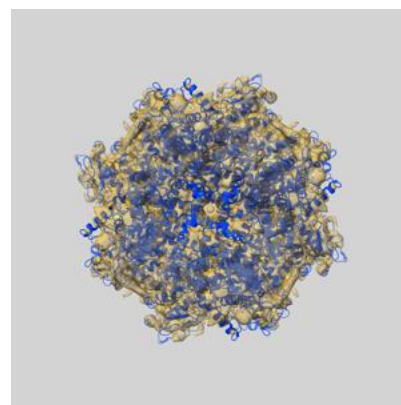
9.1 Map-model overlay [i](#)



X



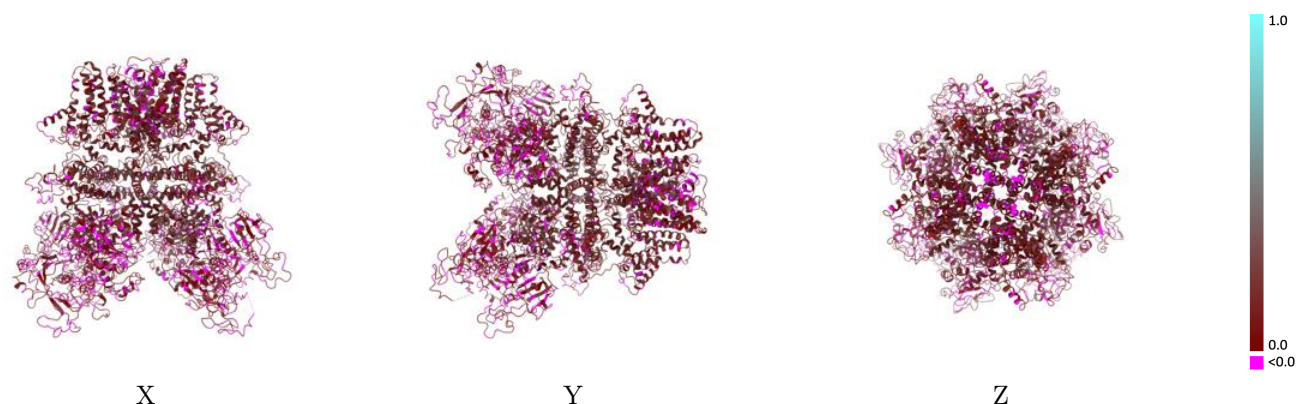
Y



Z

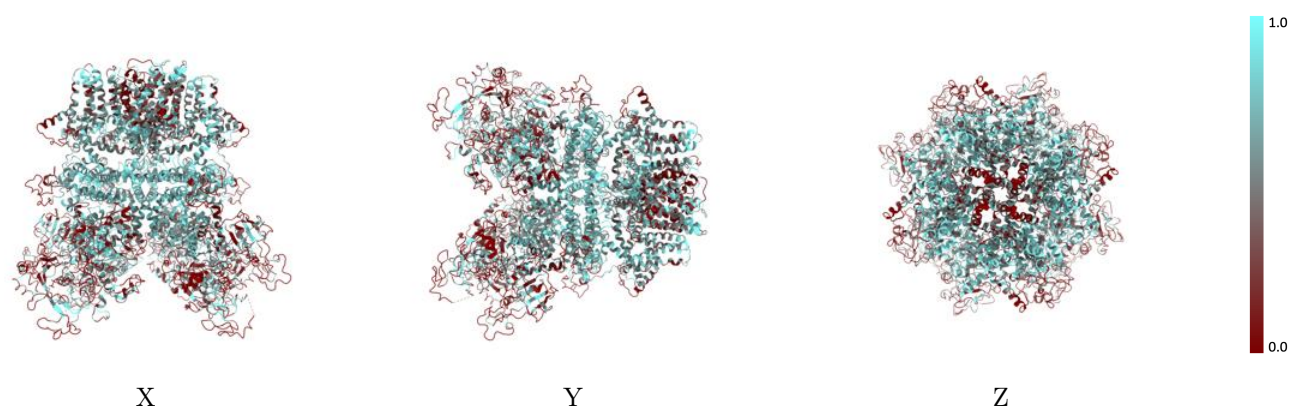
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



