



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:06 AM UTC

PDB ID : 8F79 / pdb_00008f79
EMDB ID : EMD-28898
Title : LRRC8A(T48D):C conformation 2 top focus
Authors : Kern, D.M.; Brohawn, S.G.
Deposited on : 2022-11-18
Resolution : 3.15 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

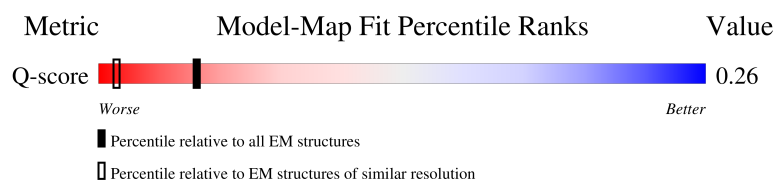
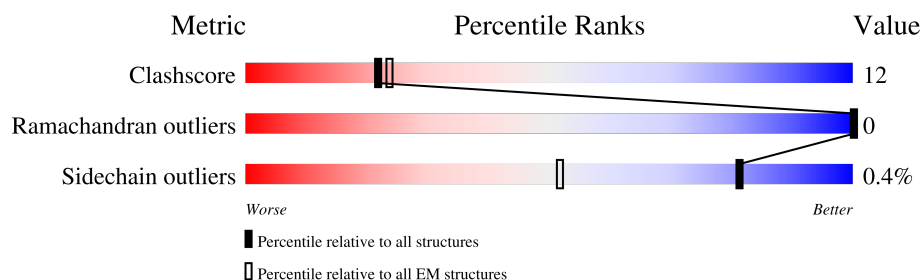
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

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	911	
1	B	911	
1	C	911	
1	D	911	

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Mol	Chain	Length	Quality of chain
1	E	911	45% 58% 21% 22%
2	F	813	46% 60% 27% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32333 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 Volume-regulated anion channel subunit LRRC8A, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	717	Total	C	N	O	S	0	0
			5916	3849	996	1046	25		
1	B	716	Total	C	N	O	S	0	0
			5912	3847	995	1045	25		
1	C	714	Total	C	N	O	S	0	0
			5898	3838	993	1042	25		
1	D	316	Total	C	N	O	S	0	0
			2648	1747	425	459	17		
1	E	715	Total	C	N	O	S	0	0
			5905	3843	994	1043	25		

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ASP	THR	engineered mutation	UNP Q80WG5
A	68O	TRP	MET	conflict	UNP P0ABE7
A	72F	ILE	HIS	conflict	UNP P0ABE7
A	72J	LEU	PRO	conflict	UNP Q80WG5
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	48	ASP	THR	engineered mutation	UNP Q80WG5
B	68O	TRP	MET	conflict	UNP P0ABE7
B	72F	ILE	HIS	conflict	UNP P0ABE7
B	72J	LEU	PRO	conflict	UNP Q80WG5
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5
C	48	ASP	THR	engineered mutation	UNP Q80WG5
C	68O	TRP	MET	conflict	UNP P0ABE7
C	72F	ILE	HIS	conflict	UNP P0ABE7
C	72J	LEU	PRO	conflict	UNP Q80WG5
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
D	48	ASP	THR	engineered mutation	UNP Q80WG5
D	68O	TRP	MET	conflict	UNP P0ABE7
D	72F	ILE	HIS	conflict	UNP P0ABE7
D	72J	LEU	PRO	conflict	UNP Q80WG5
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
E	48	ASP	THR	engineered mutation	UNP Q80WG5
E	68O	TRP	MET	conflict	UNP P0ABE7
E	72F	ILE	HIS	conflict	UNP P0ABE7
E	72J	LEU	PRO	conflict	UNP Q80WG5
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5

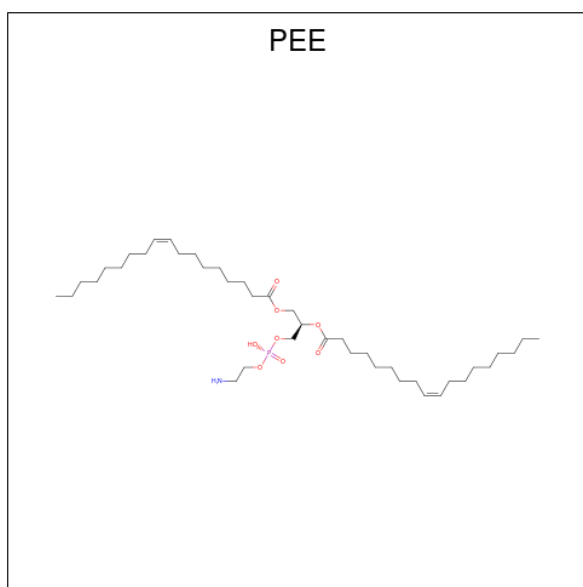
- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	704	Total	C	N	O	S	0	0
			5751	3745	940	1029	37		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			23	15	1	6	1	
3	A	1	Total	C	O			0
			13	11	2			
3	A	1	Total	C	O			0
			13	11	2			
3	B	1	Total	C	N	O	P	0
			26	18	1	6	1	
3	B	1	Total	C	O			0
			11	9	2			
3	B	1	Total	C	O			0
			10	8	2			
3	C	1	Total	C	N	O	P	0
			26	18	1	6	1	
3	C	1	Total	C	O			0
			11	9	2			
3	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	D	1	Total	C	O			0
			9	7	2			
3	D	1	Total	C	O			0
			11	9	2			
3	E	1	Total	C	N	O	P	0
			27	19	1	6	1	
3	E	1	Total	C	O			0
			10	8	2			
3	E	1	Total	C	O			0
			10	8	2			

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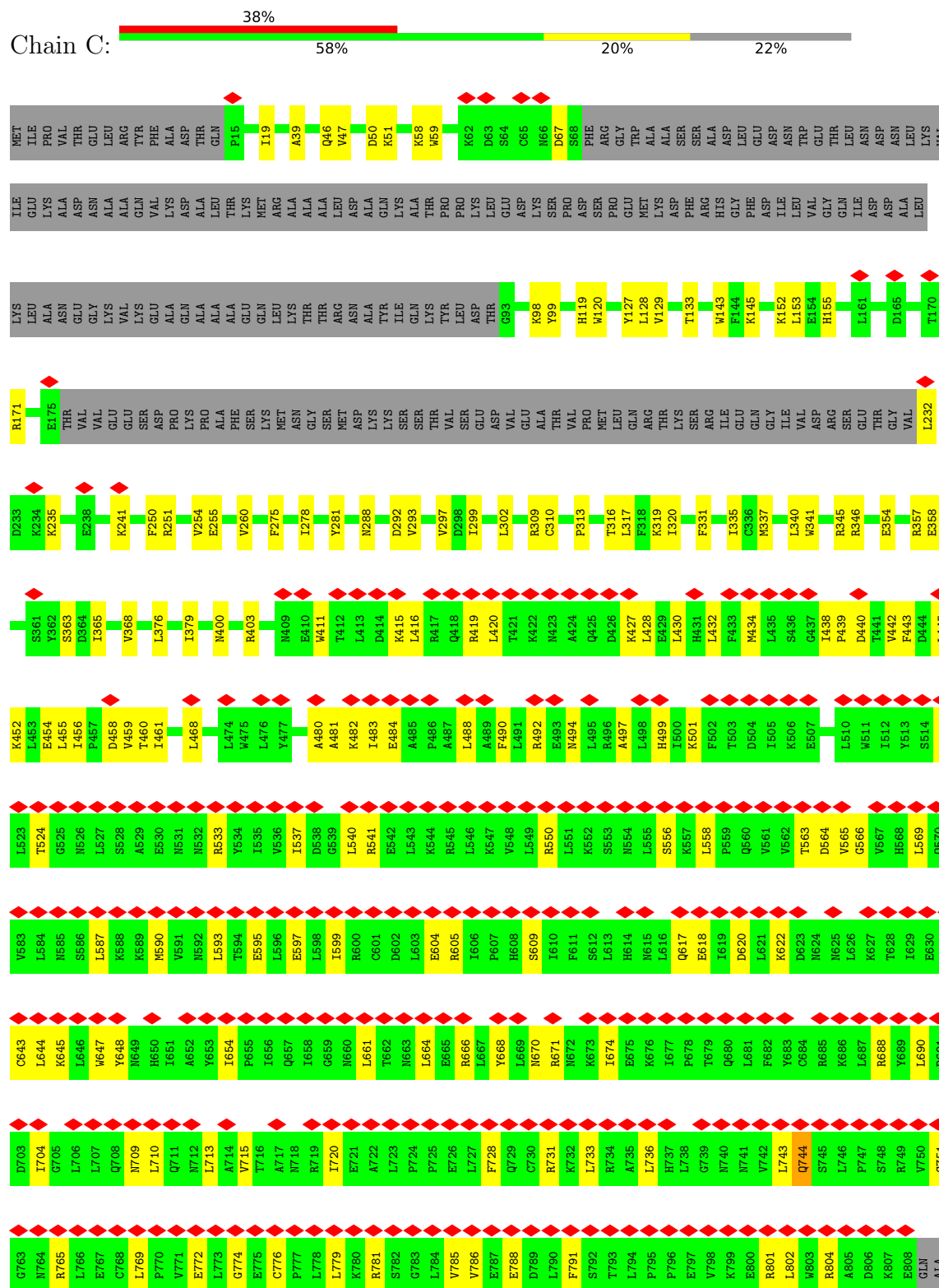
Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	F	1	Total	C	O			0
			11	9	2			
3	F	1	Total	C	O			0
			8	6	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	O	0
			1	1	
4	B	1	Total	O	0
			1	1	
4	C	1	Total	O	0
			1	1	
4	D	1	Total	O	0
			1	1	
4	E	1	Total	O	0
			1	1	
4	F	1	Total	O	0
			1	1	

