



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 8E6S / pdb_00008e6s
EMDB ID : EMD-27924
Title : Human TRPM2 ion channel in 1 mM dADPR and Ca²⁺
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on : 2022-08-23
Resolution : 4.60 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

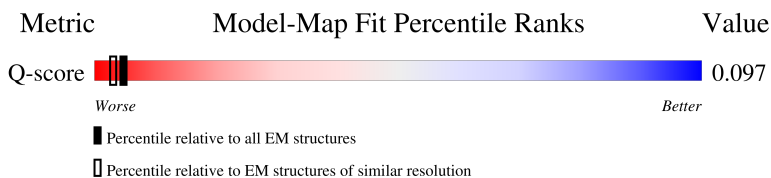
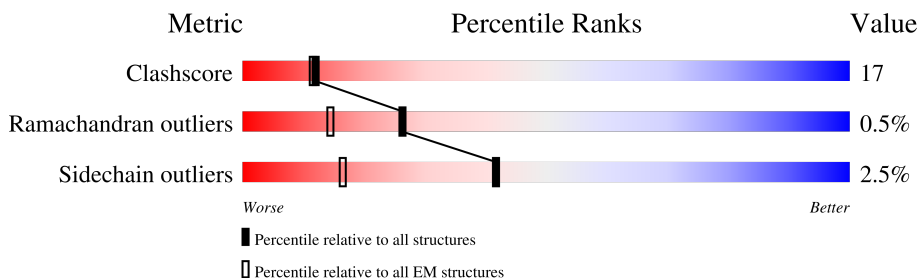
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

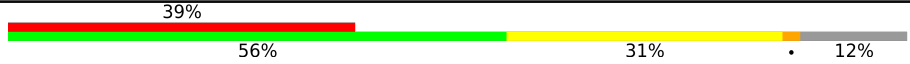
The reported resolution of this entry is 4.60 Å.

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	2407 (4.10 - 5.10)

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	 39% 56% 31% 12%
1	B	1503	 39% 56% 31% 12%
1	C	1503	 40% 56% 30% 12%
1	D	1503	 39% 56% 31% 12%

2 Entry composition [i](#)

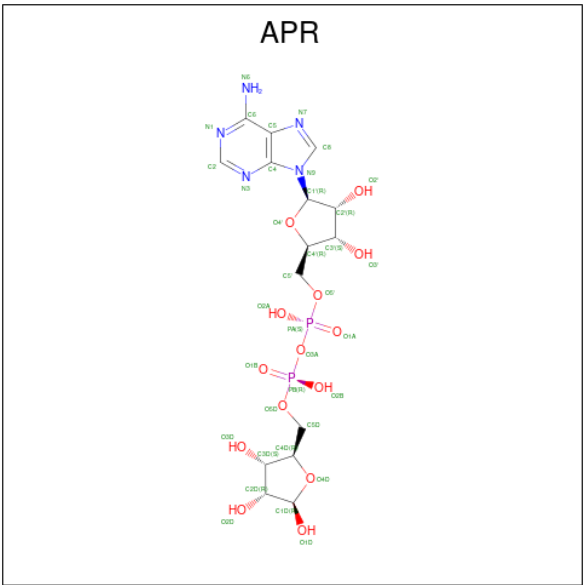
There are 5 unique types of molecules in this entry. The entry contains 42336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	1330	Total 10521	6791	1829	1851	50	0	0
1	B	1330	Total 10521	6791	1829	1851	50	0	0
1	C	1330	Total 10521	6791	1829	1851	50	0	0
1	D	1330	Total 10521	6791	1829	1851	50	0	0

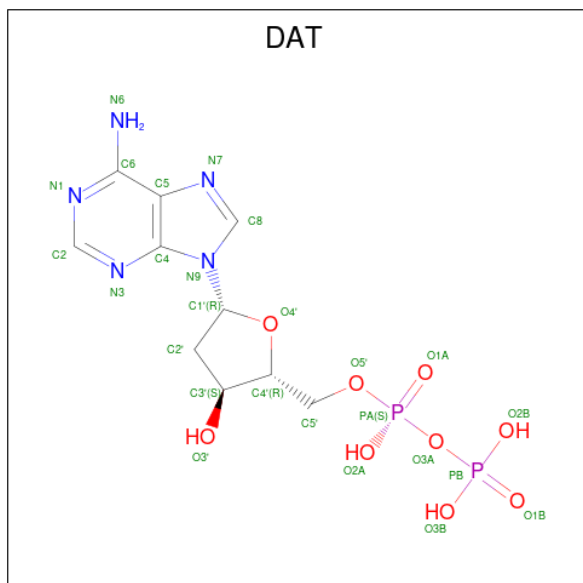
- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			35	15	5	13	2	
2	D	1	Total	C	N	O	P	0
			35	15	5	13	2	

- Molecule 3 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	

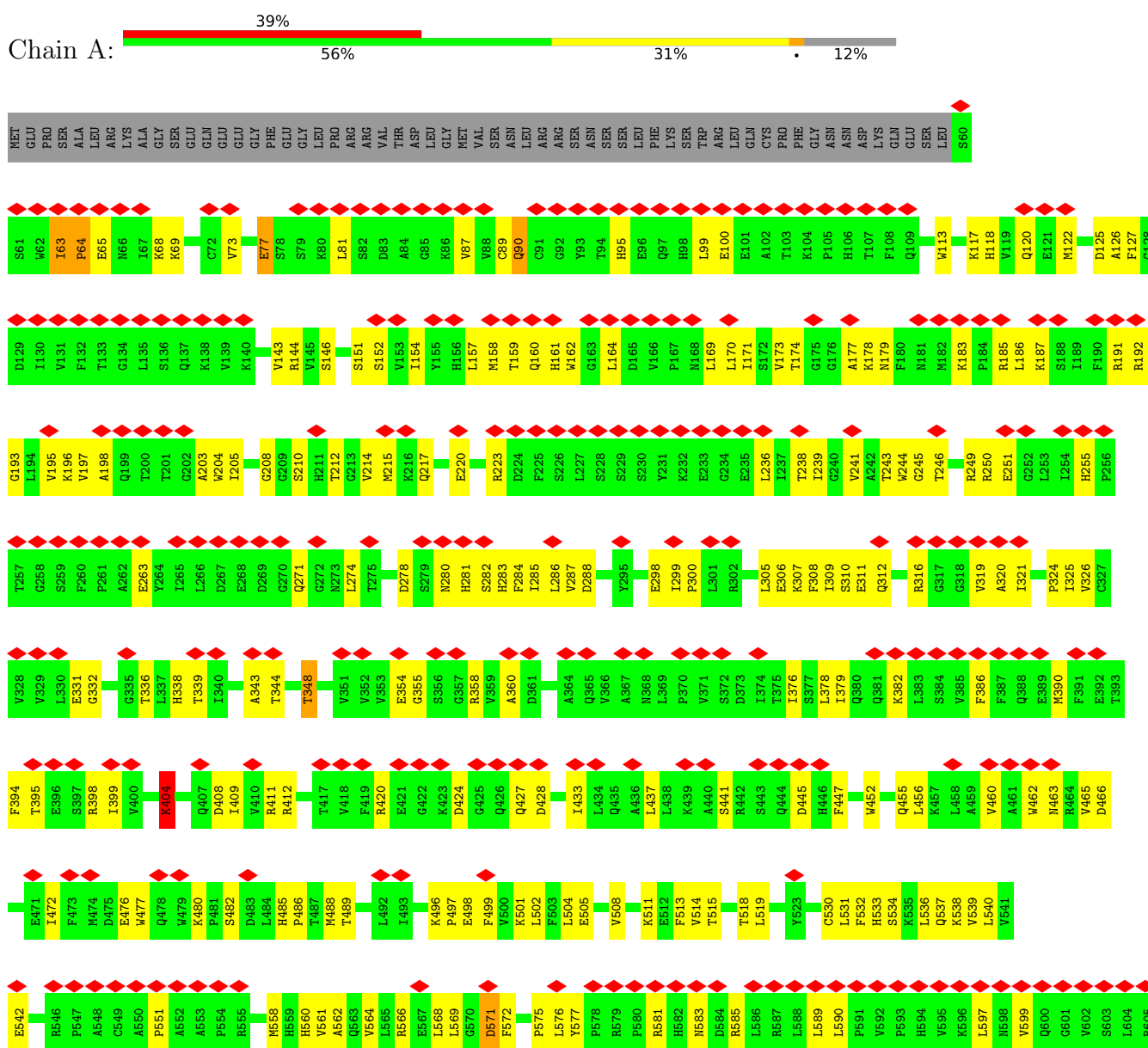
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

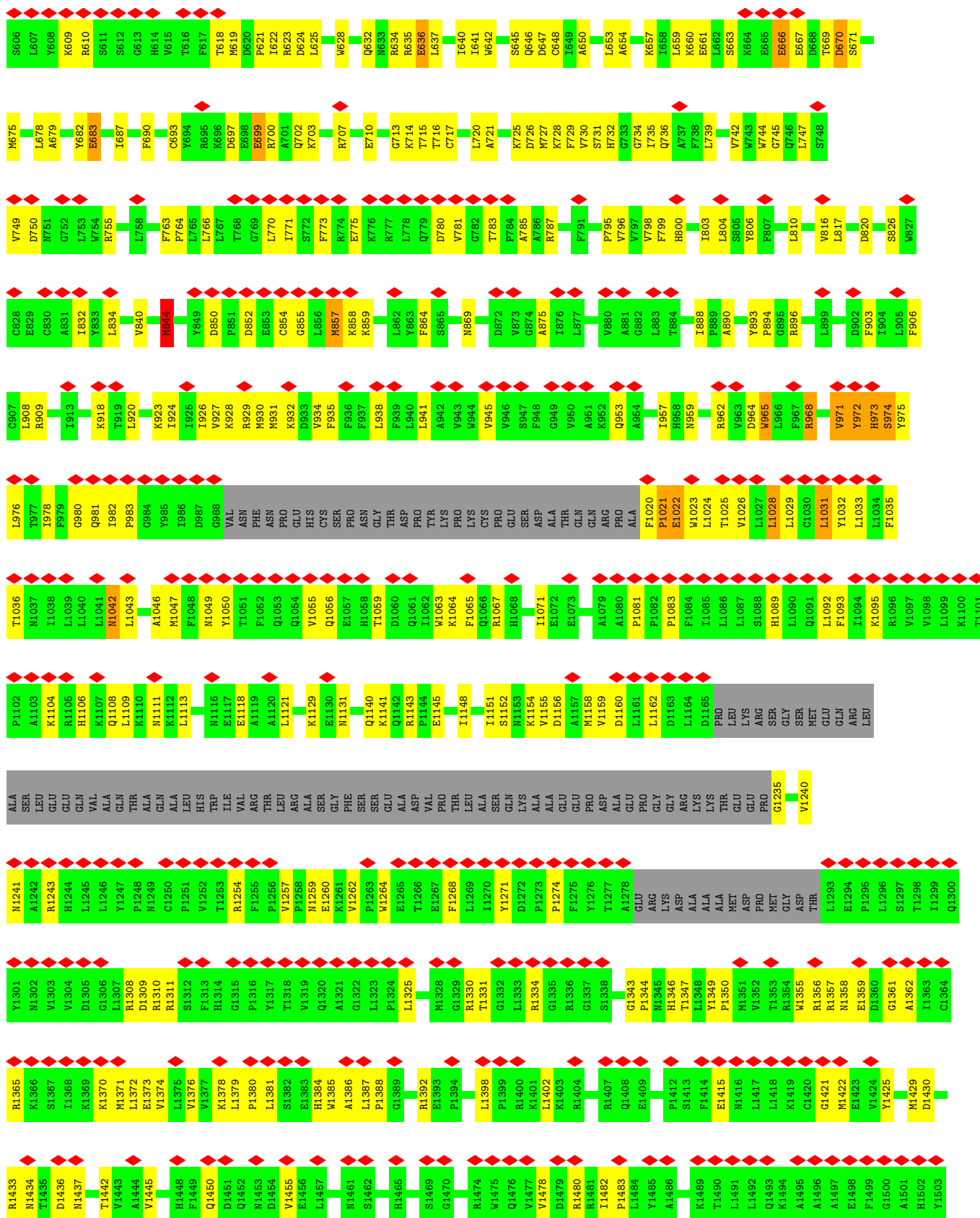
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

