



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 01:13 PM UTC

PDB ID : 5OG1 / pdb_00005og1
EMDB ID : EMD-3777
Title : Cryo EM structure of the E. coli disaggregase ClpB (BAP form, DWB mutant),
in the ATPgammaS state
Authors : Deville, C.; Carroni, M.; Franke, K.B.; Topf, M.; Bukau, B.; Mogk, A.; Saibil,
H.R.
Deposited on : 2017-07-11
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

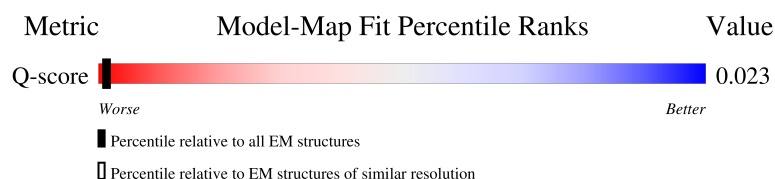
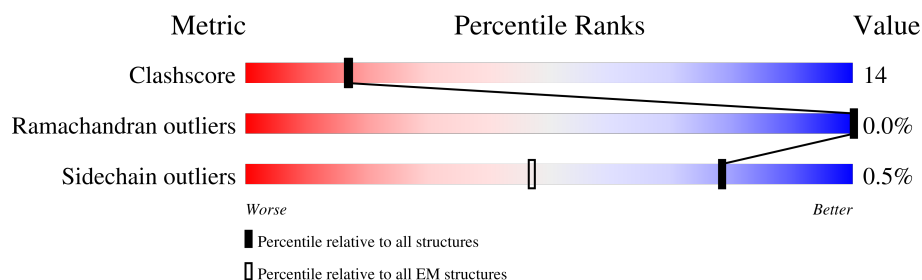
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	871	68% 68% 26% 6%
1	B	871	42% 45% 20% 34%
1	C	871	45% 45% 26% 28%
1	D	871	46% 49% 22% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	871	51% 56% 23% 21%
1	F	871	55% 53% 26% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31380 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 Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	F	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	E	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	D	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	B	572	Total	C	N	O	S	0	0
			4518	2834	823	845	16		
1	A	819	Total	C	N	O	S	0	0
			5841	3667	1118	1037	19		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	MET	-	initiating methionine	UNP P63284
C	-2	ARG	-	expression tag	UNP P63284
C	-1	GLY	-	expression tag	UNP P63284
C	0	SER	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	745	ILE	ILE	linker	UNP P0ABH9
C	746	LYS	LYS	linker	UNP P0ABH9
C	747	LYS	LYS	linker	UNP P0ABH9
C	748	ILE	ILE	linker	UNP P0ABH9
C	858	GLY	-	expression tag	UNP P63284
C	859	SER	-	expression tag	UNP P63284
C	860	ARG	-	expression tag	UNP P63284
C	861	SER	-	expression tag	UNP P63284
C	862	HIS	-	expression tag	UNP P63284
C	863	HIS	-	expression tag	UNP P63284
C	864	HIS	-	expression tag	UNP P63284

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	865	HIS	-	expression tag	UNP P63284
C	866	HIS	-	expression tag	UNP P63284
C	867	HIS	-	expression tag	UNP P63284
F	-3	MET	-	initiating methionine	UNP P63284
F	-2	ARG	-	expression tag	UNP P63284
F	-1	GLY	-	expression tag	UNP P63284
F	0	SER	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	745	ILE	ILE	linker	UNP P0ABH9
F	746	LYS	LYS	linker	UNP P0ABH9
F	747	LYS	LYS	linker	UNP P0ABH9
F	748	ILE	ILE	linker	UNP P0ABH9
F	858	GLY	-	expression tag	UNP P63284
F	859	SER	-	expression tag	UNP P63284
F	860	ARG	-	expression tag	UNP P63284
F	861	SER	-	expression tag	UNP P63284
F	862	HIS	-	expression tag	UNP P63284
F	863	HIS	-	expression tag	UNP P63284
F	864	HIS	-	expression tag	UNP P63284
F	865	HIS	-	expression tag	UNP P63284
F	866	HIS	-	expression tag	UNP P63284
F	867	HIS	-	expression tag	UNP P63284
E	-3	MET	-	initiating methionine	UNP P63284
E	-2	ARG	-	expression tag	UNP P63284
E	-1	GLY	-	expression tag	UNP P63284
E	0	SER	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	678	ALA	GLU	engineered mutation	UNP P63284
E	745	ILE	ILE	linker	UNP P0ABH9
E	746	LYS	LYS	linker	UNP P0ABH9
E	747	LYS	LYS	linker	UNP P0ABH9
E	748	ILE	ILE	linker	UNP P0ABH9
E	858	GLY	-	expression tag	UNP P63284
E	859	SER	-	expression tag	UNP P63284
E	860	ARG	-	expression tag	UNP P63284
E	861	SER	-	expression tag	UNP P63284
E	862	HIS	-	expression tag	UNP P63284
E	863	HIS	-	expression tag	UNP P63284
E	864	HIS	-	expression tag	UNP P63284
E	865	HIS	-	expression tag	UNP P63284
E	866	HIS	-	expression tag	UNP P63284

