



# wwPDB EM Validation Summary Report

Jun 24, 2023 – 02:43 PM EDT

PDB ID : 8F79  
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)

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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>.

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

EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

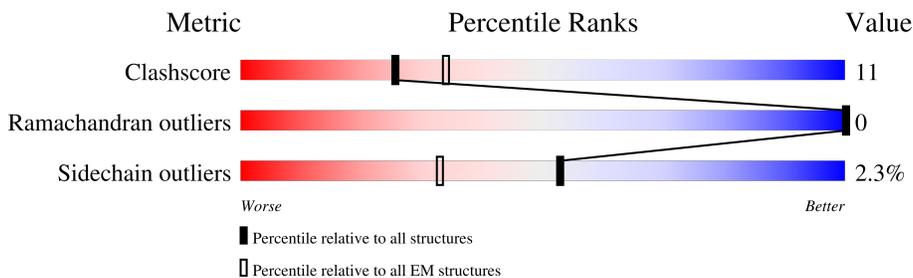
# 1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	
1	E	911	
2	F	813	

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

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

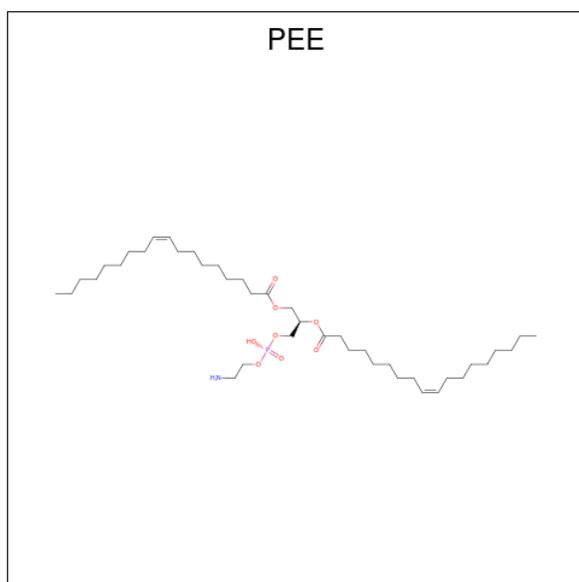
- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

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

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 (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

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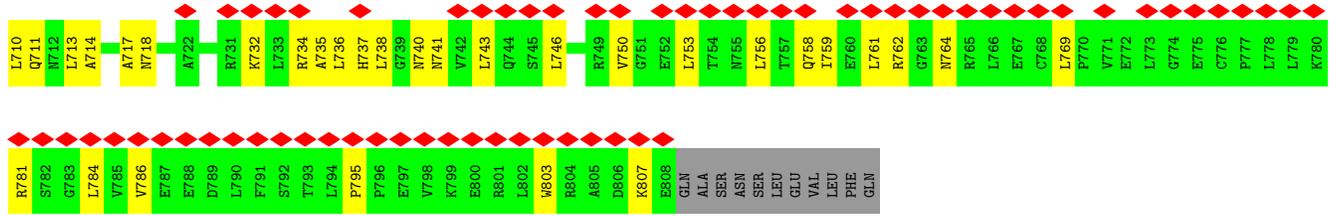
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Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	F	1	Total	C	O			0
			11	9	2			
3	F	1	Total	C	O			0
			8	6	2			

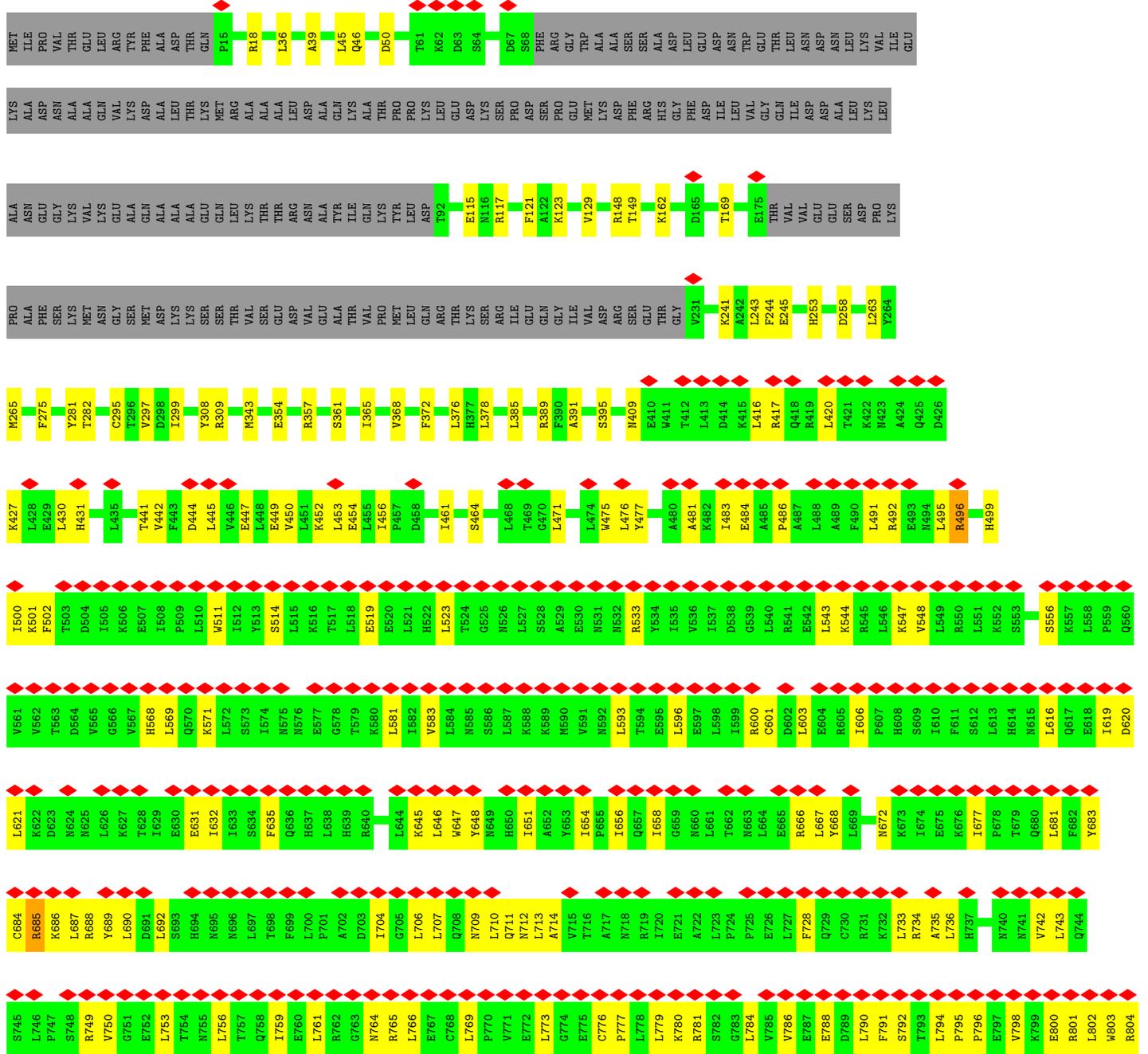
- Molecule 4 is water.