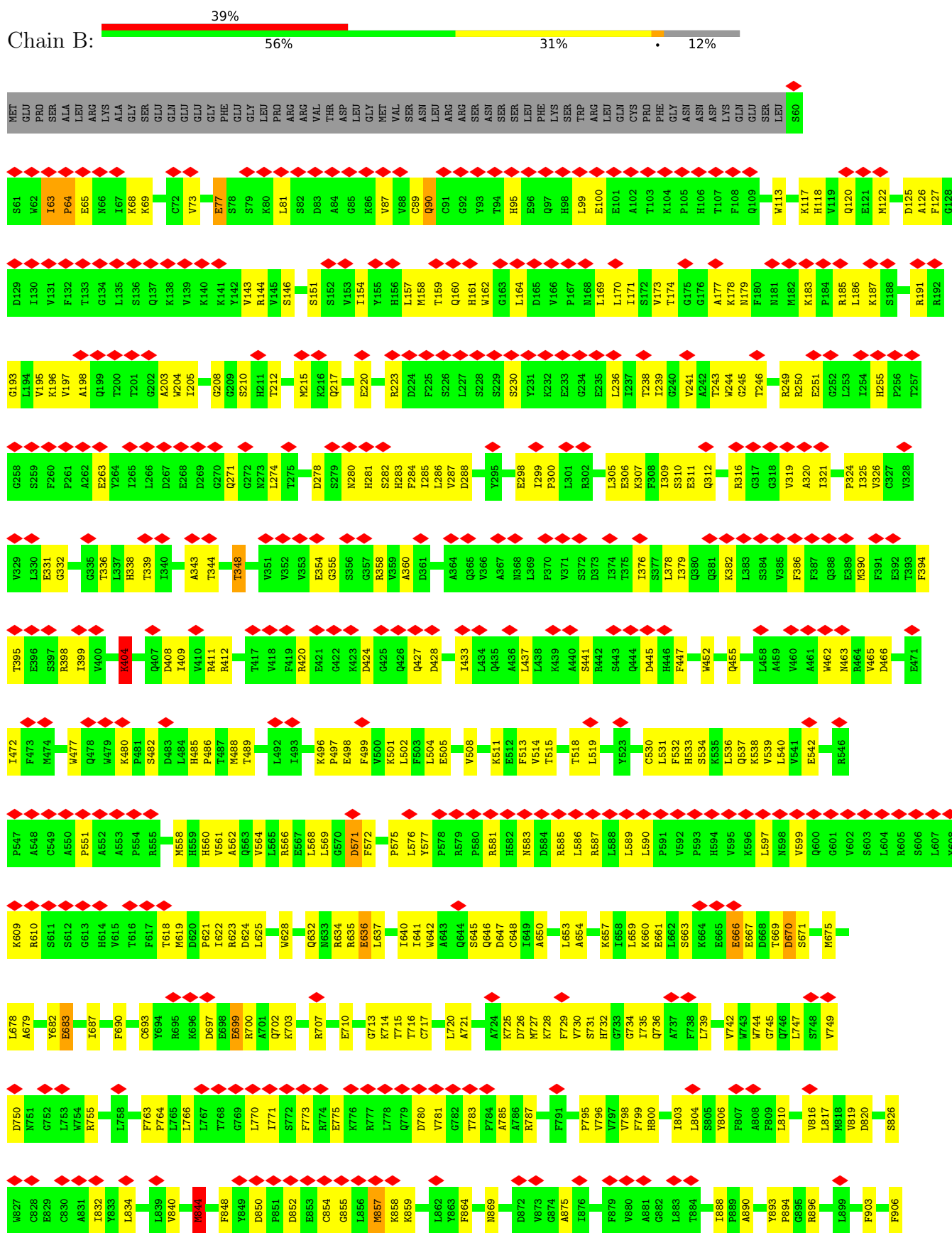
3 Residue-property plots

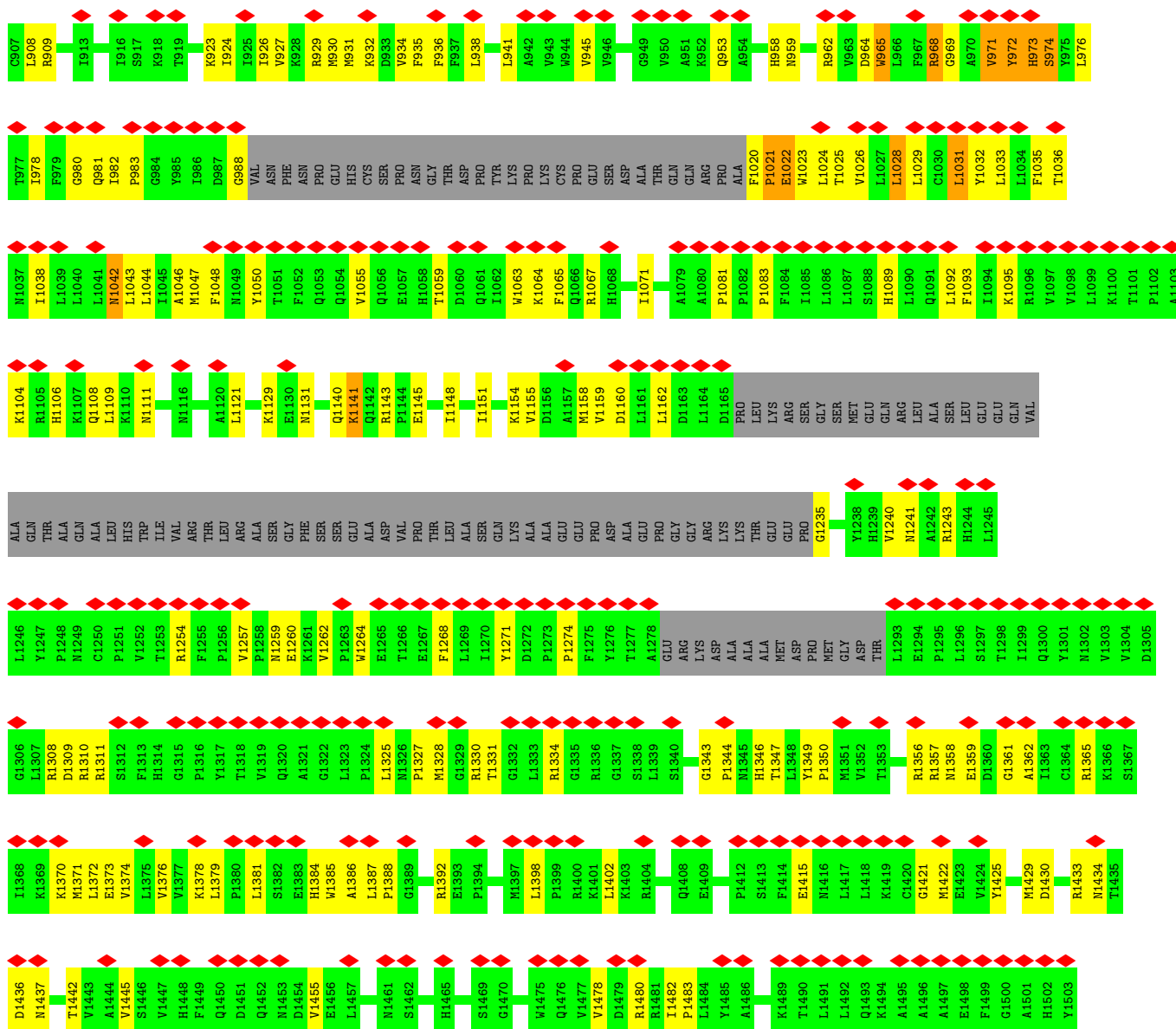
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

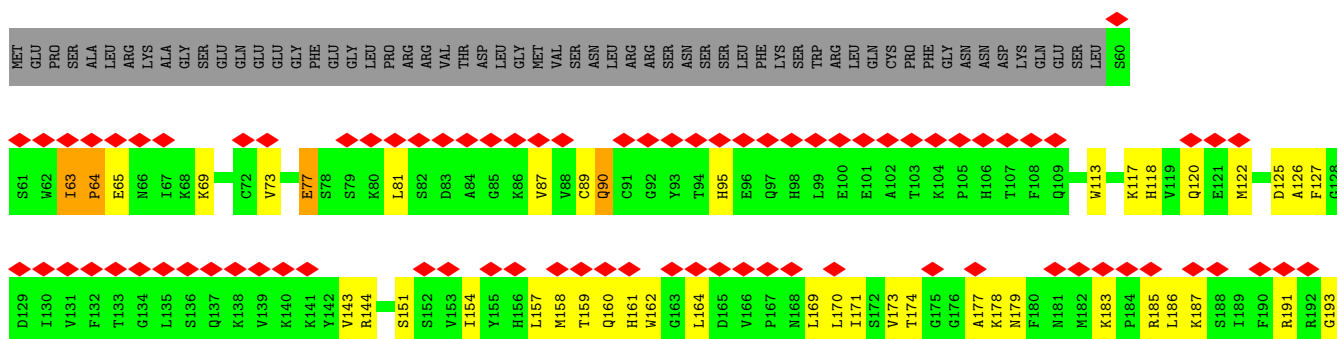
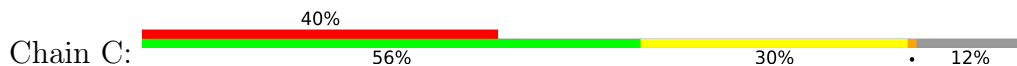