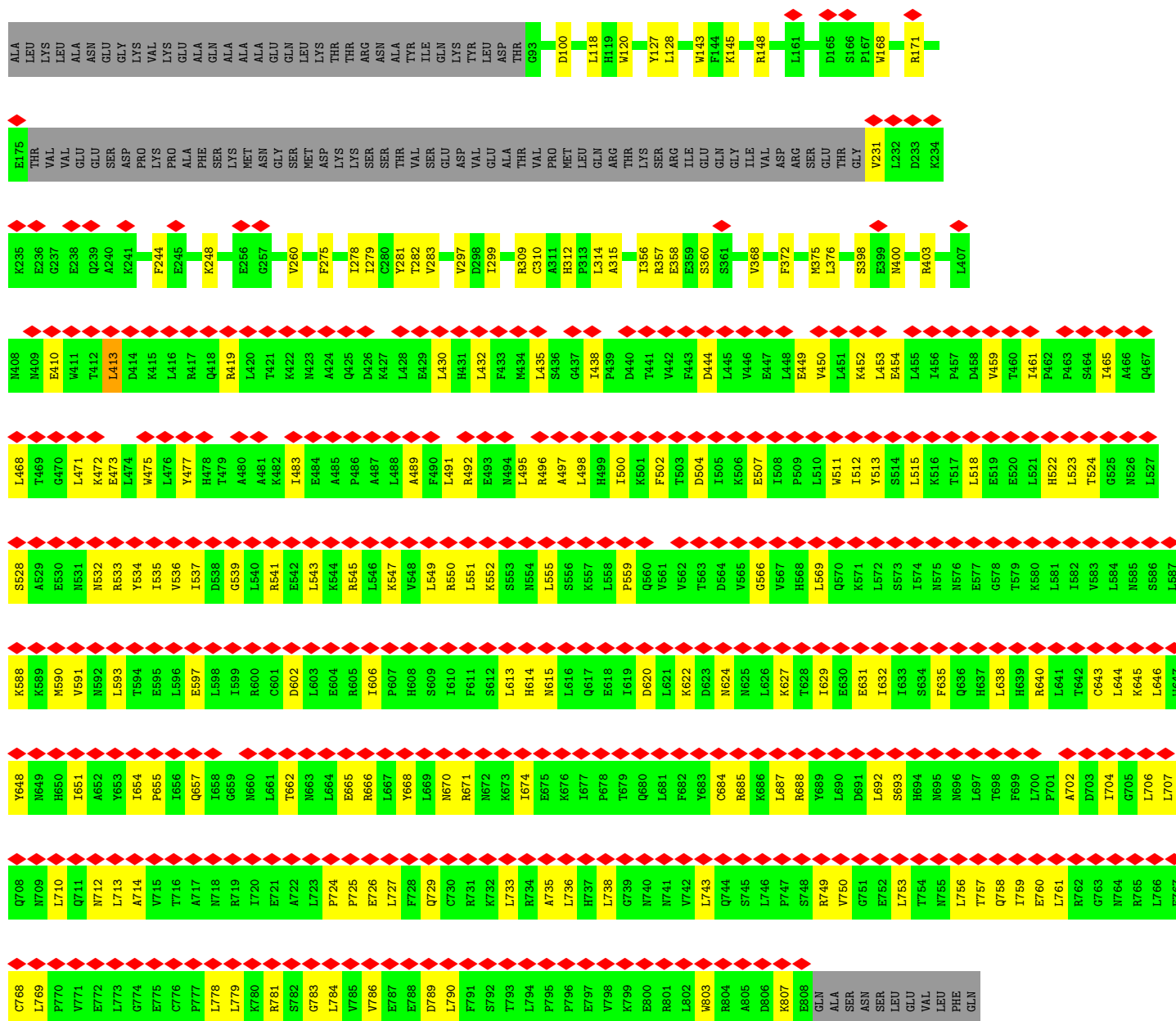
SER
ASN
SER
SER
LEU
GLU
VAL
LEU
PHE
GLN

- Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

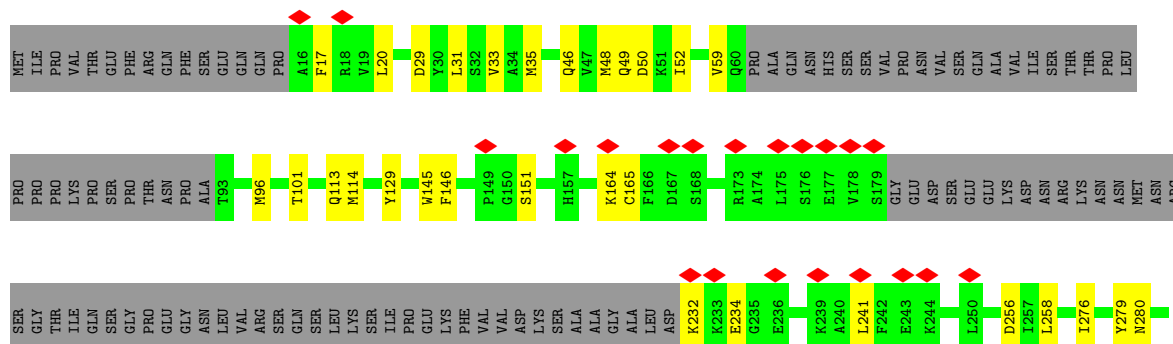


- Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562





● Molecule 2: Volume-regulated channel subunit LRRC8C



V284	R425	A485	K545	P605	L665	L725	E785
I297	L426	A486	I546	H606	F666	Y726	D786
Q298	E427	S487	L547	A607	F667	F727	A787
D299	L428	F488	S548	V608	S668	C728	L788
C308	P429	L489	S549	F609	H669	K729	F789
H309	L430	K490	K550	S610	N670	K730	E790
R310	I431	E491	S551	L611	K671	L731	T791
A313	M432	M492	N552	S612	V672	K732	L792
T363	S434	L493	V553	S613	E673	T733	P793
Q366	L436	K494	S554	L614	V674	L734	S794
E367	P437	V495	K555	Q615	L675	K735	D795
E368	T438	L496	I556	E616	P676	T736	V796
T368	T439	S497	P557	L617	S677	G737	R797
G369	V440	V498	Q558	D618	H678	K738	E798
G370	F441	K499	A559	L619	L679	W739	Q799
D362	E442	F500	V560	K620	F680	S740	N800
I363	T443	D501	V561	E621	L681	L741	K801
V366	T444	M503	D562	N622	C682	S742	A802
K367	E445	R504	V563	N623	K683	V743	D803
N368	L446	E505	S564	L624	I685	L744	SER
M373	Q447	L506	S565	K625	R686	S745	ASN
L374	S448	P507	H566	S626	Y687	F746	SER
I377	L449	P508	L567	I627	L688	K747	GLU
K378	K450	W509	Q568	E628	D689	I748	ASN
I454	L451	M510	K569	E629	L690	G749	LEU
L392	E452	Y511	M570	I630	S691	W750	PHE
S393	I455	G512	C571	V631	Y692	L751	GLN
E394	K456	L513	V572	S632	N693	L752	GLY
Q402	M457	R514	H573	F633	D694	F753	
L403	V457	N515	N574	Q634	I695	L754	
M404	M458	L516	D575	H635	R696	S755	
L405	I459	E517	G576	L636	F697	Y756	
M406	P460	E518	T577	K638	L698	L757	
M407	A461	L519	K578	L639	P699	D758	
E408	I463	Y520	L579	T640	P700	I759	
W409	A464	L521	V580	V641	E701	K760	
T410	Q465	V522	M581	L642	I702	G761	
P411	L466	G523	L582	K643	G703	M762	
D412	D467	S524	L583	L644	V704	H763	
F411	M468	L525	N584	W645	L705	F764	
K413	L469	S526	L585	Y646	Q706	E765	
K414	Q470	H527	L586	N647	S707	V766	
L415	E471	D528	K586	S648	L708	L767	
Q416	L472	I529	K587	I649	Q709	P768	
K417	C473	S530	M588	A650	Y710	P769	
L418	L474	K531	T589	Y651	F711	E770	
Q419	H475	N532	N590	L591	S712	L771	
T420	Q476	V533	L592	T592	I713	G772	
M421	S478	T534	E593	P653	T714	D773	
A422	V479	L535	L594	E654	C715	C774	
H423	K480	E536	E595	H655	M716	R775	
M424	I481	S537	L596	I656	K717	A776	
	S483	L538	V597	K657	V718	L777	
	A484	R539	H598	K658	E719	K778	
		D540	C599	L659	S720	R779	
		L541	D600	T660	P721	A780	
		S543	L601	S661	D722	G781	
		L544	E602	L662	D723	L782	
			R603	E663	E724	V783	
			I604	R664		V784	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71566	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)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.200	Depositor
Minimum map value	-1.928	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/6049	0.50	1/8198 (0.0%)
1	B	0.22	0/6045	0.52	0/8193
1	C	0.22	0/6031	0.49	0/8173
1	D	0.19	0/2723	0.40	0/3686
1	E	0.25	0/6038	0.50	0/8183
2	F	0.24	0/5877	0.51	0/7943
All	All	0.23	0/32763	0.50	1/44376 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	LEU	N-CA-C	5.20	118.08	111.69

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	5916	0	6071	145	0
1	B	5912	0	6068	149	0
1	C	5898	0	6052	126	0
1	D	2648	0	2638	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5905	0	6061	135	0
2	F	5751	0	5887	191	0
3	A	49	0	63	0	0
3	B	47	0	59	1	0
3	C	37	0	47	1	0
3	D	58	0	74	3	0
3	E	47	0	59	2	0
3	F	59	0	76	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
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	32333	0	33155	762	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 12.

The worst 5 of 762 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:D:350:LYS:HE2	1:D:369:LYS:CE	1.48	1.42
2:F:443:ILE:CG2	2:F:446:LEU:HG	1.63	1.28
1:D:350:LYS:CE	1:D:369:LYS:HE2	1.66	1.23
1:B:779:LEU:CD1	1:B:784:LEU:HD23	1.70	1.20
2:F:466:LEU:HD12	2:F:466:LEU:O	1.50	1.11

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	711/911 (78%)	686 (96%)	25 (4%)	0	100	100
1	B	710/911 (78%)	671 (94%)	39 (6%)	0	100	100
1	C	708/911 (78%)	675 (95%)	33 (5%)	0	100	100
1	D	310/911 (34%)	303 (98%)	7 (2%)	0	100	100
1	E	709/911 (78%)	674 (95%)	35 (5%)	0	100	100
2	F	698/813 (86%)	655 (94%)	43 (6%)	0	100	100
All	All	3846/5368 (72%)	3664 (95%)	182 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/830 (80%)	663 (100%)	2 (0%)	86	85
1	B	665/830 (80%)	661 (99%)	4 (1%)	78	81
1	C	663/830 (80%)	662 (100%)	1 (0%)	87	87
1	D	293/830 (35%)	293 (100%)	0	100	100
1	E	664/830 (80%)	660 (99%)	4 (1%)	78	81
2	F	659/756 (87%)	657 (100%)	2 (0%)	86	85
All	All	3609/4906 (74%)	3596 (100%)	13 (0%)	81	84

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	275	PHE
1	E	281	TYR
2	F	721	LEU
1	E	413	LEU
2	F	714	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	740	ASN
1	C	729	GLN
2	F	647	ASN
1	C	663	ASN
1	D	267	GLN

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](#)

17 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	PEE	E	902	-	9,9,50	0.62	0	9,9,55	0.79	0
3	PEE	B	902	-	10,10,50	1.64	2 (20%)	10,10,55	1.56	2 (20%)
3	PEE	A	901	-	22,22,50	1.55	3 (13%)	24,25,55	1.30	2 (8%)
3	PEE	A	903	-	12,12,50	1.10	1 (8%)	12,12,55	1.13	1 (8%)
3	PEE	F	901	-	39,39,50	1.42	4 (10%)	42,44,55	1.09	2 (4%)
3	PEE	A	902	-	12,12,50	1.11	1 (8%)	12,12,55	1.12	1 (8%)
3	PEE	D	901	-	37,37,50	1.33	3 (8%)	40,42,55	1.02	1 (2%)
3	PEE	B	901	-	25,25,50	1.53	3 (12%)	27,28,55	1.17	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEE	D	902	-	8,8,50	0.65	0	8,8,55	0.83	0
3	PEE	D	903	-	10,10,50	0.59	0	10,10,55	0.79	0
3	PEE	C	901	-	25,25,50	1.51	3 (12%)	27,28,55	1.16	1 (3%)
3	PEE	E	903	-	9,9,50	0.62	0	9,9,55	0.78	0
3	PEE	F	902	-	10,10,50	0.60	0	10,10,55	0.78	0
3	PEE	E	901	-	26,26,50	1.49	3 (11%)	28,29,55	1.15	1 (3%)
3	PEE	F	903	-	7,7,50	0.69	0	7,7,55	0.85	0
3	PEE	B	903	-	9,9,50	0.63	0	9,9,55	0.78	0
3	PEE	C	902	-	10,10,50	0.60	0	10,10,55	0.78	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	PEE	E	902	-	-	5/7/7/54	-
3	PEE	B	902	-	-	5/8/8/54	-
3	PEE	A	901	-	-	7/23/23/54	-
3	PEE	A	903	-	-	7/10/10/54	-
3	PEE	F	901	-	-	20/43/43/54	-
3	PEE	A	902	-	-	7/10/10/54	-
3	PEE	D	901	-	-	17/41/41/54	-
3	PEE	B	901	-	-	15/26/26/54	-
3	PEE	D	902	-	-	3/6/6/54	-
3	PEE	D	903	-	-	4/8/8/54	-
3	PEE	C	901	-	-	8/26/26/54	-
3	PEE	E	903	-	-	4/7/7/54	-
3	PEE	F	902	-	-	5/8/8/54	-
3	PEE	E	901	-	-	8/27/27/54	-
3	PEE	F	903	-	-	3/5/5/54	-
3	PEE	B	903	-	-	4/7/7/54	-
3	PEE	C	902	-	-	4/8/8/54	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	PEE	P-O4P	4.95	1.78	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	PEE	P-O4P	4.80	1.78	1.59
3	F	901	PEE	P-O4P	4.80	1.78	1.59
3	A	901	PEE	P-O4P	4.76	1.78	1.59
3	D	901	PEE	P-O4P	4.75	1.78	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	PEE	O2P-P-O1P	4.49	133.31	112.44
3	A	901	PEE	O2P-P-O1P	4.48	133.28	112.44
3	C	901	PEE	O2P-P-O1P	4.47	133.23	112.44
3	B	901	PEE	O2P-P-O1P	4.46	133.21	112.44
3	E	901	PEE	O2P-P-O1P	4.46	133.19	112.44

There are no chirality outliers.