Continued on next page...

Continued from previous page...

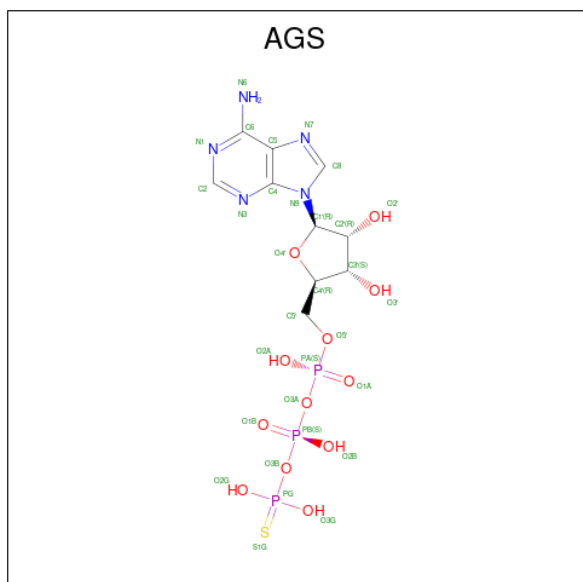
Chain	Residue	Modelled	Actual	Comment	Reference
E	867	HIS	-	expression tag	UNP P63284
D	-3	MET	-	initiating methionine	UNP P63284
D	-2	ARG	-	expression tag	UNP P63284
D	-1	GLY	-	expression tag	UNP P63284
D	0	SER	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	745	ILE	ILE	linker	UNP P0ABH9
D	746	LYS	LYS	linker	UNP P0ABH9
D	747	LYS	LYS	linker	UNP P0ABH9
D	748	ILE	ILE	linker	UNP P0ABH9
D	858	GLY	-	expression tag	UNP P63284
D	859	SER	-	expression tag	UNP P63284
D	860	ARG	-	expression tag	UNP P63284
D	861	SER	-	expression tag	UNP P63284
D	862	HIS	-	expression tag	UNP P63284
D	863	HIS	-	expression tag	UNP P63284
D	864	HIS	-	expression tag	UNP P63284
D	865	HIS	-	expression tag	UNP P63284
D	866	HIS	-	expression tag	UNP P63284
D	867	HIS	-	expression tag	UNP P63284
B	-3	MET	-	initiating methionine	UNP P63284
B	-2	ARG	-	expression tag	UNP P63284
B	-1	GLY	-	expression tag	UNP P63284
B	0	SER	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	745	ILE	ILE	linker	UNP P0ABH9
B	746	LYS	LYS	linker	UNP P0ABH9
B	747	LYS	LYS	linker	UNP P0ABH9
B	748	ILE	ILE	linker	UNP P0ABH9
B	858	GLY	-	expression tag	UNP P63284
B	859	SER	-	expression tag	UNP P63284
B	860	ARG	-	expression tag	UNP P63284
B	861	SER	-	expression tag	UNP P63284
B	862	HIS	-	expression tag	UNP P63284
B	863	HIS	-	expression tag	UNP P63284
B	864	HIS	-	expression tag	UNP P63284
B	865	HIS	-	expression tag	UNP P63284
B	866	HIS	-	expression tag	UNP P63284
B	867	HIS	-	expression tag	UNP P63284
A	-3	MET	-	initiating methionine	UNP P63284