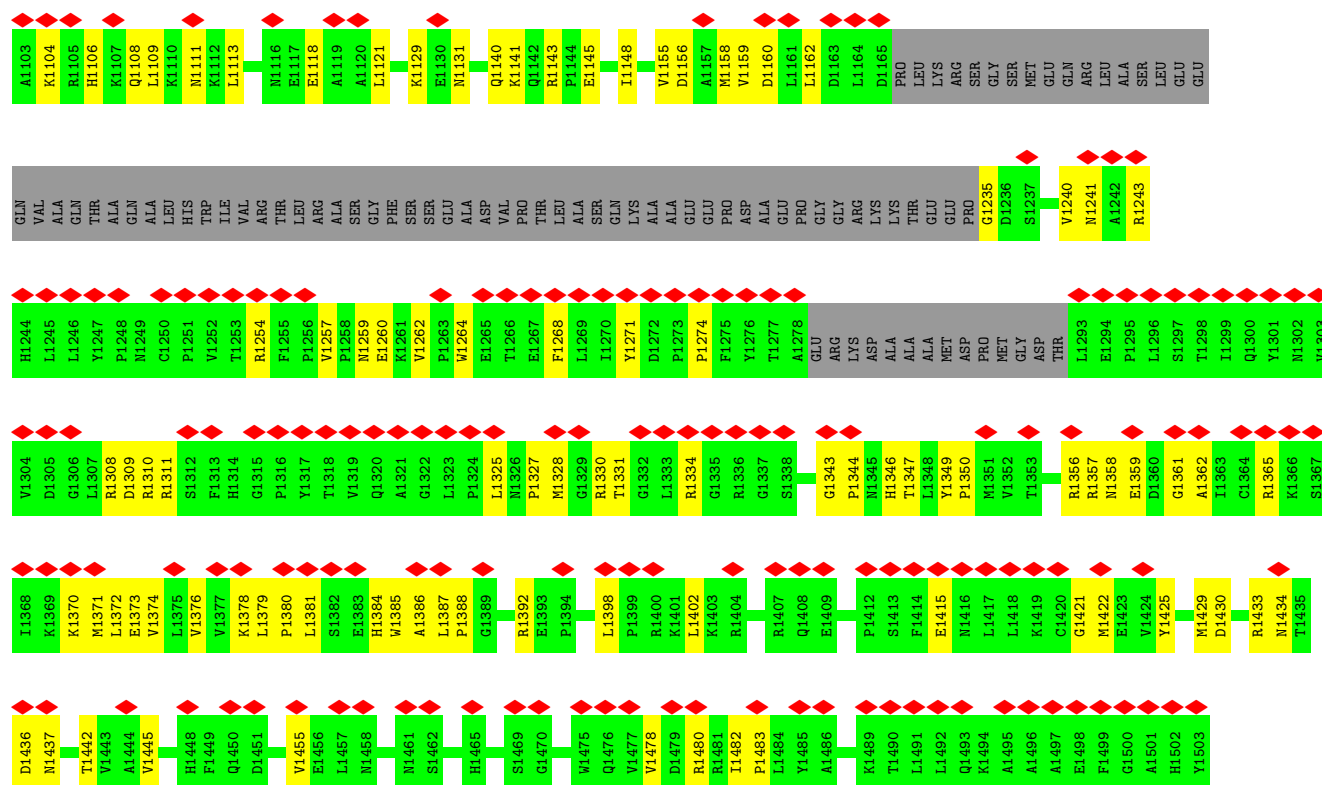




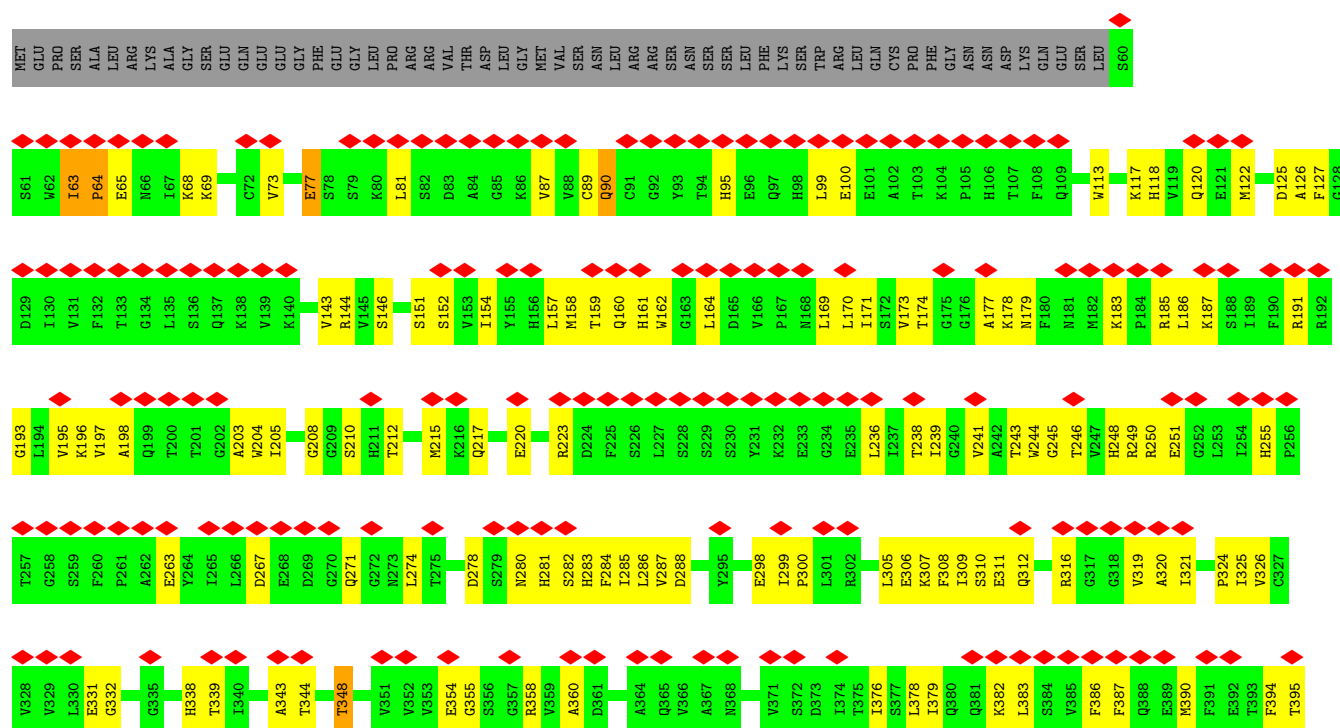
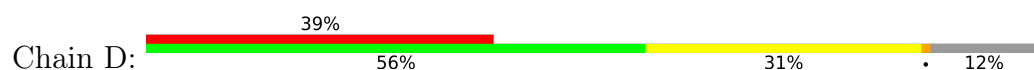
• Molecule 1: Transient receptor potential cation channel subfamily M member 2



N1037	T977	C907	S826	S748	M675	L607	R546	D475	I399	E331	L194
I1038	I978	L908	W827	V749	M676	Y608	P547	E476	V400	G332	V195
L1039	F979	R909	C828	D750	L678	K609	A548	Q477	G335	G336	K196
L1040	G980	I913	E829	W751	A679	R610	C549	Q478	E263	T336	V197
N1042	Q981	I916	C830	G752	Y682	S611	A550	Q479	Y264	L337	A198
L1043	I982	S917	A831	R755	E683	S612	P551	P481	I265	H338	Q199
L1044	P983	K918	I832	L758	E684	G613	A552	S482	I266	T339	T201
	G984	K919	Y833		I687	H614	A553	D483	I267	I340	G202
	Y985	T919	L834		F690	V615	P554	L484	E268	A343	A203
M1047	Y985				C693	T616	P555	H485	D269	T344	W204
F1048	I986	K923	V840	F763	Y694	F617	M558	T487	G270	T348	I205
N1049	D987	I924	C841	L764	R695	T618	H559	V418	Q271	G272	G208
Y1050	G988	I925	R844	L765	R696	M619	H560	F419	N273	N273	G209
T1051	VAL	I926		L766	K696	D620	V561	R420	L274	S210	G209
F1052	ASN	I927		T767	P621	P621	A562	E421	T275	H111	H111
Q1053	ASN	K928	F848	G768	D697	I622	O563	I493	D278	M215	M215
Q1054	PRD	R929	Y849	G769	E698	R623	O563	G422	S279	S279	K216
Q1055	GLU	M930	Y849	L770	E699	D624	V564	G423	N280	N280	Q217
V1055	GLU	M931	D850	L771	R700	L625	L565	D424	H281	H281	Q217
Q1056	HIS	K932	P851	S772	A701		R566	G425	S282	S282	E220
E1057	CYS	D933	D852	F773	Q702		L567	G426	H283	H283	R223
E1057	SER	V934	E853	R774	K703		L568	Q427	F284	F284	D224
H1058	PRD	P935	R774	E775	R707		L569	D428	I285	I285	D224
T1059	ASN	F935			E710		L570	I433	L286	L286	F225
D1060	THR	L938	C854	K776			L571	I434	L287	L287	S226
Q1061	ASP	F939	C855	R777			L572	Q435	D288	D288	S226
I1062	PRD	L856	L856	R778			L573	L434	Y295	Y295	S228
W1063	TYR	N857	N857	L778			Q574	L435	E298	E298	S230
K1064	LYS	K859	K859	Q779			P575	L436	I299	I299	Y231
F1065	PRD	A942	A942	D780			L576	L437	L301	L301	K232
Q1066	CYS	Y943	Y943	W781			L577	L438	E233	E233	E233
R1067	CYS	Y944	A860	C717			L578	L439	Q302	Q302	Q234
H1068	PRD	V945					L579	L440	L305	L305	E235
	GLU	V946					L580	L441	E306	E306	E235
	GLU	S947					L581	L442	K307	K307	L236
	SER	F948					L582	L443	I309	I309	I237
	ALA	G949					L583	L444	E311	E311	V241
	GLN	V950					L584	L445	Q312	Q312	A242
	GLN	K951					L585	L446	R316	R316	T243
	ARG	A875					L586	L447	G317	G317	W244
	PRD	L876					L587	L448	F386	F386	G245
	ALA	L877					L588	L449	F387	F387	T246
P1081	P1082	Q953					L589	L450	Q388	Q388	R249
P1082	P1083	A954					L590	L451	E320	E320	R250
P1083	F1084	V880					L591	L452	I321	I321	E251
F1084	C882	A881					L592	L453	P324	P324	G252
I1085	L883	L883					L593	L454	I325	I325	L253
L1086	T894	T894					L594	L455	F394	F394	I254
L1087	D964	D964					L595	L456	C327	C327	H255
S1088	Y965	Y965					L596	L457	V329	V329	P256
H1089	L966	L966					L597	L458	V329	V329	G258
L1090	P967	P967					L598	L459	L330	L330	
Q1091	C1030	C1030					L599	L460			
L1092	Y1032	Y1032					L600	L461			
F1093	L1033	L1033					L601	L462			
I1094	L1034	L1034					L602	L463			
K1095	F1035	F1035					L603	L464			
R1096	T1036	T1036					L604	L465			
V1097							L605	L466			
V1098							L606	L467			
V1099							L607	L468			
K1100							L608	L469			
T1101							L609	L470			
P1102							L610	L471			



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



E396	S397	R398	I399	V400	K404	Q407	D408	I409	V410	R411	R412	T417	V418	F419	R420	E421	Q422	K423	D424	Q425	Q426	Q427	D428	I433	L434	Q435	A436	L437	L438	K439	A440	S441	R442	S443	Q444	D445	H446	F447	W452	D453	H454	Q455	L458	A459	V460	A461	W462	M463	R464	D466	E471						
I472	F473	M474	W477	Q478	W479	K480	P481	S482	D483	L484	H485	P486	T487	M488	T489	L492	I493	K496	P497	E498	F499	V500	F572	K501	L502	F503	L504	E505	V508	K511	E512	F513	V514	T515	T518	L519	Y523	C530	L531	F532	H533	S534	K535	L536	Q537	K538	V539	L540	Y541	E542	R546						
P547	A548	C549	A550	P551	A552	A553	P554	R555	M558	H559	H560	V561	A562	Q563	V564	L565	R566	E567	L568	L569	G570	D571	F572	T573	Q574	P575	L576	Y577	P578	R579	P580	R581	H582	N583	D584	R585	L586	R587	L588	L589	P591	V592	F593	H594	V595	K596	L597	N598	V599	Q600	G601	V602	S603	L604	R605	S606	L607
Y608	K609	R610	S611	S612	G613	H614	V615	T616	F617	T618	M619	D620	V621	I622	R623	D624	L625	W628	V631	Q632	N633	R634	R635	E636	L637	I640	I641	W642	A643	Q644	S645	Q646	D647	C648	I649	A650	L653	A654	K657	L658	K659	E661	L662	S663	W664	K664	E665	E666	E667	D668	T669	D670	S671				
M675	L678	A679	Y682	E683	I687	F690	C693	D697	E698	E699	R700	Q701	R703	R707	E710	G713	K714	T715	T716	C717	L720	A721	K725	T726	M727	K728	F729	S731	H732	G733	G734	I735	Q736	F738	L739	V742	W743	W744	G745	Q746	L747	S748	V749	D750													
R755	L758	F763	P764	L765	L766	L767	T768	G769	L770	I771	E772	R773	R774	E775	K776	L778	Q779	D780	V781	G782	T783	P784	A785	A786	R787	T793	A794	P795	V796	V797	F798	F799	H800	L803	L804	S805	Y806	L810	C811	L812	V816	L817	D820	S826	C830	A831	I832	Y833									
L834	W840	C841	R844	R845	F848	H849	D850	P851	D852	E853	C854	G855	L856	M857	K858	K859	A860	A861	L862	T863	F864	S865	R869	K870	L871	D872	W873	L876	L877	L878	F879	V880	A881	C882	L883	T884	T888	P889	A890	H893	P894	G895	R896	L899	F903	I904	L905	F906	C907	L908							
R909	L910	I913	K918	T919	L920	I924	I925	I926	V927	R928	R929	H930	H931	K932	P933	V934	F935	F936	F937	L938	F939	L940	L941	A942	V943	V944	V945	V946	S947	F948	G949	V950	A951	K952	Q953	A954	V959	R962	D964	V965	L966	F967	R968	G969	A970	V971	Y972	H973	S974	L976	T977	I978					
F979	G980	Q981	I982	P983	Q984	Y985	I986	D987	G988	VAL	ASN	PHE	ASN	PRO	GLU	HIS	CYS	SER	PRO	ASN	GLY	THR	ASP	PRO	LYS	CYS	PRO	GLU	SER	ASP	ALA	THR	GLN	ARG	PRO	ALA	F1020	P1021	E1022	W1023	T1024	T1025	V1026	L1027	L1028	L1029	C1030	L1031	G1032	Y1033	L1034	F1035	T1036	N1037	I1038		
L1039	L1040	L1041	N1042	L1043	M1047	F1048	N1049	Y1050	T1051	F1052	Q1053	Q1054	V1055	Q1056	E1057	H1058	T1059	D1060	Q1061	I1062	W1063	K1064	F1065	Q1066	R1067	H1068	I1071	E1072	E1073	A1079	A1080	P1081	P1082	P1083	F1084	I1085	L1086	L1087	S1088	H1089	L1090	Q1091	L1092	F1093	I1094	K1095	R1096	V1097	V1098	L1099	K1100	P1102	A1103	K1104	R1105		
H1106	K1107	Q1108	L1109	K1110	M1111	K1112	M1116	L1121	K1129	E1130	M1131	Q1140	K1141	Q1142	R1143	P1144	E1145	I1148	K1154	V1155	D1156	A1157	M1158	V1159	D1160	L1161	L1162	D1163	L1164	D1165	PRO	LEU	LYS	ARG	GLY	SER	MET	GLN	GLU	ARG	LEU	ALA	SER	LEU	GLU	VAL	ALA	THR	ALA								
GLN	ALA	HIS	TRP	ILE	VAL	ARG	LEU	ALA	SER	GLY	PHE	SER	GLU	ALA	ASP	VAL	PRO	THR	LEU	ALA	SER	GLN	LYS	ALA	GLU	PRO	ASP	ALA	GLY	ALA	ALA	ALA	MET	ASP	PRO	THR	THR	GLU	GLU	PRO	G1235	V1240	N1241	A1242	R1243	H1244	L1245	L1246	Y1247	P1248	N1249	C1250	P1251				
V1252	T1253	R1254	F1255	P1256	V1257	N1258	E1259	E1260	K1261	V1262	P1263	E1264	E1265	T1266	E1267	F1268	L1269	I1270	Y1271	D1272	P1273	P1274	F1275	V1276	T1277	A1278	GLU	ARG	LYS	ASP	ALA	GLY	ALA	ALA	MET	ASP	PRO	THR	L1293	E1294	P1295	L1296	S1297	T1298	L1299	Q1300	Y1301	N1302	V1303	V1304	D1305	G1306	L1307	R1308	D1309	R1310	R1311