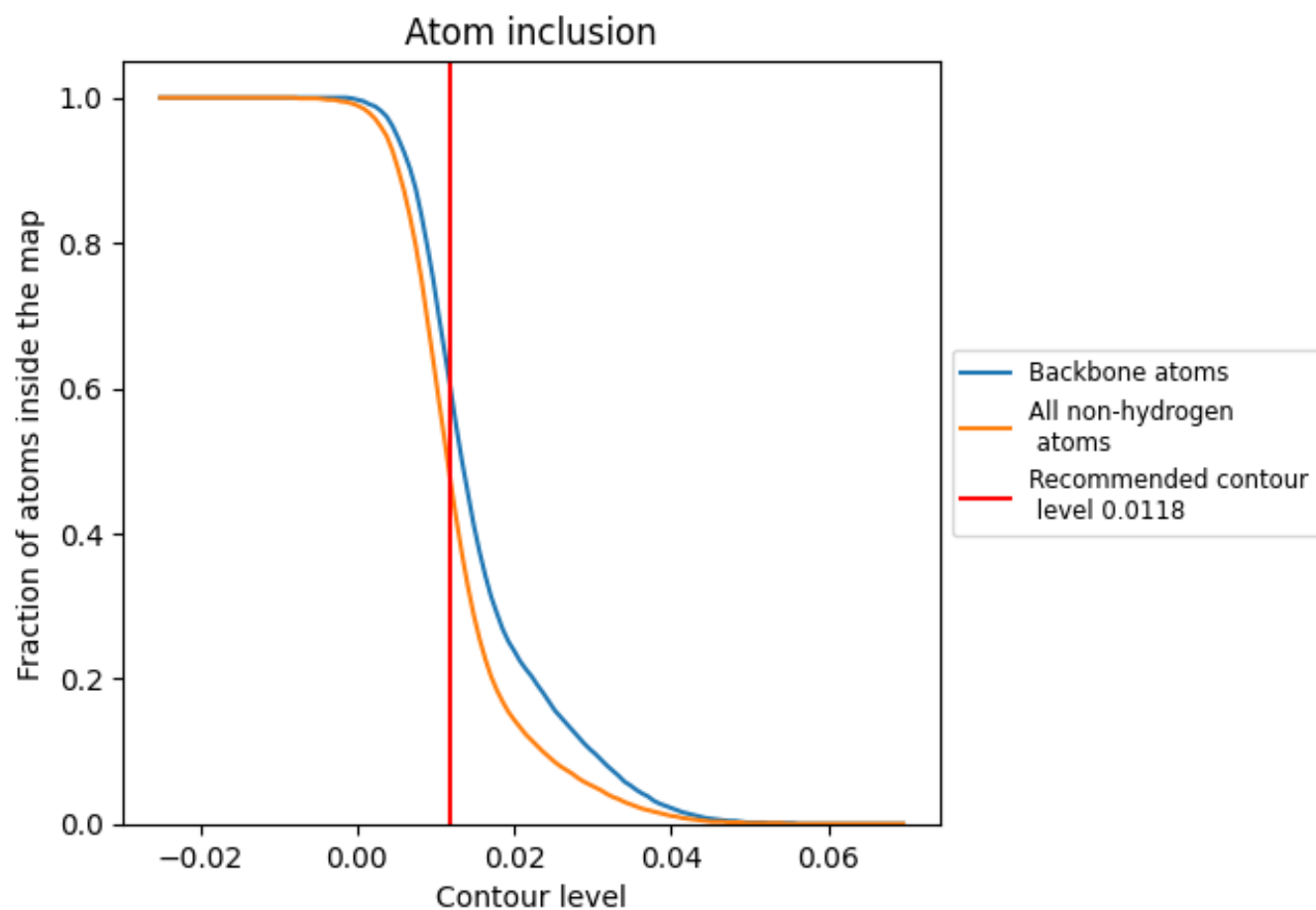
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 48% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4790	0.1230
A	0.4810	0.1250
B	0.4770	0.1220
C	0.4820	0.1240
D	0.4770	0.1210