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP P63284
A	-1	GLY	-	expression tag	UNP P63284
A	0	SER	-	expression tag	UNP P63284
A	279	ALA	GLU	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	745	ILE	ILE	linker	UNP P0ABH9
A	746	LYS	LYS	linker	UNP P0ABH9
A	747	LYS	LYS	linker	UNP P0ABH9
A	748	ILE	ILE	linker	UNP P0ABH9
A	858	GLY	-	expression tag	UNP P63284
A	859	SER	-	expression tag	UNP P63284
A	860	ARG	-	expression tag	UNP P63284
A	861	SER	-	expression tag	UNP P63284
A	862	HIS	-	expression tag	UNP P63284
A	863	HIS	-	expression tag	UNP P63284
A	864	HIS	-	expression tag	UNP P63284
A	865	HIS	-	expression tag	UNP P63284
A	866	HIS	-	expression tag	UNP P63284
A	867	HIS	-	expression tag	UNP P63284

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

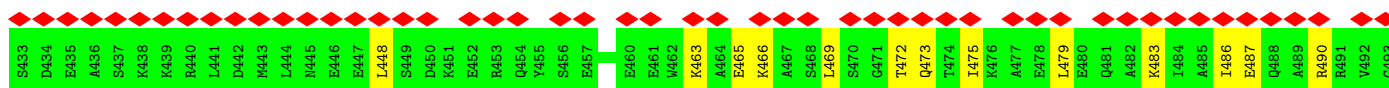


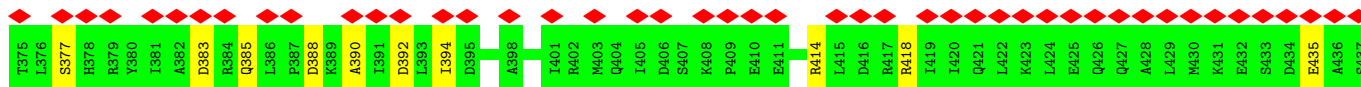
Mol	Chain	Residues	Atoms					AltConf	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

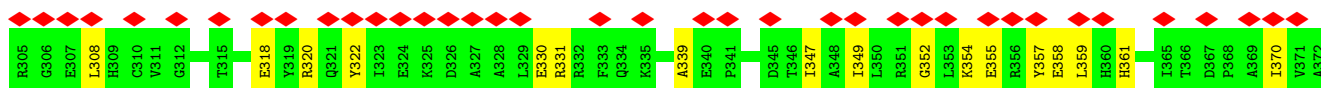
Continued on next page...

Continued from previous page...

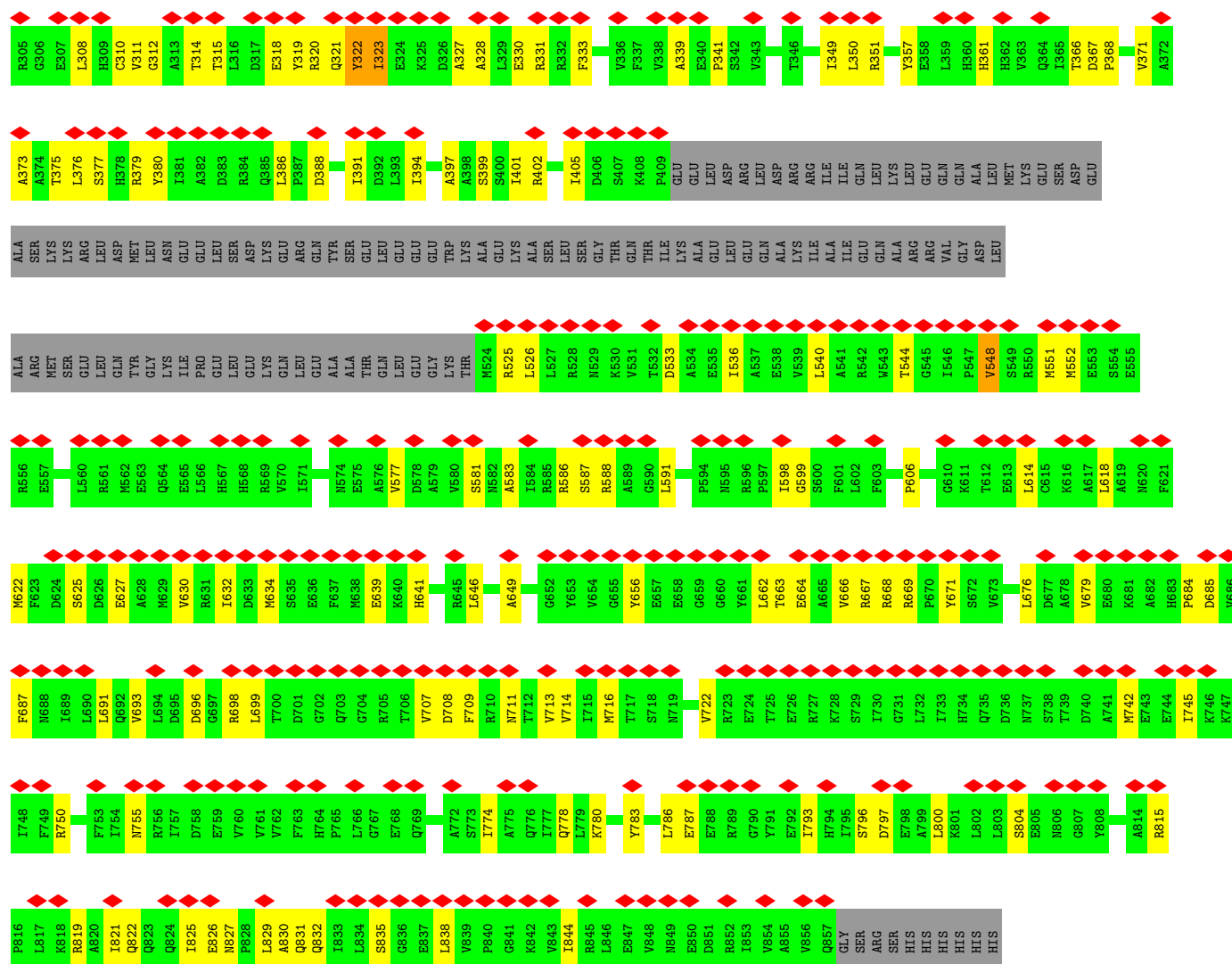
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0