HI448	FI449	QI450	DI451	QI452	NI453	DI454	VI455	EI456	LI457	MI458	NI461	SI462	HI465	SI469	GI470	WI475	QI476	VI477	VI478	DI479	RI480	LI481	LI482	PI483	LI484	YI485	A1486	KI489	TI490	LI491	LI492	QI493	KI494	A1495	A1496	A1497	EI498	F1499	GI500	A1501	HI502	YI503															
LI375	VI376	VI377	KI378	LI379	PI380	LI381	SI382	EI383	HI384	WI385	AI386	LI387	PI388	GI389	LI392	EI393	PI394	LI398	PI399	RI400	KI401	LI402	KI403	RI404	QI408	EI409	PI412	SI413	FI414	EI415	NI416	LI417	LI418	KI419	CI420	GI421	MI422	EI423	VI424	YI425	MI429	DI430	DI431	PI432	RI433	NI434	TI435	DI436	NI437	TI442	VI443	A1444					
SI312	FI313	HI314	GI315	PI316	YI317	LI318	VI319	QI320	AI321	GI322	LI323	PI324	LI325	NI326	PI327	MI328	GI329	RI330	TI331	GI332	LI333	RI334	GI335	RI336	GI337	SI338	GI343	PI344	NI345	HI346	TI347	LI348	YI349	PI350	MI351	VI352	TI353	RI354	WI355	RI356	RI357	NI358	EI359	DI360	GI361	A1362	TI363	CI364	RI365	KI366	SI367	TI368	KI369	MI370	LI372	EI373	VI374

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95674	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	22000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.852	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.169	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: ZN, CA, APR, DAT

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	0.18	0/10787	0.52	6/14658 (0.0%)
1	B	0.18	0/10787	0.52	6/14658 (0.0%)
1	C	0.18	0/10787	0.52	6/14658 (0.0%)
1	D	0.18	0/10787	0.52	6/14658 (0.0%)
All	All	0.18	0/43148	0.52	24/58632 (0.0%)

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	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	974	SER	N-CA-C	5.98	121.14	113.18
1	B	974	SER	N-CA-C	5.96	121.11	113.18
1	D	974	SER	N-CA-C	5.96	121.10	113.18
1	A	974	SER	N-CA-C	5.93	121.07	113.18
1	A	404	LYS	CB-CG-CD	5.82	124.69	111.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ILE	Peptide
1	A	666	GLU	Peptide
1	A	965	TRP	Peptide
1	A	968	ARG	Peptide
1	A	971	VAL	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	10521	0	10407	395	0
1	B	10521	0	10407	409	0
1	C	10521	0	10407	392	0
1	D	10521	0	10407	373	0
2	A	35	0	19	1	0
2	B	35	0	19	1	0
2	C	35	0	19	1	0
2	D	35	0	19	0	0
3	A	26	0	12	1	0
3	B	26	0	12	1	0
3	C	26	0	12	1	0
3	D	26	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	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	42336	0	41752	1451	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 17.

The worst 5 of 1451 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:GLU:HB3	1:D:975:TYR:N	1.66	1.09
1:A:1024:LEU:H	1:B:972:TYR:C	1.70	0.99
1:C:1022:GLU:HB3	1:D:975:TYR:H	0.84	0.99
1:C:1022:GLU:CB	1:D:975:TYR:H	1.78	0.95
1:B:981:GLN:NE2	1:C:981:GLN:OE1	1.99	0.95

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	1322/1503 (88%)	1169 (88%)	147 (11%)	6 (0%)	24	63
1	B	1322/1503 (88%)	1170 (88%)	145 (11%)	7 (0%)	24	63
1	C	1322/1503 (88%)	1171 (89%)	144 (11%)	7 (0%)	24	63
1	D	1322/1503 (88%)	1171 (89%)	145 (11%)	6 (0%)	24	63
All	All	5288/6012 (88%)	4681 (88%)	581 (11%)	26 (0%)	26	63

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	87	VAL
1	B	64	PRO
1	B	87	VAL
1	C	64	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	B	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	C	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	D	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
All	All	4436/5272 (84%)	4324 (98%)	112 (2%)	42	62

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	195	VAL
1	D	1371	MET
1	C	834	LEU
1	D	1160	ASP
1	D	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	732	HIS
1	D	732	HIS
1	C	118	HIS
1	D	684	HIS
1	D	1437	ASN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	APR	D	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)
3	DAT	D	1602	-	27,28,28	0.59	0	41,43,43	0.66	0
3	DAT	B	1602	-	27,28,28	0.58	0	41,43,43	0.66	0
2	APR	A	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)
2	APR	C	1601	-	38,38,39	0.47	0	54,58,60	0.68	1 (1%)
2	APR	B	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)
3	DAT	A	1602	-	27,28,28	0.59	0	41,43,43	0.66	0
3	DAT	C	1602	-	27,28,28	0.59	0	41,43,43	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APR	D	1601	-	-	0/22/50/54	0/4/4/4
3	DAT	D	1602	-	-	2/16/28/28	0/3/3/3
3	DAT	B	1602	-	-	2/16/28/28	0/3/3/3
2	APR	A	1601	-	-	0/22/50/54	0/4/4/4
2	APR	C	1601	-	-	0/22/50/54	0/4/4/4
2	APR	B	1601	-	-	0/22/50/54	0/4/4/4
3	DAT	A	1602	-	-	2/16/28/28	0/3/3/3
3	DAT	C	1602	-	-	2/16/28/28	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1601	APR	C1D-C2D-C3D	-3.04	98.54	102.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	APR	C1D-C2D-C3D	-3.04	98.55	102.29
2	B	1601	APR	C1D-C2D-C3D	-3.02	98.57	102.29
2	C	1601	APR	C1D-C2D-C3D	-3.01	98.59	102.29

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

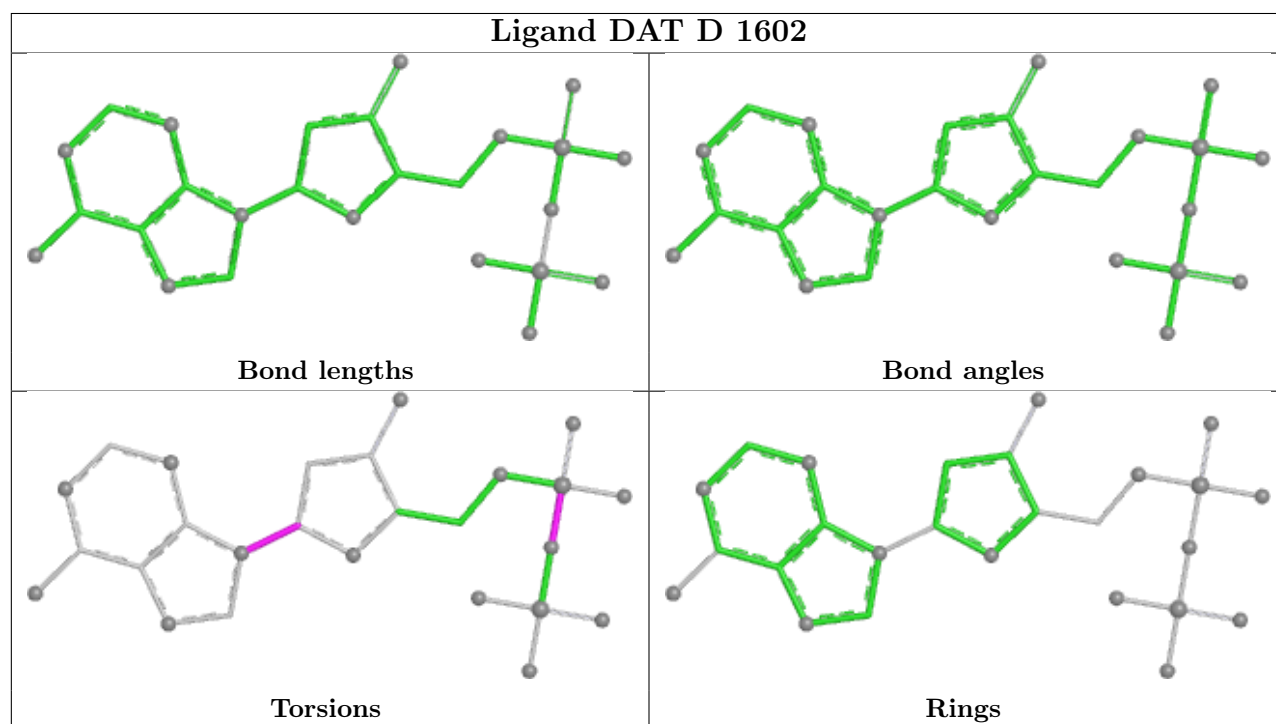
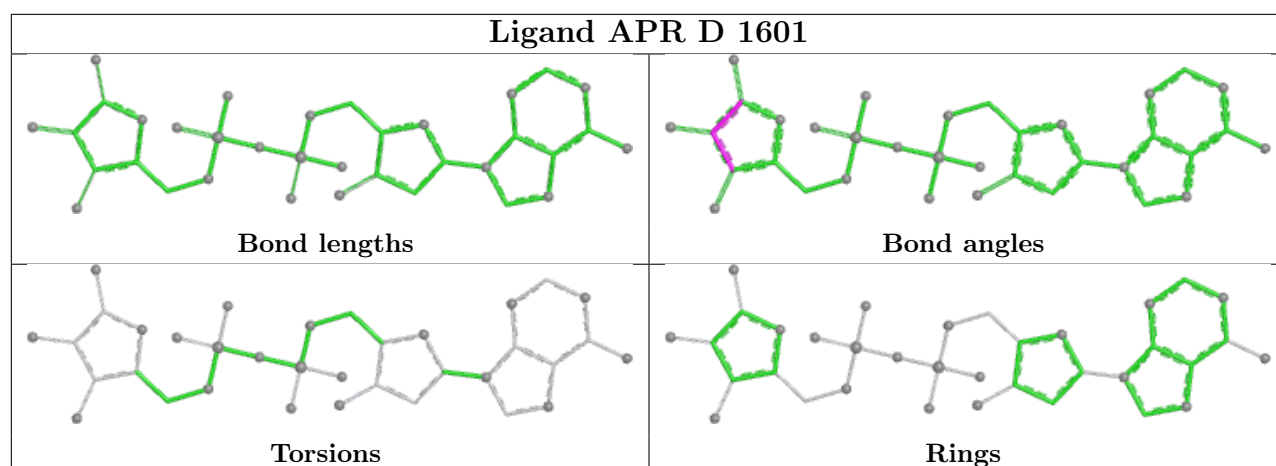
Mol	Chain	Res	Type	Atoms
3	A	1602	DAT	PB-O3A-PA-O5'
3	B	1602	DAT	PB-O3A-PA-O5'
3	C	1602	DAT	PB-O3A-PA-O5'
3	D	1602	DAT	PB-O3A-PA-O5'
3	A	1602	DAT	C2'-C1'-N9-C4