5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	PEE	C17-C18-C19-C20
3	A	901	PEE	C4-O4P-P-O2P
3	A	901	PEE	O4P-C4-C5-N
3	B	901	PEE	C1-O3P-P-O1P
3	B	901	PEE	C1-O3P-P-O4P

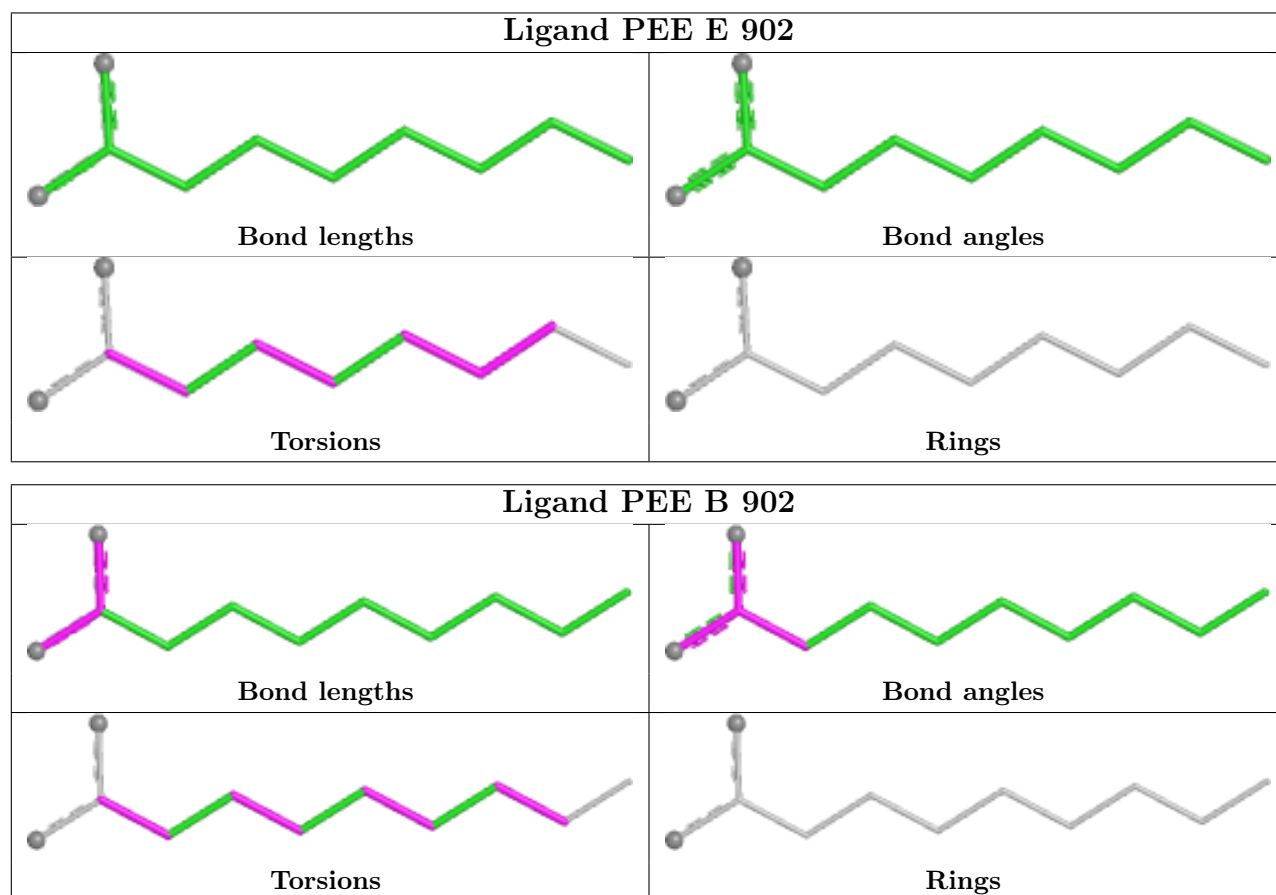
There are no ring outliers.

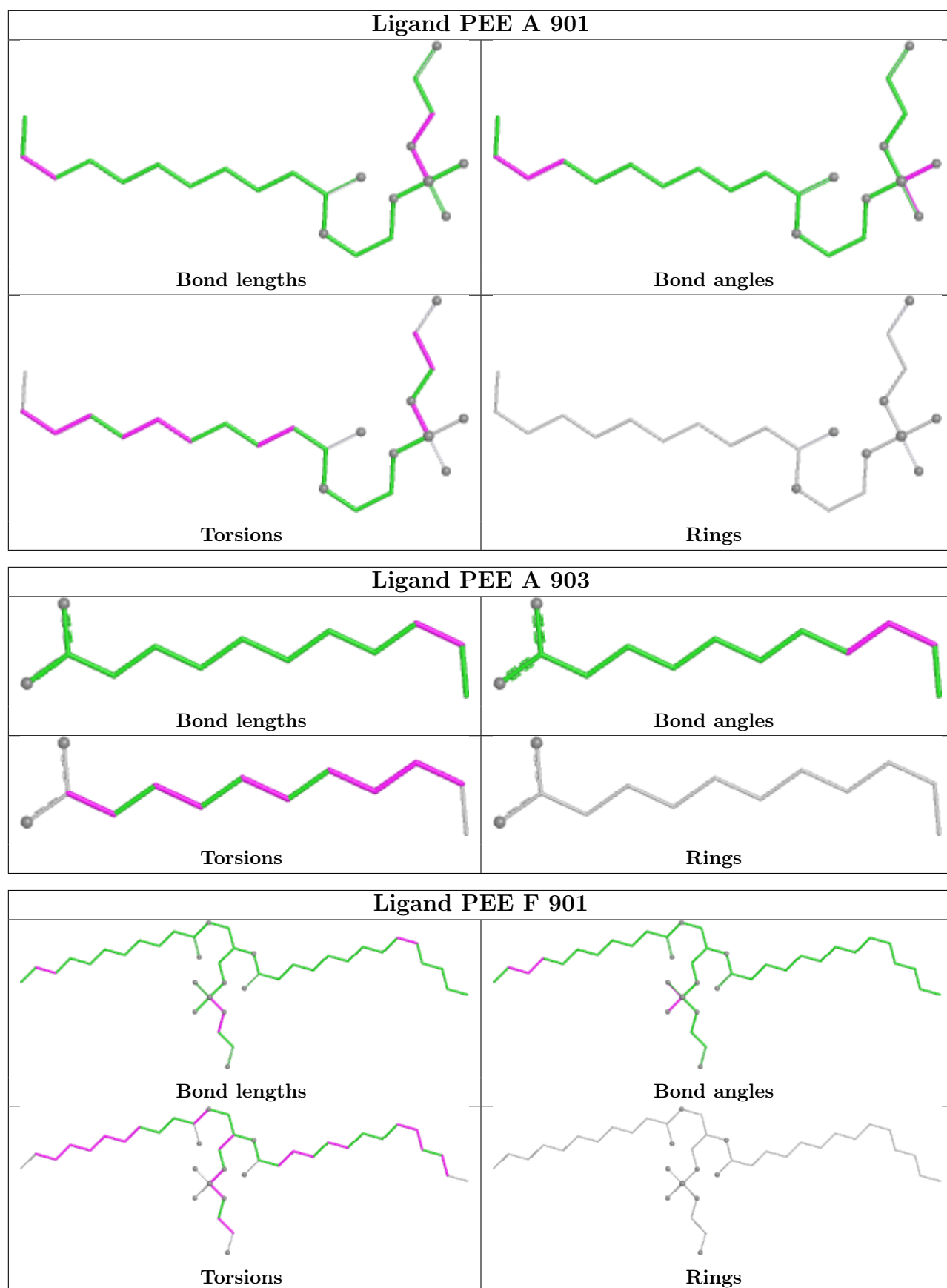
6 monomers are involved in 8 short contacts:

