



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 02:40 AM JST

PDB ID : 24VN / pdb_000024vn
EMDB ID : EMD-69845
Title : Cryo-EM structure of the human wild-type KCNQ2/KCNQ3 heterotetramer (2:2 stoichiometry) in apo state (M2323 WT, without symmetry expansion)
Authors : Wang, Y.F.; Yang, H.; Qu, Y.N.; Shen, H.Z.
Deposited on : 2026-03-22
Resolution : 3.58 Å(reported)

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

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

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

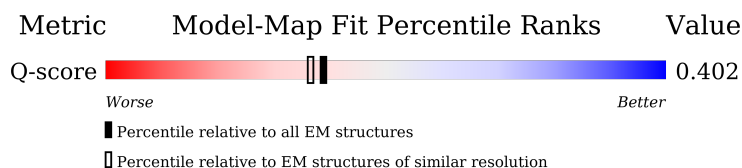
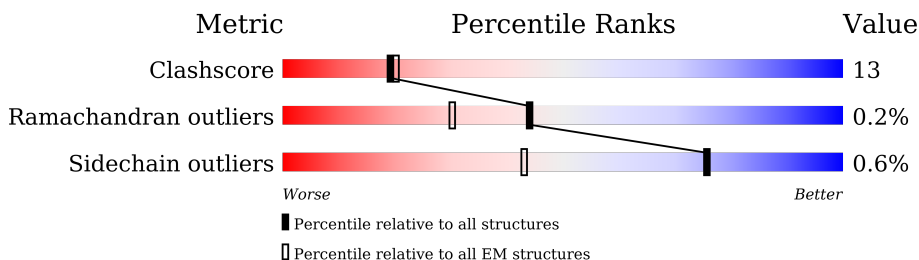
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

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	892	
1	C	892	
2	B	1142	
2	D	1142	

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
4	YJ0	B	901	X	-	-	-
4	YJ0	D	901	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8056 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		
1	C	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O43525
A	-18	ALA	-	expression tag	UNP O43525
A	-17	SER	-	expression tag	UNP O43525
A	-16	ASP	-	expression tag	UNP O43525
A	-15	TYR	-	expression tag	UNP O43525
A	-14	LYS	-	expression tag	UNP O43525
A	-13	ASP	-	expression tag	UNP O43525
A	-12	HIS	-	expression tag	UNP O43525
A	-11	ASP	-	expression tag	UNP O43525
A	-10	ILE	-	expression tag	UNP O43525
A	-9	ASP	-	expression tag	UNP O43525
A	-8	TYR	-	expression tag	UNP O43525
A	-7	LYS	-	expression tag	UNP O43525
A	-6	ASP	-	expression tag	UNP O43525
A	-5	ASP	-	expression tag	UNP O43525
A	-4	ASP	-	expression tag	UNP O43525
A	-3	ASP	-	expression tag	UNP O43525
A	-2	LYS	-	expression tag	UNP O43525
A	-1	GLY	-	expression tag	UNP O43525
A	0	THR	-	expression tag	UNP O43525
C	-19	MET	-	initiating methionine	UNP O43525
C	-18	ALA	-	expression tag	UNP O43525
C	-17	SER	-	expression tag	UNP O43525
C	-16	ASP	-	expression tag	UNP O43525
C	-15	TYR	-	expression tag	UNP O43525
C	-14	LYS	-	expression tag	UNP O43525

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	ASP	-	expression tag	UNP O43525
C	-12	HIS	-	expression tag	UNP O43525
C	-11	ASP	-	expression tag	UNP O43525
C	-10	ILE	-	expression tag	UNP O43525
C	-9	ASP	-	expression tag	UNP O43525
C	-8	TYR	-	expression tag	UNP O43525
C	-7	LYS	-	expression tag	UNP O43525
C	-6	ASP	-	expression tag	UNP O43525
C	-5	ASP	-	expression tag	UNP O43525
C	-4	ASP	-	expression tag	UNP O43525
C	-3	ASP	-	expression tag	UNP O43525
C	-2	LYS	-	expression tag	UNP O43525
C	-1	GLY	-	expression tag	UNP O43525
C	0	THR	-	expression tag	UNP O43525

- Molecule 2 is a protein called Green fluorescent protein,Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	243	Total	C	N	O	S	0	0
			1982	1318	332	323	9		
2	D	247	Total	C	N	O	S	0	0
			2006	1333	336	328	9		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-270	MET	-	initiating methionine	UNP P42212
B	-269	ALA	-	expression tag	UNP P42212
B	-268	MET	-	expression tag	UNP P42212
B	-267	HIS	-	expression tag	UNP P42212
B	-266	HIS	-	expression tag	UNP P42212
B	-265	HIS	-	expression tag	UNP P42212
B	-264	HIS	-	expression tag	UNP P42212
B	-263	HIS	-	expression tag	UNP P42212
B	-262	HIS	-	expression tag	UNP P42212
B	-261	HIS	-	expression tag	UNP P42212
B	-260	HIS	-	expression tag	UNP P42212
B	-259	GLY	-	expression tag	UNP P42212
B	-258	GLY	-	expression tag	UNP P42212
B	-257	SER	-	expression tag	UNP P42212
B	-256	MET	-	expression tag	UNP P42212

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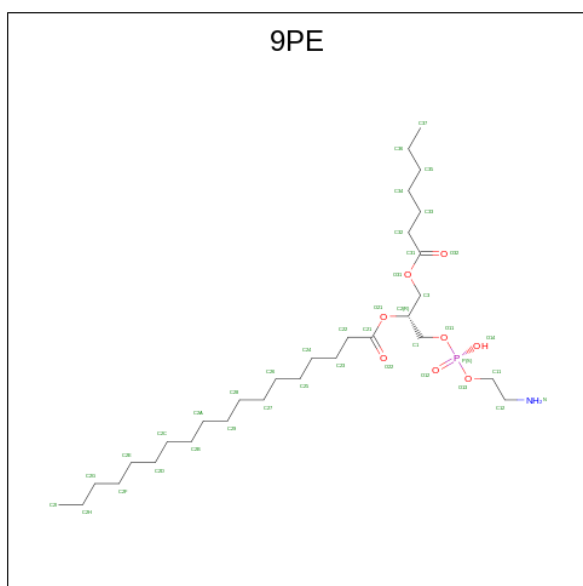
Chain	Residue	Modelled	Actual	Comment	Reference
B	-255	VAL	-	expression tag	UNP P42212
B	-192	LEU	PHE	conflict	UNP P42212
B	-191	THR	SER	conflict	UNP P42212
B	-149	THR	LYS	conflict	UNP P42212
B	-50	LYS	ALA	conflict	UNP P42212
B	-25	LEU	HIS	conflict	UNP P42212
B	-17	SER	-	linker	UNP P42212
B	-16	GLY	-	linker	UNP P42212
B	-15	LEU	-	linker	UNP P42212
B	-14	ARG	-	linker	UNP P42212
B	-13	SER	-	linker	UNP P42212
B	-12	GLY	-	linker	UNP P42212
B	-11	LEU	-	linker	UNP P42212
B	-10	GLU	-	linker	UNP P42212
B	-9	VAL	-	linker	UNP P42212
B	-8	LEU	-	linker	UNP P42212
B	-7	PHE	-	linker	UNP P42212
B	-6	GLN	-	linker	UNP P42212
B	-5	GLY	-	linker	UNP P42212
B	-4	PRO	-	linker	UNP P42212
B	-3	GLY	-	linker	UNP P42212
B	-2	GLY	-	linker	UNP P42212
B	-1	ARG	-	linker	UNP P42212
D	-270	MET	-	initiating methionine	UNP P42212
D	-269	ALA	-	expression tag	UNP P42212
D	-268	MET	-	expression tag	UNP P42212
D	-267	HIS	-	expression tag	UNP P42212
D	-266	HIS	-	expression tag	UNP P42212
D	-265	HIS	-	expression tag	UNP P42212
D	-264	HIS	-	expression tag	UNP P42212
D	-263	HIS	-	expression tag	UNP P42212
D	-262	HIS	-	expression tag	UNP P42212
D	-261	HIS	-	expression tag	UNP P42212
D	-260	HIS	-	expression tag	UNP P42212
D	-259	GLY	-	expression tag	UNP P42212
D	-258	GLY	-	expression tag	UNP P42212
D	-257	SER	-	expression tag	UNP P42212
D	-256	MET	-	expression tag	UNP P42212
D	-255	VAL	-	expression tag	UNP P42212
D	-192	LEU	PHE	conflict	UNP P42212
D	-191	THR	SER	conflict	UNP P42212
D	-149	THR	LYS	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	LYS	ALA	conflict	UNP P42212
D	-25	LEU	HIS	conflict	UNP P42212
D	-17	SER	-	linker	UNP P42212
D	-16	GLY	-	linker	UNP P42212
D	-15	LEU	-	linker	UNP P42212
D	-14	ARG	-	linker	UNP P42212
D	-13	SER	-	linker	UNP P42212
D	-12	GLY	-	linker	UNP P42212
D	-11	LEU	-	linker	UNP P42212
D	-10	GLU	-	linker	UNP P42212
D	-9	VAL	-	linker	UNP P42212
D	-8	LEU	-	linker	UNP P42212
D	-7	PHE	-	linker	UNP P42212
D	-6	GLN	-	linker	UNP P42212
D	-5	GLY	-	linker	UNP P42212
D	-4	PRO	-	linker	UNP P42212
D	-3	GLY	-	linker	UNP P42212
D	-2	GLY	-	linker	UNP P42212
D	-1	ARG	-	linker	UNP P42212

- Molecule 3 is (1R)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P) (labeled as "Ligand of Interest" by depositor).



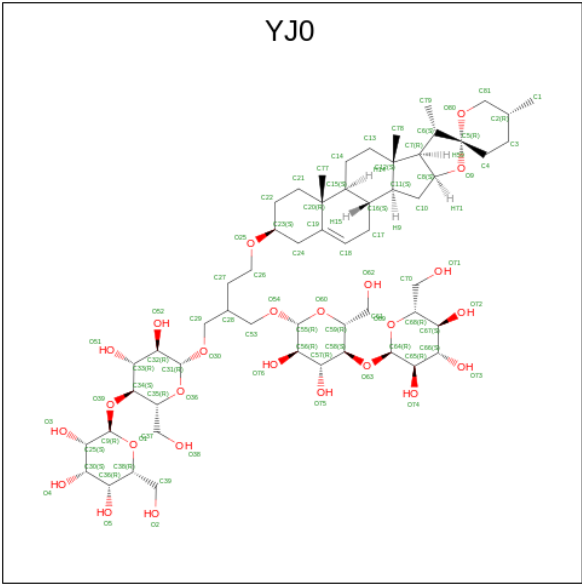
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	P
			40	30	1	8	1
							0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	C	1	40	30	1	8	1	0

- Molecule 4 is (2R)-2-{[(4-O-hexopyranosyl-beta-D-glucopyranosyl)oxy]methyl}-4-{[(25R)-5beta,14beta,17beta-spirostan-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: YJ0) (formula: C₅₆H₉₂O₂₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	B	1	81	56	25	0
4	D	1	81	56	25	0

[illegible]