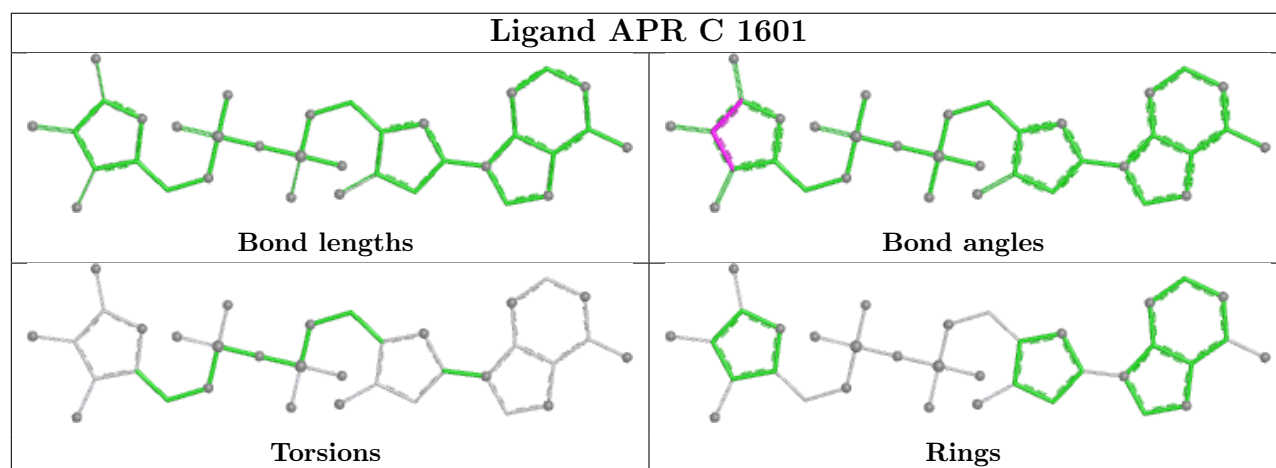
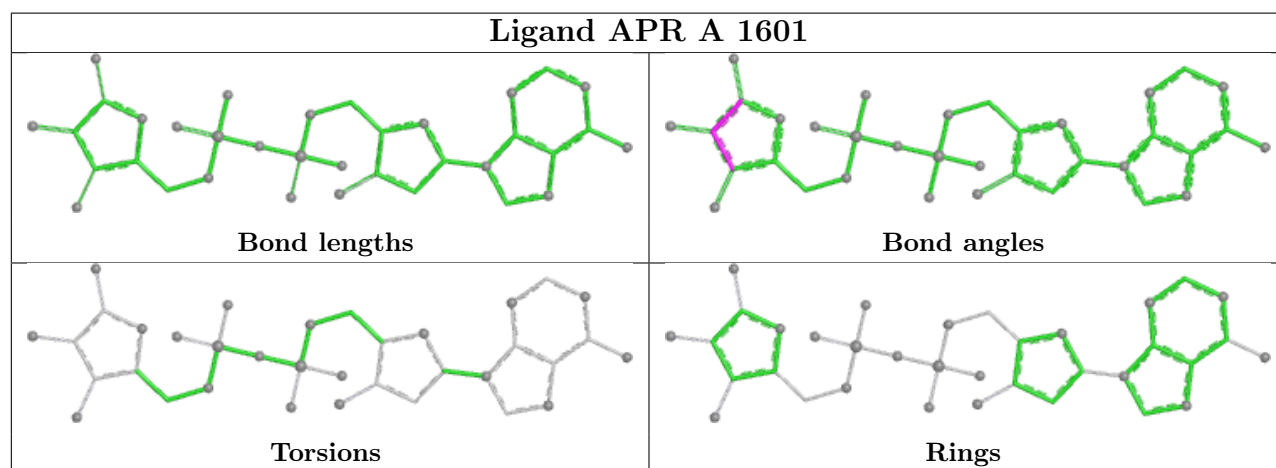
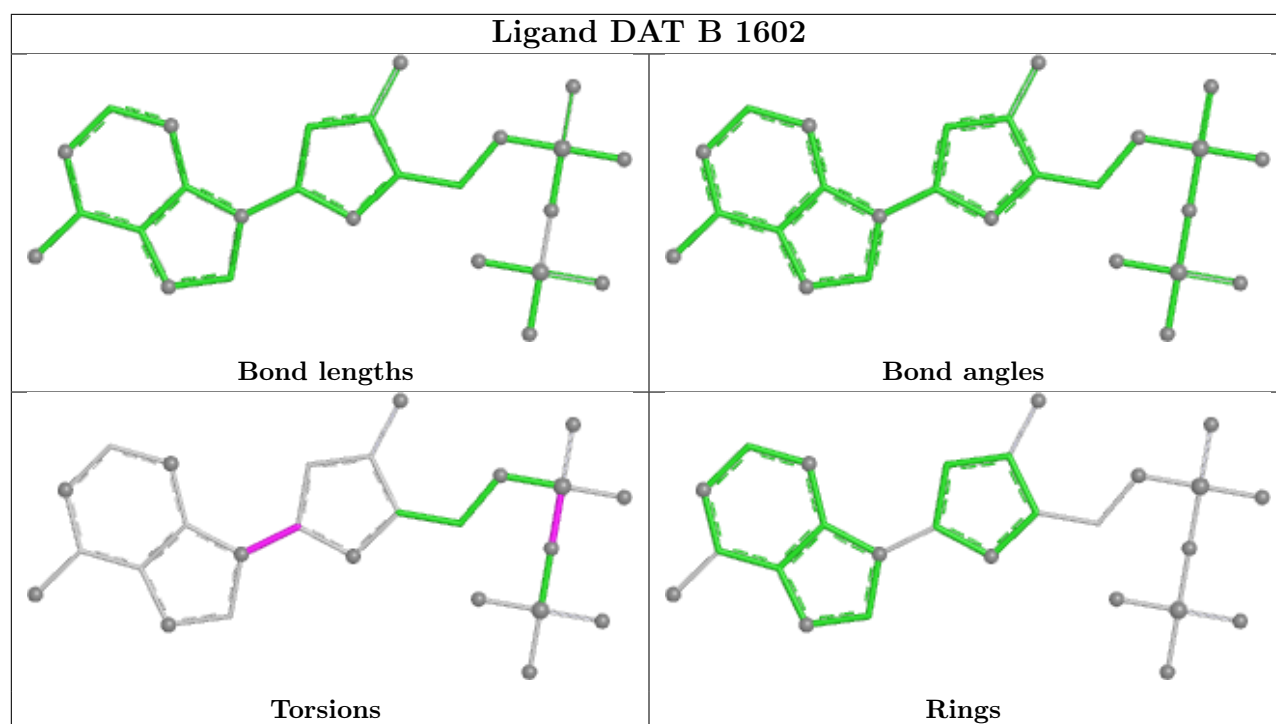
There are no ring outliers.

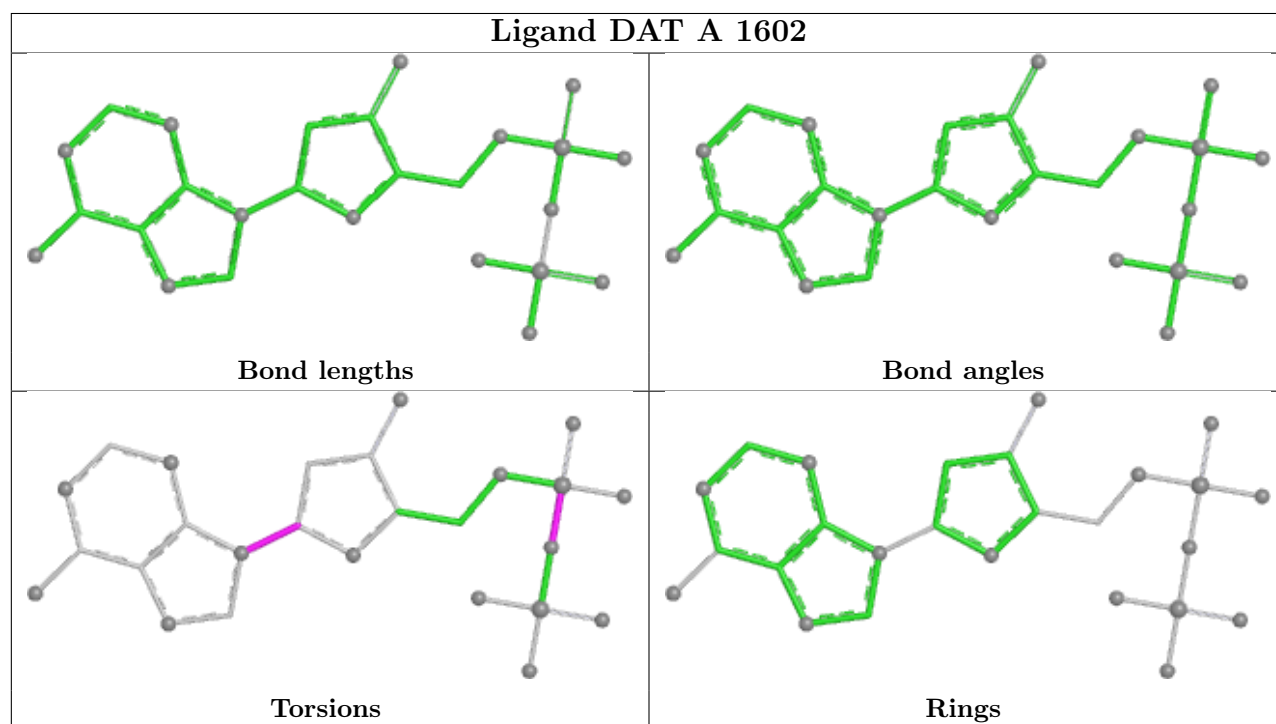
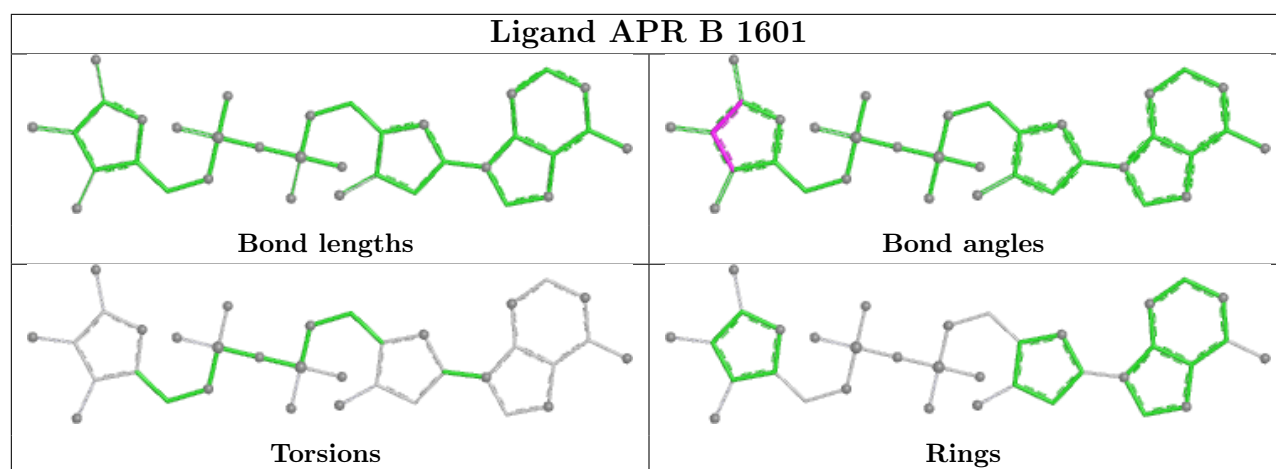
7 monomers are involved in 7 short contacts:

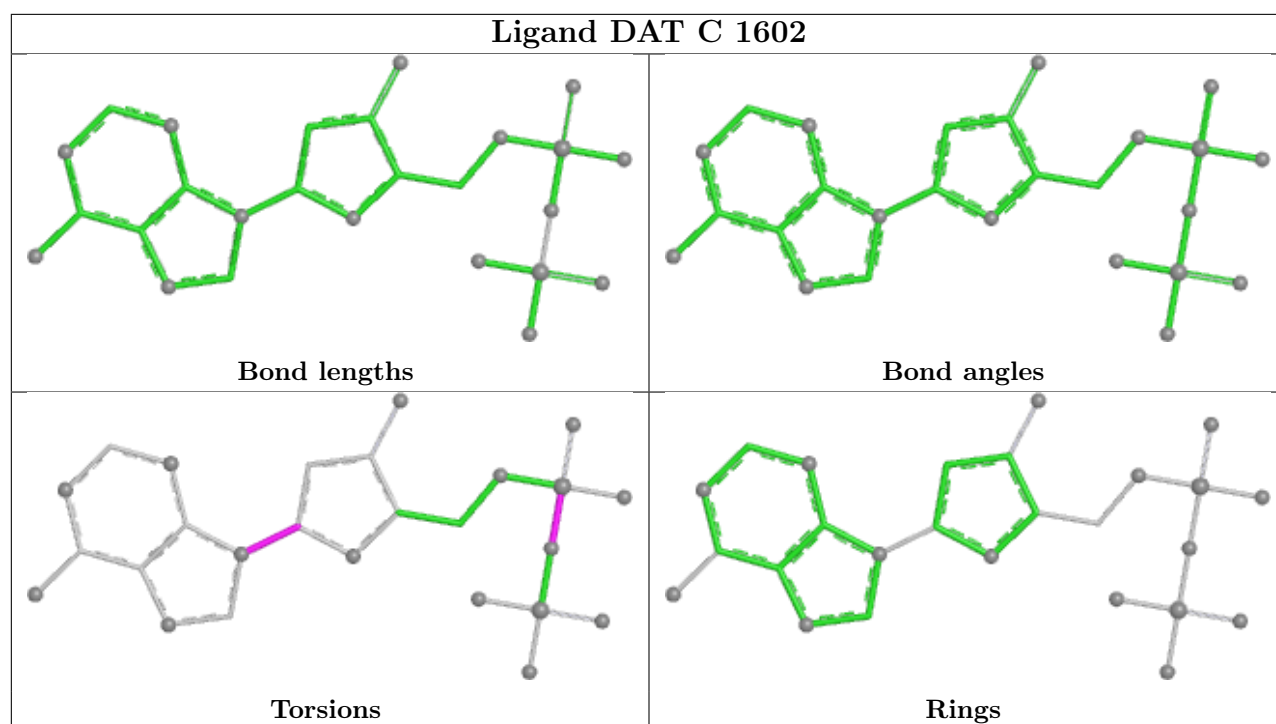
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1602	DAT	1	0
3	B	1602	DAT	1	0
2	A	1601	APR	1	0
2	C	1601	APR	1	0
2	B	1601	APR	1	0
3	A	1602	DAT	1	0
3	C	1602	DAT	1	0

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.