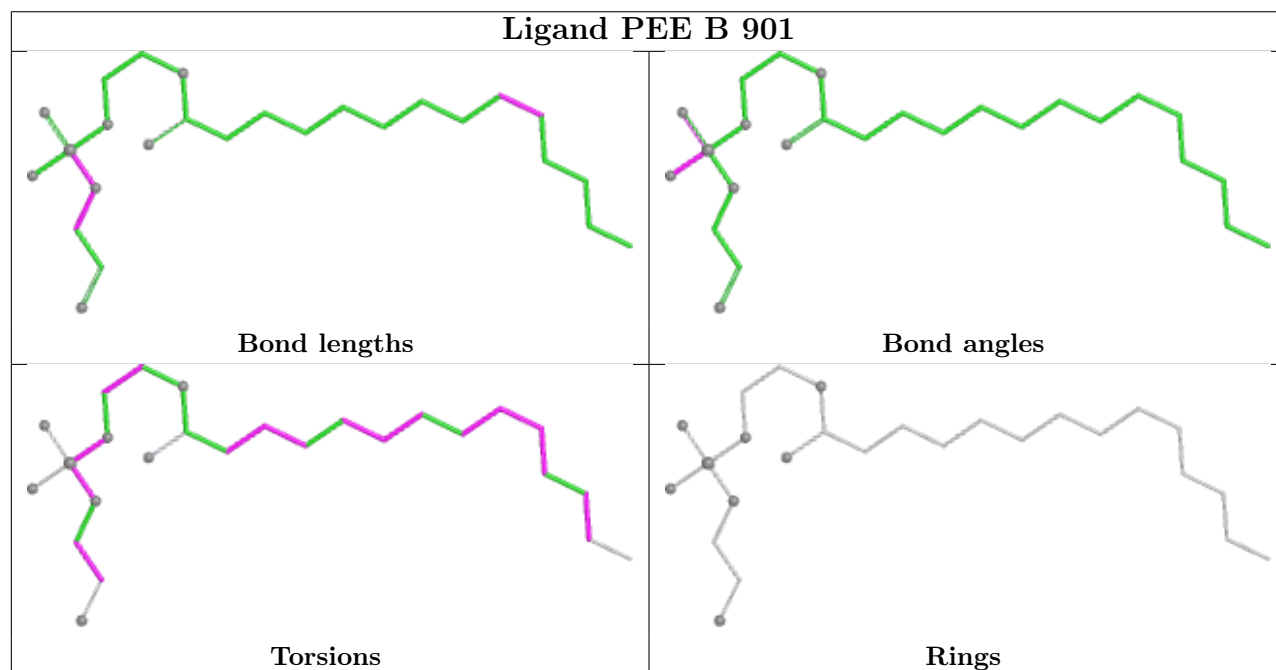
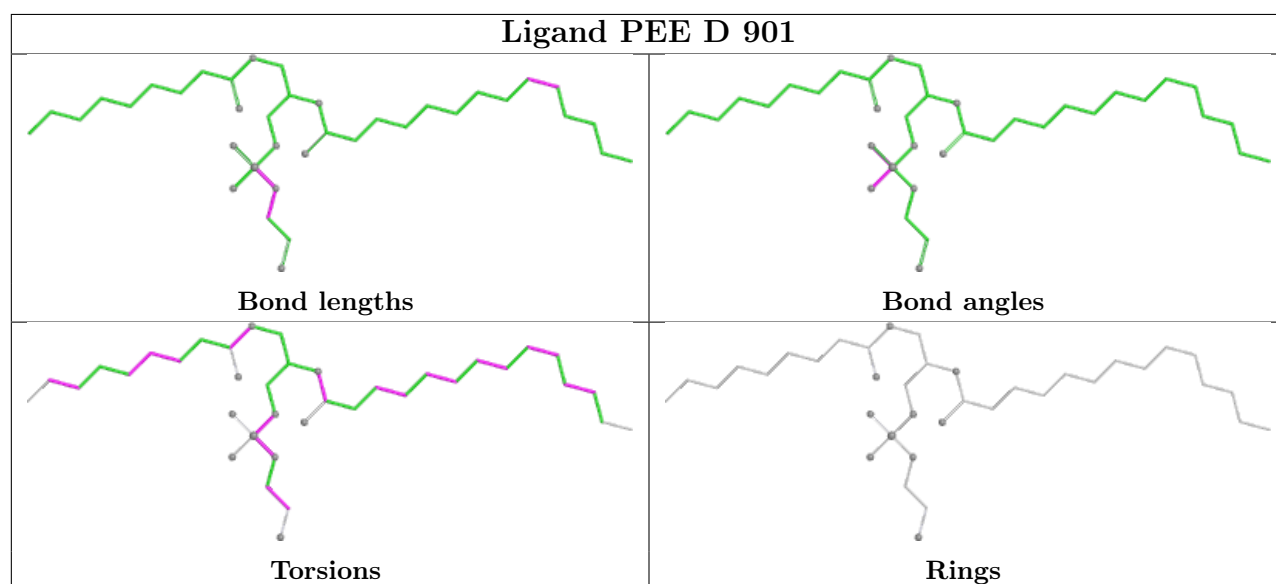
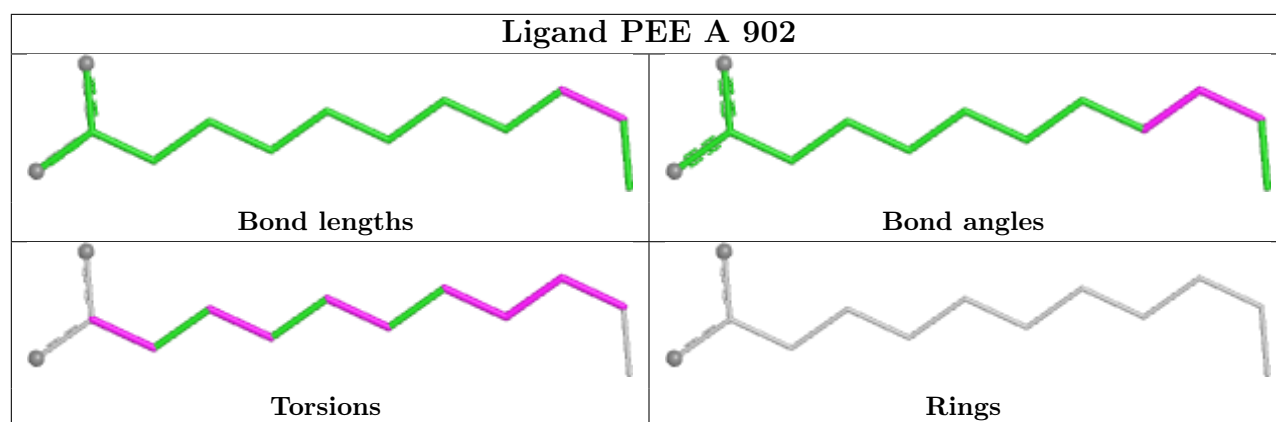
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	902	PEE	1	0
3	F	901	PEE	1	0
3	D	901	PEE	3	0
3	B	901	PEE	1	0
3	C	901	PEE	1	0
3	E	901	PEE	1	0

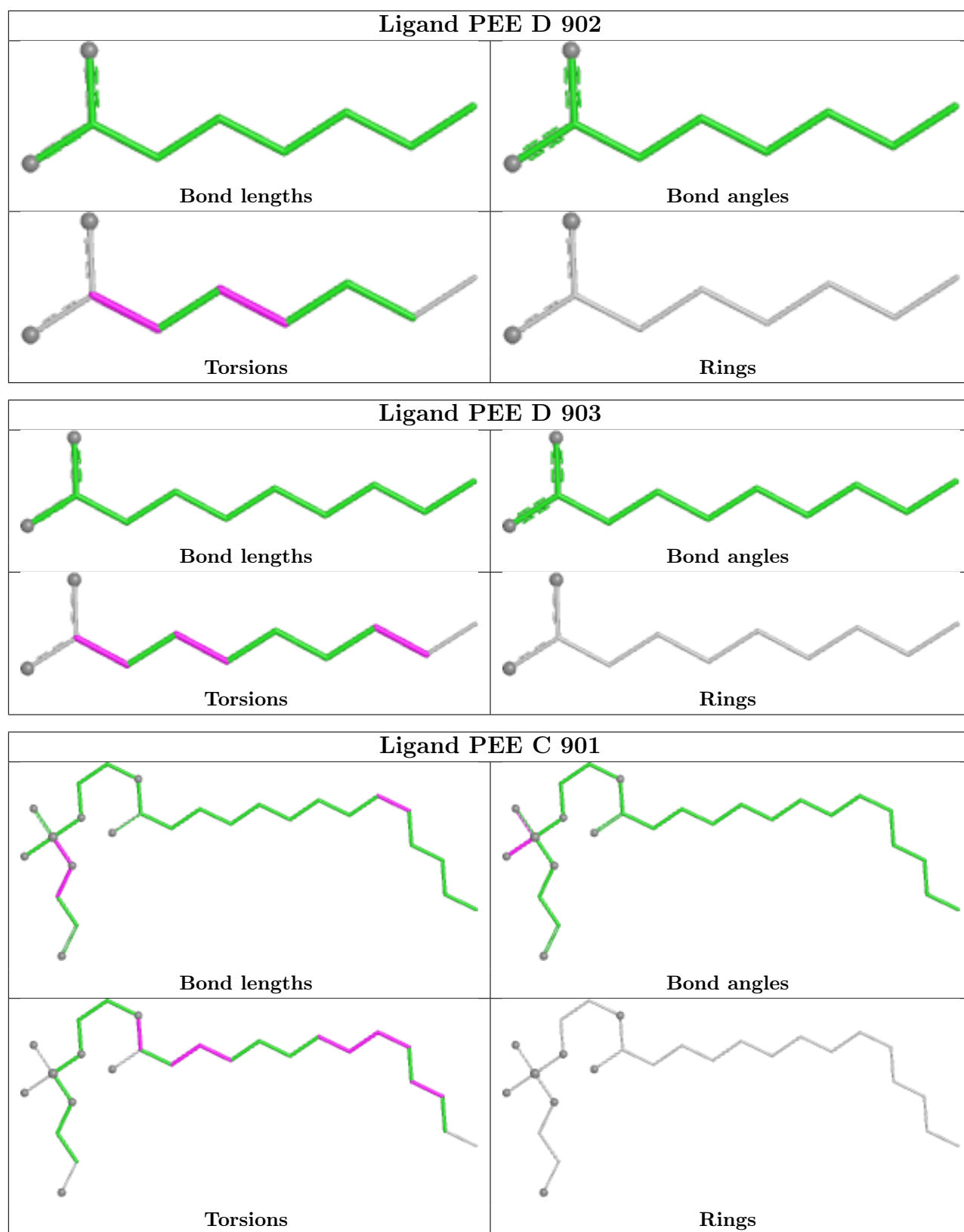
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

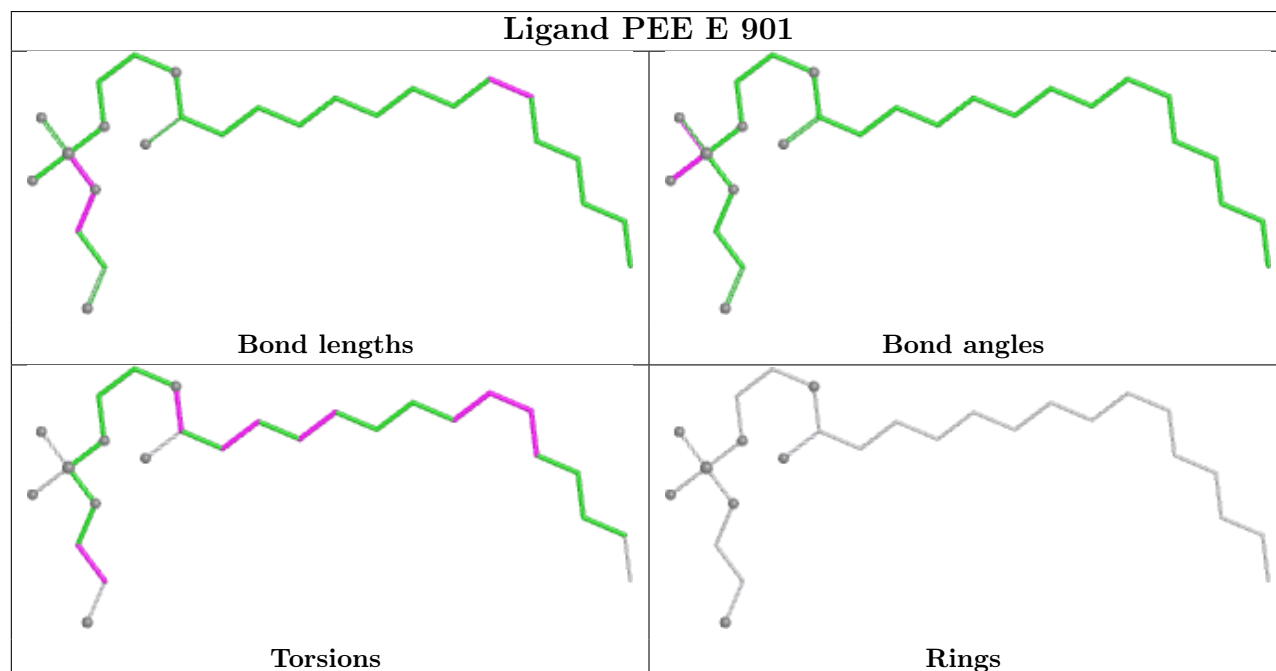
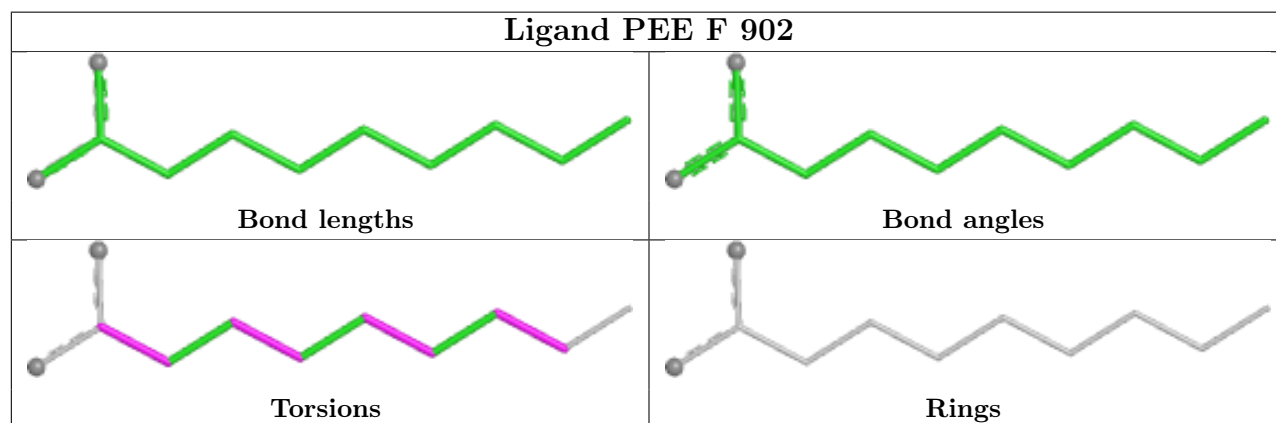
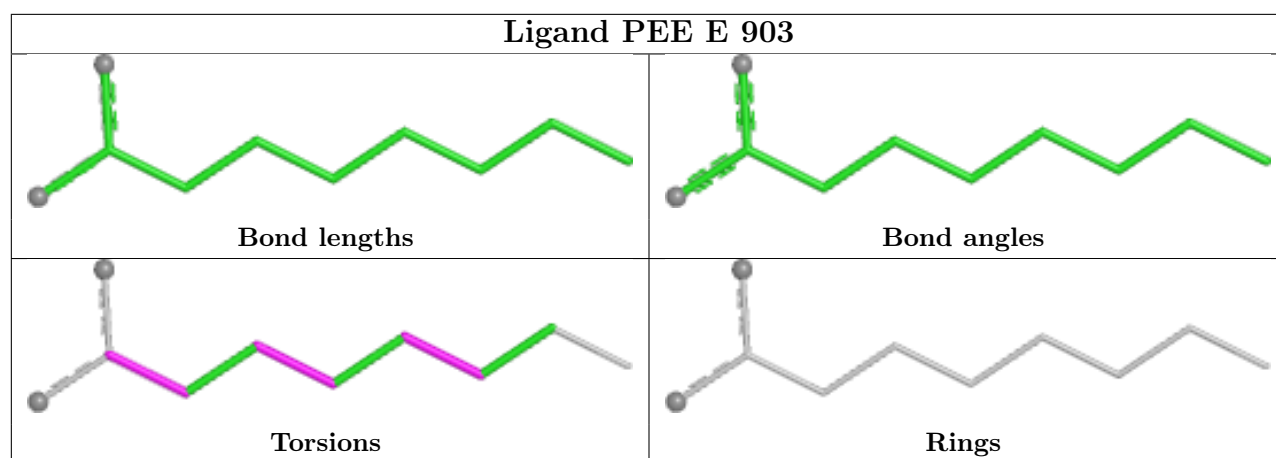
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