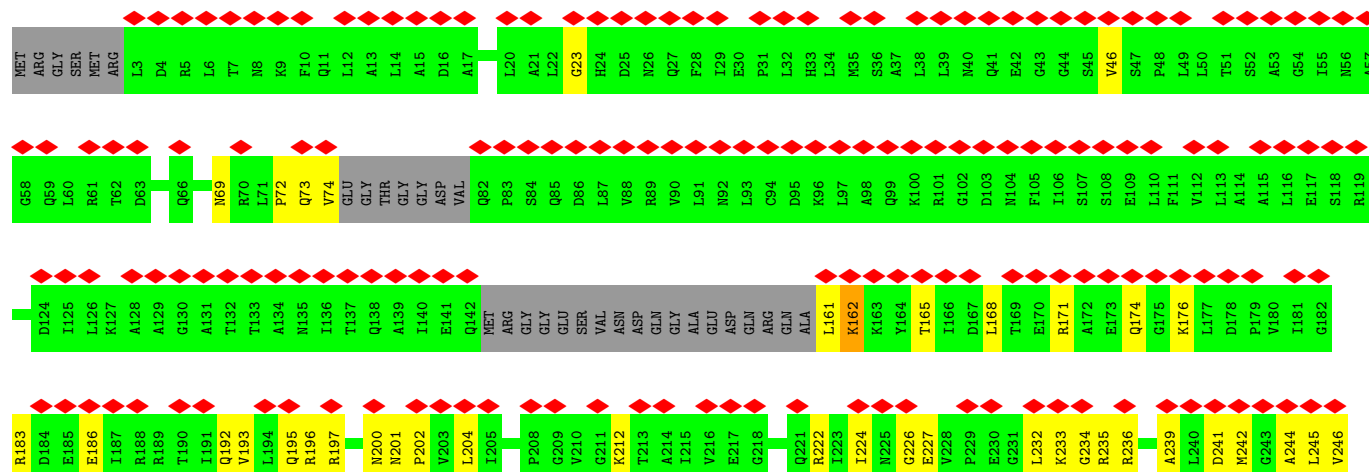




[illegible]



- Molecule 1: Chaperone protein ClpB, ATP-dependent Clp protease ATP-binding subunit ClpA, Chaperone protein ClpB