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 3



MET	SER	ASP	TYR	LYS	ASP	HIS	ASP	ILE	ASP	TYR	LYS	ASP	GLY	THR	MET	GLY	LEU	LYS	ALA	ARG	ALA	ALA	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN	PRO	ALA	ALA	ALA	GLY	ASP	GLU	GLN
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ARG	LYS	VAL	GLY	LEU	ALA	PRO	GLY	ASP	VAL	GLU	GLN	VAL	THR	LEU	ALA	GLY	LEU	LEU	GLU	GLY	GLY	GLY	ARG	ASP	GLU	GLY	GLN	ARG	ARG	THR	THR	PRO	GLN	GLY	ILE	GLY	GLY	LEU	LEU	SER	ARG	PRO	VAL	LYS	ARG	ASN
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ASN	ASN
L173	L110
R174	I111
I175	Y112
W176	D113
A177	A114
A178	E115
G179	R116
C180	R117
C181	P118
C182	G120
R183	W121
Y184	A122
W187	L124
R188	Y125
G189	H126
R190	A127
L191	L128
K192	F129
A194	V130
R195	V133
K196	L134
P197	G135
L198	A140
C199	T143
M200	T144
L201	F145
D202	K146
E203	E149
F204	D154
V205	W155
L206	L156
I207	L159
A208	E160
S209	F162
VAL	F165
PRO	I166
VAL	A169
VAL	E170
VAL	F171
ALA	A172
VAL	
GLY	
ASN	
GLN	
VAL	
ALA	
THR	
SER	
LEU	
ARG	
S228	
L229	
R230	
Q233	

R236	R237	L238	R239	M240	K259	E260	T263	E263	K264	D285	V286	P287	E288	V289	D290	A291	D292	G293	E294	E295	M296	K297	E298	E299	L311	A315	L316	T317	G318	L319	G320	D321	K322	T326	A333	G365	K366	H367	P368	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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ALA	ALA	GLU	LEU	ILE	GLN	ALA	ALA	TRP	TRP	TYR	TYR	ALA	ALA	ASN	ASN	ARG	ASP	LEU	VAL	ALA	THR	TRP	ARG	PHE	TYR	GLY	SER	VAL	VAL	SER	PHE	PHE	PHE	ARG	LYS	GLU	GLN	LEU	GLU	ALA	ALA	LEU	GLY	SER	SER	SER	GLN	LYS	LEU	LEU	LEU	ASP	ARG	VAL	ARG	LEU	ALA	ARG	SER	ASN
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PRO	ARG	GLY	SER	ASN	THR	LYS	GLY	LEU	PHE	THR	PRO	PRO	LEU	ASN	VAL	ASP	ALA	ILE	GLU	GLU	SER	PRO	PRO	GLY	LYS	VAL	GLY	LEU	ASN	ASN	LYS	GLU	ARG	PHE	THR	THR	PHE	ARG	MET	LYS	ALA	ALA	TYR	ALA	PHE	GLU	ASP	ALA	GLY	GLY	ASP
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[illegible]

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

[illegible]

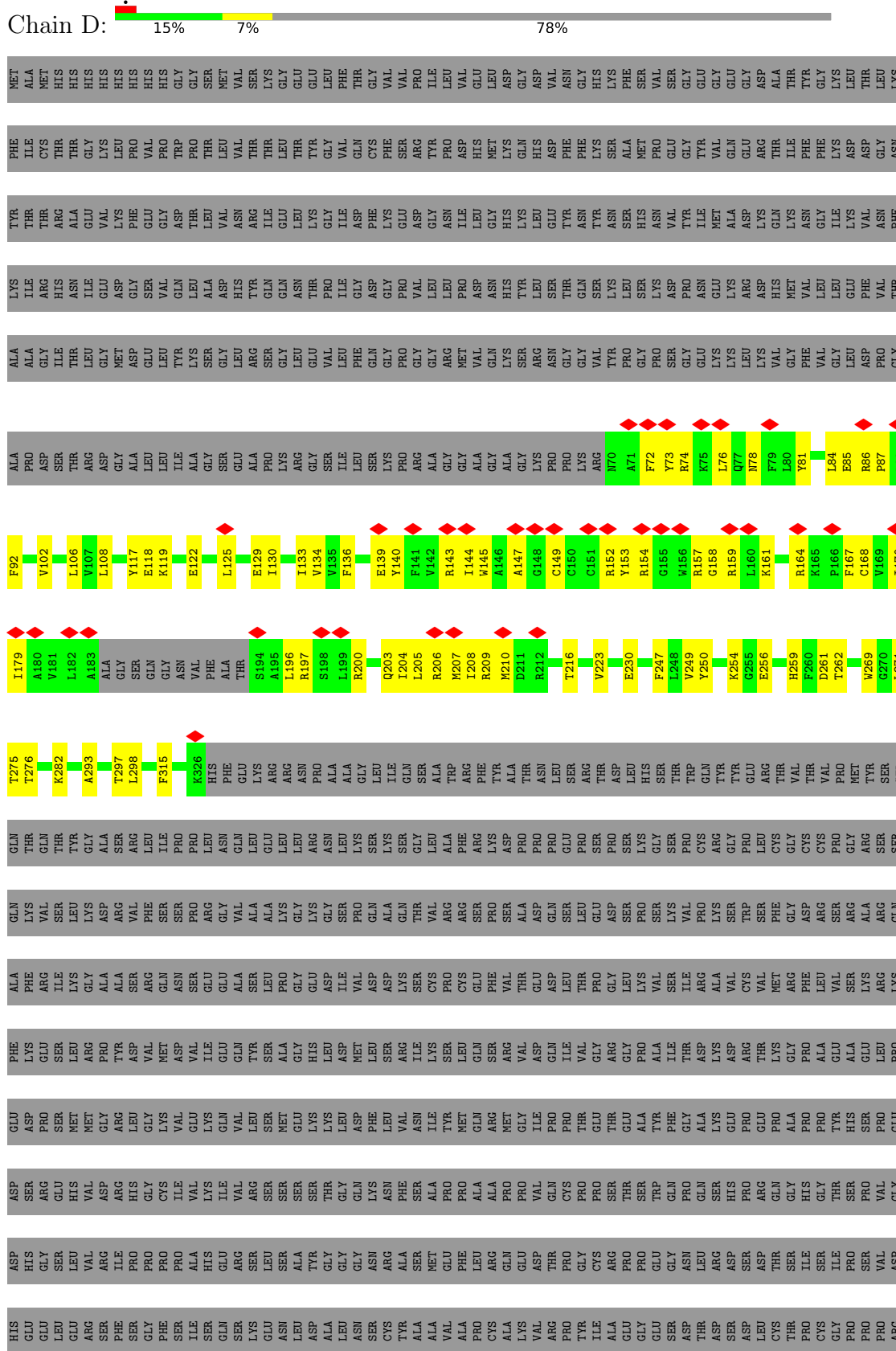
PRO	SER	ALA	THR	THR	TYR	VAL	ARG	PRO	THR	VAL	LEU	PRO	LEU	THR	LEU	ASP	SER	ARG	VAL	SER	CYS	HIS	ILEN	ALA	ASP	LEU	ILEN	PRO	TYR	SER	ASP	ARG	LEU	SER	PRO	ILEN	ARG	ARG	ARG	SER	LEU	THR	THR	ARG	ASP	SER	ASP	THR	PRO	LEU	LEU	THR	TRP
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AL	SN	IS	LU	EU	LU	RG	ER	ER	LY	HE	ER	LE	ER	LN	SP	RG	SP	SP	YR	PHE	LY	SN	LY	ER	RP	RG	YS	RG	EU	LU	LY	HR	SP	HR	SP	SP	HR	RO	HE	PRO	ER	LY	TET	TET	EU
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THR
GLY
ASP
GLY
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SER
ASN
LYS
PRO
ILE

● Molecule 2: Green fluorescent protein, Potassium voltage-gated channel subfamily KQT member 2





SER
ALA
THR
GLY
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GLY
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PHE
GLY
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VAL
GLY
TRP
ALA
GLY
PRO
ARG
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.965	Depositor
Minimum map value	-2.457	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.494	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9PE, YJ0

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	0.16	0/1960	0.45	0/2653
1	C	0.15	0/1960	0.46	0/2653
2	B	0.22	0/2036	0.40	0/2757
2	D	0.16	0/2060	0.41	0/2790
All	All	0.17	0/8016	0.43	0/10853

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

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	1913	0	1970	47	0
1	C	1913	0	1970	48	0
2	B	1982	0	2020	61	0
2	D	2006	0	2046	63	0
3	A	40	0	59	1	0
3	C	40	0	59	1	0
4	B	81	0	0	1	0
4	D	81	0	0	0	0
All	All	8056	0	8124	205	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 13.