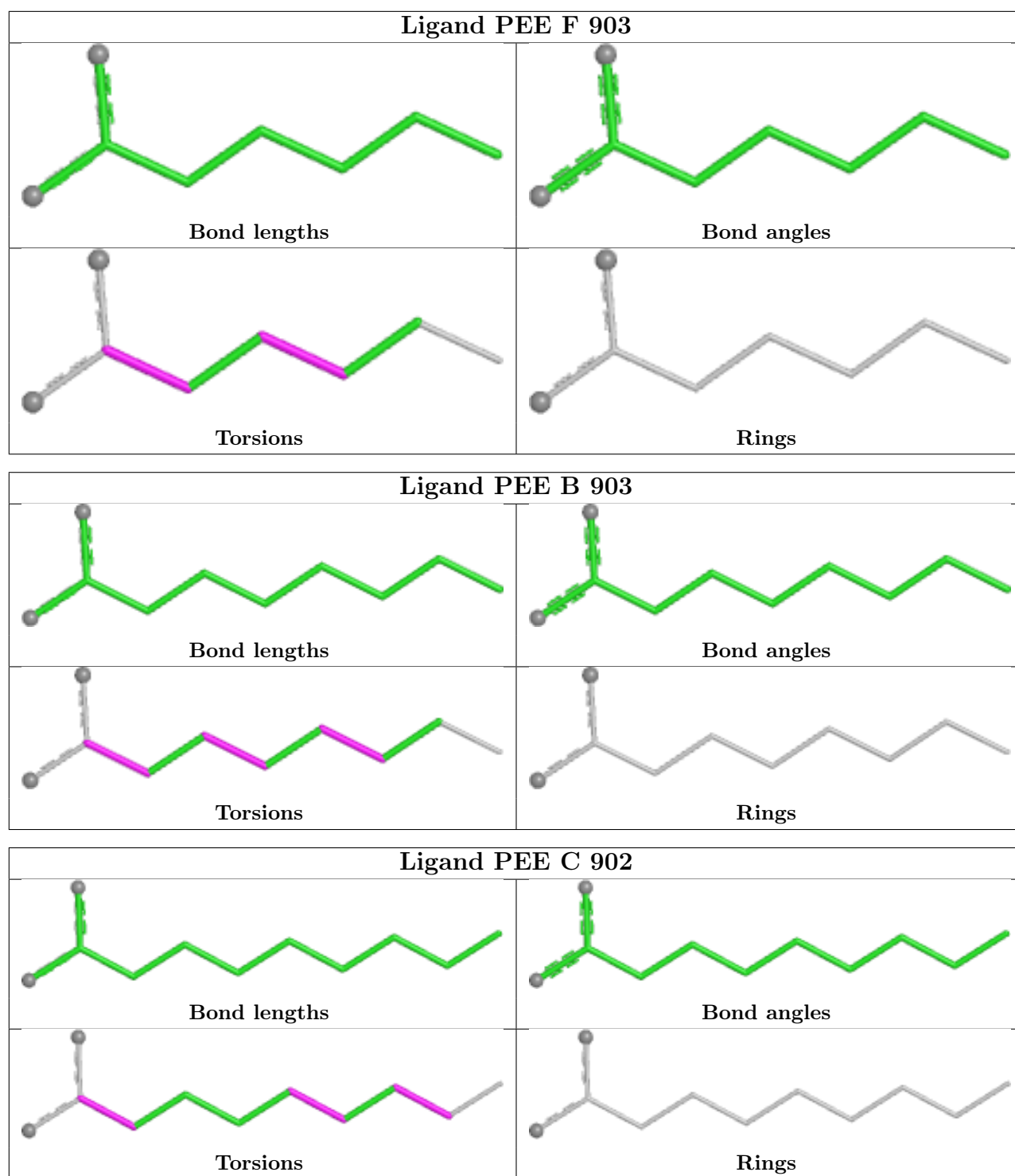












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

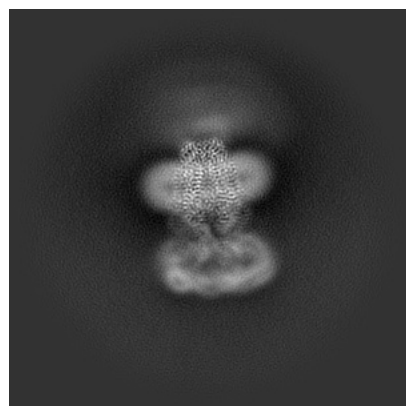
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28898. These allow visual inspection of the internal detail of the map and identification of artifacts.

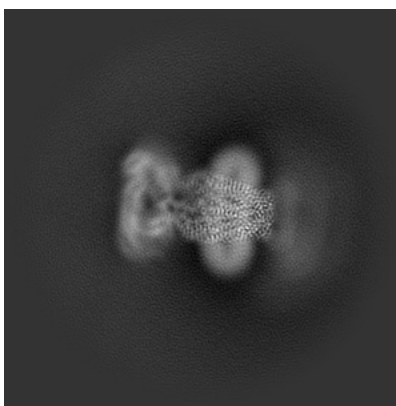
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

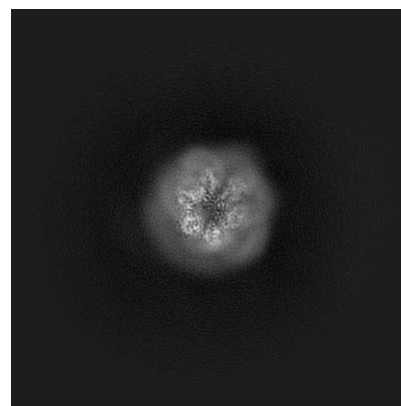
6.1.1 Primary map



X

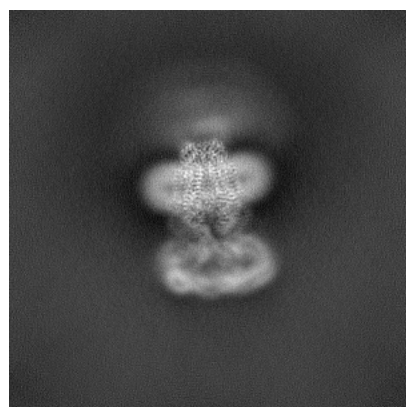


Y

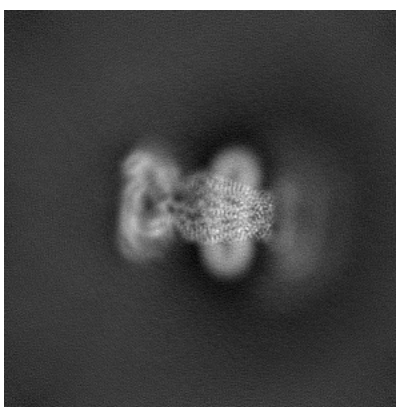


Z

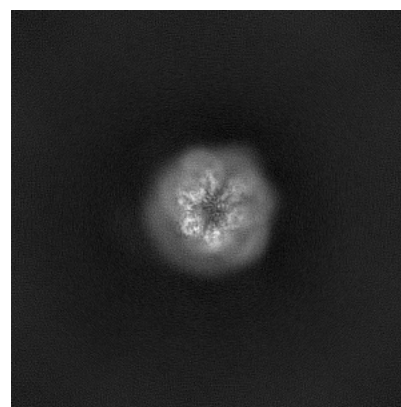
6.1.2 Raw map



X



Y

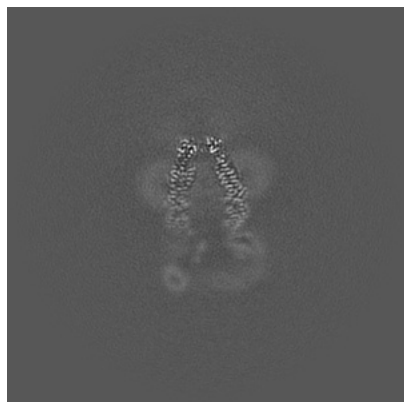


Z

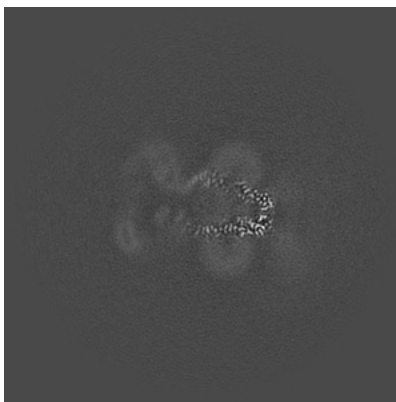
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