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	



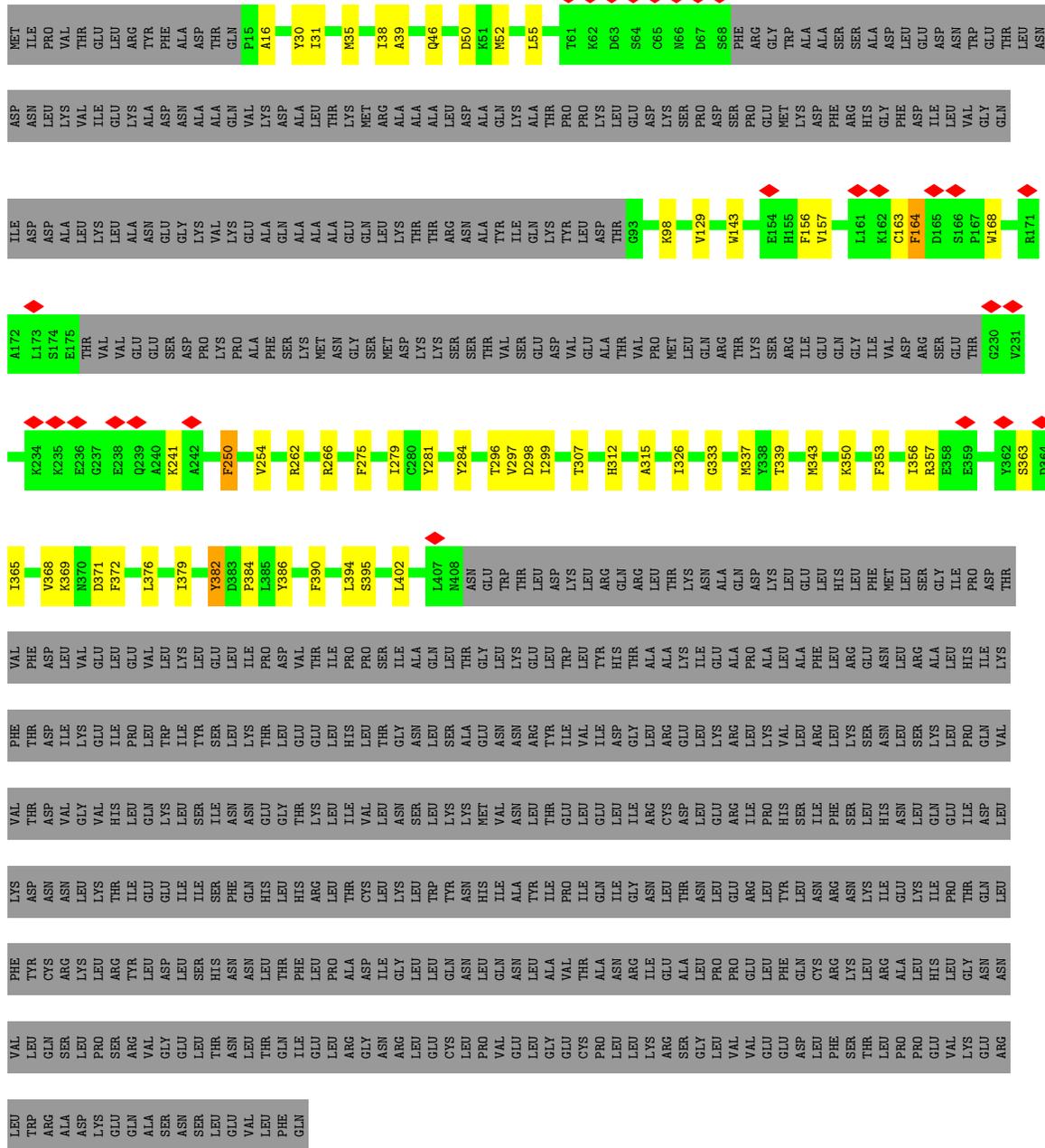


• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562





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



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





P769	F769	Q709	I649	T589	I529	L469	W409	L258	ARG
E770	E770	Y710	A650	N690	S630	Q470	T410	F273	LYS
L771	L771	F711	Y651	L591	K531	E471	P411	L274	ASN
G772	G772	S712	I652	T592	N532	L472	K412	I275	MET
D773	D773	I713	P653	E593	V533	C473	K413	I276	ASN
C774	C774	T714	E654	L594	T534	L474	K414	Y279	ARG
R775	R775	C715	H655	E595	L535	H475	R415	N280	ARG
A776	A776	N716	I656	L596	E536	Q476	Q416	Y284	GLY
L777	L777	K717	K657	V597	S537	C477	K417	V284	THR
K778	K778	V718	K658	H598	L538	S478	L418	I297	GLN
R779	R779	E719	L659	H598	R539	K480	Q419	Q298	GLY
A780	A780	S720	T660	C599	D540	I481	T420	D299	PRO
G781	G781	D600	S661	L601	L541	H482	M421	C308	GLY
L782	L782	E602	L662	E602	K542	S483	A422	N309	ASN
V783	V783	R603	E663	R603	S543	A484	H423	H310	LEU
W784	W784	I604	R664	I604	L544	A485	M424	H310	VAL
E785	E785	P605	L665	P605	L544	L486	R425	A313	ARG
D786	D786	H606	F666	H606	I546	S487	L426	L426	SER
A787	A787	A607	F667	A607	L547	F488	L428	Y343	GLN
L788	L788	V608	S668	V608	S548	L489	P429	Y353	LEU
F789	F789	H609	H669	H609	I549	K490	L430	Q356	SER
E790	E790	S610	M670	S610	K550	E491	L431	E357	LYS
T791	T791	L611	V672	L611	S551	M492	I431	T358	PRO
L792	L792	L612	E673	L612	N552	L493	M432	G359	GLU
P793	P793	S613	V674	S613	V553	K494	L433	D362	LYS
S794	S794	L614	L675	L614	S554	V495	S434	I363	PHE
D795	D795	Q615	L676	Q615	S554	L496	Q435	D362	VAL
W796	W796	E616	P676	E616	K555	S497	L436	I363	VAL
R797	R797	L617	S677	L617	I556	V498	P437	V366	ASP
Q798	Q798	H678	H678	H678	P557	K499	D438	K367	LYS
N800	N800	D618	L679	D618	Q558	F500	T439	N368	ALA
R801	R801	L619	F680	L619	A559	D501	V440	D369	ALA
A802	A802	K620	L681	K620	V560	D502	F441	F370	GLY
D803	D803	E621	C682	E621	V561	M503	T444	M373	ALA
SER	SER	N622	N683	N622	D562	R504	E445	L374	LEU
ASN	ASN	G623	K684	G623	V563	E505	L446	I377	LEU
GLU	GLU	L624	I685	L624	S564	L506	Q447	E234	LEU
ASN	ASN	K625	R686	K625	S564	P507	S448	E236	ASP
TYR	TYR	S626	R687	S626	H566	P508	L449	G236	ASP
LEU	LEU	I627	Y688	I627	L567	W509	K450	K233	ASP
TYR	TYR	E628	D689	E628	Q568	M510	L451	K233	ASP
PHE	PHE	G629	L690	G629	K569	Y511	E452	E240	ASP
GLN	GLN	I630	S691	I630	M570	G512	I453	L241	ASP
GLY	GLY	V631	Y692	V631	C571	L513	I454	F242	ASP
		S632	N693	S632	V572	R514	K455	K244	ASP
		D694	D694	D694	H573	N515	M456	L250	ASP
		I695	R696	I695	N574	L516	V457	D256	ASP
		Y756	F697	Y756	D575	E517	M458	L405	ASP
		D758	F697	D758	E518	E518	I459	L405	ASP
		I759	I698	I759	L519	L519	P460	M406	ASP
		P699	P699	P699	Y520	Y520	T462	M407	ASP
		P700	P700	P700	K578	L521	I463	E408	ASP
		E701	E701	E701	L579	V522	A464		
		I702	I702	I702	V580	G523	Q465		
		G703	G703	G703	M581	S524	L466		
		V704	V704	V704	L582	L525	D467		
		E765	E765	E765	N583	S526	M468		
		V766	V766	V766	N584	H527			
		L767	L767	L767	L585	D528			
		P768	P768	P768	K586				
					K587				
					M588				

## 4 Experimental information i

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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.29	0/6049	0.56	0/8198
1	B	0.28	0/6045	0.57	0/8193
1	C	0.27	0/6031	0.54	0/8173
1	D	0.27	0/2723	0.48	0/3686
1	E	0.28	0/6038	0.54	0/8183
2	F	0.28	0/5877	0.55	0/7943
All	All	0.28	0/32763	0.55	0/44376

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5916	0	6071	143	0
1	B	5912	0	6068	146	0
1	C	5898	0	6052	122	0
1	D	2648	0	2638	40	0
1	E	5905	0	6061	133	0
2	F	5751	0	5887	189	0
3	A	49	0	63	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	47	0	59	1	0
3	C	37	0	47	1	0
3	D	58	0	74	2	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	747	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 11.

The worst 5 of 747 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	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	665/830 (80%)	650 (98%)	15 (2%)	50	76
1	B	665/830 (80%)	651 (98%)	14 (2%)	53	78
1	C	663/830 (80%)	653 (98%)	10 (2%)	65	84
1	D	293/830 (35%)	283 (97%)	10 (3%)	37	68
1	E	664/830 (80%)	652 (98%)	12 (2%)	59	81
2	F	659/756 (87%)	637 (97%)	22 (3%)	38	69
All	All	3609/4906 (74%)	3526 (98%)	83 (2%)	53	76

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	433	PHE
2	F	343	TYR
1	E	647	TRP
2	F	146	PHE
2	F	509	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	522	HIS
2	F	112	ASN
2	F	113	GLN
1	A	758	GLN
1	A	592	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 monosaccharides 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	903	-	9,9,50	0.62	0	9,9,55	0.80	0
3	PEE	B	901	-	25,25,50	1.49	2 (8%)	27,28,55	1.14	1 (3%)
3	PEE	C	901	-	25,25,50	1.47	3 (12%)	27,28,55	1.13	1 (3%)
3	PEE	B	902	-	10,10,50	1.61	2 (20%)	10,10,55	1.55	2 (20%)
3	PEE	A	903	-	12,12,50	1.08	1 (8%)	12,12,55	1.11	1 (8%)
3	PEE	E	901	-	26,26,50	1.45	2 (7%)	28,29,55	1.11	1 (3%)
3	PEE	A	902	-	12,12,50	1.09	1 (8%)	12,12,55	1.10	1 (8%)
3	PEE	F	901	-	39,39,50	1.39	3 (7%)	42,44,55	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEE	D	902	-	8,8,50	0.64	0	8,8,55	0.85	0
3	PEE	D	903	-	10,10,50	0.59	0	10,10,55	0.80	0
3	PEE	F	902	-	10,10,50	0.59	0	10,10,55	0.80	0
3	PEE	C	902	-	10,10,50	0.60	0	10,10,55	0.79	0
3	PEE	E	902	-	9,9,50	0.62	0	9,9,55	0.81	0
3	PEE	B	903	-	9,9,50	0.62	0	9,9,55	0.79	0
3	PEE	D	901	-	37,37,50	1.31	2 (5%)	40,42,55	0.99	1 (2%)
3	PEE	A	901	-	22,22,50	1.51	3 (13%)	24,25,55	1.26	2 (8%)
3	PEE	F	903	-	7,7,50	0.68	0	7,7,55	0.87	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	903	-	-	4/7/7/54	-
3	PEE	B	901	-	-	15/26/26/54	-
3	PEE	C	901	-	-	8/26/26/54	-
3	PEE	B	902	-	-	5/8/8/54	-
3	PEE	A	903	-	-	7/10/10/54	-
3	PEE	E	901	-	-	8/27/27/54	-
3	PEE	A	902	-	-	7/10/10/54	-
3	PEE	F	901	-	-	21/43/43/54	-
3	PEE	D	902	-	-	3/6/6/54	-
3	PEE	D	903	-	-	4/8/8/54	-
3	PEE	F	902	-	-	5/8/8/54	-
3	PEE	C	902	-	-	4/8/8/54	-
3	PEE	E	902	-	-	5/7/7/54	-
3	PEE	B	903	-	-	4/7/7/54	-
3	PEE	D	901	-	-	17/41/41/54	-
3	PEE	A	901	-	-	7/23/23/54	-
3	PEE	F	903	-	-	3/5/5/54	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	PEE	P-O4P	4.81	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	4.67	1.78	1.59
3	F	901	PEE	P-O4P	4.66	1.78	1.59
3	A	901	PEE	P-O4P	4.62	1.78	1.59
3	D	901	PEE	P-O4P	4.62	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	4.26	133.31	112.24
3	A	901	PEE	O2P-P-O1P	4.26	133.28	112.24
3	C	901	PEE	O2P-P-O1P	4.25	133.23	112.24
3	B	901	PEE	O2P-P-O1P	4.24	133.21	112.24
3	E	901	PEE	O2P-P-O1P	4.24	133.19	112.24

There are no chirality outliers.