All (205) 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:A:182:CYS:SG	1:A:183:ARG:N	2.56	0.78
1:C:182:CYS:SG	1:C:183:ARG:N	2.55	0.78
2:D:144:ILE:HG22	2:D:159:ARG:HD3	1.68	0.74
1:A:193:PHE:O	1:A:196:LYS:NZ	2.21	0.74
2:B:259:HIS:HB3	2:B:282:LYS:HG2	1.70	0.72
1:A:355:LEU:HD22	2:D:230:GLU:HG2	1.73	0.70
2:B:176:ILE:HA	2:B:179:ILE:HD12	1.74	0.70
1:C:333:ALA:O	1:C:337:SER:HB3	1.95	0.67
2:B:136:PHE:HE2	2:B:206:ARG:HD3	1.60	0.67
1:A:193:PHE:HD1	1:A:196:LYS:HZ1	1.43	0.65
1:A:179:GLY:HA2	1:A:184:TYR:CE1	2.31	0.65
1:A:179:GLY:HA2	1:A:184:TYR:CD1	2.32	0.64
1:A:263:THR:HG23	2:B:216:THR:HG23	1.79	0.64
1:A:333:ALA:O	1:A:337:SER:HB3	1.96	0.64
2:B:172:ILE:O	2:B:176:ILE:HG12	1.98	0.64
2:B:151:CYS:O	2:B:154:ARG:NH2	2.31	0.63
2:B:287:TRP:CD1	2:D:117:TYR:HH	2.16	0.63
2:D:256:GLU:N	2:D:256:GLU:OE2	2.31	0.63
1:A:130:PHE:HA	1:A:133:VAL:HG12	1.81	0.63
1:C:233:GLN:HG3	1:C:236:ARG:HH22	1.64	0.62
1:C:144:THR:HG21	2:B:263:TYR:H	1.64	0.62
1:C:239:ARG:O	1:C:239:ARG:NH1	2.32	0.62
1:C:311:LEU:HD11	2:B:298:LEU:HD21	1.80	0.61
2:D:259:HIS:HB3	2:D:282:LYS:HG2	1.82	0.61
2:D:74:ARG:O	2:D:78:ASN:ND2	2.34	0.61
2:D:149:CYS:O	2:D:154:ARG:NH1	2.33	0.61
2:D:130:ILE:O	2:D:134:VAL:HG23	2.00	0.61
1:A:118:PRO:HB2	1:A:119:ARG:HD3	1.84	0.60
2:D:130:ILE:HA	2:D:133:ILE:HD12	1.83	0.60
1:A:338:LEU:HD21	2:B:271:LEU:HD11	1.83	0.60
2:D:203:GLN:OE1	2:D:206:ARG:NH2	2.34	0.59
1:A:311:LEU:HD11	2:D:298:LEU:HD21	1.84	0.59
1:C:233:GLN:OE1	1:C:233:GLN:N	2.33	0.59
1:A:128:LEU:O	1:A:132:ILE:HG12	2.04	0.58
2:D:250:TYR:OH	2:D:254:LYS:NZ	2.36	0.58
2:D:157:ARG:HH12	2:D:161:LYS:HD3	1.69	0.58
1:A:239:ARG:O	1:A:239:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:GLU:O	2:D:122:GLU:HG2	2.04	0.57
1:C:113:ASP:N	1:C:113:ASP:OD1	2.36	0.57
1:A:156:LEU:O	1:A:160:GLU:HG2	2.05	0.57
2:B:173:MET:SD	2:B:173:MET:N	2.77	0.57
1:C:130:PHE:HE1	1:C:240:MET:HA	1.69	0.56
2:B:250:TYR:OH	2:B:254:LYS:NZ	2.39	0.56
1:C:118:PRO:HB2	1:C:119:ARG:HD3	1.86	0.56
2:B:70:ASN:OD1	2:B:71:ALA:N	2.40	0.55
2:B:168:CYS:O	2:B:172:ILE:HD12	2.07	0.55
1:C:156:LEU:O	1:C:160:GLU:HG2	2.08	0.53
1:C:338:LEU:HD21	2:D:271:LEU:HD11	1.89	0.53
2:D:261:ASP:OD1	2:D:262:THR:HG23	2.08	0.53
1:A:174:ARG:HG3	1:A:193:PHE:HZ	1.74	0.53
1:A:134:LEU:HD22	1:A:237:MET:HE1	1.91	0.53
2:B:70:ASN:O	2:B:74:ARG:HG3	2.08	0.53
1:A:295:GLU:O	1:A:296:MET:HG2	2.08	0.53
2:D:72:PHE:O	2:D:76:LEU:HG	2.10	0.52
2:B:139:GLU:O	2:B:142:VAL:N	2.43	0.52
2:D:154:ARG:H	2:D:158:GLY:HA3	1.73	0.52
2:B:136:PHE:CE2	2:B:206:ARG:HD3	2.43	0.52
2:D:167:PHE:O	2:D:170:ILE:HG12	2.10	0.52
1:A:130:PHE:O	1:A:134:LEU:HG	2.09	0.52
1:C:193:PHE:O	1:C:196:LYS:NZ	2.43	0.52
2:D:172:ILE:O	2:D:176:ILE:HG12	2.10	0.51
2:D:204:ILE:HD12	2:D:207:MET:HE3	1.91	0.51
1:A:261:LEU:HD11	1:A:351:LEU:HD11	1.92	0.51
1:C:134:LEU:HD22	1:C:237:MET:HE1	1.91	0.51
2:B:140:TYR:O	2:B:144:ILE:HG12	2.10	0.51
2:D:140:TYR:O	2:D:144:ILE:HG13	2.10	0.51
1:C:319:TYR:OH	2:B:273:THR:OG1	2.25	0.51
2:B:80:LEU:O	2:B:84:LEU:HG	2.11	0.51
1:C:112:TYR:O	1:C:116:GLU:HG3	2.11	0.51
2:D:140:TYR:CD1	2:D:172:ILE:HD11	2.46	0.51
1:C:174:ARG:HH22	1:C:199:CYS:HA	1.74	0.51
2:B:203:GLN:OE1	2:B:206:ARG:NH1	2.44	0.50
2:D:85:GLU:OE1	2:D:86:ARG:HG2	2.09	0.50
2:B:167:PHE:O	2:B:170:ILE:HG13	2.12	0.50
2:D:157:ARG:NH1	2:D:161:LYS:HD3	2.25	0.50
2:D:152:ARG:HE	2:D:153:TYR:HD2	1.59	0.50
2:D:161:LYS:HA	2:D:164:ARG:HG2	1.94	0.50
2:D:140:TYR:CE2	2:D:144:ILE:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:PHE:HA	2:B:106:LEU:HG	1.94	0.50
1:A:202:ASP:O	1:A:206:LEU:HG	2.10	0.50
1:C:169:ALA:O	1:C:173:LEU:HG	2.11	0.50
1:C:173:LEU:O	1:C:177:ALA:HB3	2.12	0.49
1:C:202:ASP:O	1:C:206:LEU:HG	2.11	0.49
1:C:130:PHE:HA	1:C:133:VAL:HG12	1.93	0.49
1:A:260:GLU:HG3	2:B:219:LEU:HD21	1.94	0.49
2:B:108:LEU:HB3	2:B:125:LEU:HG	1.95	0.48
2:B:157:ARG:HA	2:B:160:LEU:HD12	1.96	0.48
2:D:85:GLU:CD	2:D:86:ARG:HG2	2.38	0.48
1:A:126:HIS:O	1:A:130:PHE:HD2	1.96	0.48
2:B:156:TRP:HD1	2:B:157:ARG:NH1	2.11	0.48
2:D:73:TYR:OH	2:D:145:TRP:NE1	2.46	0.48
1:A:186:GLY:O	1:A:190:ARG:NH1	2.46	0.48
1:C:130:PHE:O	1:C:134:LEU:HG	2.14	0.48
2:D:205:LEU:HA	2:D:208:ILE:HG22	1.95	0.47
2:B:83:VAL:HG23	2:B:84:LEU:HD23	1.96	0.47
2:B:204:ILE:O	2:B:208:ILE:HG22	2.14	0.47
2:D:154:ARG:N	2:D:158:GLY:HA3	2.29	0.47
1:C:230:ARG:HD2	2:B:247:PHE:CE1	2.50	0.47
1:C:355:LEU:HB3	2:B:230:GLU:HG2	1.96	0.47
1:C:171:PHE:O	1:C:174:ARG:HG2	2.14	0.47
2:D:176:ILE:HA	2:D:179:ILE:HG22	1.97	0.46
1:A:176:TRP:HZ3	1:A:190:ARG:HD3	1.80	0.46
1:A:284:LYS:O	1:A:287:PRO:HD2	2.15	0.46
1:A:299:GLU:HB3	1:A:322:LYS:HG2	1.97	0.46
2:B:141:PHE:HD1	2:B:144:ILE:HD11	1.80	0.46
1:C:260:GLU:HA	1:C:263:THR:HB	1.97	0.46
1:A:182:CYS:O	1:A:185:LYS:N	2.38	0.46
1:C:194:ALA:HA	1:C:199:CYS:SG	2.56	0.46
1:C:284:LYS:O	1:C:287:PRO:HD2	2.14	0.46
2:B:141:PHE:CD1	2:B:144:ILE:HD11	2.51	0.46
1:A:182:CYS:HB3	1:A:184:TYR:CE2	2.51	0.46
1:A:315:ALA:O	1:A:317:ILE:N	2.49	0.46
2:D:167:PHE:HZ	2:D:209:ARG:HA	1.81	0.46
1:C:171:PHE:O	1:C:175:ILE:HG22	2.16	0.46
2:D:108:LEU:HB3	2:D:125:LEU:HG	1.97	0.46
2:D:81:TYR:HD2	2:D:147:ALA:HB3	1.81	0.45
2:D:139:GLU:O	2:D:143:ARG:HG2	2.16	0.45
2:D:125:LEU:HD13	2:D:200:ARG:NH2	2.31	0.45
1:A:301:GLU:HG3	1:A:302:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:HA	1:C:259:LYS:HD2	1.77	0.45
2:D:125:LEU:HD23	2:D:125:LEU:HA	1.78	0.45
2:D:168:CYS:O	2:D:172:ILE:HG12	2.16	0.45
2:B:166:PRO:O	2:B:170:ILE:HG12	2.16	0.45
1:A:180:CYS:H	1:A:184:TYR:HE1	1.65	0.45
1:A:239:ARG:O	1:A:239:ARG:HG2	2.17	0.45
1:C:175:ILE:HA	1:C:193:PHE:HE2	1.81	0.45
2:B:169:VAL:HA	2:B:172:ILE:HD12	1.99	0.45
2:B:80:LEU:HA	2:B:83:VAL:HG22	1.99	0.45
2:D:129:GLU:O	2:D:133:ILE:HG13	2.16	0.45
2:D:207:MET:O	2:D:210:MET:HE3	2.17	0.45
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.82	0.44
2:D:136:PHE:CZ	2:D:206:ARG:HD2	2.52	0.44
2:B:212:ARG:HG2	2:B:213:ARG:HG3	1.98	0.44
2:B:118:GLU:O	2:B:122:GLU:HG2	2.18	0.44
2:D:223:VAL:HG21	2:D:315:PHE:CE1	2.53	0.44
2:D:196:LEU:HD22	2:D:200:ARG:HD2	1.99	0.44
2:B:139:GLU:O	2:B:140:TYR:C	2.58	0.44
2:B:144:ILE:O	2:B:159:ARG:NH2	2.46	0.44
2:B:174:VAL:HG13	2:B:202:LEU:HB3	1.99	0.44
1:C:180:CYS:SG	1:C:181:CYS:N	2.91	0.44
1:C:364:ARG:HH11	1:C:364:ARG:HG2	1.82	0.44
2:B:173:MET:HE3	2:B:176:ILE:HD11	1.99	0.43
2:B:274:LEU:HD22	2:B:300:GLY:HA3	2.00	0.43
1:A:138:ILE:O	1:A:142:LEU:HD22	2.18	0.43
1:C:140:ALA:O	1:C:143:THR:HG22	2.18	0.43
2:B:293:ALA:O	2:B:297:THR:HB	2.18	0.43
2:D:206:ARG:O	2:D:209:ARG:HG2	2.17	0.43
3:A:1001:9PE:H2EA	3:A:1001:9PE:H2HA	1.85	0.43
2:B:84:LEU:HD12	2:B:143:ARG:HH11	1.83	0.43
1:A:202:ASP:HA	1:A:205:VAL:HG22	2.00	0.43
1:C:149:GLU:OE2	1:C:149:GLU:N	2.42	0.43
1:A:319:TYR:OH	2:D:273:THR:OG1	2.28	0.43
2:D:140:TYR:CZ	2:D:144:ILE:HD11	2.52	0.43
2:D:275:THR:O	2:D:276:THR:HB	2.19	0.43
2:B:209:ARG:O	4:B:901:YJ0:O75	2.37	0.43
2:B:127:ILE:O	2:B:131:VAL:HG23	2.18	0.43
1:A:194:ALA:HA	1:A:199:CYS:SG	2.60	0.42
2:D:102:VAL:O	2:D:106:LEU:HG	2.19	0.42
1:C:117:ARG:HA	1:C:117:ARG:HD3	1.81	0.42
1:C:193:PHE:HD1	1:C:196:LYS:NZ	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LEU:HB3	2:D:197:ARG:H	1.76	0.42
3:C:1001:9PE:H2FA	3:C:1001:9PE:H2C	1.78	0.42
1:A:261:LEU:HD21	1:A:351:LEU:HD13	2.01	0.42
2:B:105:CYS:HB2	2:B:128:LEU:HD21	2.01	0.42
2:B:134:VAL:O	2:B:138:VAL:HG23	2.19	0.42
2:D:81:TYR:HB2	2:D:147:ALA:HB2	2.02	0.42
2:D:158:GLY:HA2	2:D:161:LYS:HE3	2.02	0.42
2:D:249:VAL:HG21	2:D:269:TRP:CH2	2.55	0.42
2:B:240:LEU:HD23	2:B:240:LEU:HA	1.82	0.42
1:A:180:CYS:SG	1:A:181:CYS:N	2.93	0.42
2:D:293:ALA:O	2:D:297:THR:HB	2.20	0.42
1:A:138:ILE:O	1:A:141:VAL:HB	2.19	0.42
1:A:174:ARG:HG3	1:A:193:PHE:CZ	2.53	0.42
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.87	0.41
1:C:174:ARG:NH2	1:C:199:CYS:HA	2.34	0.41
2:B:291:LEU:O	2:B:295:THR:HG23	2.18	0.41
1:A:180:CYS:SG	1:A:184:TYR:OH	2.70	0.41
1:C:171:PHE:HA	1:C:174:ARG:HD3	2.03	0.41
1:C:315:ALA:O	1:C:317:ILE:N	2.51	0.41
2:D:119:LYS:HE2	2:D:119:LYS:HB3	1.89	0.41
2:B:293:ALA:O	2:B:297:THR:CB	2.69	0.41
1:C:321:ASP:OD1	1:C:321:ASP:N	2.54	0.41
1:A:286:VAL:HB	1:A:287:PRO:HD3	2.02	0.41
1:C:286:VAL:HB	1:C:287:PRO:HD3	2.02	0.41
2:B:299:ILE:HD13	2:B:299:ILE:HA	1.88	0.41
2:D:261:ASP:OD1	2:D:261:ASP:C	2.63	0.41
1:C:260:GLU:HG2	2:D:315:PHE:CD1	2.56	0.41
1:C:283:GLU:OE1	1:C:326:THR:OG1	2.23	0.41
1:C:366:LYS:C	1:C:366:LYS:HD3	2.46	0.41
2:B:125:LEU:HD23	2:B:125:LEU:HA	1.90	0.41
2:B:223:VAL:HG21	2:B:315:PHE:CE1	2.55	0.41
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.89	0.41
2:D:84:LEU:HD13	2:D:143:ARG:HD2	2.02	0.41
2:D:153:TYR:HB2	2:D:158:GLY:O	2.21	0.41
1:C:263:THR:HG23	2:D:216:THR:HG23	2.03	0.40
2:B:84:LEU:HD13	2:B:143:ARG:HD2	2.02	0.40
2:B:288:ASN:O	2:B:292:LEU:HG	2.21	0.40
2:B:326:LYS:HB3	2:B:326:LYS:HE2	1.74	0.40
2:D:87:PRO:HB2	2:D:92:PHE:CE1	2.56	0.40
1:A:230:ARG:HD2	2:D:247:PHE:CE1	2.56	0.40
1:A:179:GLY:HA2	1:A:184:TYR:HD1	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HB3	1:C:119:ARG:HH22	1.87	0.40
1:C:299:GLU:HB3	1:C:322:LYS:HG2	2.03	0.40
2:B:249:VAL:HG21	2:B:269:TRP:CH2	2.56	0.40
2:B:165:LYS:HB2	2:B:168:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/892 (26%)	215 (92%)	19 (8%)	1 (0%)	30	60
1	C	235/892 (26%)	214 (91%)	21 (9%)	0	100	100
2	B	239/1142 (21%)	223 (93%)	15 (6%)	1 (0%)	30	60
2	D	243/1142 (21%)	228 (94%)	15 (6%)	0	100	100
All	All	952/4068 (23%)	880 (92%)	70 (7%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	156	TRP
1	A	296	MET