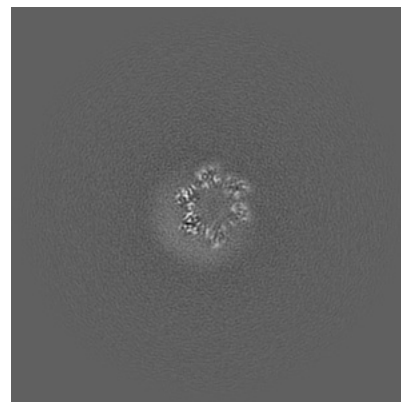
6.2.1 Primary map



X Index: 208

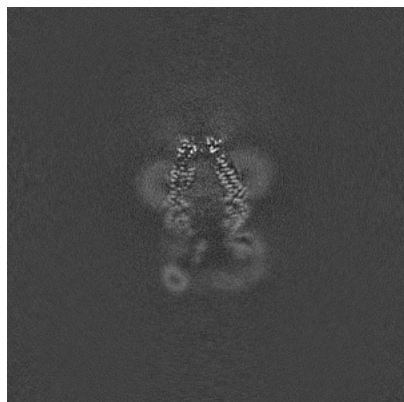


Y Index: 208

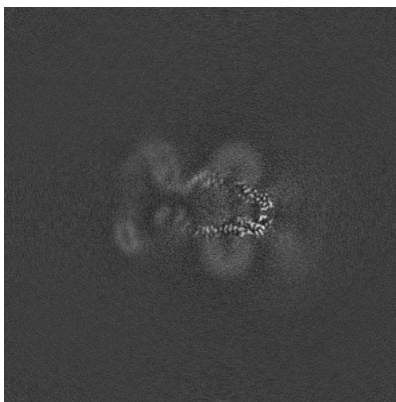


Z Index: 208

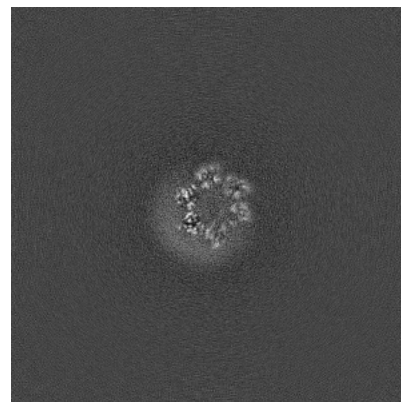
6.2.2 Raw map



X Index: 208



Y Index: 208

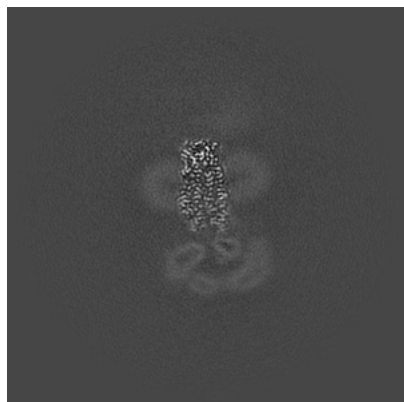


Z Index: 208

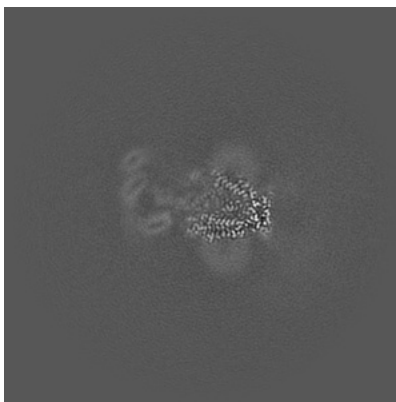
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

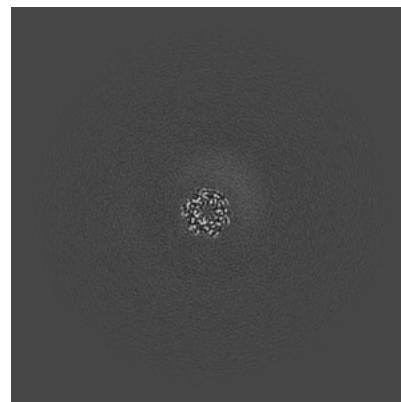
6.3.1 Primary map



X Index: 187

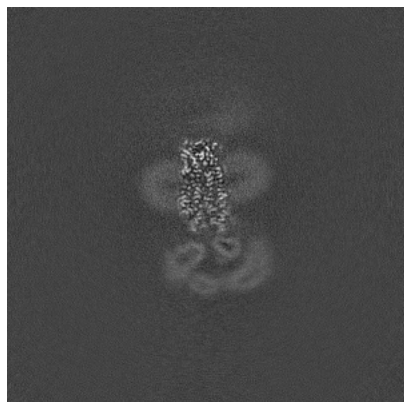


Y Index: 188

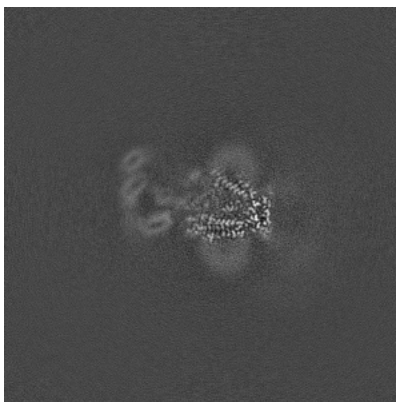


Z Index: 265

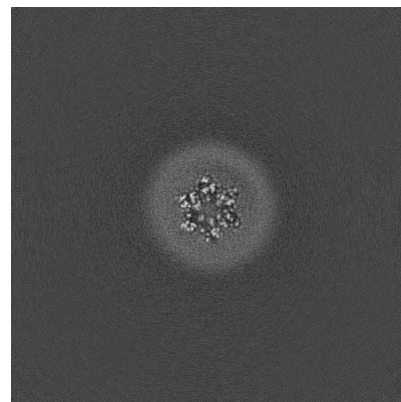
6.3.2 Raw map



X Index: 187



Y Index: 188

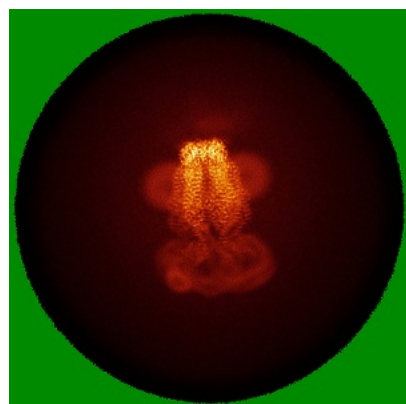


Z Index: 247

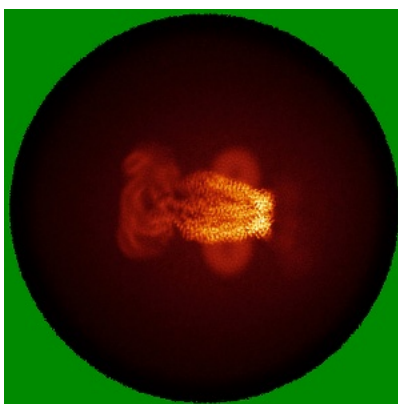
The images above show the largest variance slices of the map in three orthogonal directions.

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

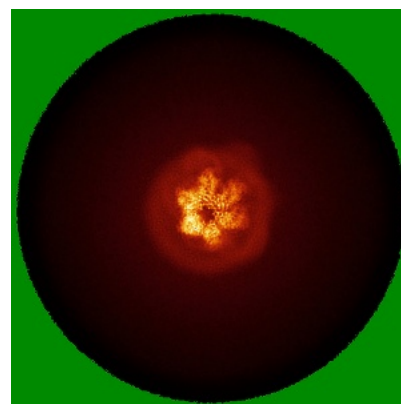
6.4.1 Primary map



X

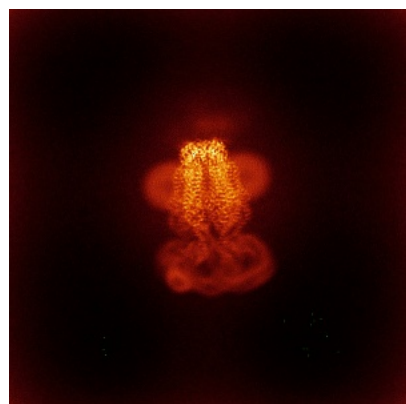


Y

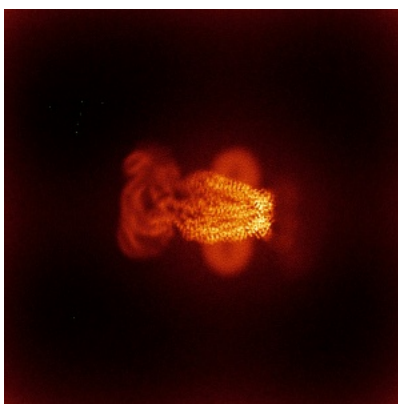


Z

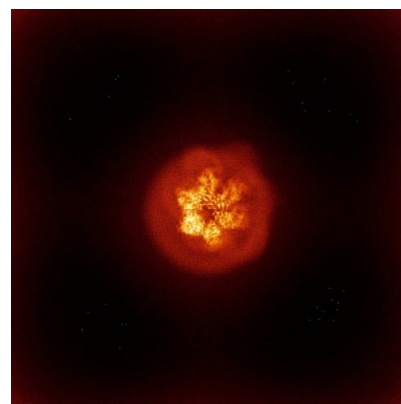
6.4.2 Raw map



X



Y

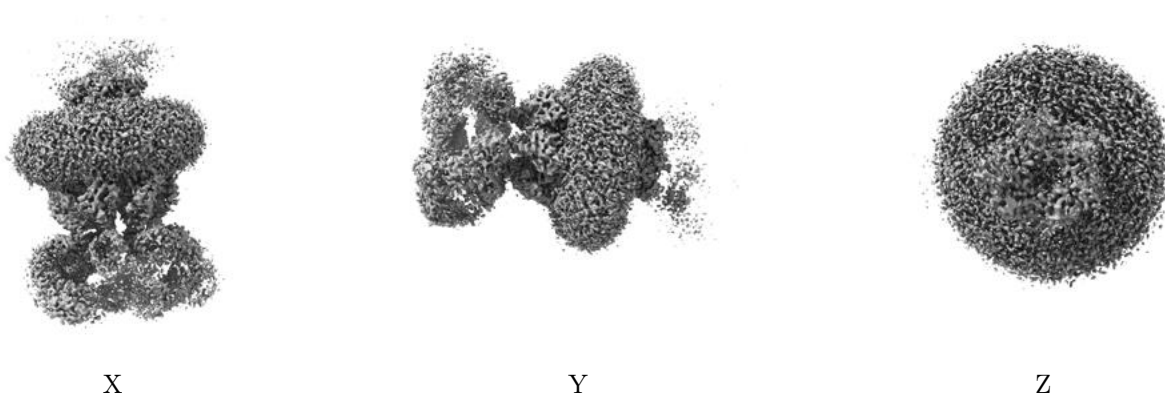


Z

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.

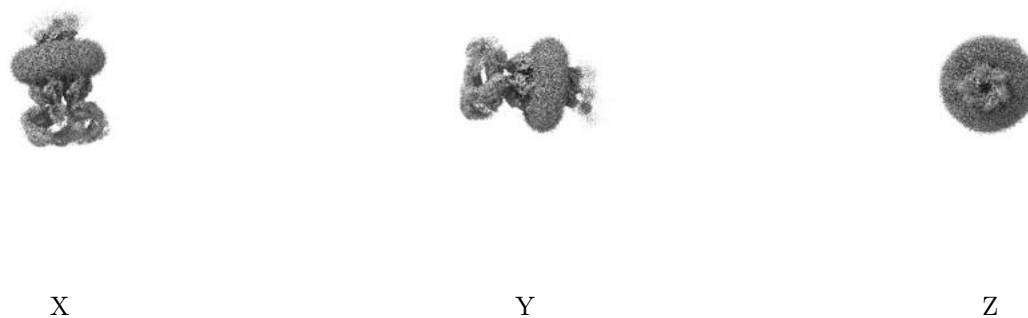
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