5 of 127 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	C4-O4P-P-O3P

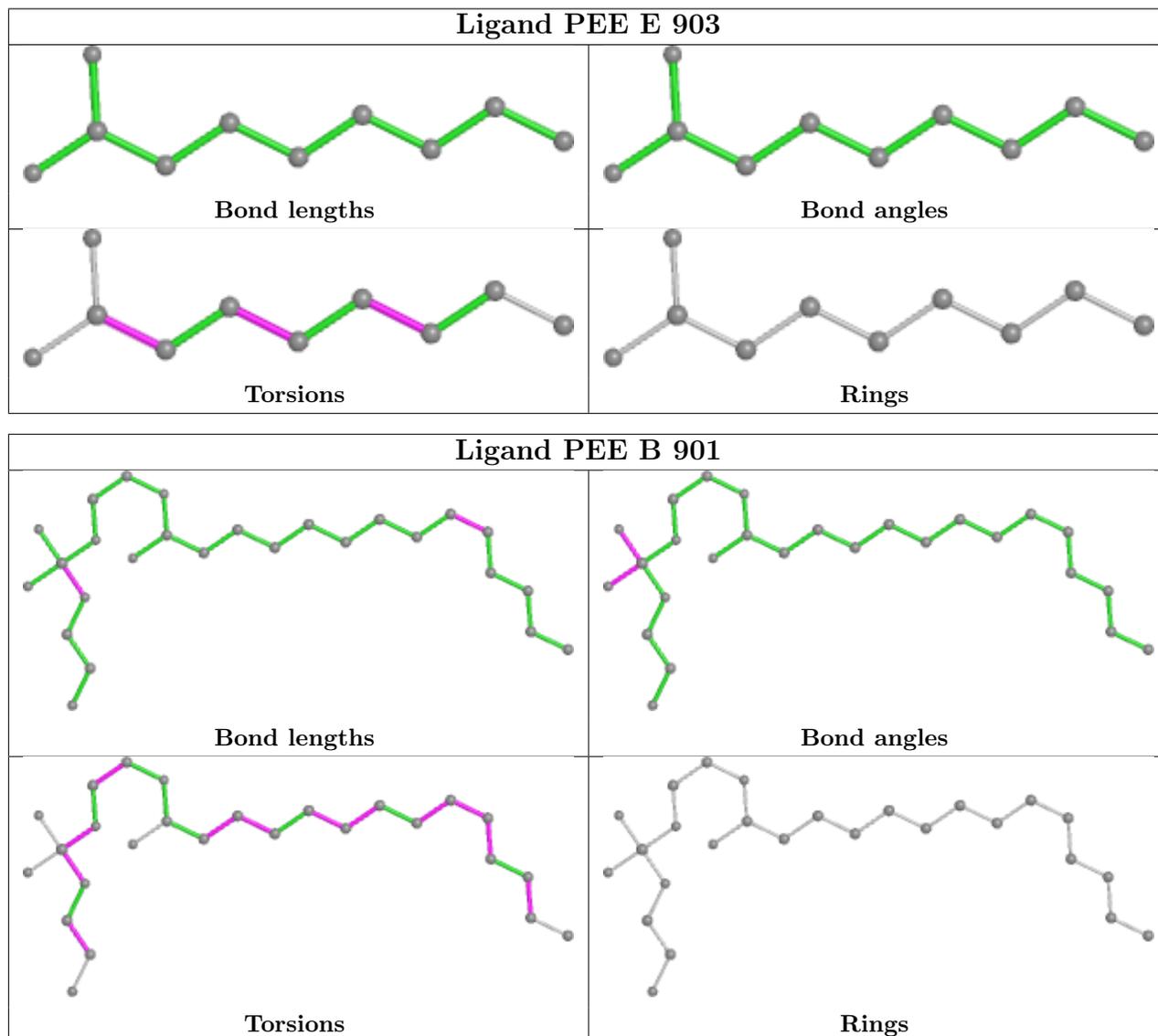
There are no ring outliers.

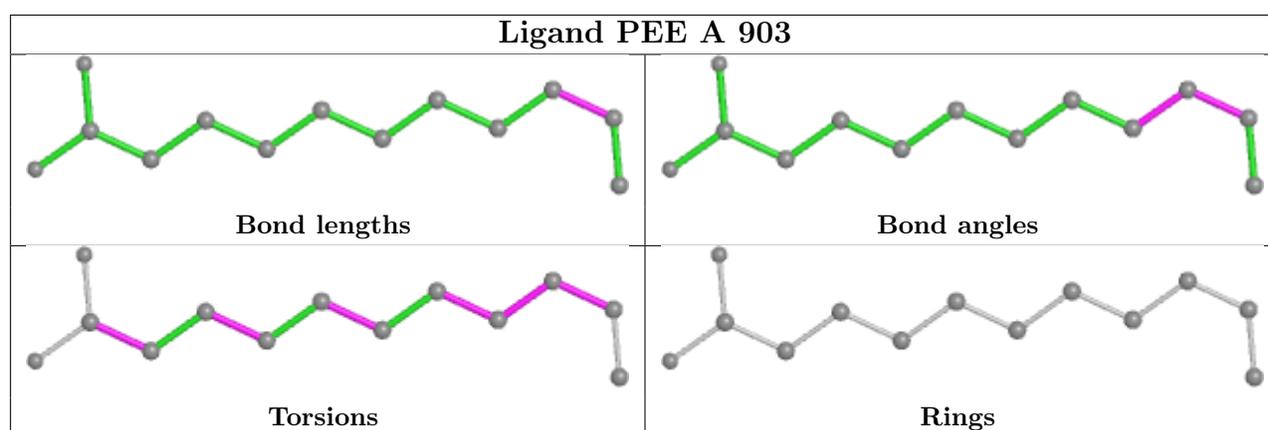
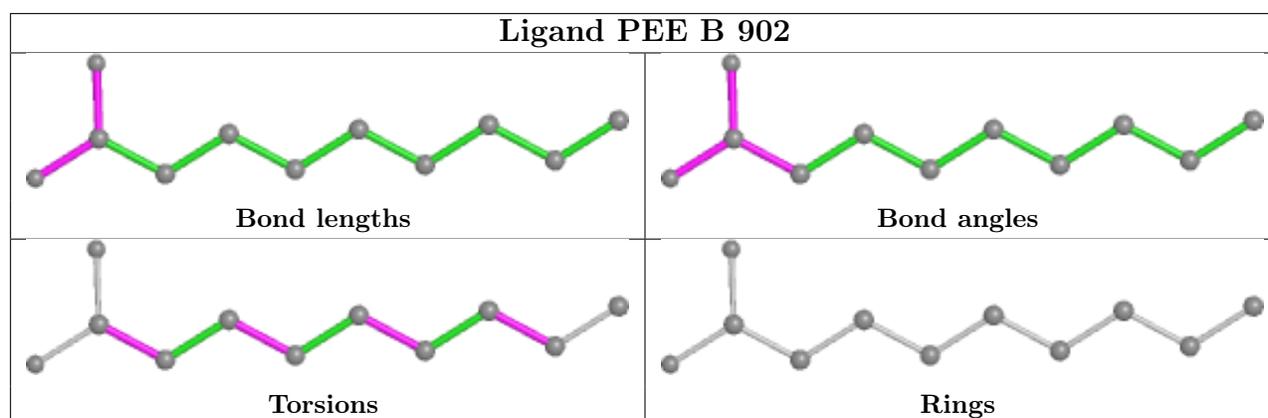
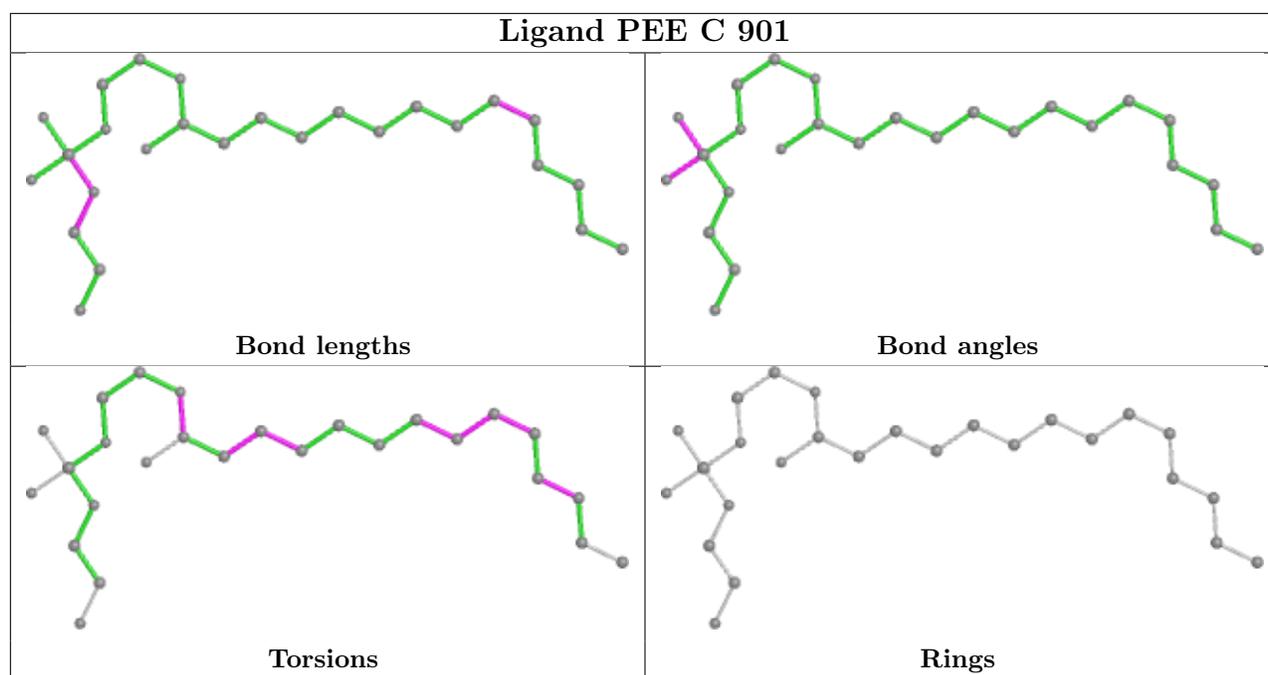
6 monomers are involved in 7 short contacts:

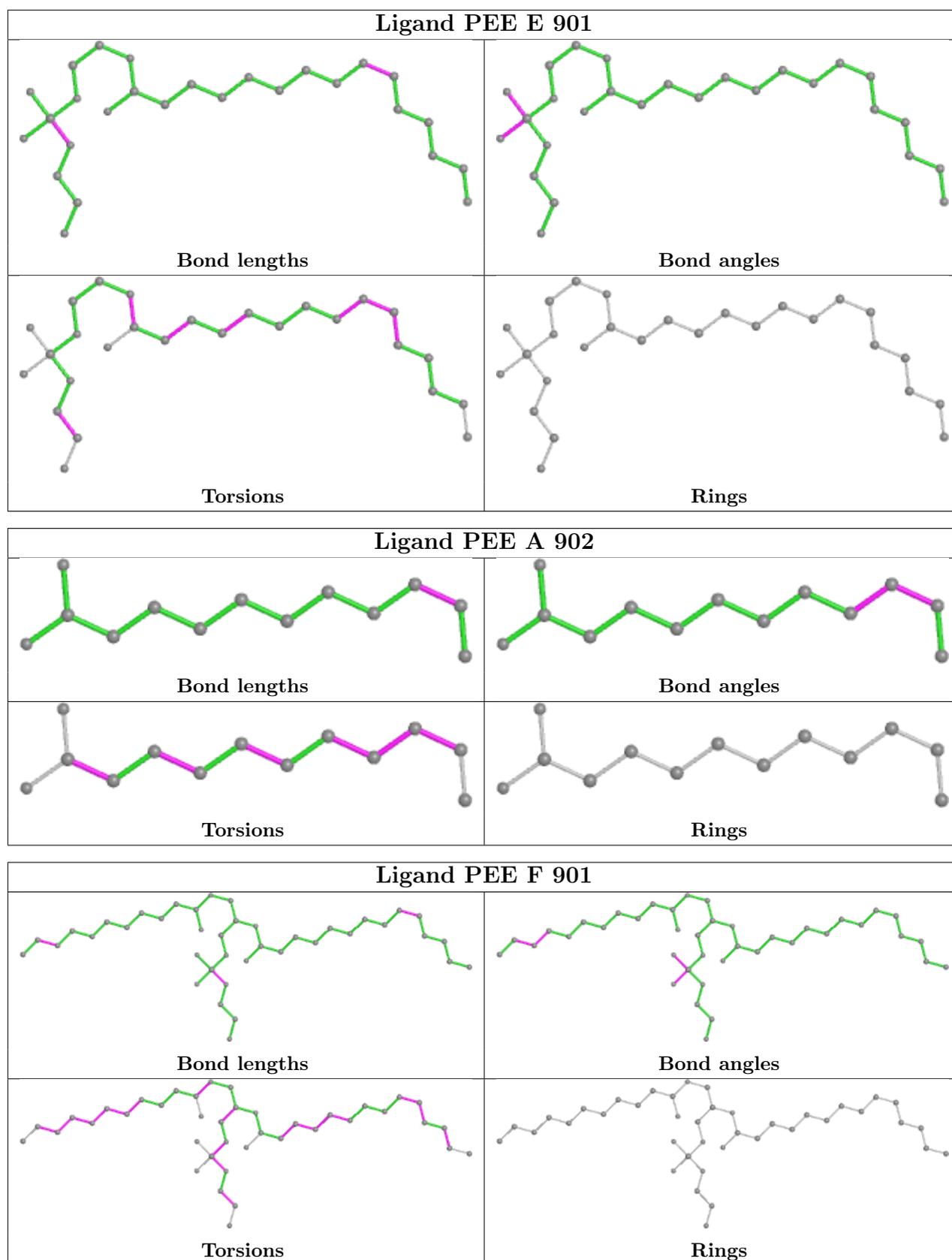
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	PEE	1	0
3	C	901	PEE	1	0
3	E	901	PEE	1	0
3	F	901	PEE	1	0
3	E	902	PEE	1	0
3	D	901	PEE	2	0