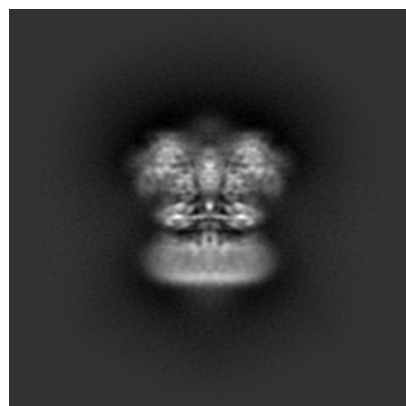
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27924. These allow visual inspection of the internal detail of the map and identification of artifacts.

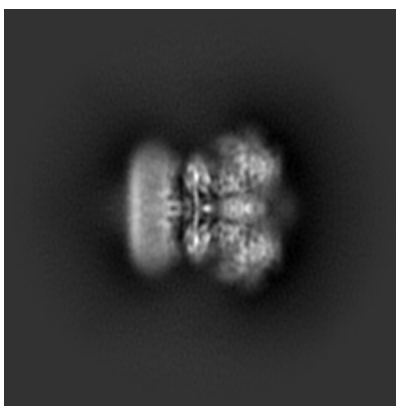
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

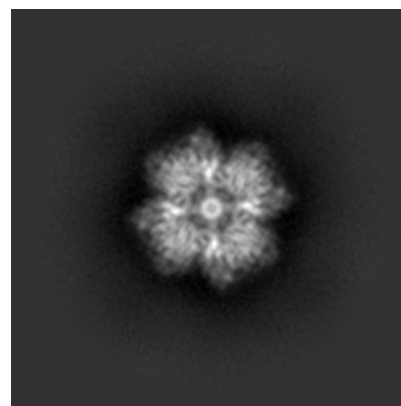
6.1.1 Primary map



X

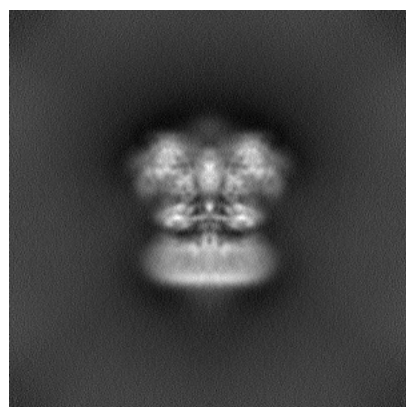


Y

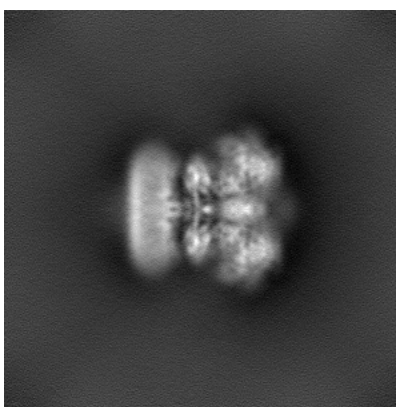


Z

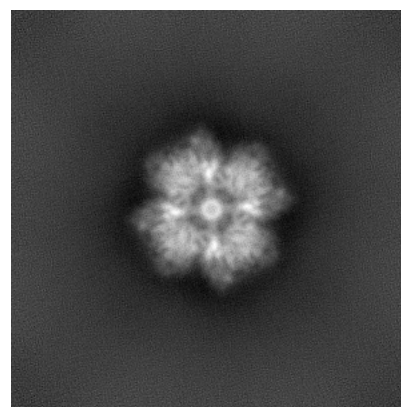
6.1.2 Raw map



X



Y

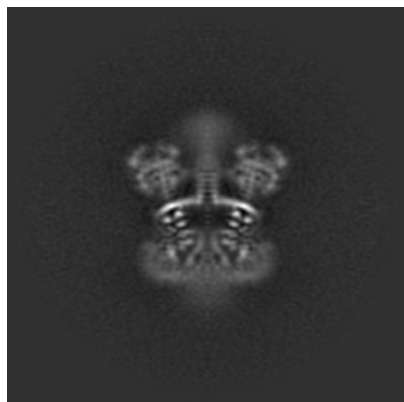


Z

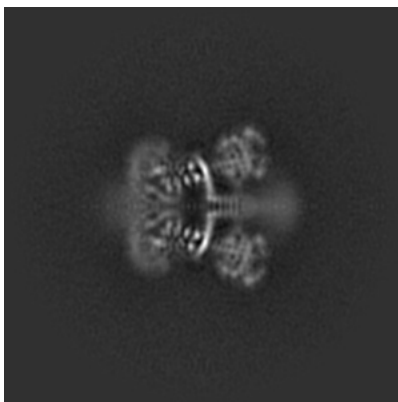
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

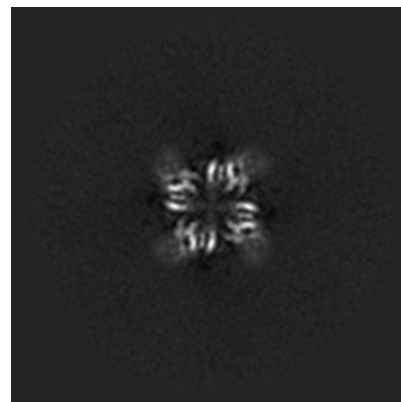
6.2.1 Primary map



X Index: 180

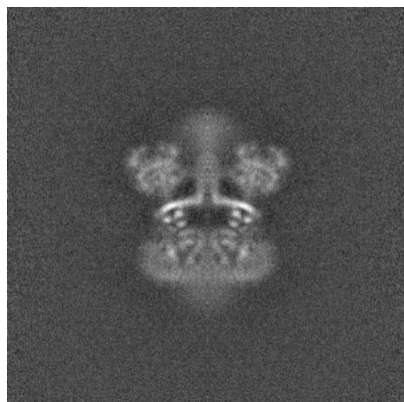


Y Index: 180

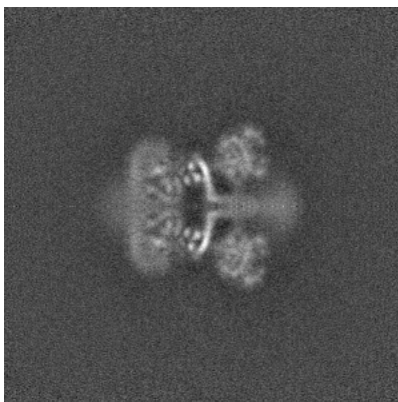


Z Index: 180

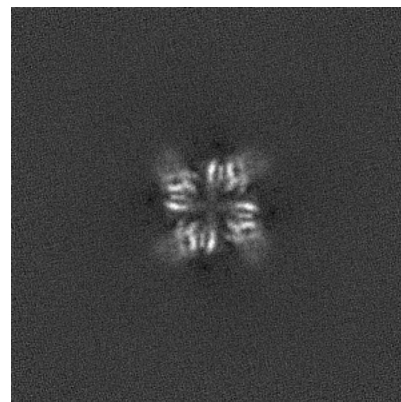
6.2.2 Raw map



X Index: 180



Y Index: 180

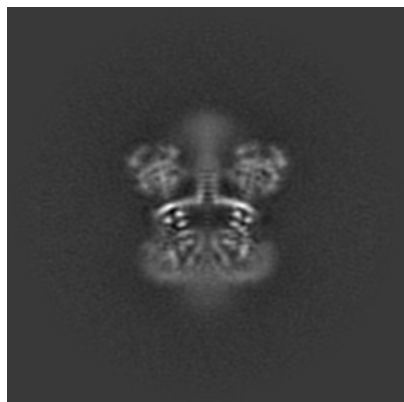


Z Index: 180

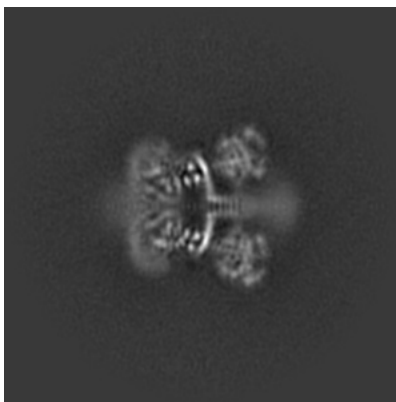
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

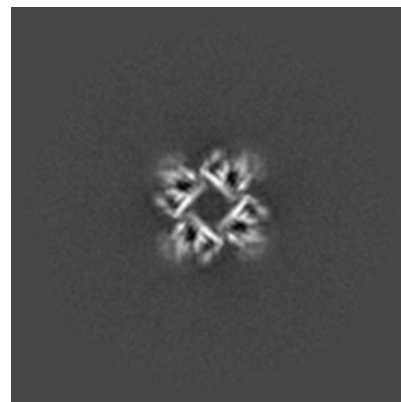
6.3.1 Primary map



X Index: 179

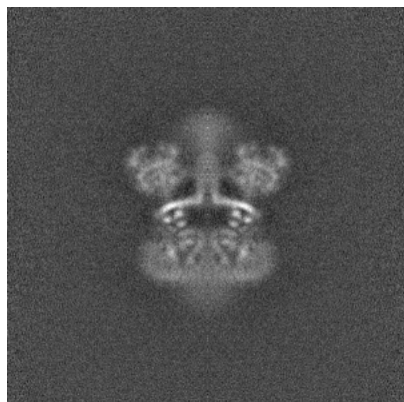


Y Index: 179

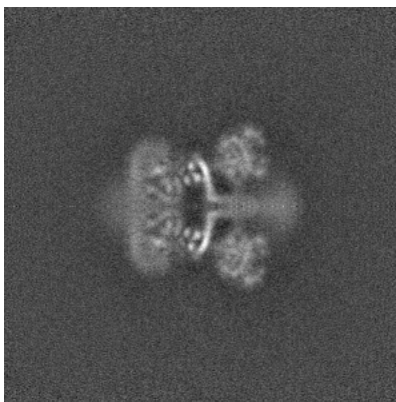


Z Index: 173

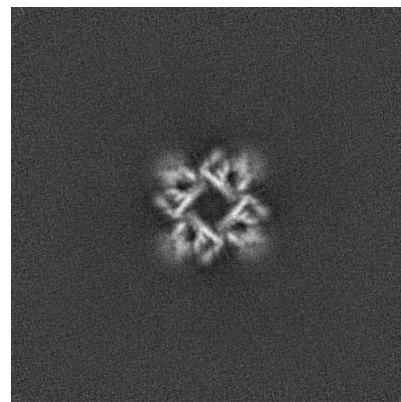
6.3.2 Raw map



X Index: 180



Y Index: 180

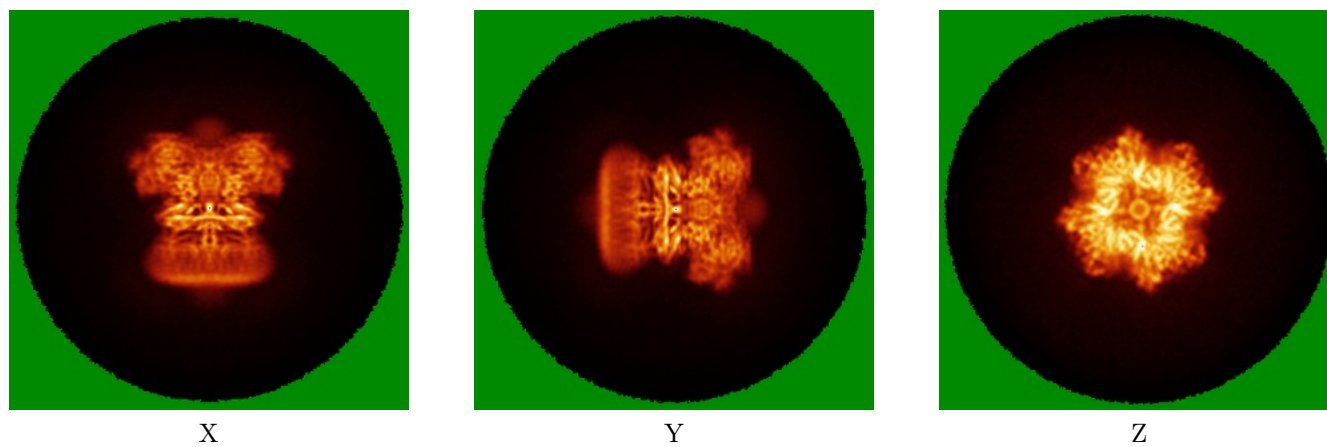


Z Index: 173

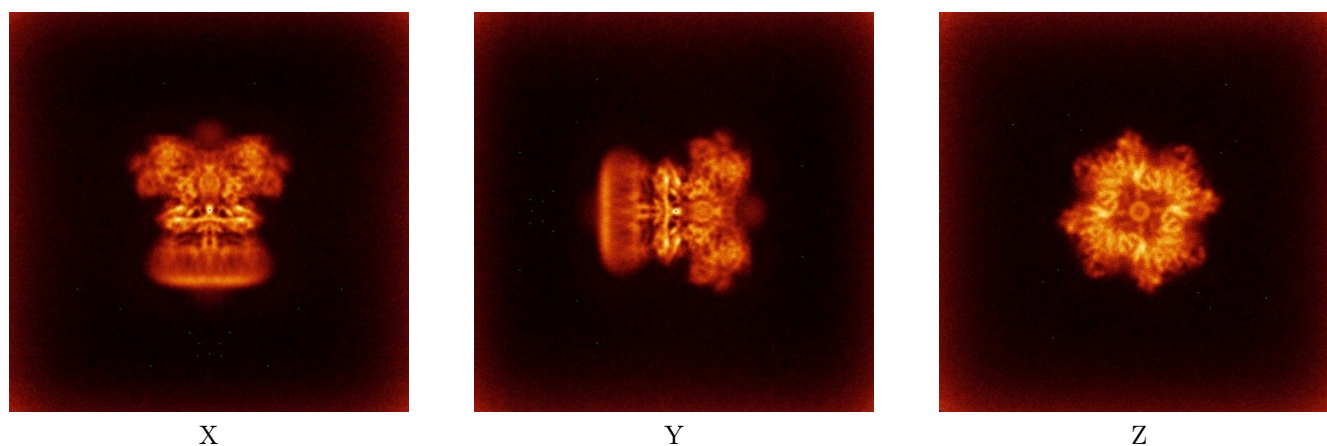
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