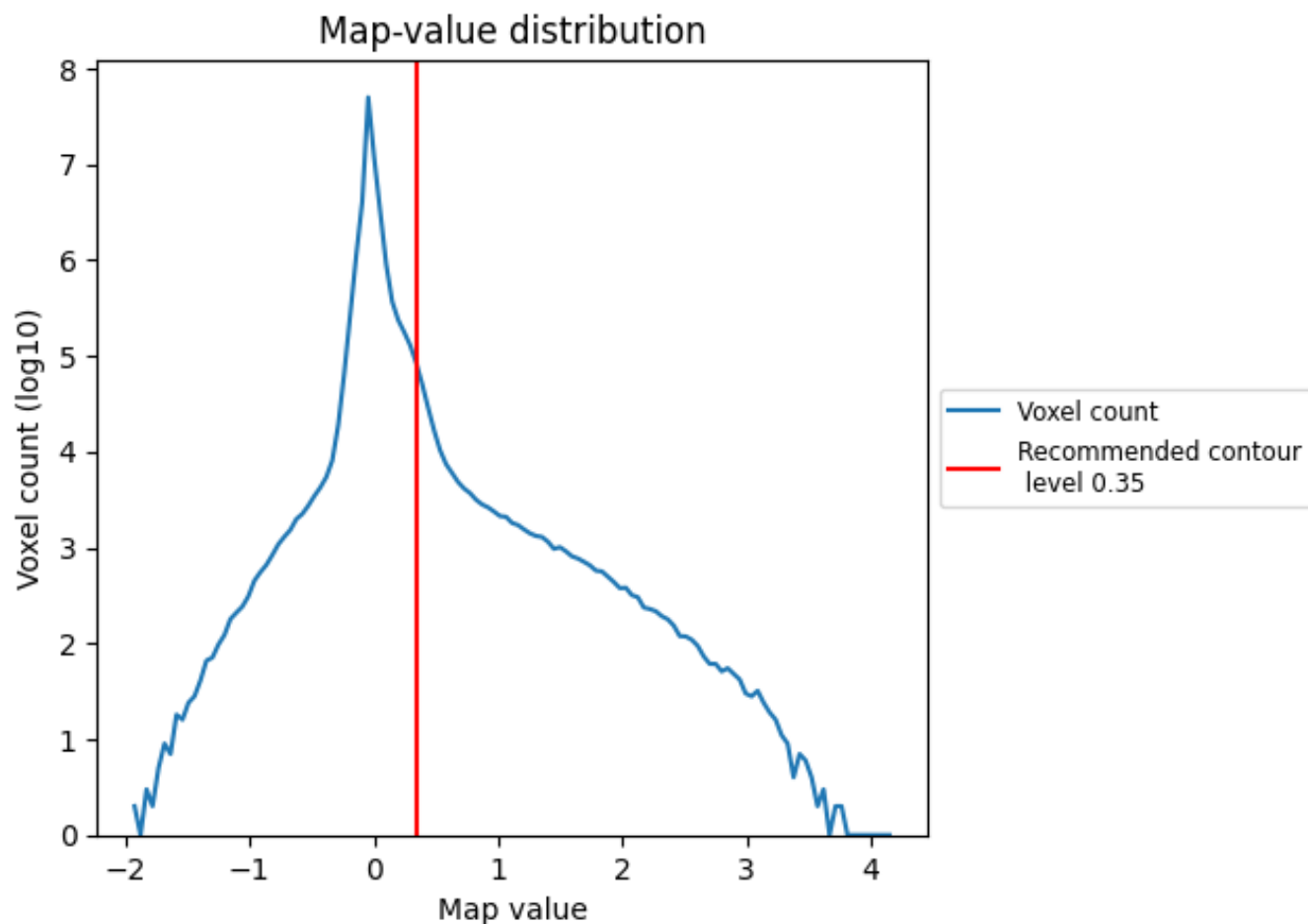
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

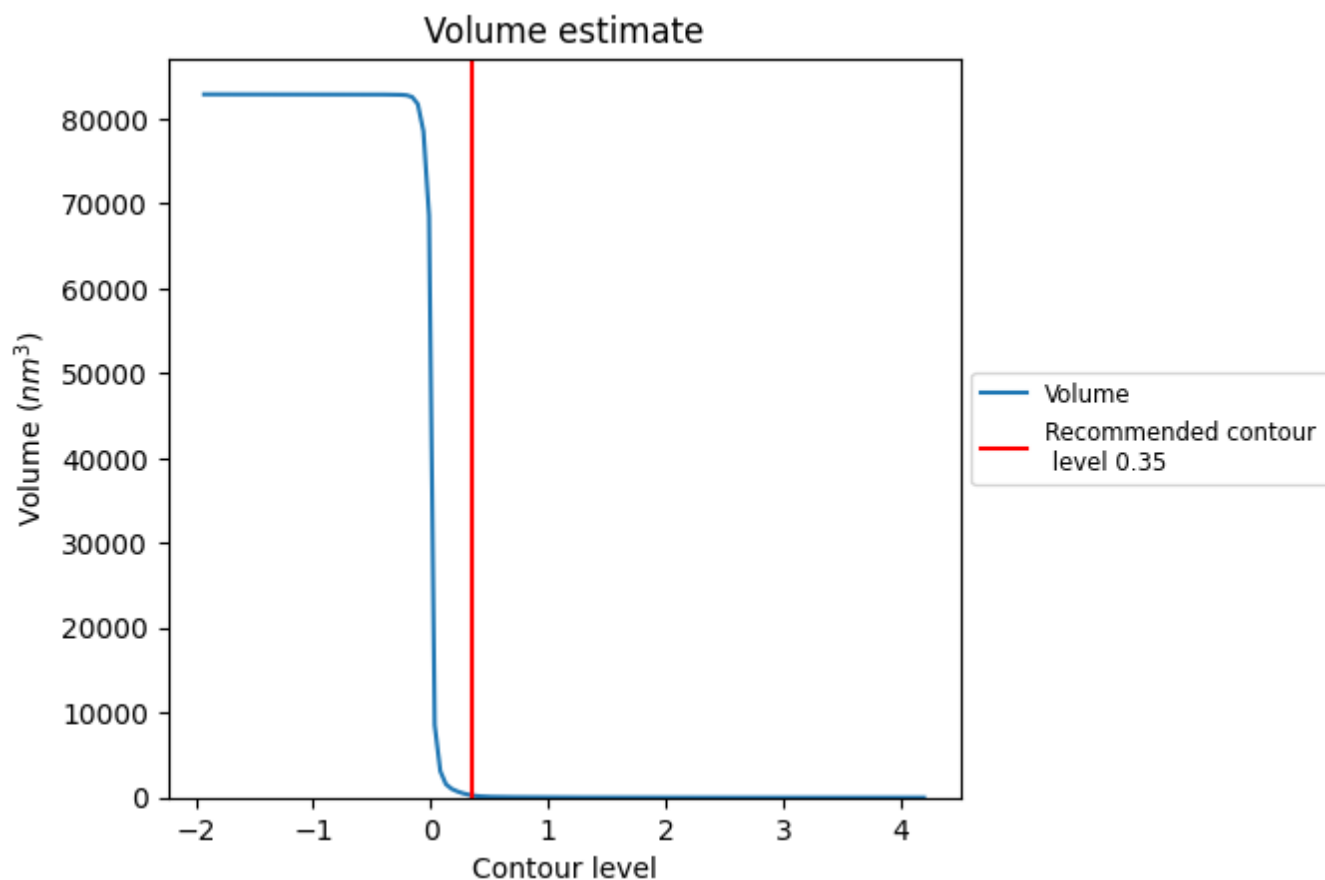
This section contains the results of statistical analysis of the map.

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.

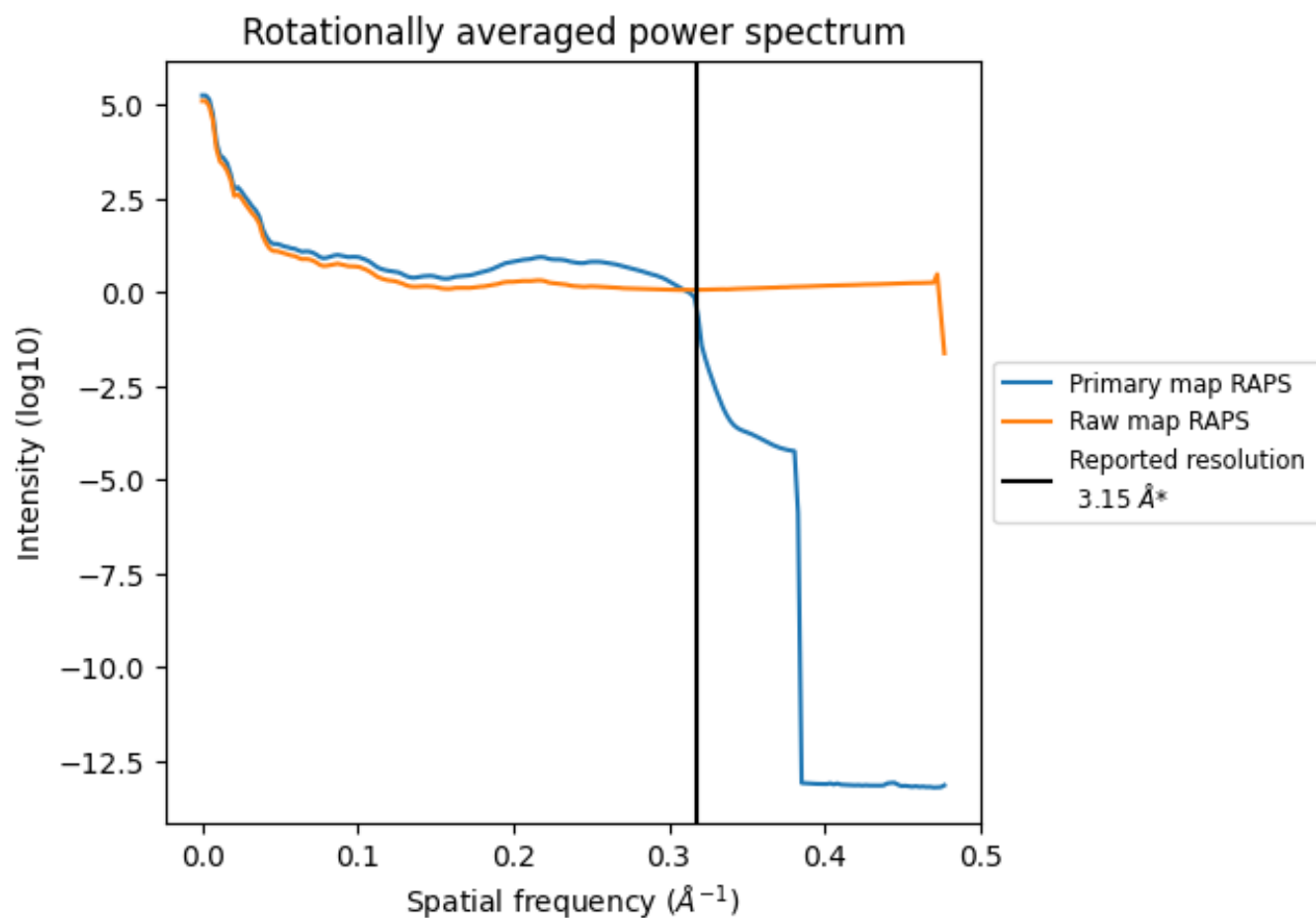
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm^3 ; this corresponds to an approximate mass of 247 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 ⓘ