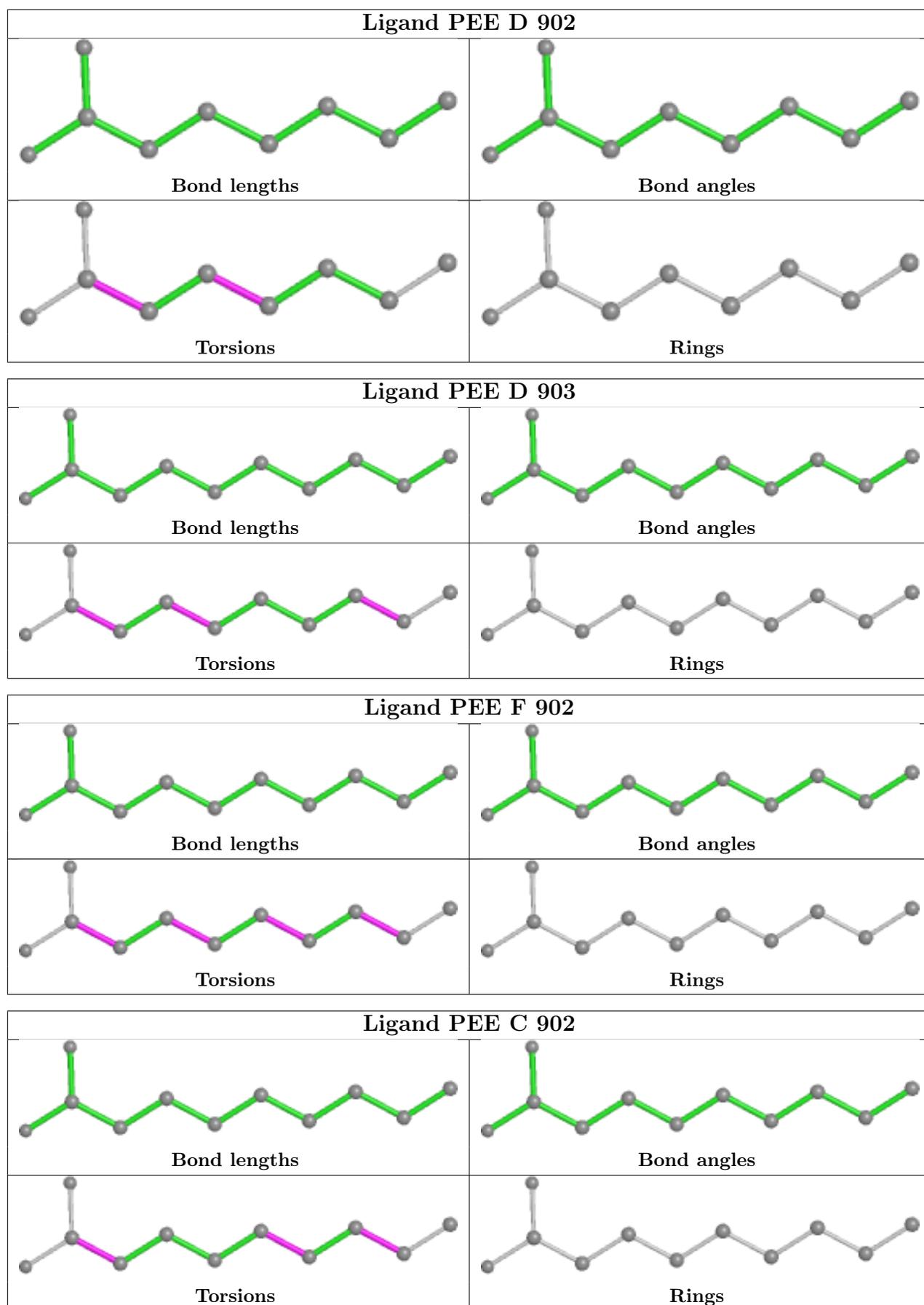
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

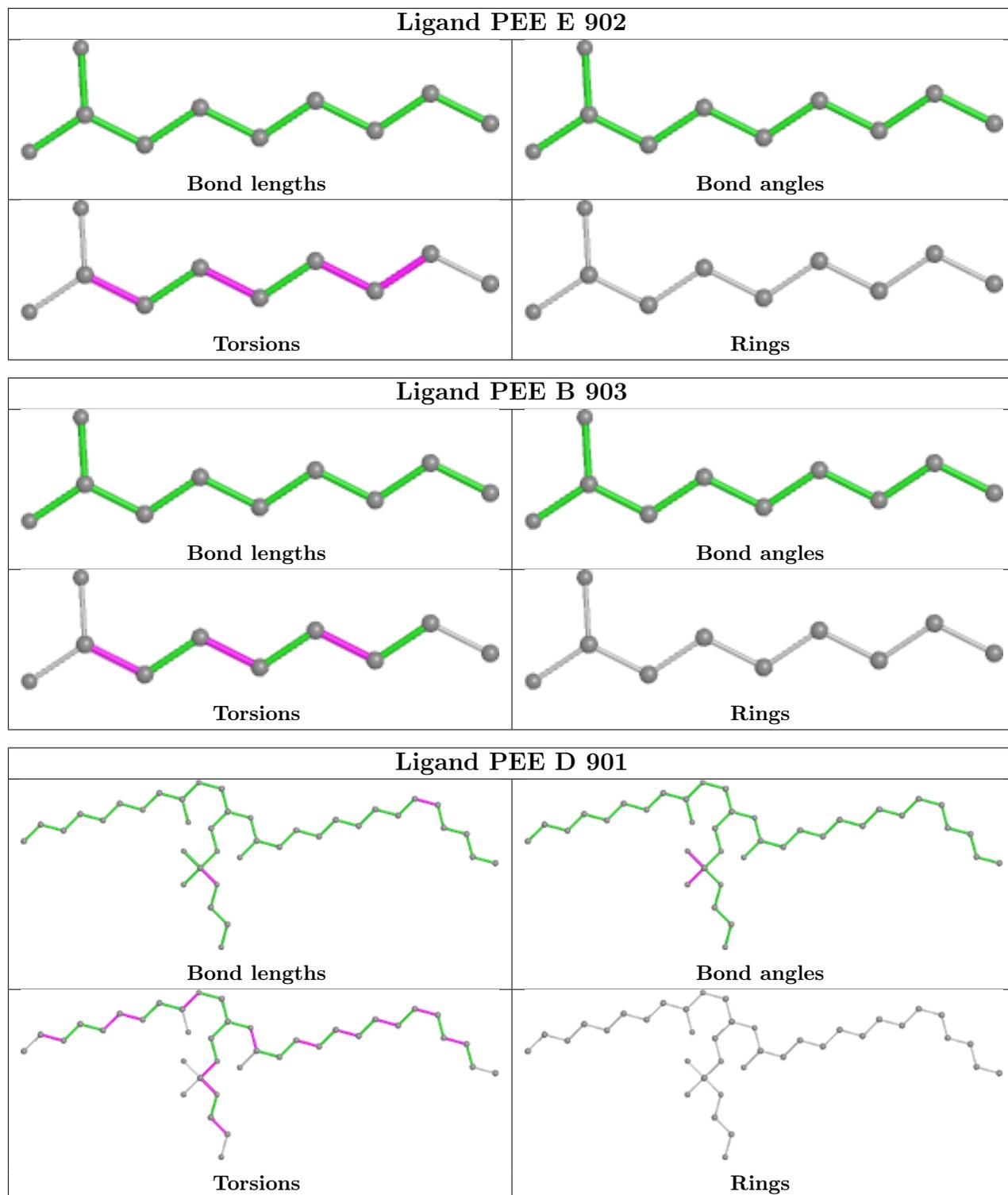
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