G807	Y808	D809	P810	G813	A814	R815	P816	L817	R818	R819	A820	I821	Q822	Q823	Q824	I825	E826	N827	P828	L829	A830	Q831	Q832	I833	L834	S835	G836	E837	P840	G841	K842	W843	L844	R845	L846	E847	W848	N849	E850	D851	R852	I853	W854	Q857	GLY	SER	ARG	SER	HIS	HIS	HIS	HIS	HIS						
I745	I748	F749	R750	F751	E752	F753	I754	W755	R756	I757	D758	E759	V760	V761	V762	F763	H764	F765	L766	G767	E768	Q769	H770	I771	A772	S773	I774	A775	Q776	I777	W778	L779	K780	R781	L782	Y783	K784	E787	E788	R789	G790	Y791	E792	I793	H794	I795	S796	D797	E798	A799	L800	K801	L802	L803	S804	E805	N806		
H683	V686	F687	N688	L689	L690	L691	Q692	V693	L694	D695	D696	L699	T700	D701	G702	Q703	G704	R705	T706	S642	V707	F709	R710	W711	T712	V713	W714	T715	W716	T717	S718	W719	L720	G721	V722	R723	E724	T725	E726	R727	K728	S729	I730	G731	L732	I733	H734	Q735	D736	W737	S738	T739	D740	A741	W742	E743	E744		
N620	F621	M622	F623	D624	S625	D626	E627	A628	M629	V630	R631	L632	D633	E636	F637	M638	E639	K640	H641	S642	V643	L646	V647	G648	A649	P650	P651	G652	Y653	G654	Y655	Y656	E657	E658	G659	G660	Y661	L662	T663	E664	A665	V666	R667	R668	R669	P670	Y671	S672	V673	I674	L675	L676	D677	E680	K681	A682			
R556	E557	K558	L559	L560	R561	M562	E563	Q564	E565	L566	H567	H568	R569	V570	I571	G572	Q573	N574	E575	A576	V577	D578	N582	A583	I584	R585	R586	S587	R588	A589	G590	L591	A592	D593	P594	N595	R596	I598	G599	S600	F601	L602	F603	L604	G605	P606	V609	G610	E613	L614	C615	K616	A617	L618	A619				
A496	R497	M498	S499	E500	L501	Q502	Y503	G504	K505	I506	P507	E508	L509	E510	K511	Q512	L513	E514	A515	A516	T517	Q518	L519	E520	G521	K522	T523	M524	R525	L526	L527	R528	N529	K530	V531	T532	D533	A534	E535	I536	A537	E538	V539	L540	A541	R542	W543	T544	G545	I546	P547	V548	S549	R550	M551	M552	E553	S554	E555
A436	S437	K438	K439	R440	L441	D442	M443	L444	N445	E446	E447	L448	S449	D450	K451	E452	R453	Q454	Y455	A456	E457	L458	E459	E460	E461	W462	K463	A464	E465	K466	A467	S468	L469	S470	G471	T472	Q473	R474	I475	K476	A477	E478	L479	E480	Q481	A482	K483	I484	A485	L486	E487	Q488	A489	R490	R491	V492	D494	L495	
L376	S377	H378	R379	Y380	I381	A382	D442	R383	Q385	L386	P387	D388	K389	A390	I391	L393	I394	D395	E396	A397	A398	S399	S400	I401	M403	Q404	I405	D406	S407	K408	P409	E410	E411	L412	D413	R414	L415	D416	R417	R418	I419	I420	Q421	L422	K423	L424	A425	Q426	Q427	A428	L429	M430	K431	E432	A433	S434	D434	E435	
E307	L308	H309	C310	V311	G312	A313	T314	T315	L316	D317	E318	Y319	R320	Q321	Y322	I323	E324	K325	D326	A327	A328	L329	E330	R331	R332	F333	Q334	K335	V336	F337	V338	A339	E340	P341	D345	L350	R351	K354	E355	R356	L359	H360	H361	H362	V363	T366	D367	P368	A369	I370	V371	A372	A373						
A247	G248	A249	K250	Y251	R252	G253	E254	F255	E256	E257	R258	L259	K260	G261	V262	L263	N264	D265	L266	A267	K268	Q269	E270	G271	N272	V273	I274	L275	F276	I277	D278	A279	L280	H281	T282	M283	VAL	GLY	ALA	GLY	LYS	ALA	ASP	GLY	ALA	MET	ASP	A295	G296	N297	M298	L299	K300	P301	A302	L303	A304	R305	G306

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.757	Depositor
Minimum map value	-1.595	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.225	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/5909	0.73	4/7815 (0.1%)
1	B	0.33	0/4582	0.76	6/6178 (0.1%)
1	C	0.32	0/5025	0.77	5/6766 (0.1%)
1	D	0.30	0/5025	0.74	5/6766 (0.1%)
1	E	0.29	0/5512	0.68	1/7420 (0.0%)
1	F	0.31	0/5512	0.73	4/7420 (0.1%)
All	All	0.31	0/31565	0.73	25/42365 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	2
All	All	0	11