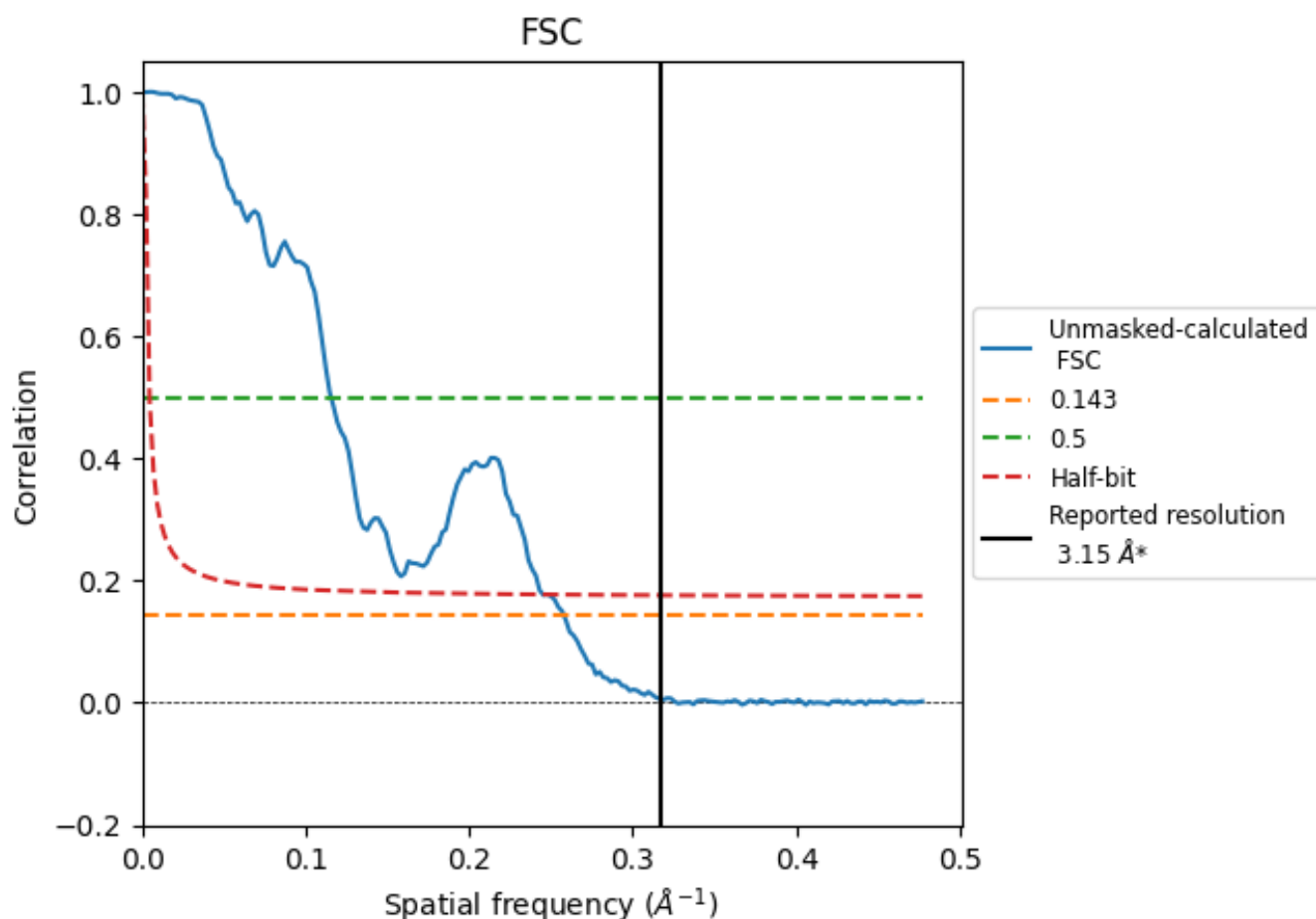


*Reported resolution corresponds to spatial frequency of $0.317 \text{ \AA}^{-1}$

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 0.317 Å⁻¹

8.2 Resolution estimates [i](#)

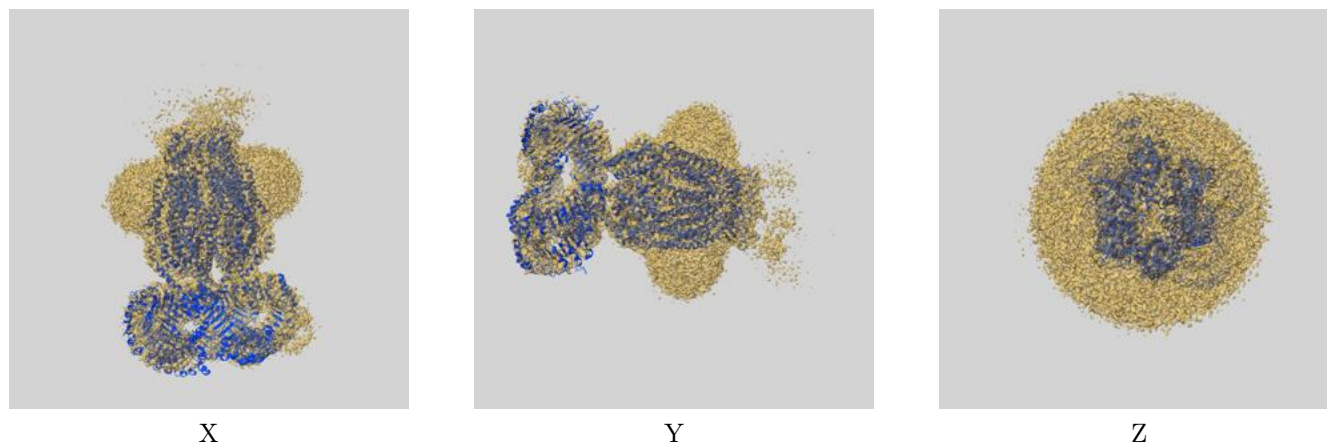
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	8.66	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.15 by more than 10 %

9 Map-model fit [i](#)

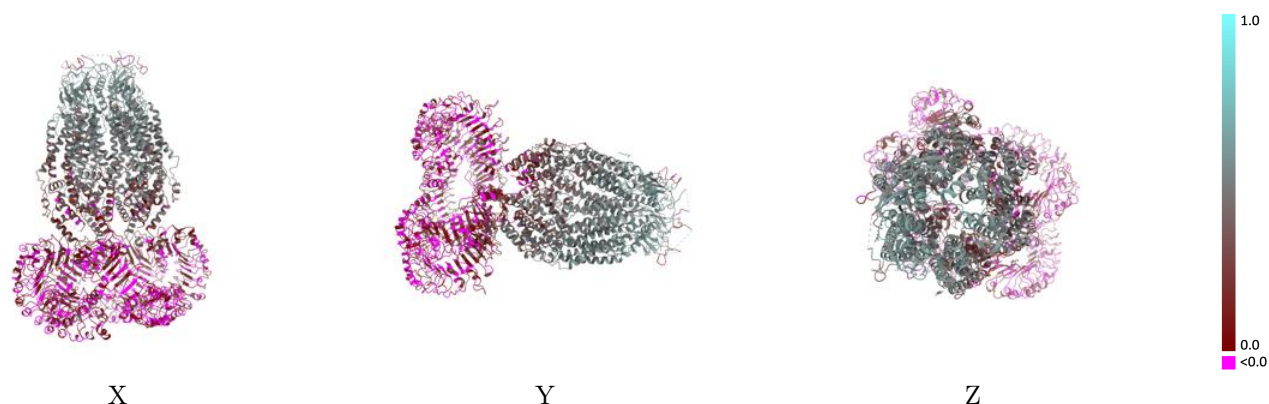
This section contains information regarding the fit between EMDB map EMD-28898 and PDB model 8F79. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



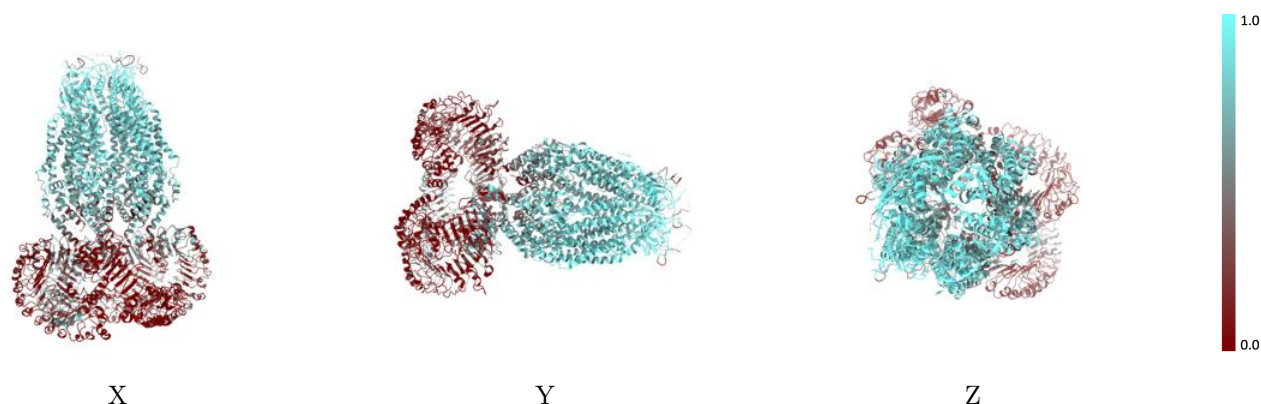
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



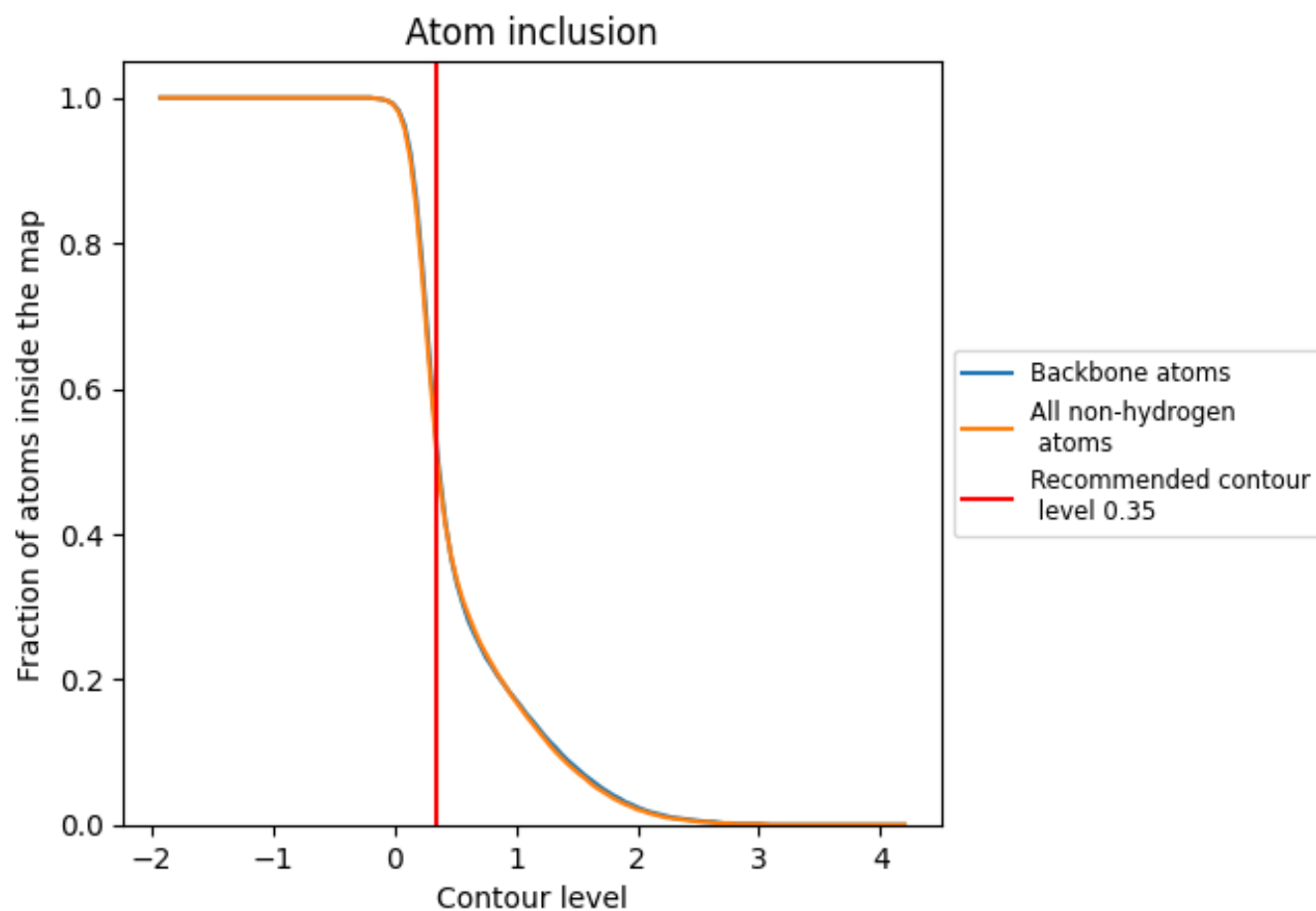
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 50% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5030	0.2600
A	0.6150	0.2830
B	0.5120	0.2710
C	0.4720	0.2430
D	0.7750	0.4420
E	0.3850	0.2070
F	0.4370	0.2110

1.0

0.0

<0.0