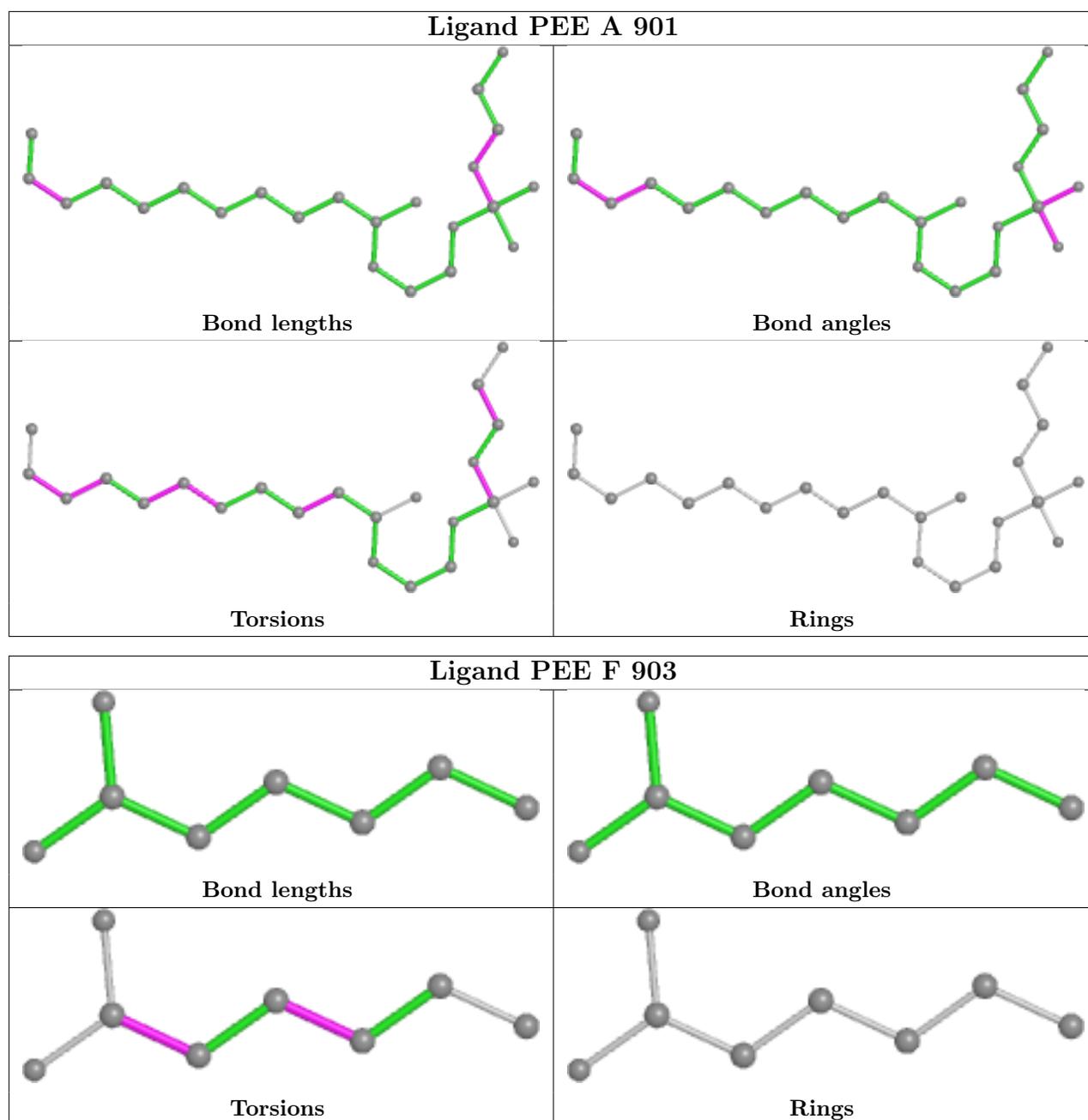












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

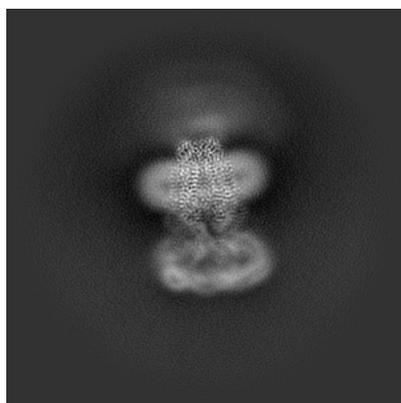
## 6 Map visualisation [i](#)

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

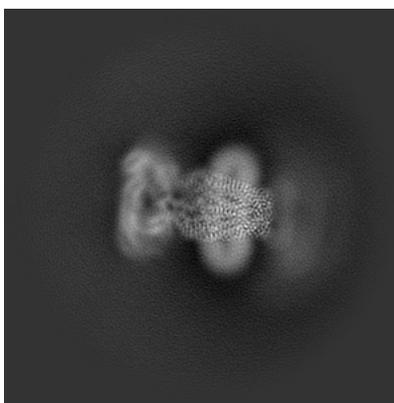
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

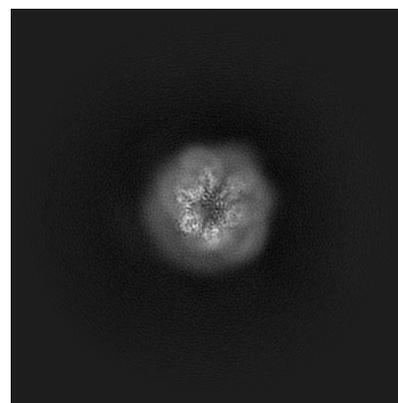
#### 6.1.1 Primary map



X

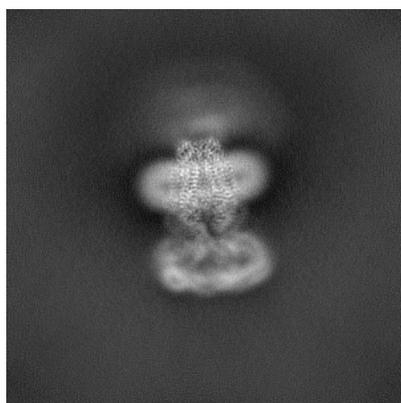


Y

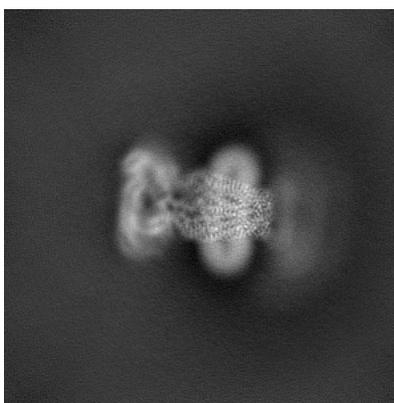


Z

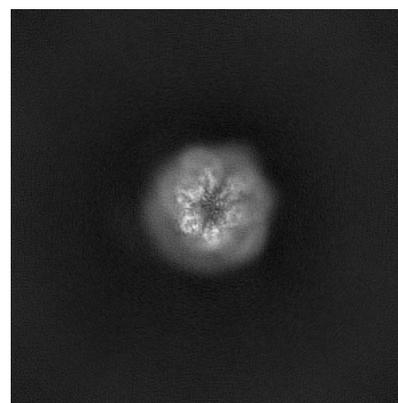
#### 6.1.2 Raw map



X



Y

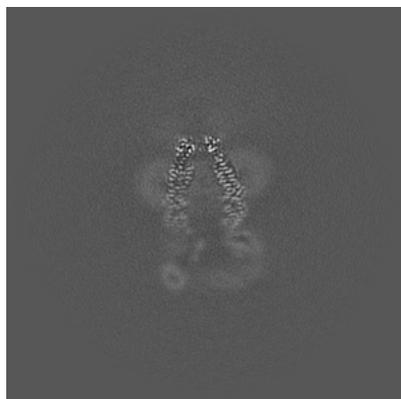


Z

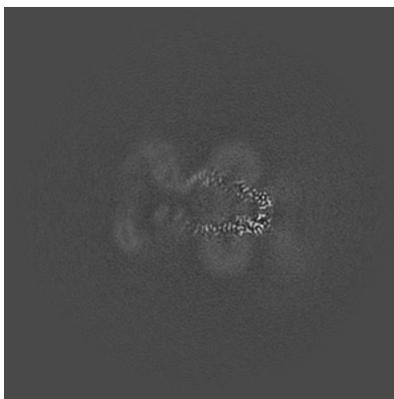
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

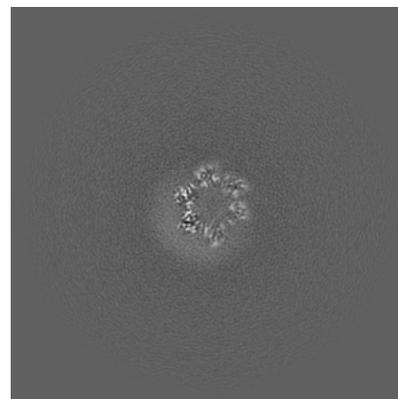
### 6.2.1 Primary map



X Index: 208

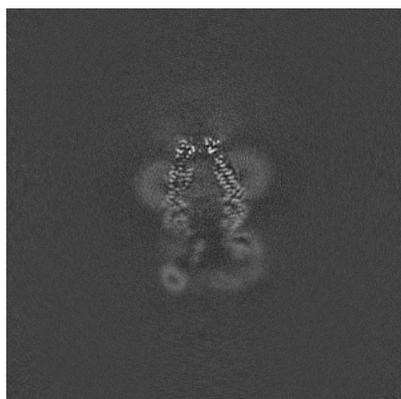


Y Index: 208

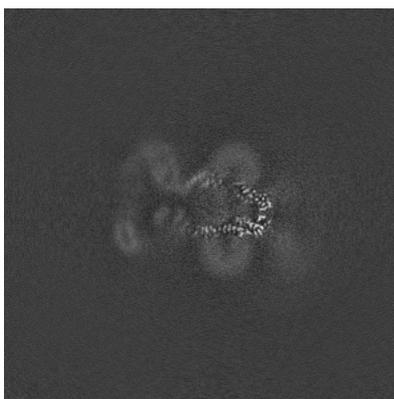


Z Index: 208

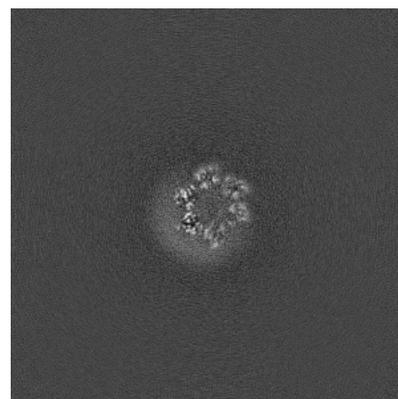
### 6.2.2 Raw map



X Index: 208



Y Index: 208

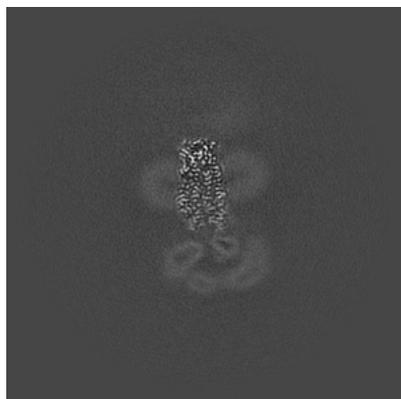


Z Index: 208

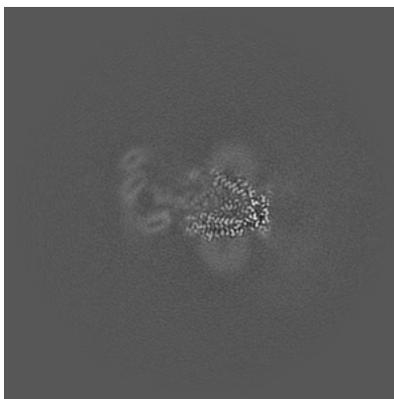
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