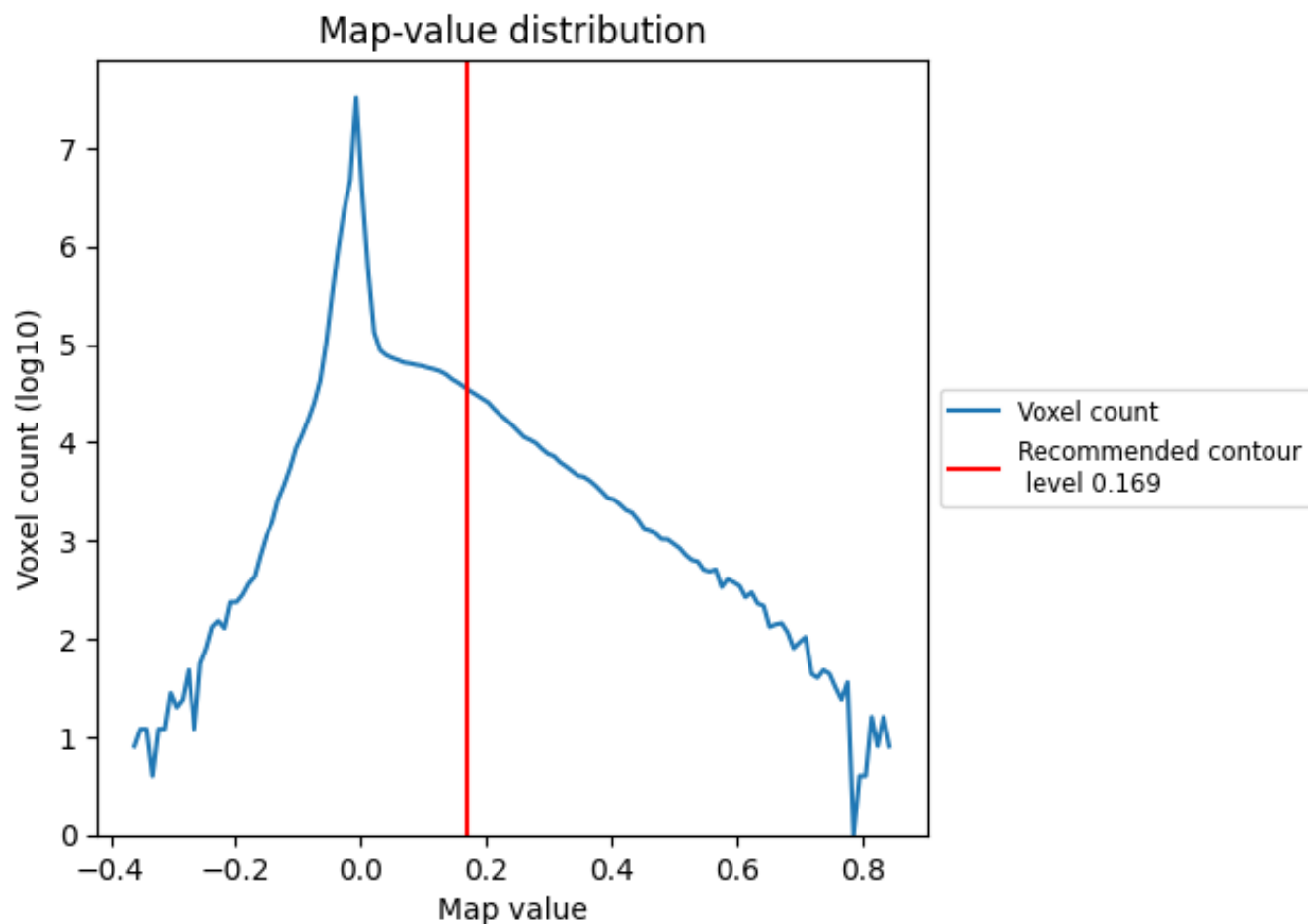
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

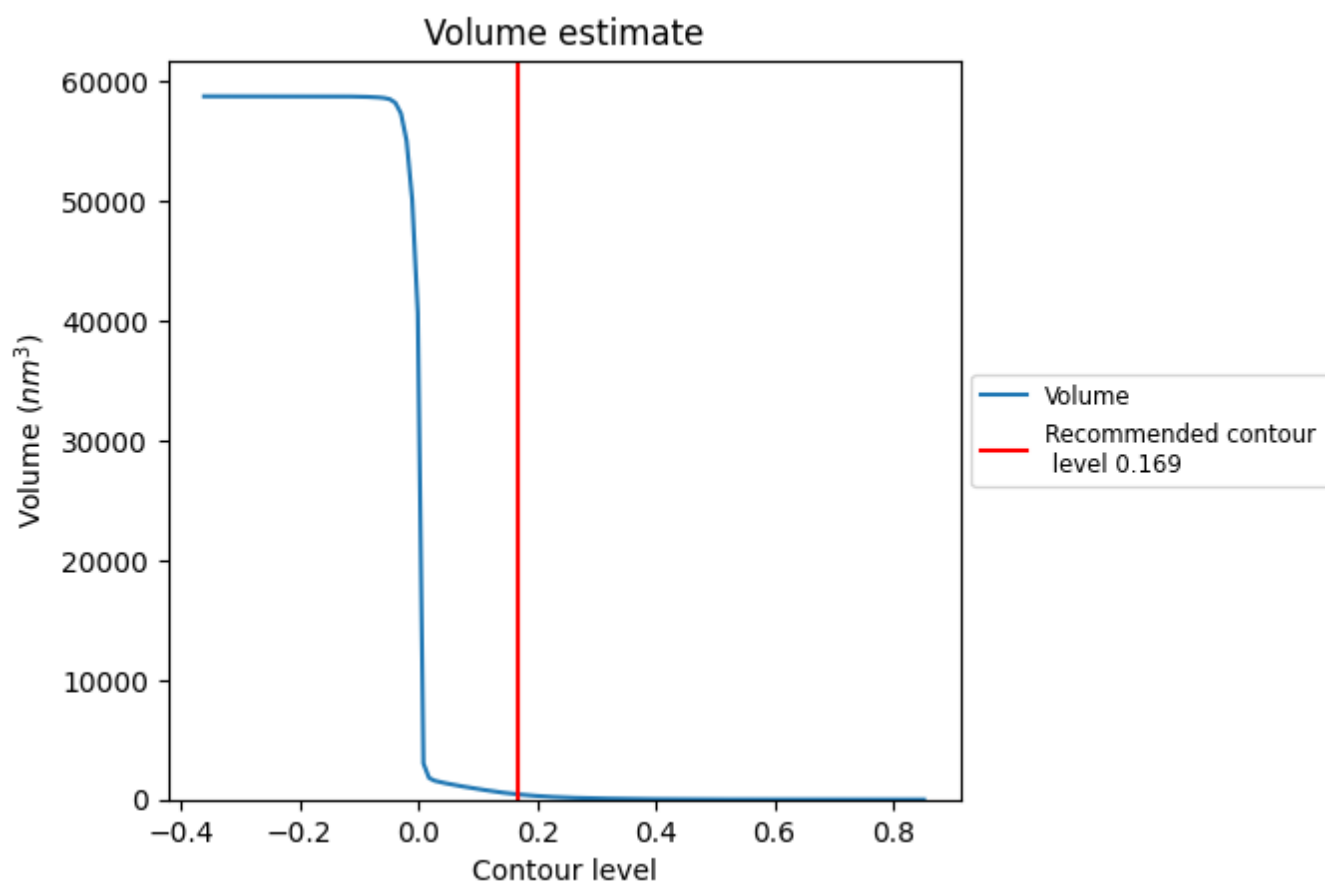
This section contains the results of statistical analysis of the map.

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.

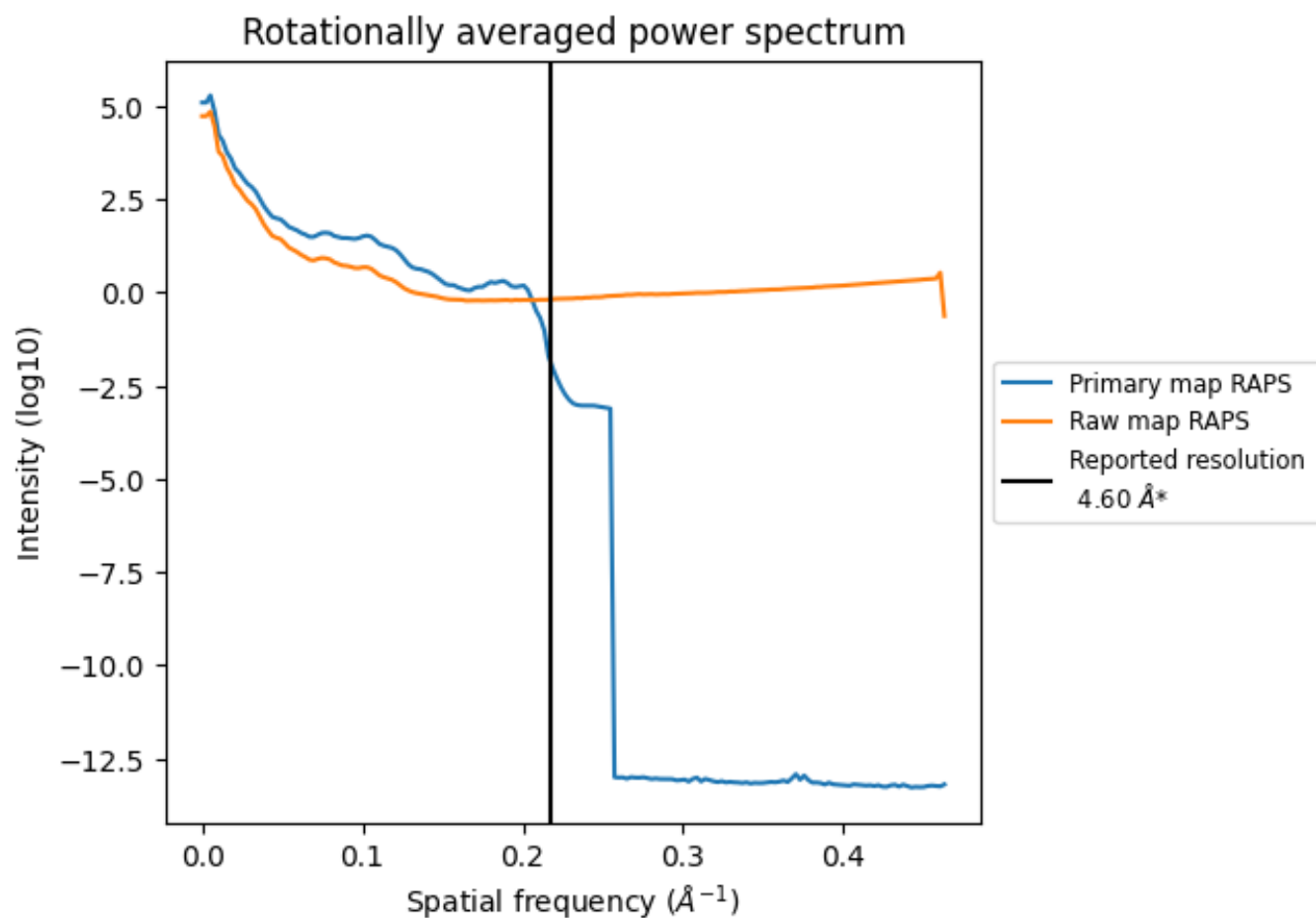
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm^3 ; this corresponds to an approximate mass of 390 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 ⓘ