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	196/743 (26%)	193 (98%)	3 (2%)	57	70
1	C	196/743 (26%)	196 (100%)	0	100	100
2	B	204/961 (21%)	202 (99%)	2 (1%)	68	75
2	D	206/961 (21%)	206 (100%)	0	100	100
All	All	802/3408 (24%)	797 (99%)	5 (1%)	76	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	151	VAL
1	A	272	LEU
2	B	167	PHE
2	B	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	78	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](#)

4 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
3	9PE	C	1001	-	39,39,39	0.97	4 (10%)	42,44,44	0.94	2 (4%)
3	9PE	A	1001	-	39,39,39	0.97	4 (10%)	42,44,44	0.96	2 (4%)
4	YJ0	B	901	-	90,90,90	0.30	0	136,138,138	1.01	9 (6%)
4	YJ0	D	901	-	90,90,90	0.20	0	136,138,138	0.53	1 (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	9PE	C	1001	-	-	15/43/43/43	-
3	9PE	A	1001	-	-	25/43/43/43	-
4	YJ0	B	901	-	14/14/33/34	15/32/200/200	1/10/10/10
4	YJ0	D	901	-	9/9/33/34	11/32/200/200	1/10/10/10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	9PE	O21-C2	-2.52	1.40	1.46
3	A	1001	9PE	O21-C2	-2.49	1.40	1.46
3	C	1001	9PE	O31-C31	2.42	1.40	1.33
3	A	1001	9PE	O31-C31	2.40	1.40	1.33
3	A	1001	9PE	O21-C21	2.14	1.40	1.34
3	C	1001	9PE	O21-C21	2.12	1.40	1.34
3	C	1001	9PE	O31-C3	-2.11	1.40	1.45
3	A	1001	9PE	O31-C3	-2.10	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	YJ0	C12-C7-C8	-5.15	97.90	104.13
3	A	1001	9PE	O21-C21-C22	4.03	120.19	111.50
3	C	1001	9PE	O21-C21-C22	3.99	120.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	YJ0	C10-C8-C7	-3.53	100.16	107.52
4	B	901	YJ0	O9-C8-C7	-3.37	100.10	105.07
4	B	901	YJ0	C10-C11-C12	2.81	107.65	103.91
4	B	901	YJ0	O9-C8-C10	2.73	118.89	112.36
4	B	901	YJ0	C12-C7-C6	2.70	129.75	120.56
3	C	1001	9PE	O31-C31-C32	2.59	120.03	111.91
3	A	1001	9PE	O31-C31-C32	2.57	119.96	111.91
4	B	901	YJ0	C17-C16-C15	2.52	112.77	109.71
4	B	901	YJ0	C20-C15-C16	2.24	116.10	112.73
4	D	901	YJ0	C53-C28-C29	2.20	114.52	111.00
4	B	901	YJ0	C5-O9-C8	-2.07	102.51	108.28

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	901	YJ0	C16
4	B	901	YJ0	C5
4	B	901	YJ0	C55
4	B	901	YJ0	C59
4	B	901	YJ0	C34
4	B	901	YJ0	C58
4	B	901	YJ0	C8
4	B	901	YJ0	C64
4	B	901	YJ0	C6
4	B	901	YJ0	C23
4	B	901	YJ0	C11
4	B	901	YJ0	C68
4	B	901	YJ0	C31
4	B	901	YJ0	C35
4	D	901	YJ0	C16
4	D	901	YJ0	C5
4	D	901	YJ0	C59
4	D	901	YJ0	C57
4	D	901	YJ0	C6
4	D	901	YJ0	C32
4	D	901	YJ0	C15
4	D	901	YJ0	C12
4	D	901	YJ0	C65

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	9PE	C1-O11-P-O12
3	A	1001	9PE	C11-O13-P-O14
3	A	1001	9PE	O13-C11-C12-N
3	A	1001	9PE	C22-C21-O21-C2
3	C	1001	9PE	C11-O13-P-O12
3	C	1001	9PE	O13-C11-C12-N
4	B	901	YJ0	C53-C28-C29-O30
4	B	901	YJ0	C28-C29-O30-C31
4	D	901	YJ0	O36-C31-O30-C29
4	D	901	YJ0	O60-C55-O54-C53
4	B	901	YJ0	C57-C58-O63-C64
3	A	1001	9PE	O22-C21-O21-C2
3	C	1001	9PE	O22-C21-O21-C2
3	C	1001	9PE	C22-C21-O21-C2
4	D	901	YJ0	C56-C55-O54-C53
3	C	1001	9PE	C31-C32-C33-C34
3	A	1001	9PE	C11-O13-P-O11
3	C	1001	9PE	C2C-C2D-C2E-C2F
3	A	1001	9PE	C2A-C2B-C2C-C2D
3	A	1001	9PE	C21-C22-C23-C24
4	D	901	YJ0	C27-C26-O25-C23
3	A	1001	9PE	C31-C32-C33-C34
3	A	1001	9PE	C24-C25-C26-C27
3	C	1001	9PE	C2B-C2C-C2D-C2E
4	B	901	YJ0	C27-C28-C29-O30
3	A	1001	9PE	C32-C31-O31-C3
4	D	901	YJ0	C32-C31-O30-C29
4	B	901	YJ0	O60-C59-C61-O62
3	A	1001	9PE	C33-C34-C35-C36
3	A	1001	9PE	C1-C2-C3-O31
3	C	1001	9PE	C2A-C2B-C2C-C2D
3	A	1001	9PE	O32-C31-O31-C3
3	A	1001	9PE	C2F-C2G-C2H-C2I
3	A	1001	9PE	C29-C2A-C2B-C2C
4	B	901	YJ0	C35-C34-O39-C9
4	B	901	YJ0	C33-C34-O39-C9
3	A	1001	9PE	C32-C33-C34-C35
3	C	1001	9PE	C25-C26-C27-C28
3	A	1001	9PE	C1-O11-P-O13
4	B	901	YJ0	C29-C28-C53-O54
4	D	901	YJ0	O1-C9-O39-C34
3	C	1001	9PE	C11-O13-P-O11
4	B	901	YJ0	O69-C64-O63-C58

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Mol	Chain	Res	Type	Atoms
3	A	1001	9PE	C1-O11-P-O14
3	C	1001	9PE	C12-C11-O13-P
4	D	901	YJ0	C59-C58-O63-C64
4	D	901	YJ0	C57-C58-O63-C64
4	D	901	YJ0	C28-C29-O30-C31
4	D	901	YJ0	C25-C9-O39-C34
3	A	1001	9PE	O21-C2-C3-O31
4	B	901	YJ0	C59-C58-O63-C64
3	C	1001	9PE	C26-C27-C28-C29
3	A	1001	9PE	C2C-C2D-C2E-C2F
4	D	901	YJ0	C22-C23-O25-C26
4	B	901	YJ0	C27-C26-O25-C23
3	C	1001	9PE	C32-C33-C34-C35
3	A	1001	9PE	C2E-C2F-C2G-C2H
3	C	1001	9PE	C29-C2A-C2B-C2C
4	B	901	YJ0	C65-C64-O63-C58
4	B	901	YJ0	C26-C27-C28-C29
3	C	1001	9PE	O11-C1-C2-C3
3	A	1001	9PE	O21-C21-C22-C23
3	A	1001	9PE	C2B-C2C-C2D-C2E
4	B	901	YJ0	C26-C27-C28-C53
4	B	901	YJ0	O25-C26-C27-C28
3	A	1001	9PE	O22-C21-C22-C23

All (2) ring outliers are listed below:

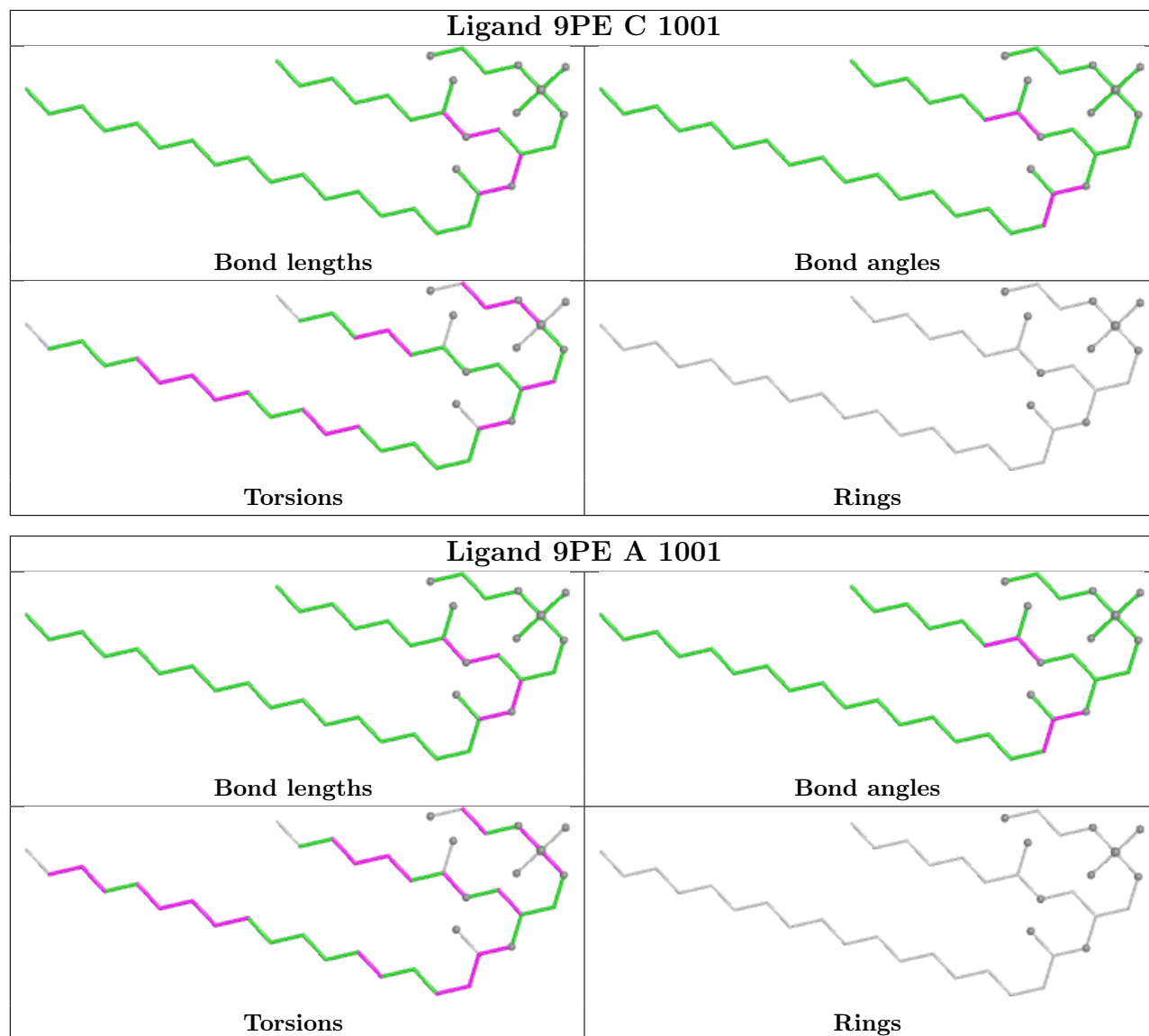
Mol	Chain	Res	Type	Atoms
4	D	901	YJ0	C2-C3-C4-C5-C81-O80
4	B	901	YJ0	C2-C3-C4-C5-C81-O80