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	702	GLY	N-CA-C	7.45	121.65	112.64
1	F	339	ALA	CA-C-N	7.33	134.87	120.94
1	F	339	ALA	C-N-CA	7.33	134.87	120.94
1	A	271	GLY	CA-C-N	7.17	134.61	121.70
1	A	271	GLY	C-N-CA	7.17	134.61	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	409	PRO	Peptide
1	D	550	ARG	Peptide
1	E	850	GLU	Peptide
1	F	636	GLU	Peptide
1	F	638	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5696	171	0
1	B	4518	0	4613	125	0
1	C	4960	0	5051	179	0
1	D	4960	0	5051	143	0
1	E	5442	0	5552	146	0
1	F	5442	0	5551	178	0
2	B	31	0	12	4	0
2	C	62	0	24	4	0
2	D	62	0	24	5	0
2	E	62	0	24	9	0
All	All	31380	0	31598	872	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 14.

The worst 5 of 872 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:E:251:TYR:CE1	1:A:73:GLN:N	2.07	1.22
1:E:614:LEU:O	1:E:618:LEU:HB2	1.54	1.06
1:B:663:THR:O	1:B:667:ARG:HB2	1.59	1.03
1:F:663:THR:O	1:F:667:ARG:HB2	1.57	1.01
1:C:357:TYR:O	1:C:361:HIS:HB2	1.58	1.01

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	811/871 (93%)	764 (94%)	47 (6%)	0	100	100
1	B	566/871 (65%)	520 (92%)	45 (8%)	1 (0%)	43	77
1	C	618/871 (71%)	560 (91%)	58 (9%)	0	100	100
1	D	618/871 (71%)	572 (93%)	46 (7%)	0	100	100
1	E	682/871 (78%)	637 (93%)	45 (7%)	0	100	100
1	F	682/871 (78%)	630 (92%)	52 (8%)	0	100	100
All	All	3977/5226 (76%)	3683 (93%)	293 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	ILE

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	582/726 (80%)	577 (99%)	5 (1%)	70	76
1	B	483/726 (66%)	480 (99%)	3 (1%)	78	80
1	C	533/726 (73%)	531 (100%)	2 (0%)	84	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	533/726 (73%)	530 (99%)	3 (1%)	78	80
1	E	582/726 (80%)	581 (100%)	1 (0%)	87	85
1	F	582/726 (80%)	579 (100%)	3 (0%)	81	81
All	All	3295/4356 (76%)	3278 (100%)	17 (0%)	78	81

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	LEU
1	A	646	LEU
1	D	432	GLU
1	D	571	ILE
1	B	273	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
1	A	364	GLN
1	D	737	ASN
1	A	297	ASN
1	A	574	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	D	902	-	32,33,33	0.63	1 (3%)	45,52,52	0.90	1 (2%)
2	AGS	E	902	-	32,33,33	0.83	1 (3%)	45,52,52	1.10	3 (6%)
2	AGS	C	902	-	32,33,33	0.88	2 (6%)	45,52,52	0.93	1 (2%)
2	AGS	D	901	-	32,33,33	0.76	2 (6%)	45,52,52	0.94	2 (4%)
2	AGS	E	901	-	32,33,33	0.58	1 (3%)	45,52,52	1.07	4 (8%)
2	AGS	B	901	-	32,33,33	0.73	1 (3%)	45,52,52	0.78	2 (4%)
2	AGS	C	901	-	32,33,33	0.56	0	45,52,52	1.09	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	D	902	-	-	4/21/38/38	0/3/3/3
2	AGS	E	902	-	-	5/21/38/38	0/3/3/3
2	AGS	C	902	-	-	1/21/38/38	0/3/3/3
2	AGS	D	901	-	-	5/21/38/38	0/3/3/3
2	AGS	E	901	-	-	13/21/38/38	0/3/3/3
2	AGS	B	901	-	-	8/21/38/38	0/3/3/3
2	AGS	C	901	-	-	9/21/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	902	AGS	PB-O3B	-2.92	1.56	1.59
2	C	902	AGS	PB-O3A	-2.64	1.56	1.59
2	B	901	AGS	PG-S1G	2.36	1.95	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	AGS	PB-O3A	-2.27	1.57	1.59
2	D	902	AGS	PG-S1G	2.16	1.95	1.90