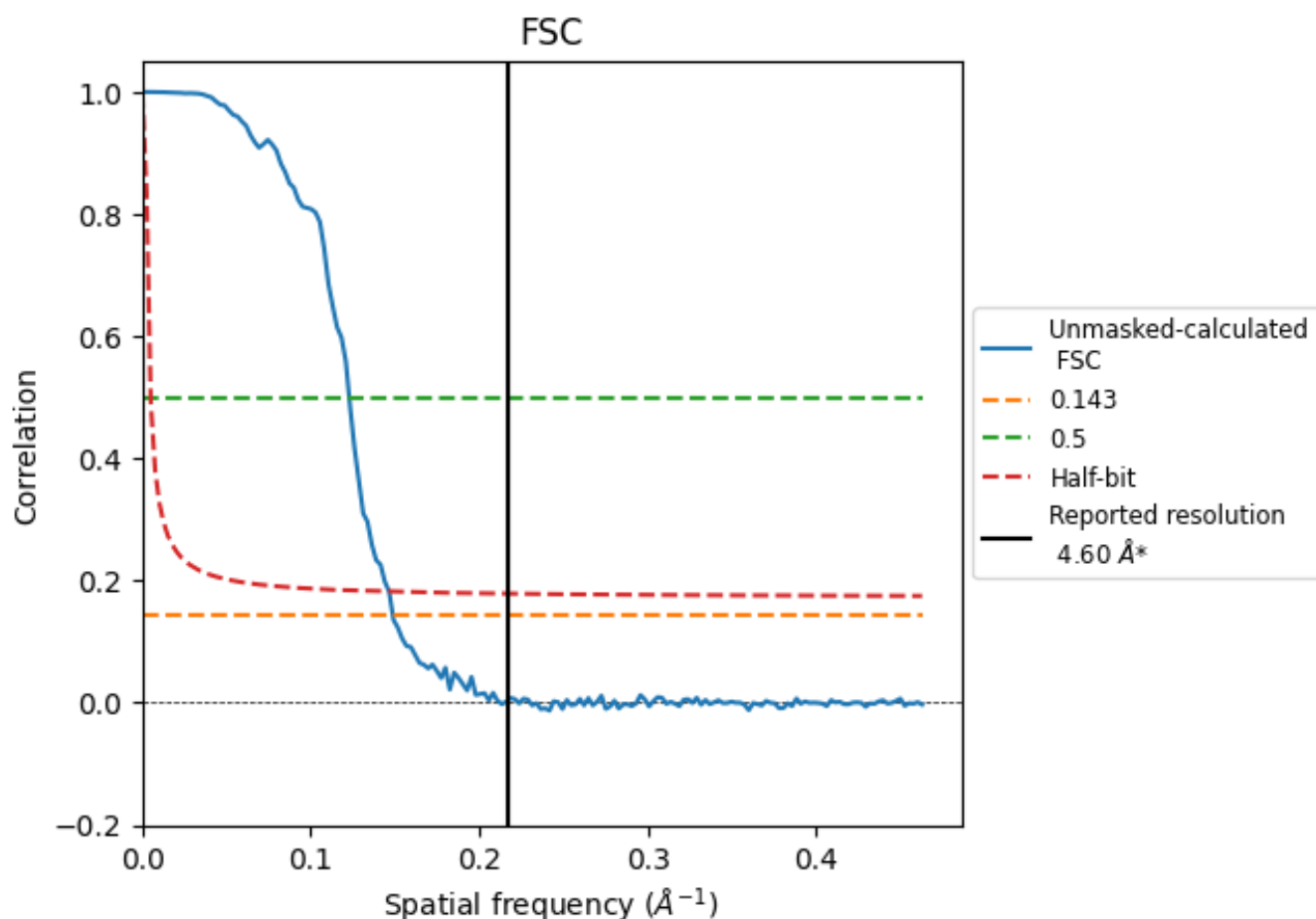


*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

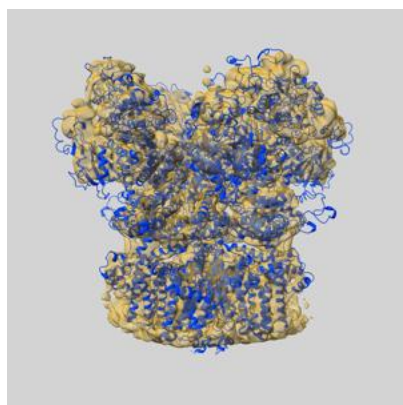
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.14	6.82

*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 6.72 differs from the reported value 4.6 by more than 10 %

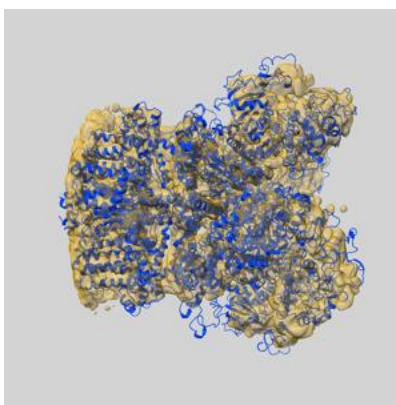
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27924 and PDB model 8E6S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

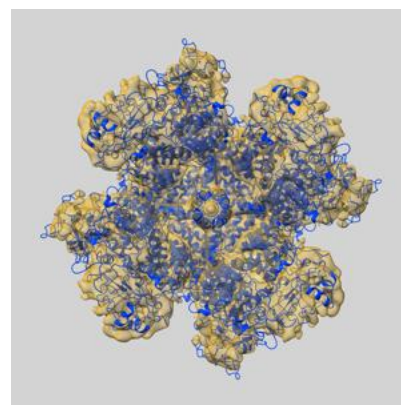
9.1 Map-model overlay [i](#)



X



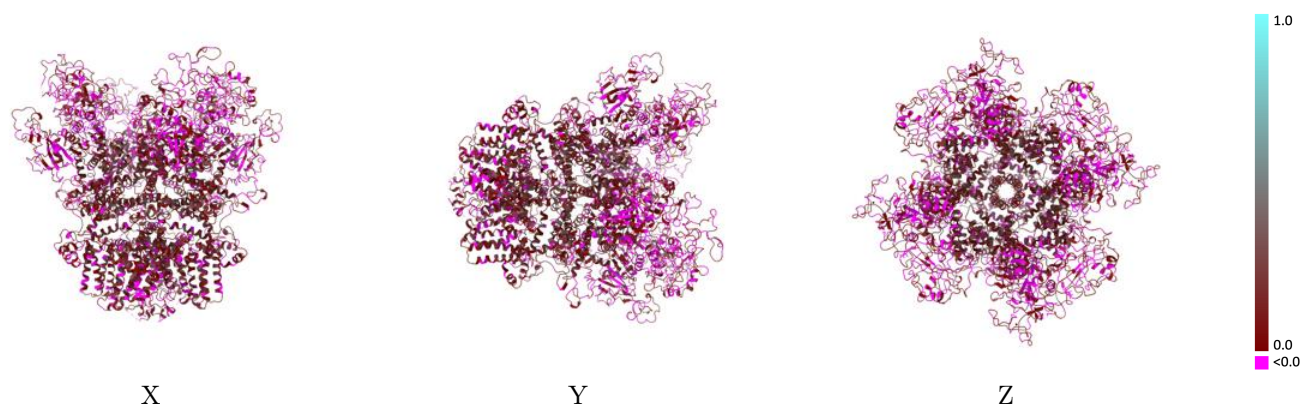
Y



Z

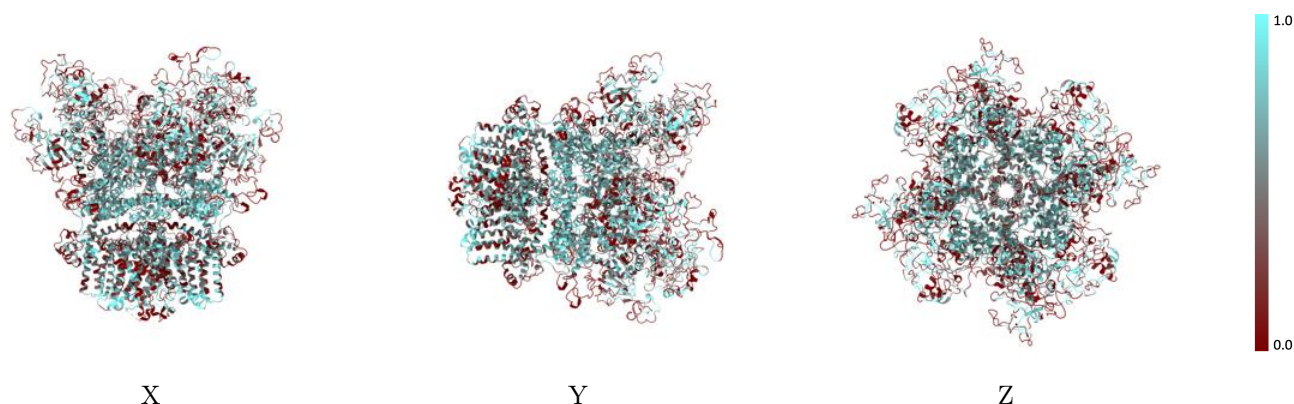
The images above show the 3D surface view of the map at the recommended contour level 0.169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



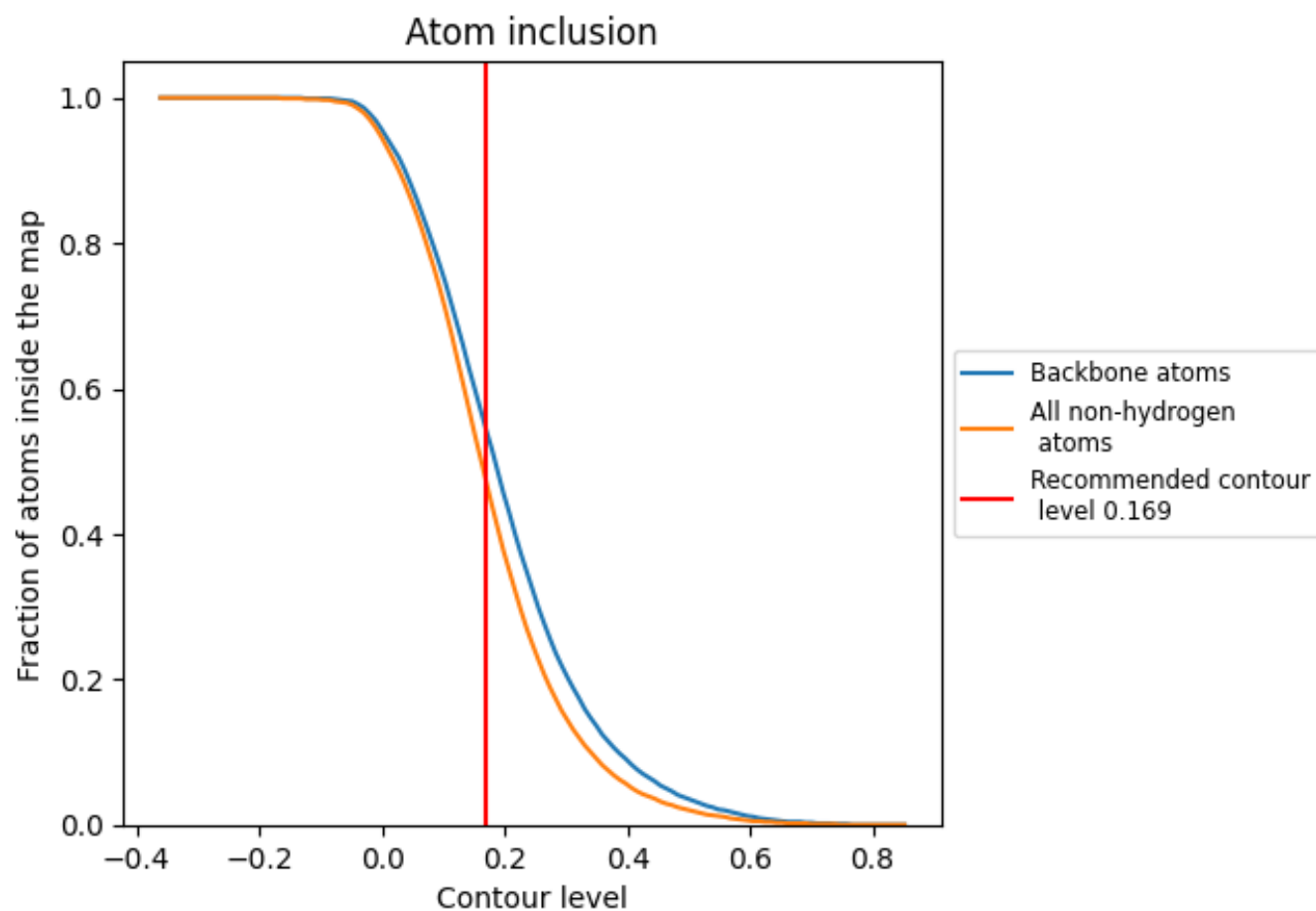
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.169).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% 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 (0.169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.0970
A	0.4750	0.0990
B	0.4760	0.0970
C	0.4710	0.0940
D	0.4760	0.0970