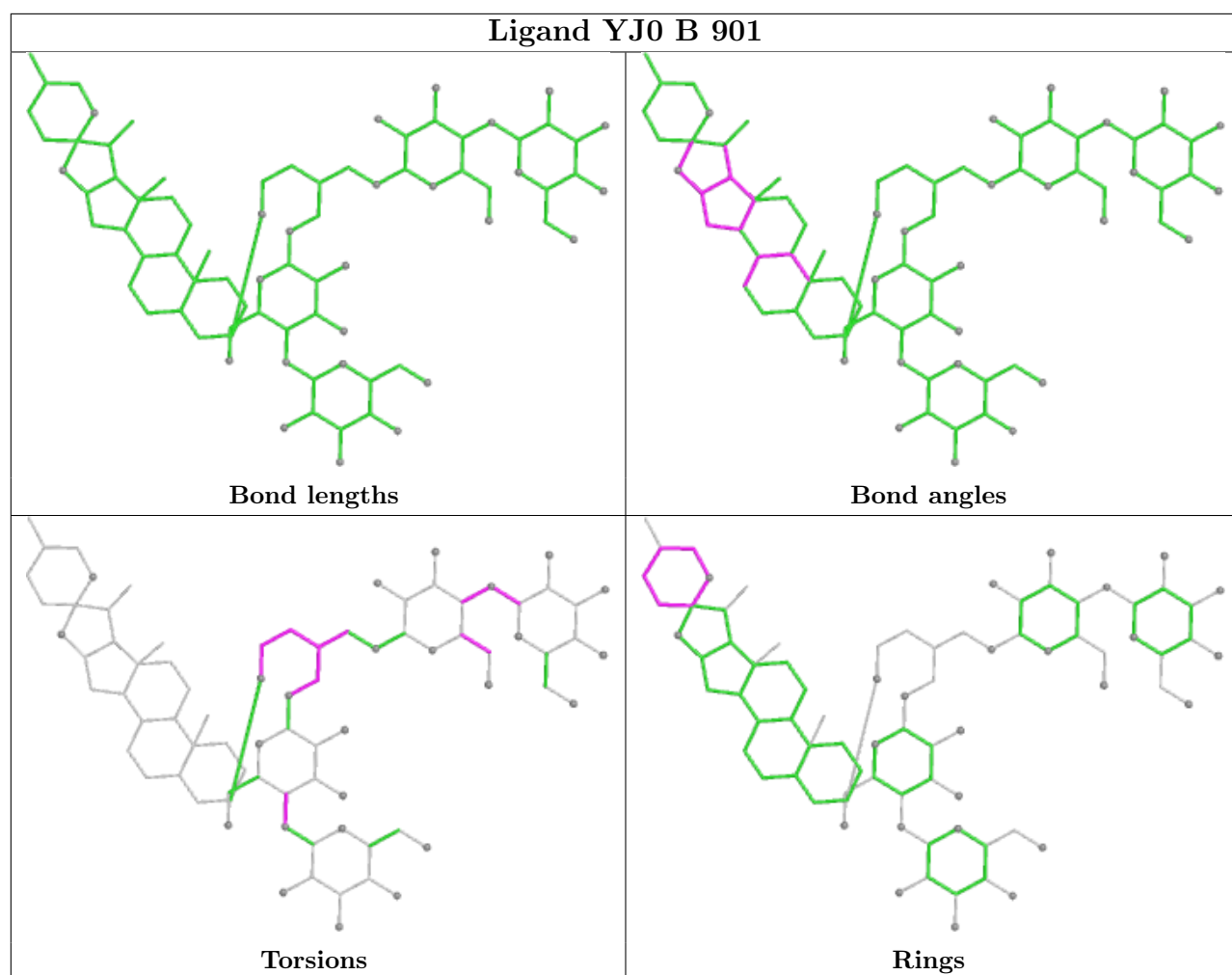
3 monomers are involved in 3 short contacts:

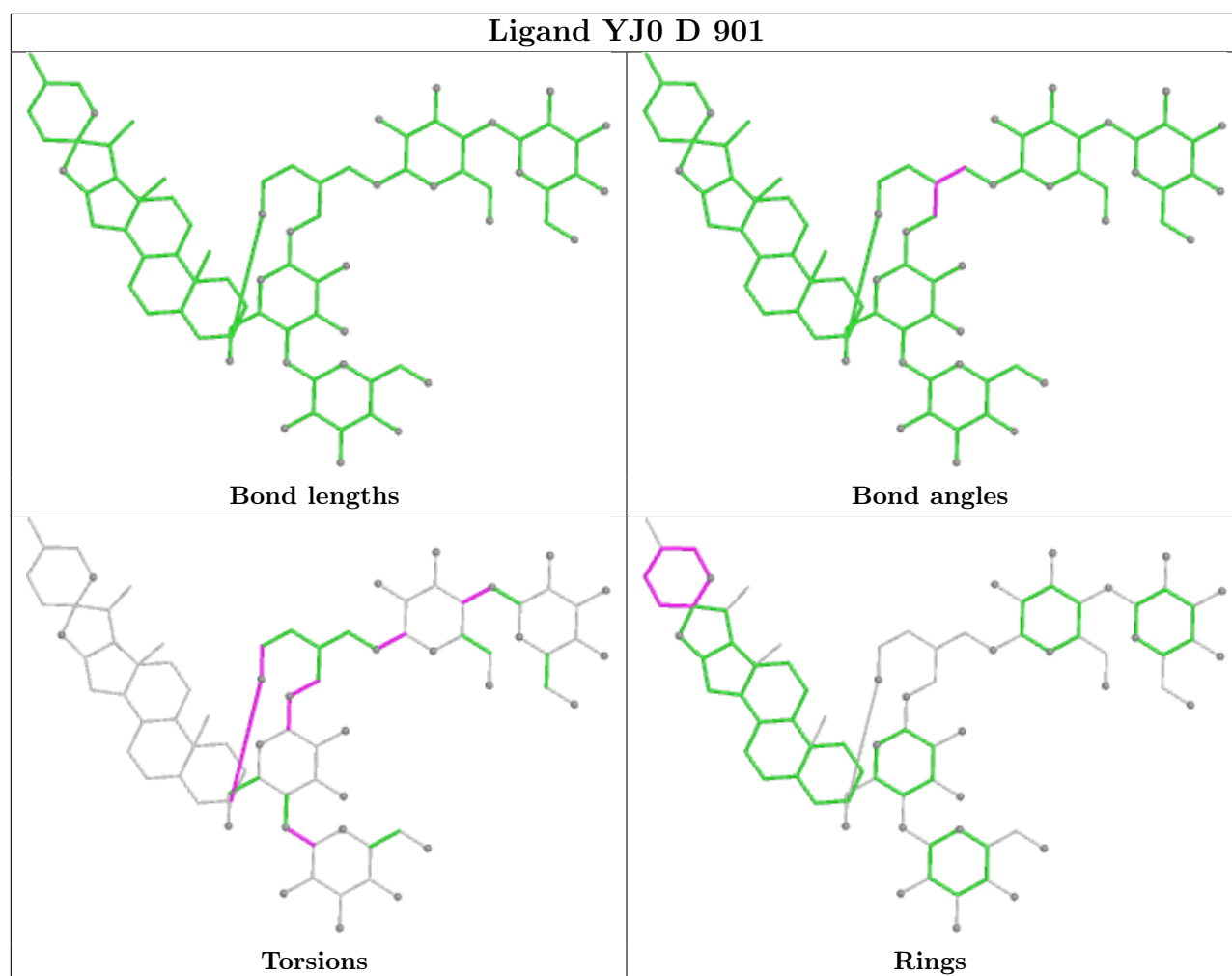
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	9PE	1	0
3	A	1001	9PE	1	0
4	B	901	YJ0	1	0

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.

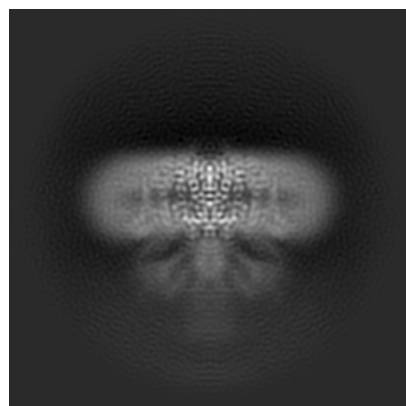
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69845. These allow visual inspection of the internal detail of the map and identification of artifacts.

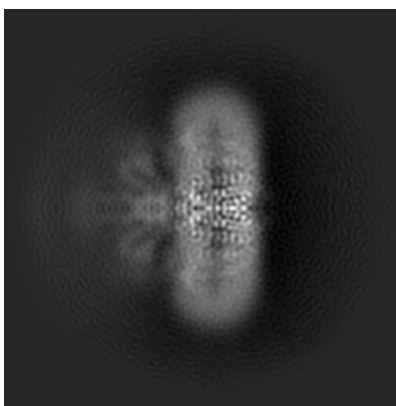
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