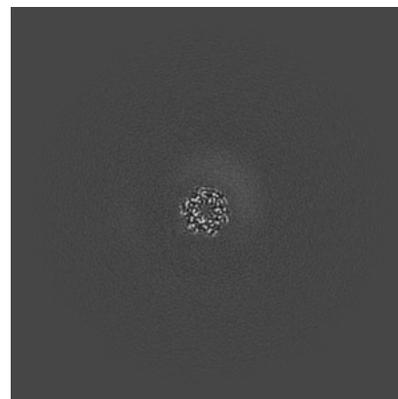
### 6.3.1 Primary map



X Index: 187

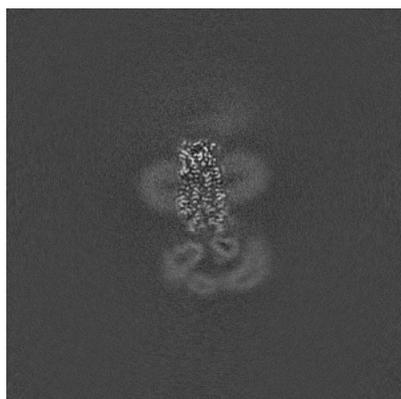


Y Index: 188

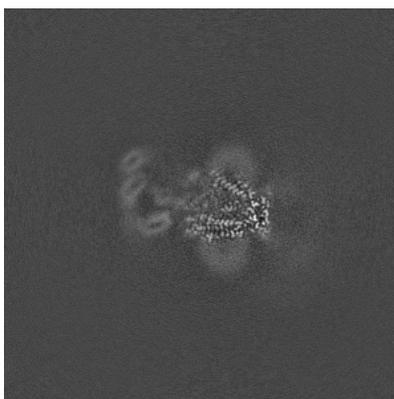


Z Index: 265

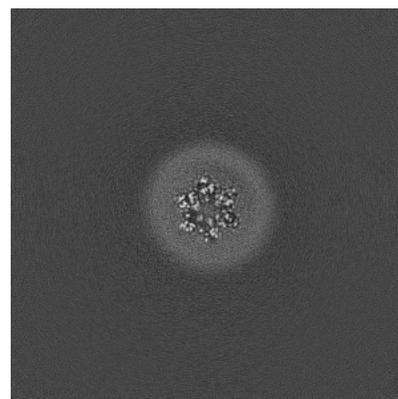
### 6.3.2 Raw map



X Index: 187



Y Index: 188

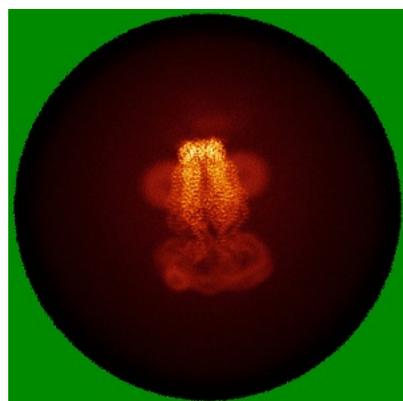


Z Index: 247

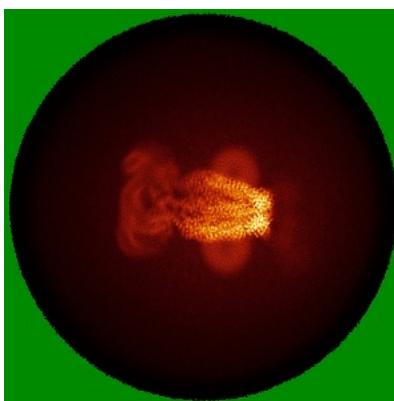
The images above show the largest variance slices of the map in three orthogonal directions.

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

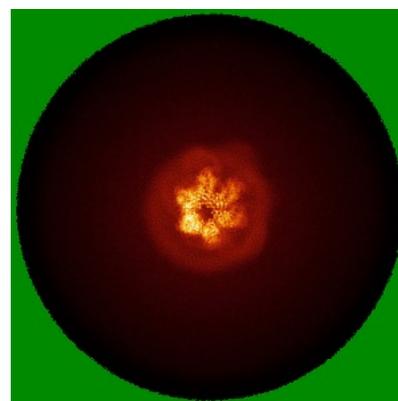
### 6.4.1 Primary map



X

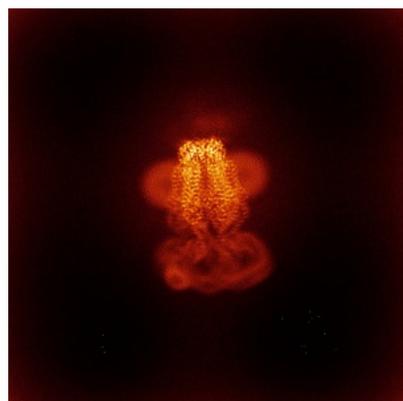


Y

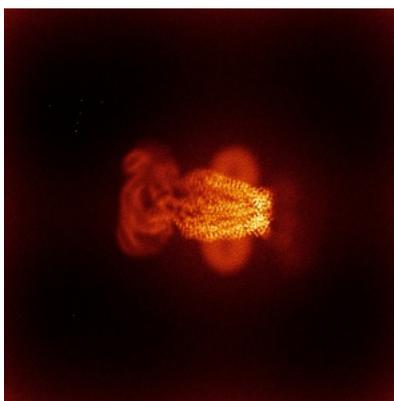


Z

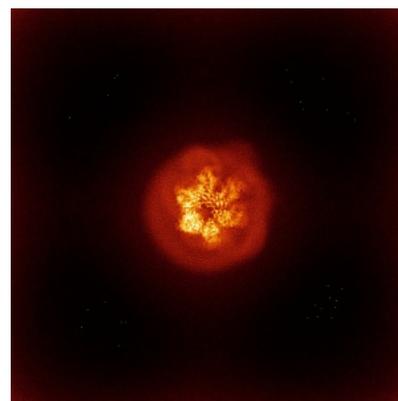
### 6.4.2 Raw map



X



Y

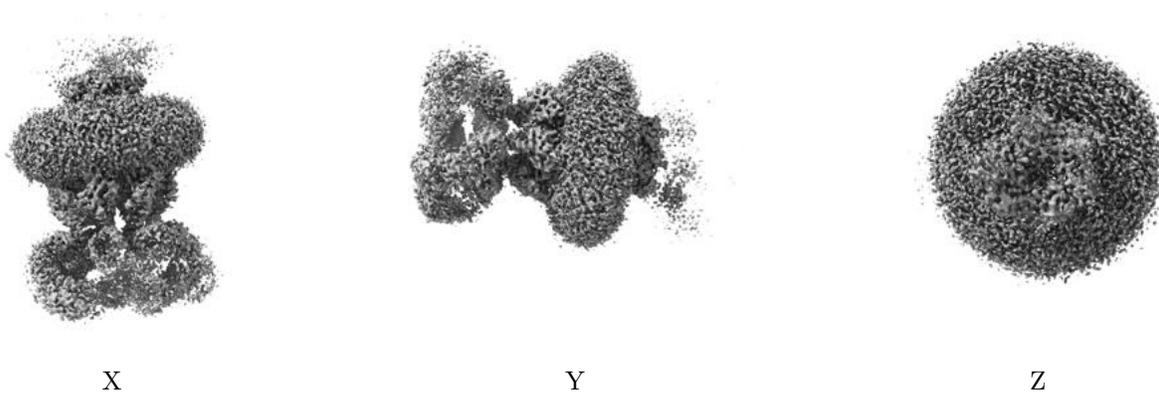


Z

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.

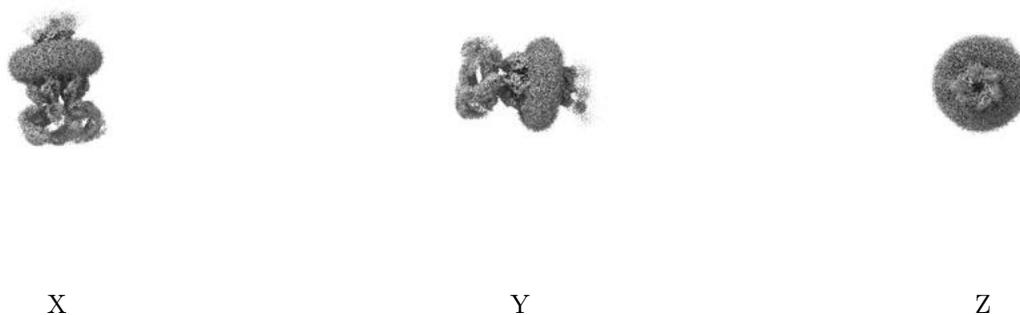
## 6.5 Orthogonal surface views [i](#)

### 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.

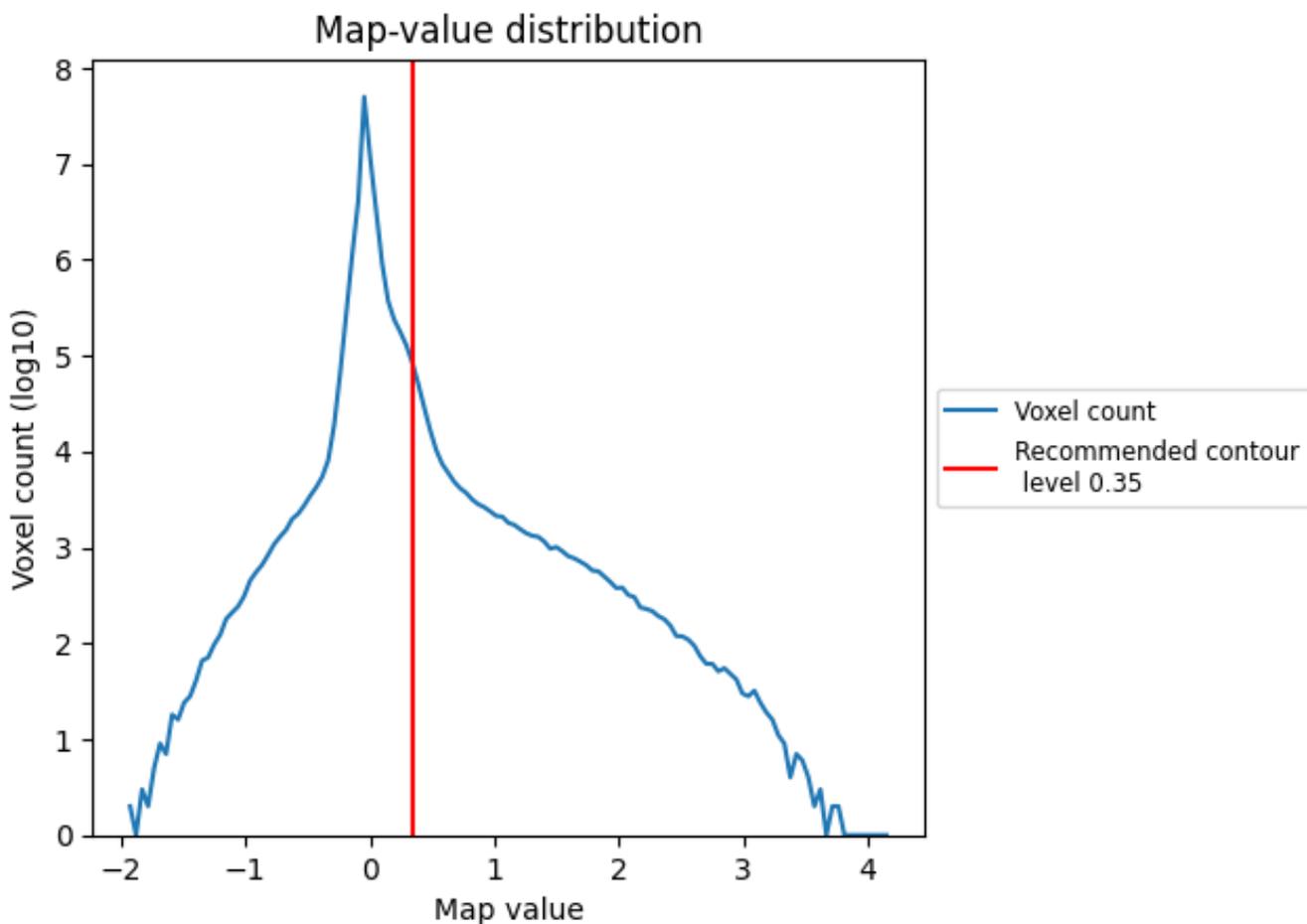
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