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	902	AGS	PB-O3B-PG	-5.53	112.94	133.17
2	C	902	AGS	PB-O3B-PG	-4.35	117.24	133.17
2	E	901	AGS	PB-O3B-PG	-4.15	117.98	133.17
2	D	902	AGS	PB-O3B-PG	-4.04	118.39	133.17
2	D	901	AGS	PB-O3B-PG	-3.89	118.93	133.17

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	AGS	C5'-O5'-PA-O1A
2	C	901	AGS	C5'-O5'-PA-O2A
2	C	901	AGS	C5'-O5'-PA-O3A
2	E	901	AGS	C5'-O5'-PA-O1A
2	E	901	AGS	C5'-O5'-PA-O2A

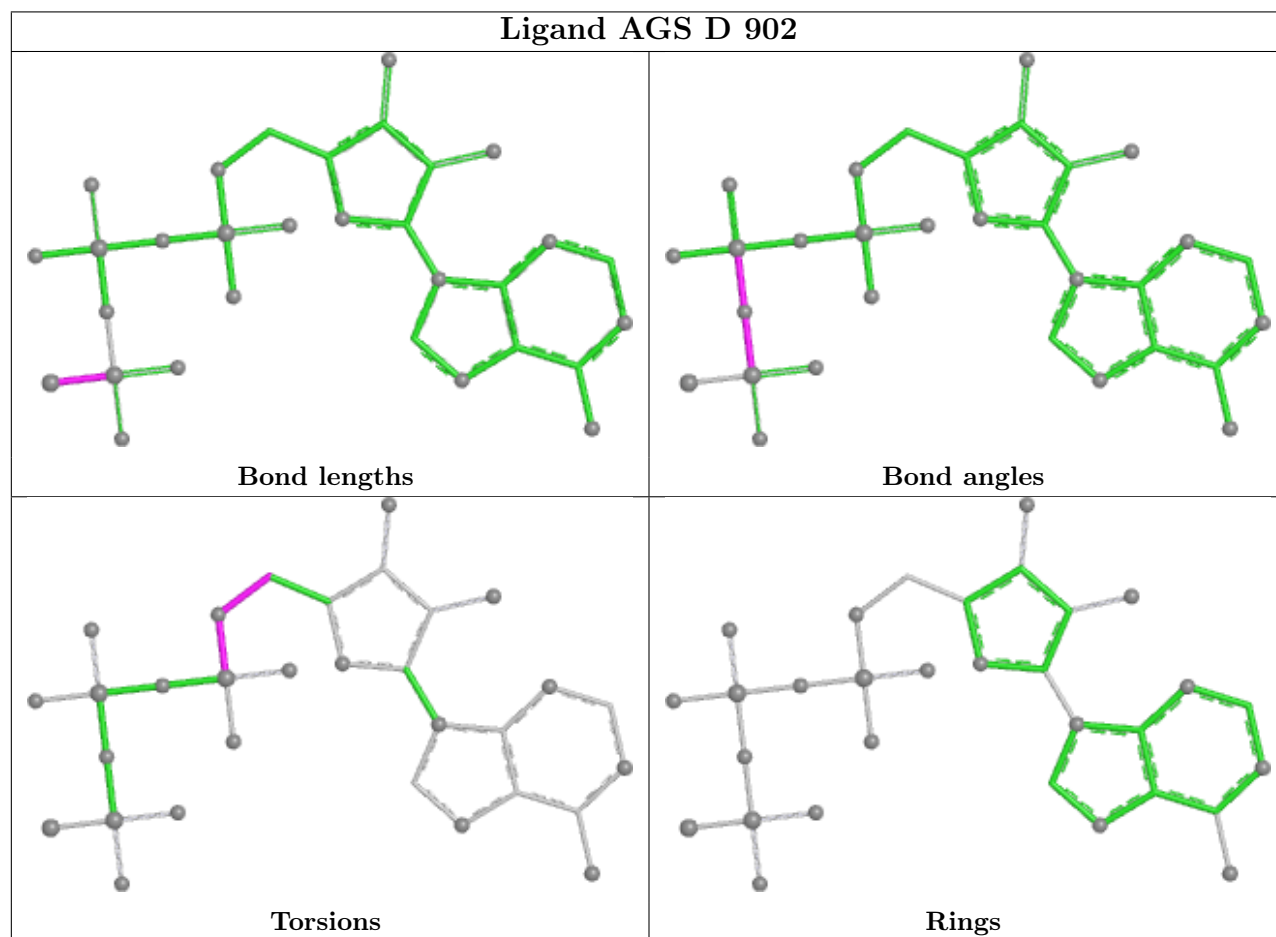
There are no ring outliers.