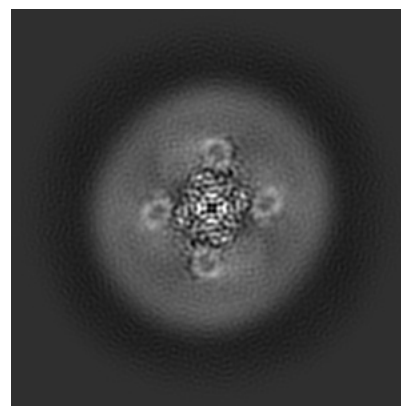
6.1.1 Primary map



X

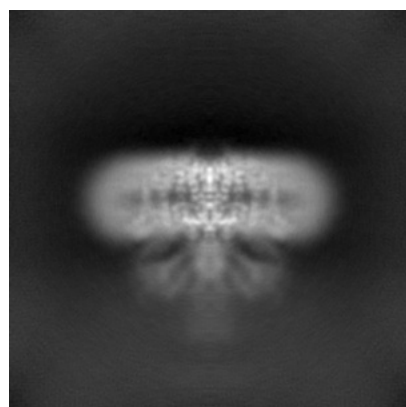


Y

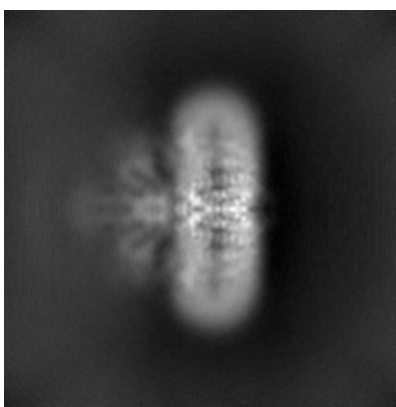


Z

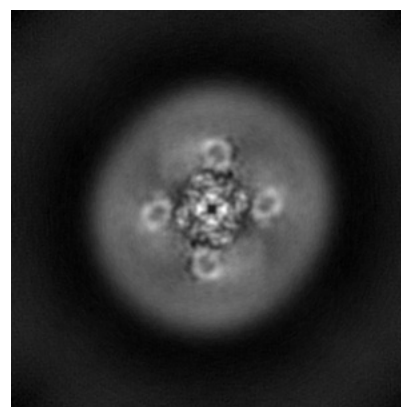
6.1.2 Raw map



X



Y

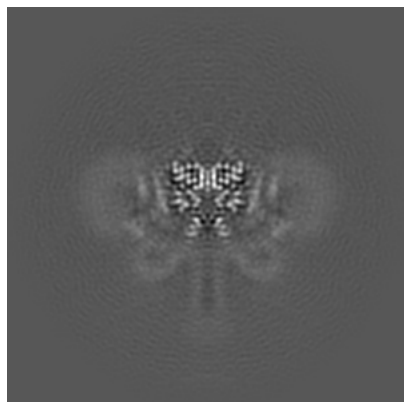


Z

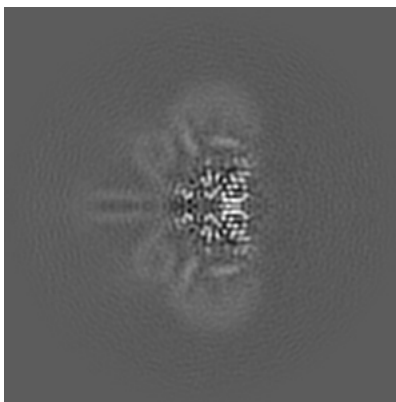
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

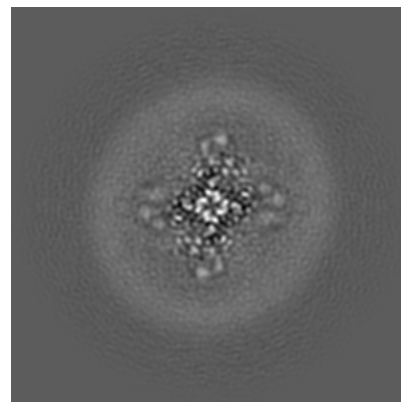
6.2.1 Primary map



X Index: 120

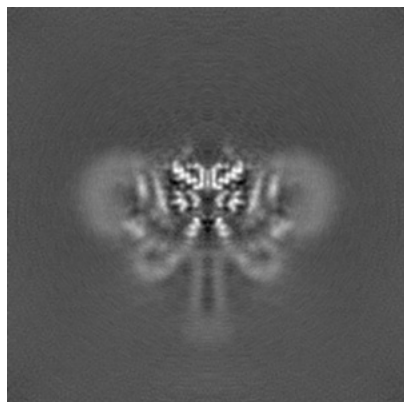


Y Index: 120

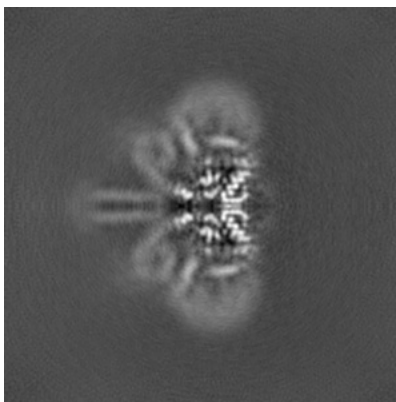


Z Index: 120

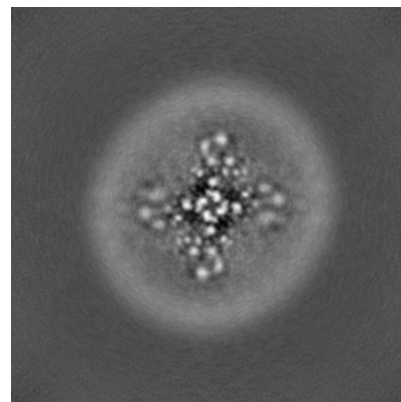
6.2.2 Raw map



X Index: 120



Y Index: 120

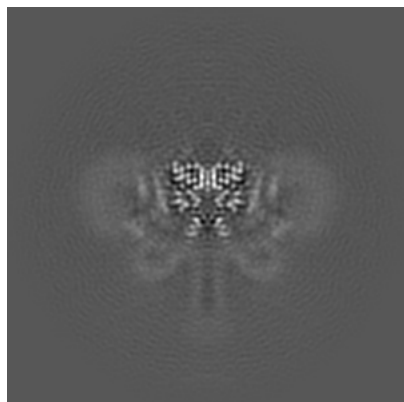


Z Index: 120

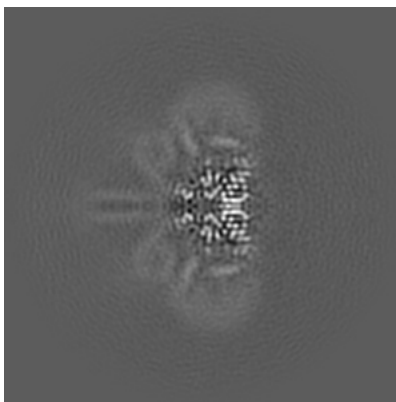
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

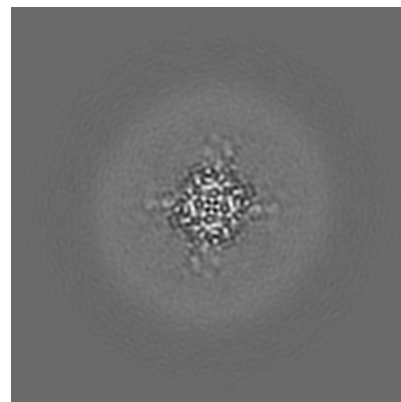
6.3.1 Primary map



X Index: 120

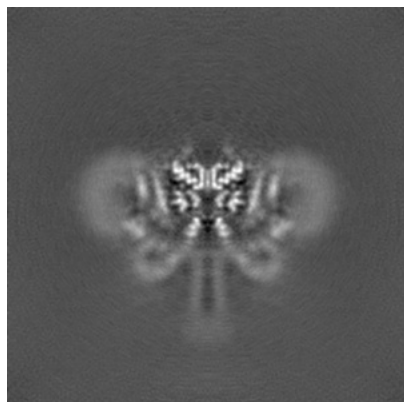


Y Index: 120

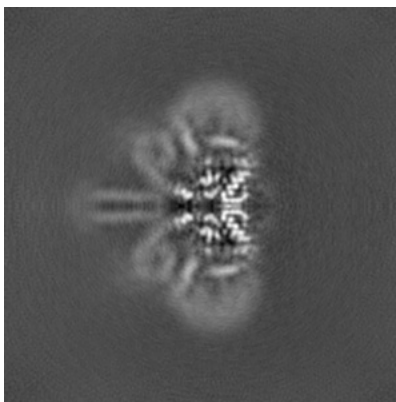


Z Index: 139

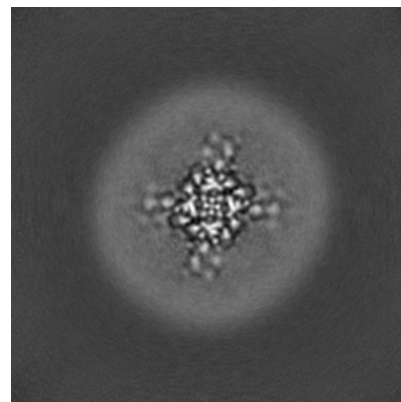
6.3.2 Raw map



X Index: 120



Y Index: 120

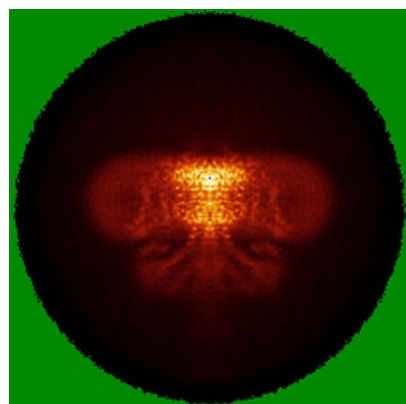


Z Index: 139

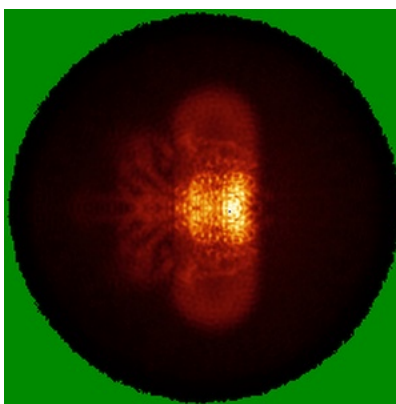
The images above show the largest variance slices of the map in three orthogonal directions.

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

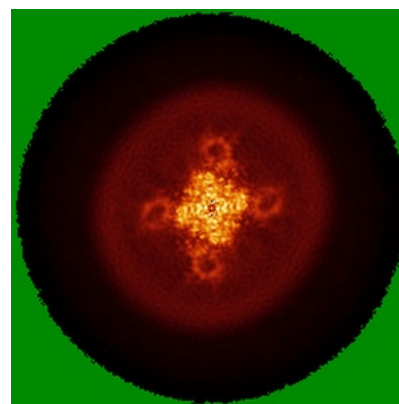
6.4.1 Primary map



X

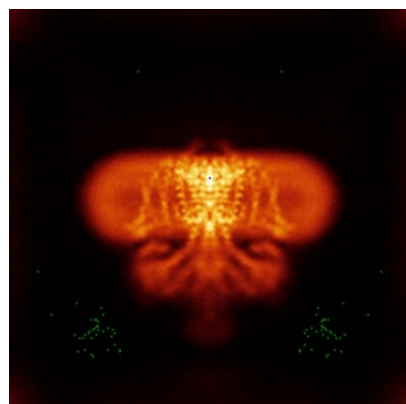


Y

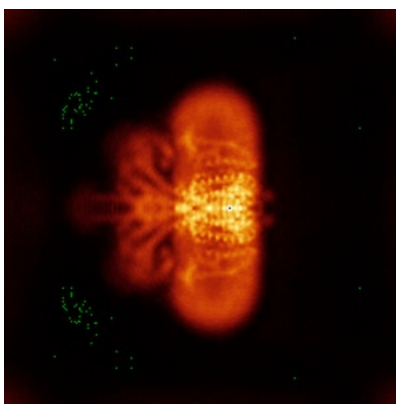


Z

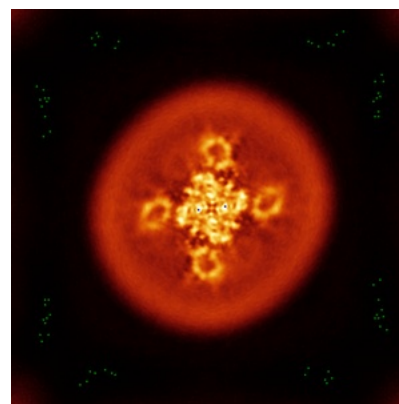
6.4.2 Raw map



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.