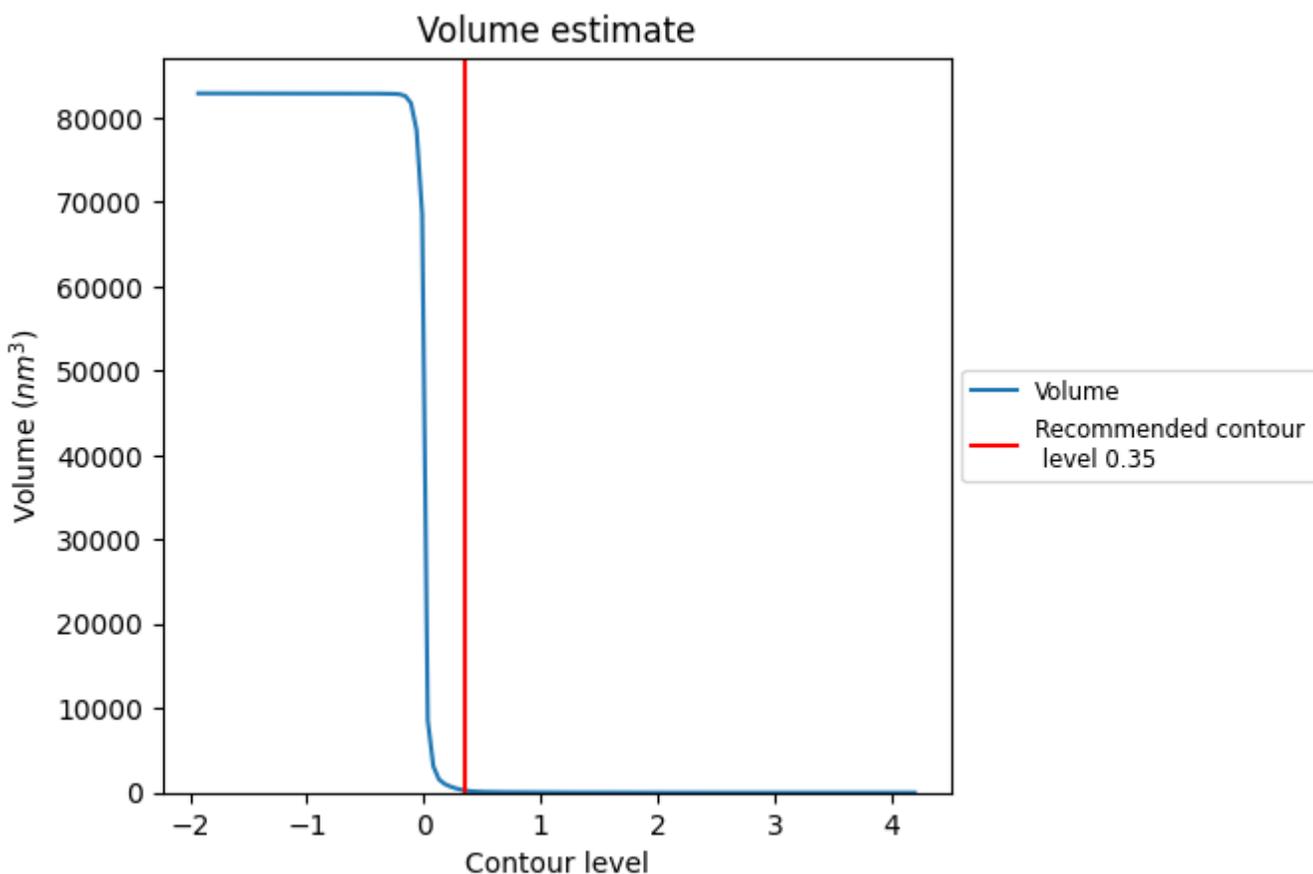
This section contains the results of statistical analysis of the map.

### 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.

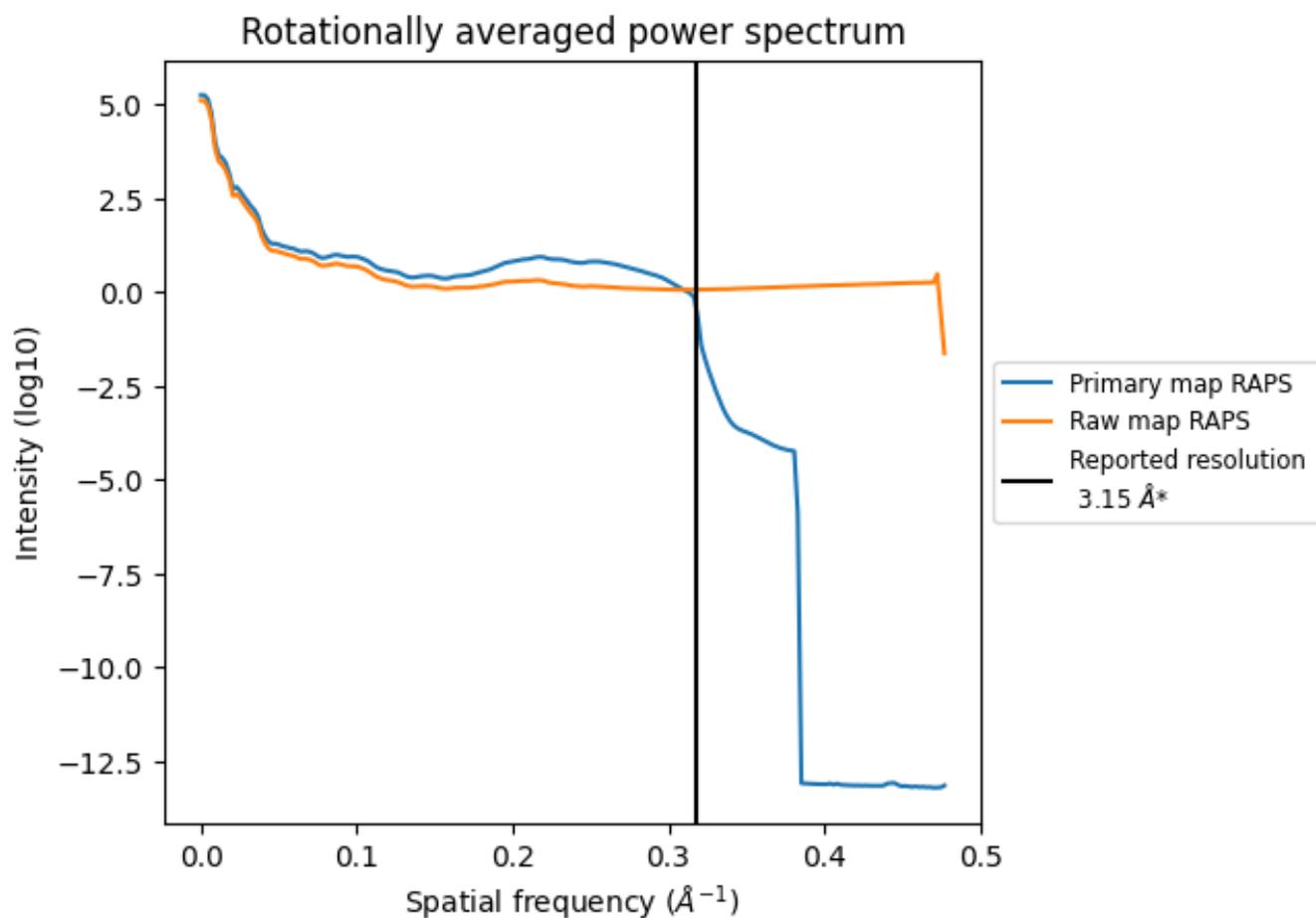
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 273 nm<sup>3</sup>; 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 [i](#)