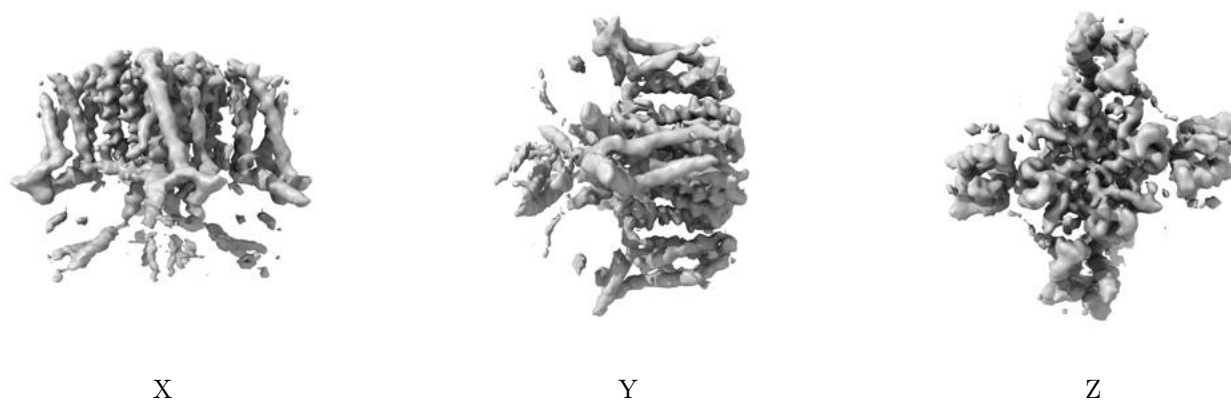
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.494. 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.

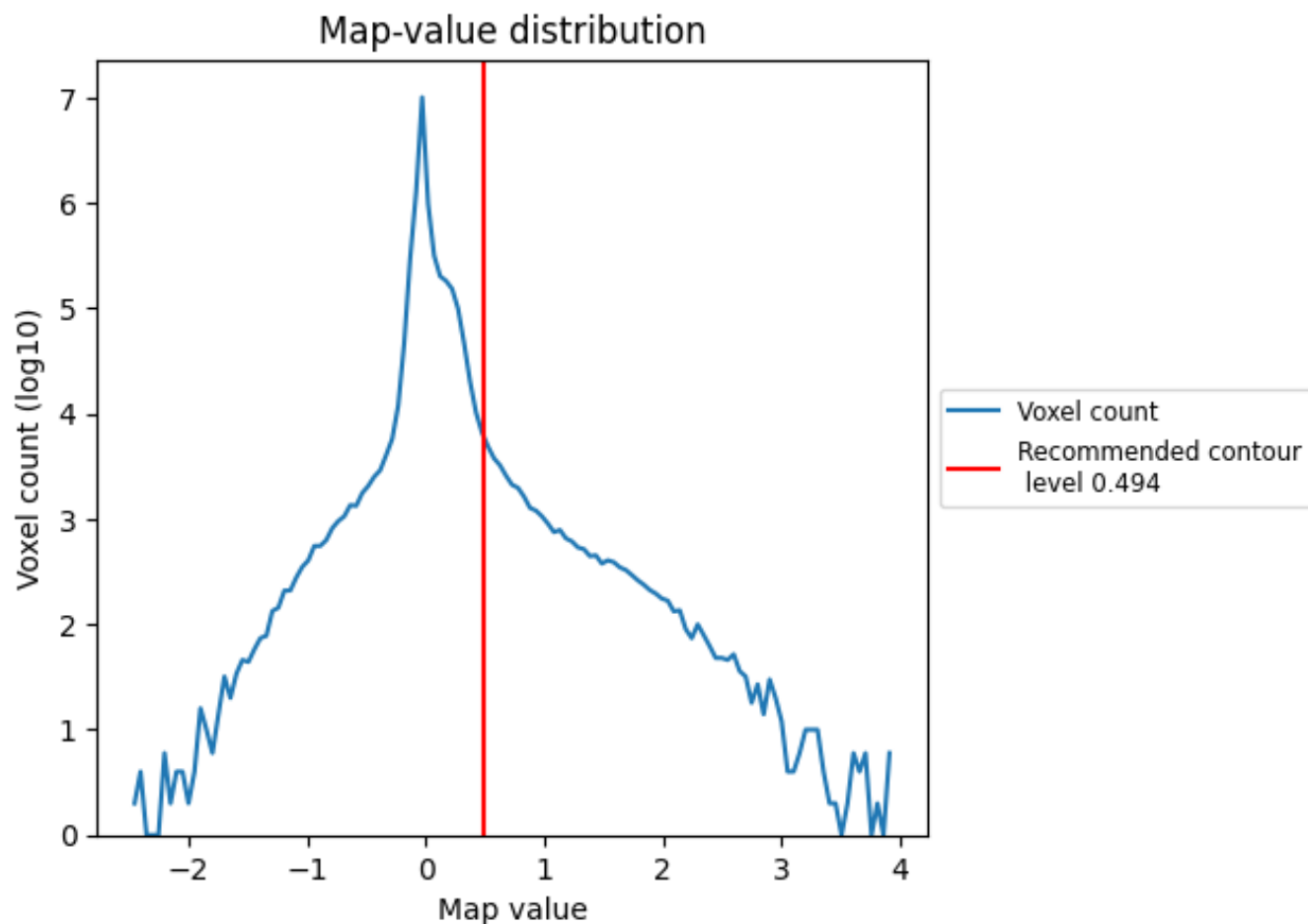
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

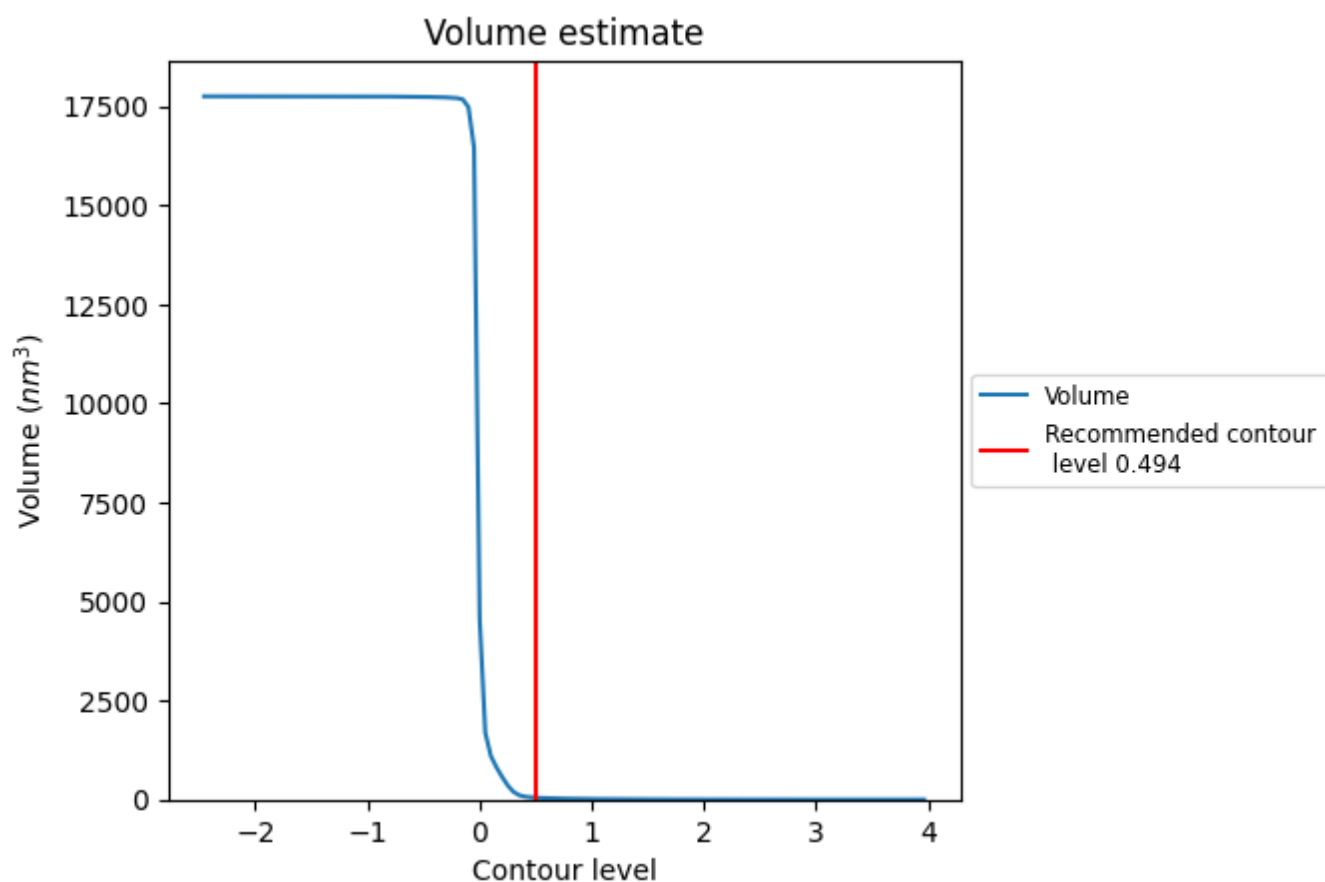
This section contains the results of statistical analysis of the map.

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.

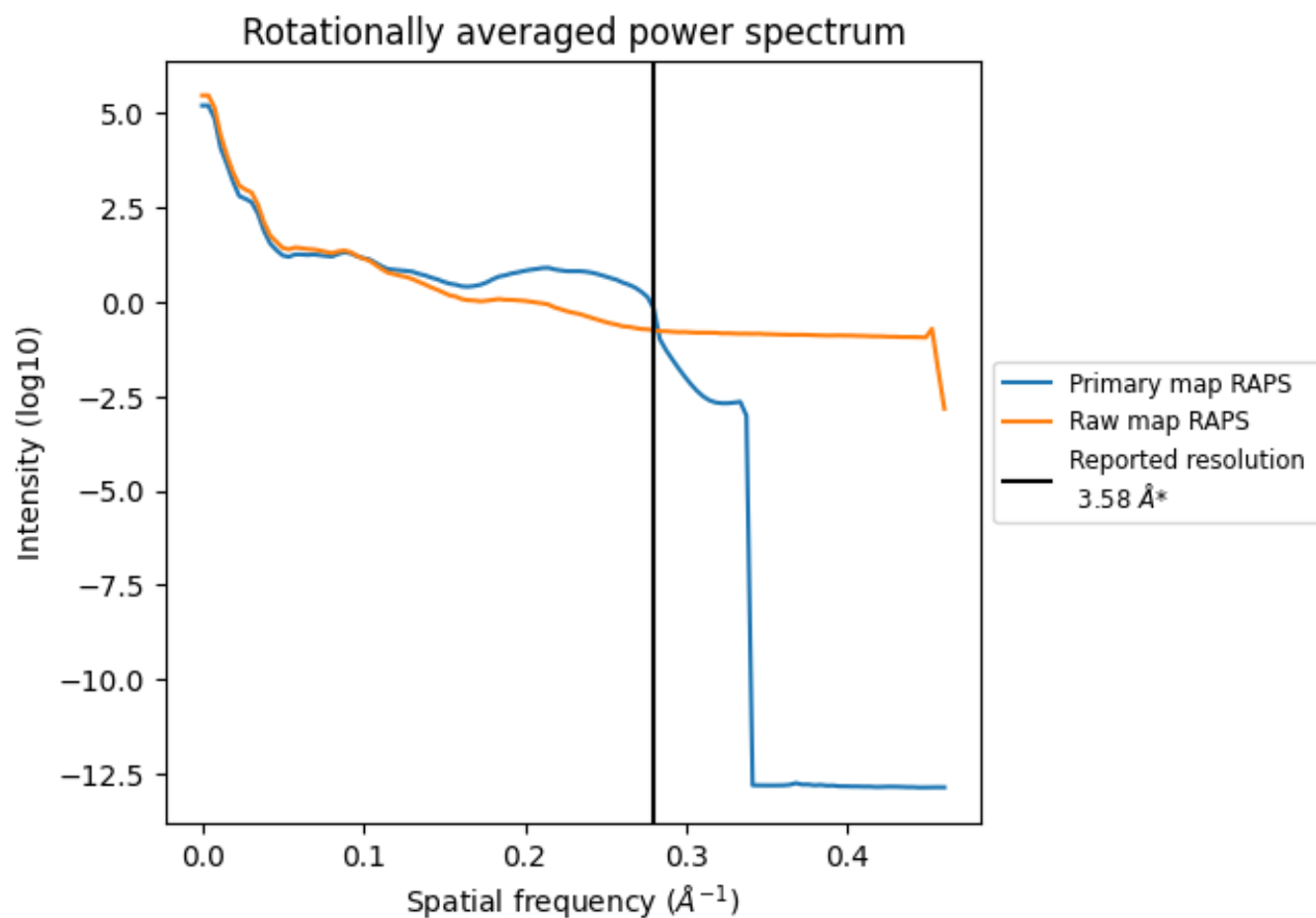
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 44 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 ⓘ