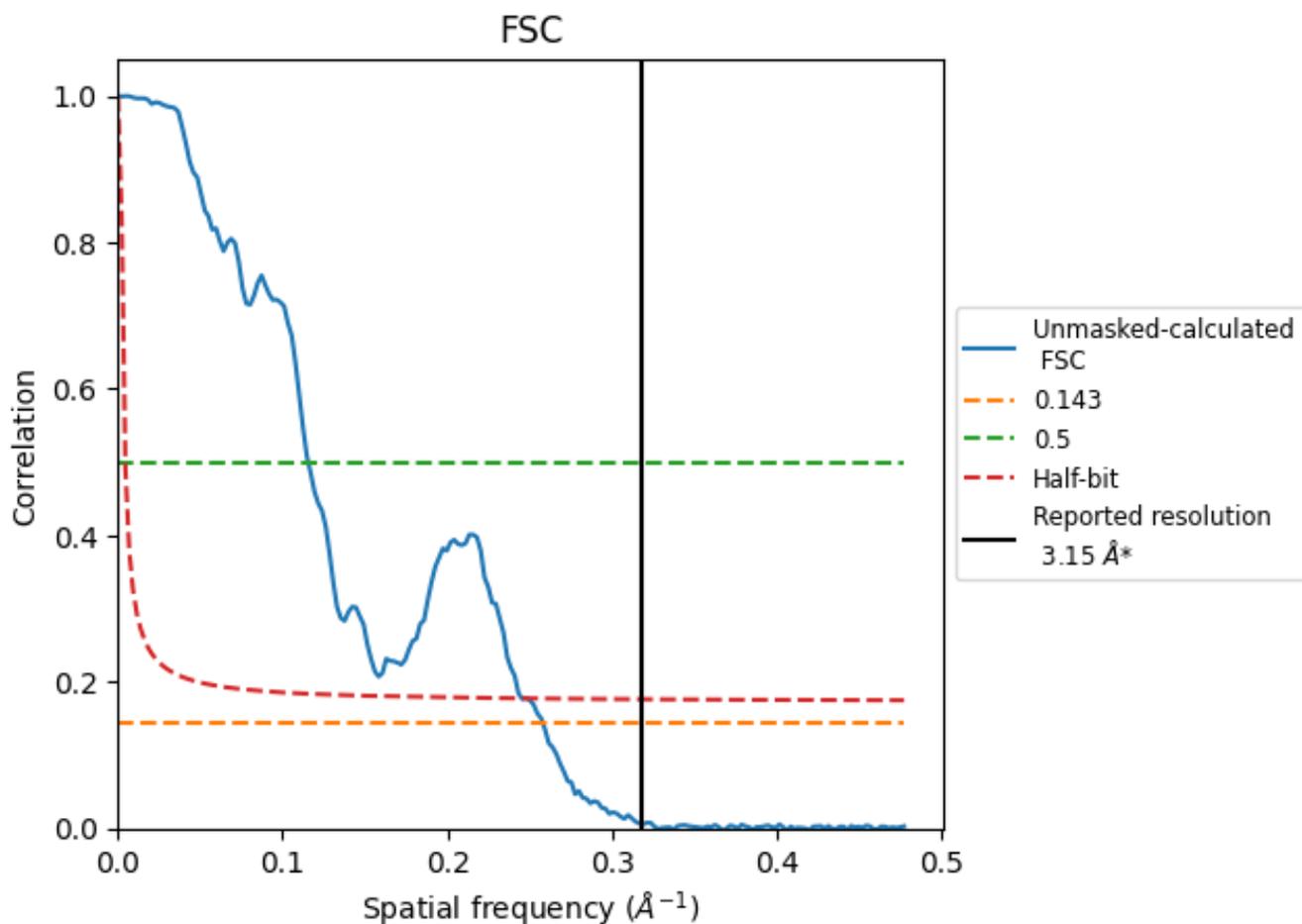


\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

## 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  $0.317 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

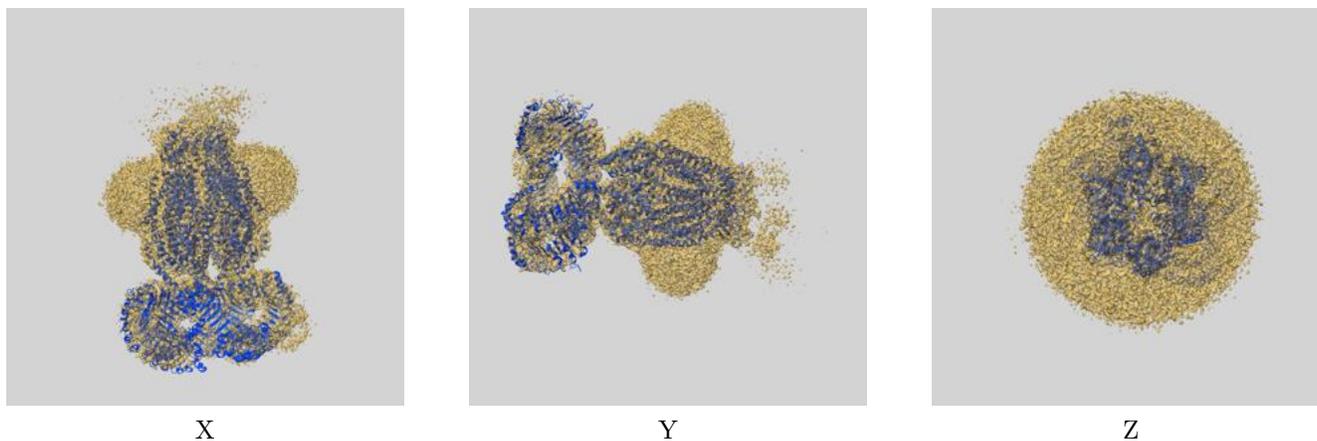
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	8.66	4.08

\*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](#)

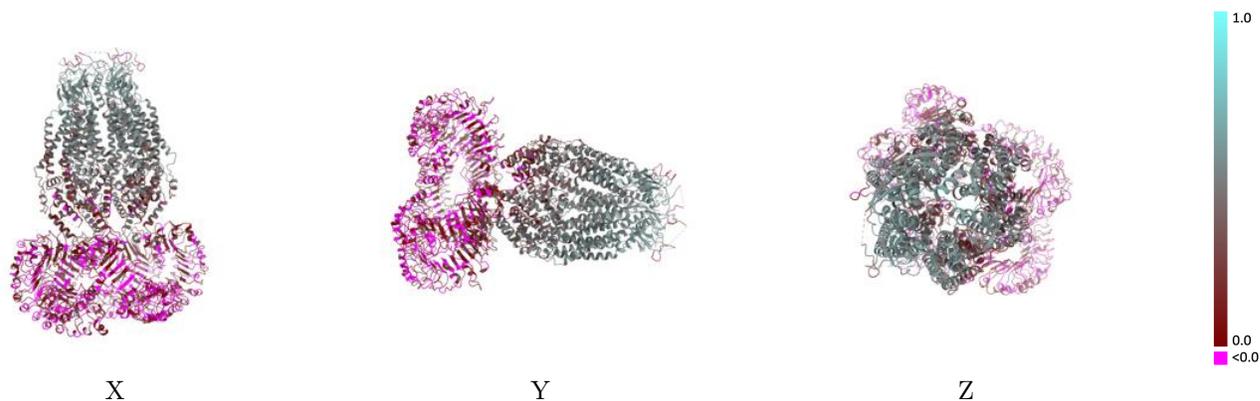
This section contains information regarding the fit between EMDB map EMD-28898 and PDB model 8F79. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



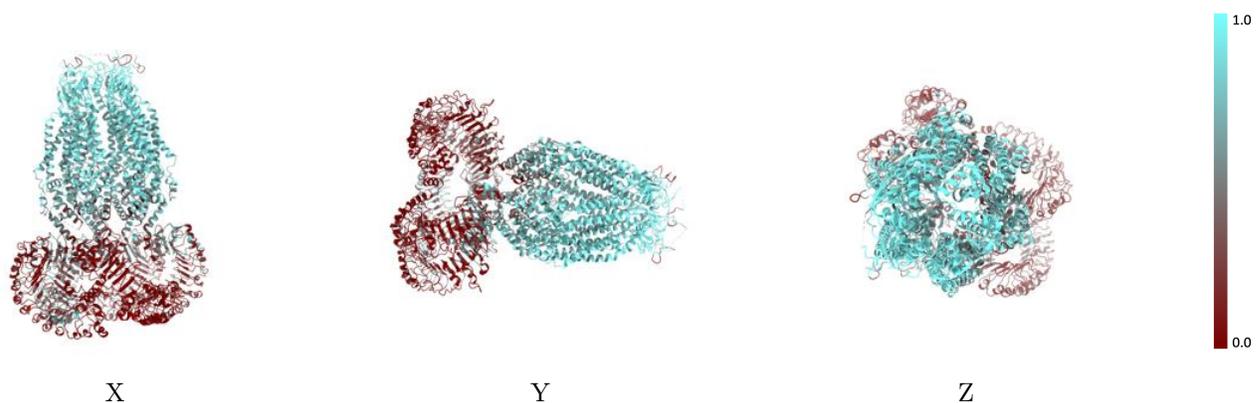
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



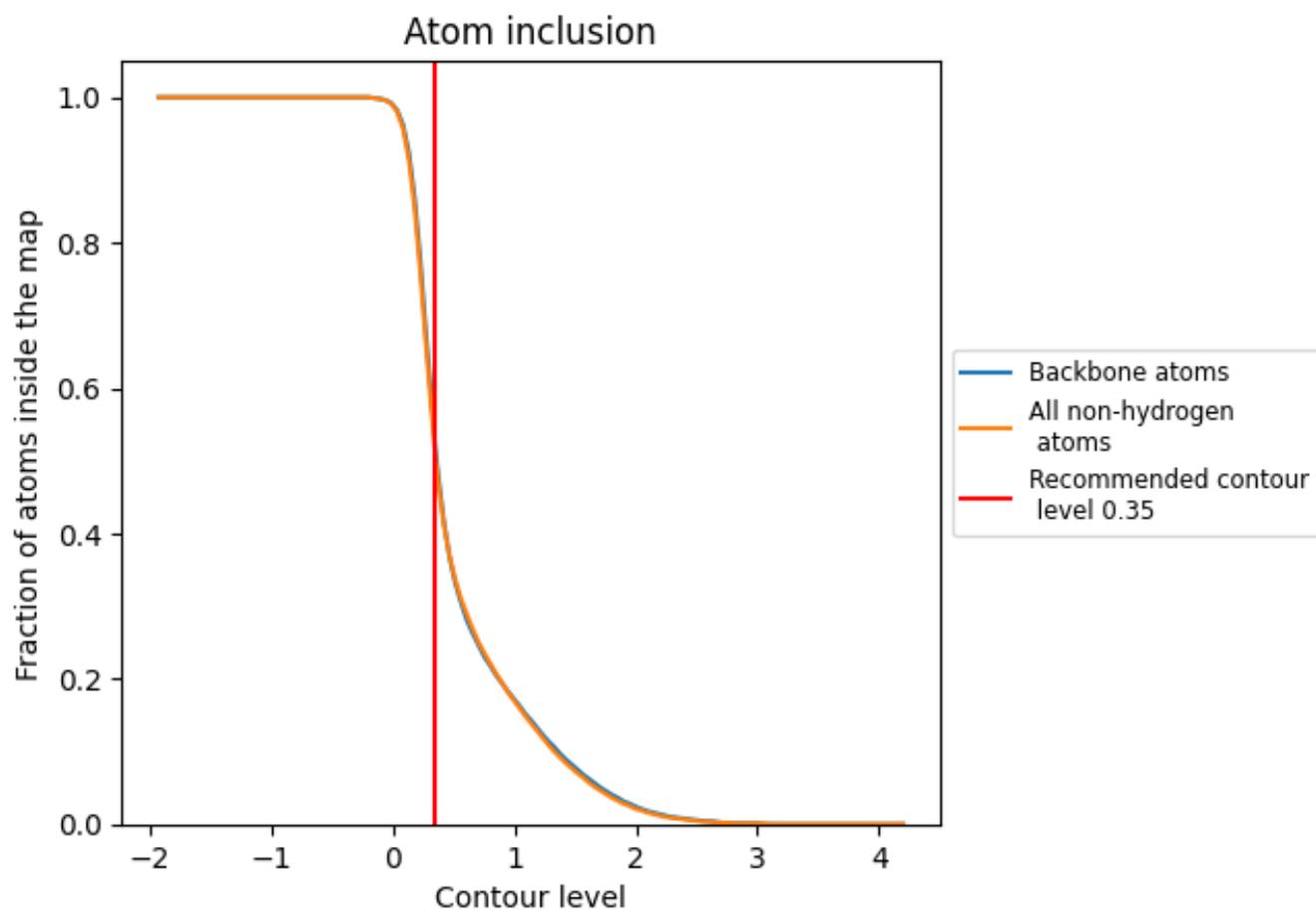
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 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