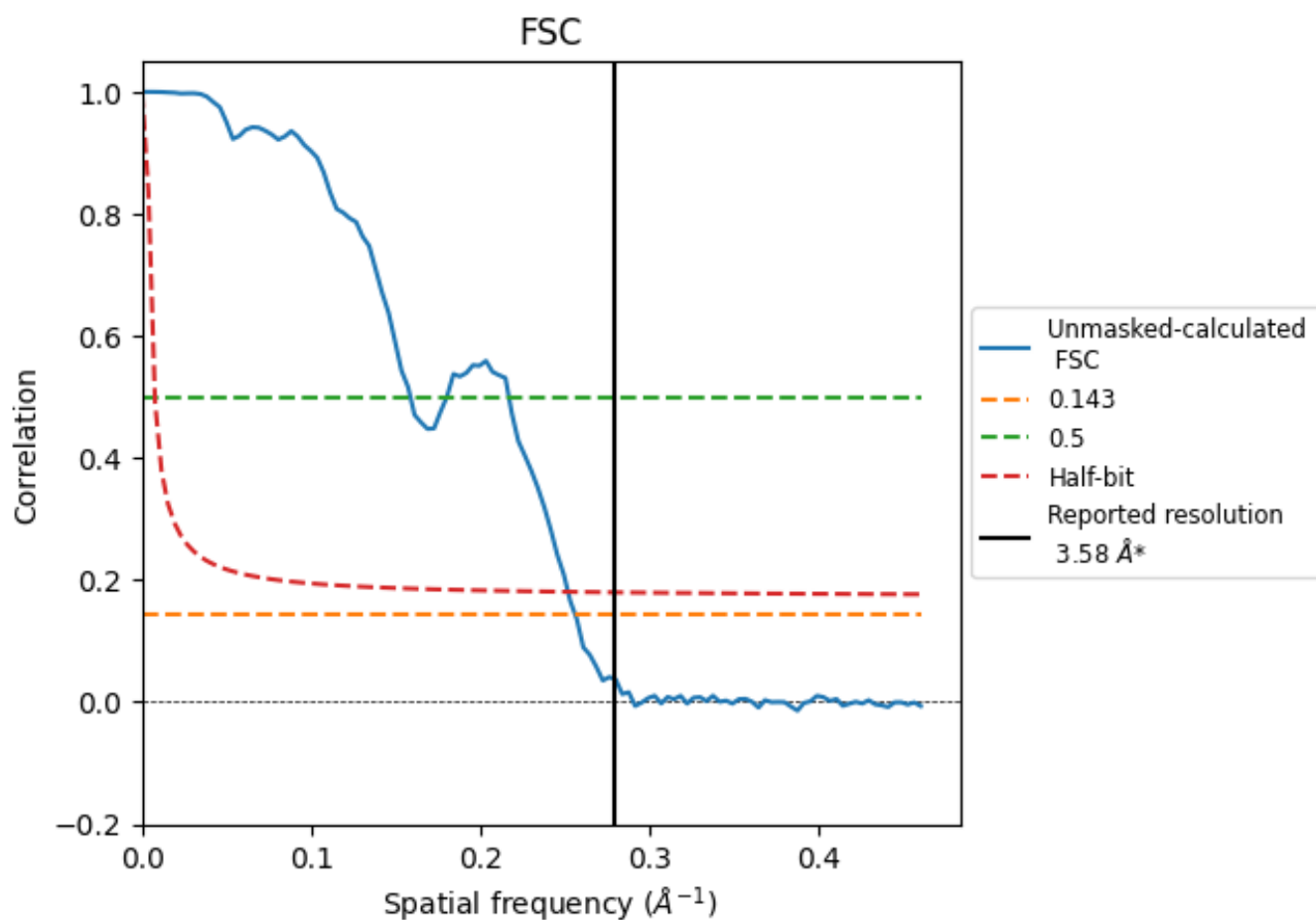


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 $0.279 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

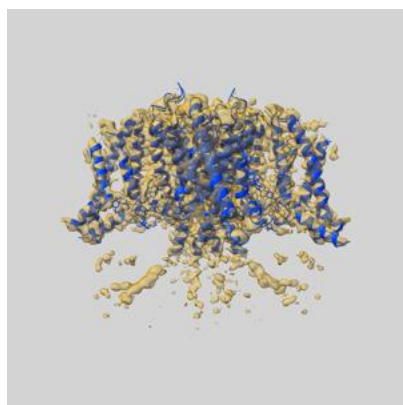
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.31	3.97

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

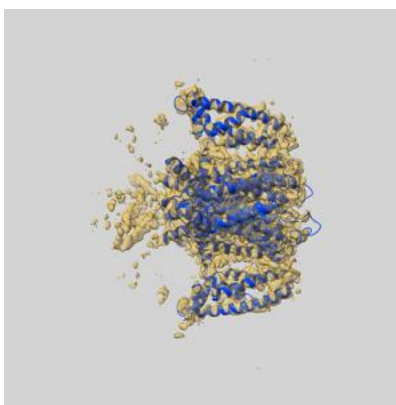
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69845 and PDB model 24VN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

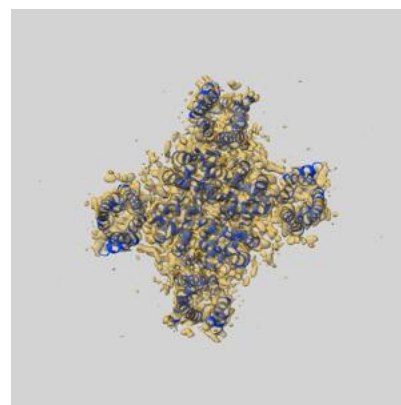
9.1 Map-model overlay [i](#)



X



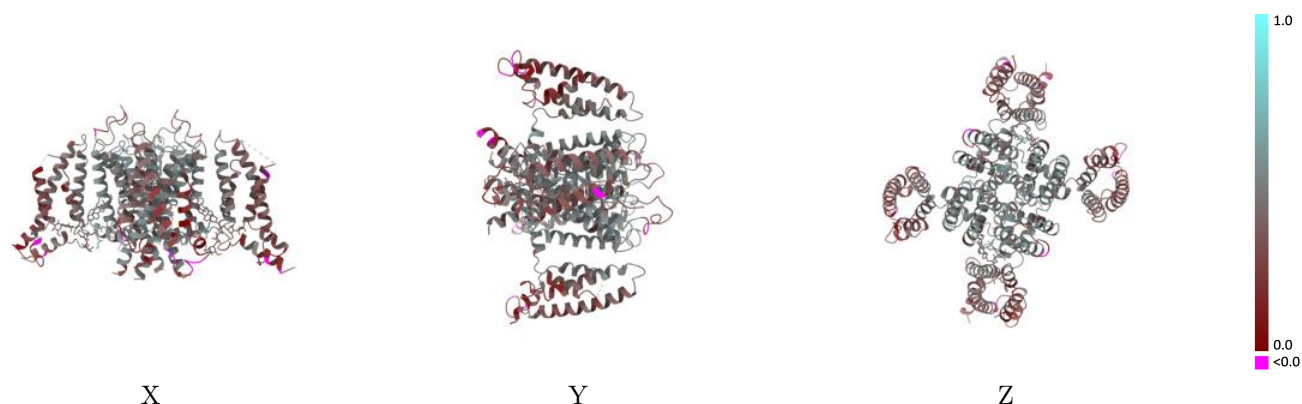
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.494 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](#)



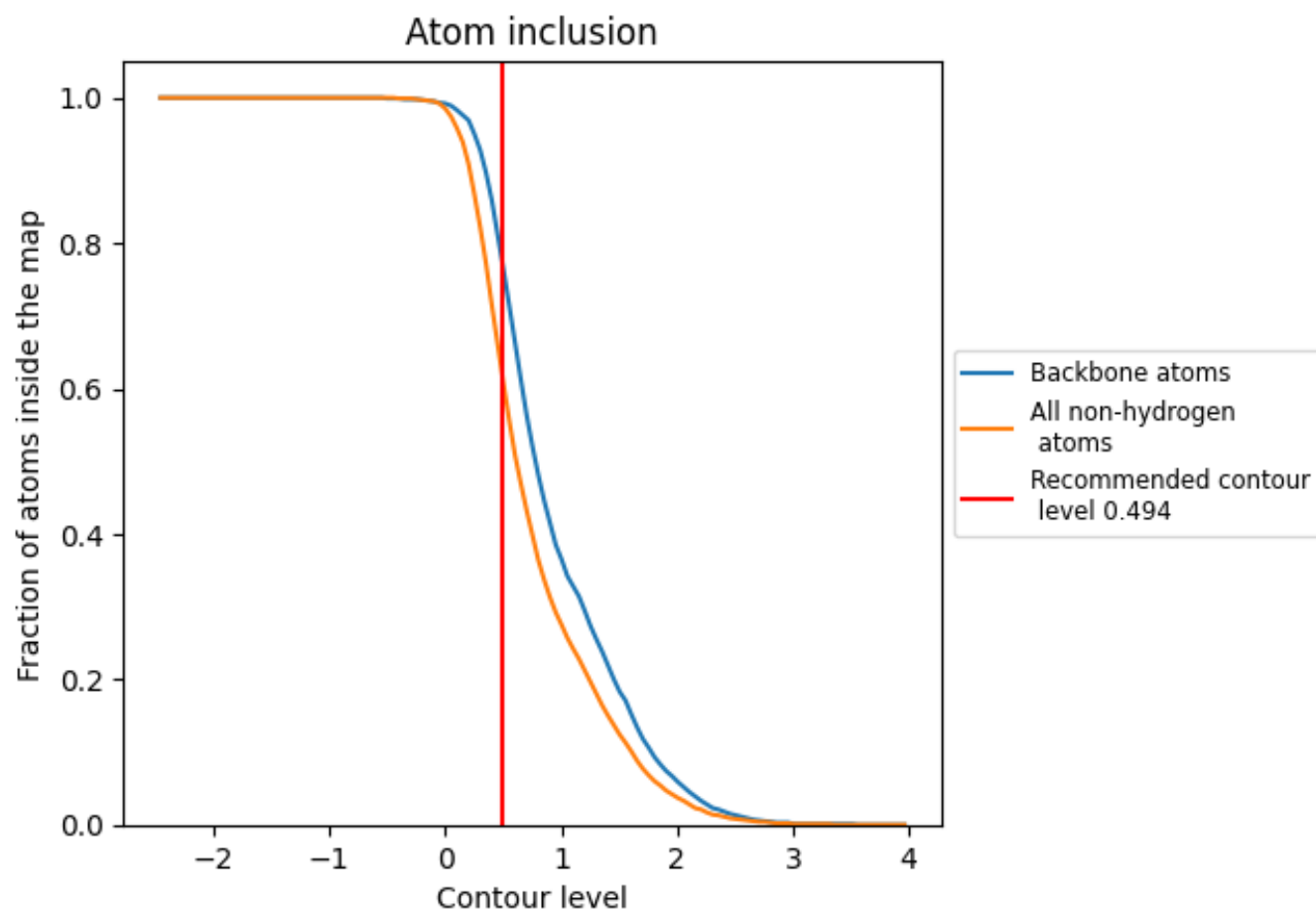
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.494).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.494) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.4020
A	0.5870	0.3900
B	0.6480	0.4140
C	0.5910	0.3900
D	0.6370	0.4110