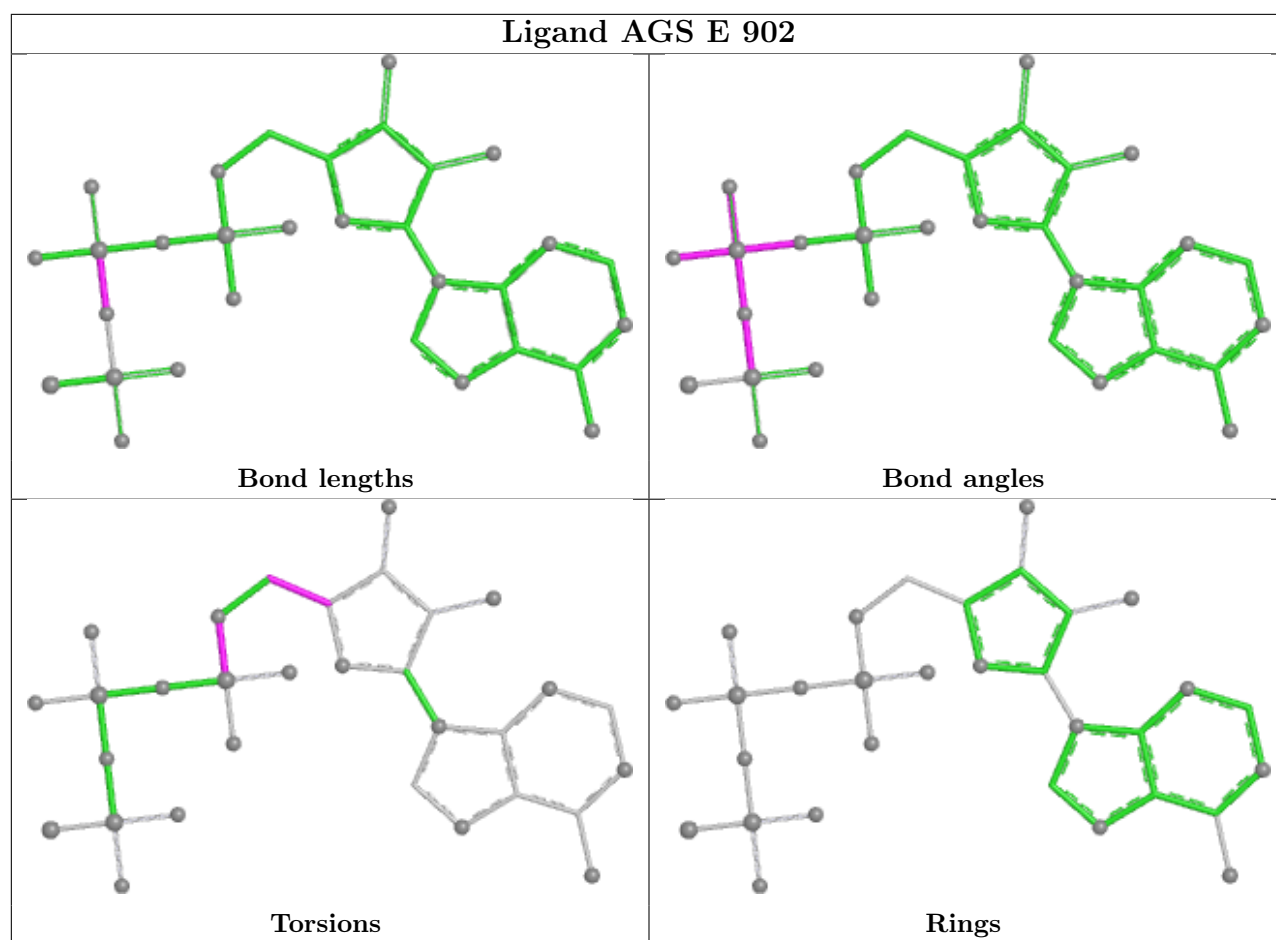
7 monomers are involved in 22 short contacts:

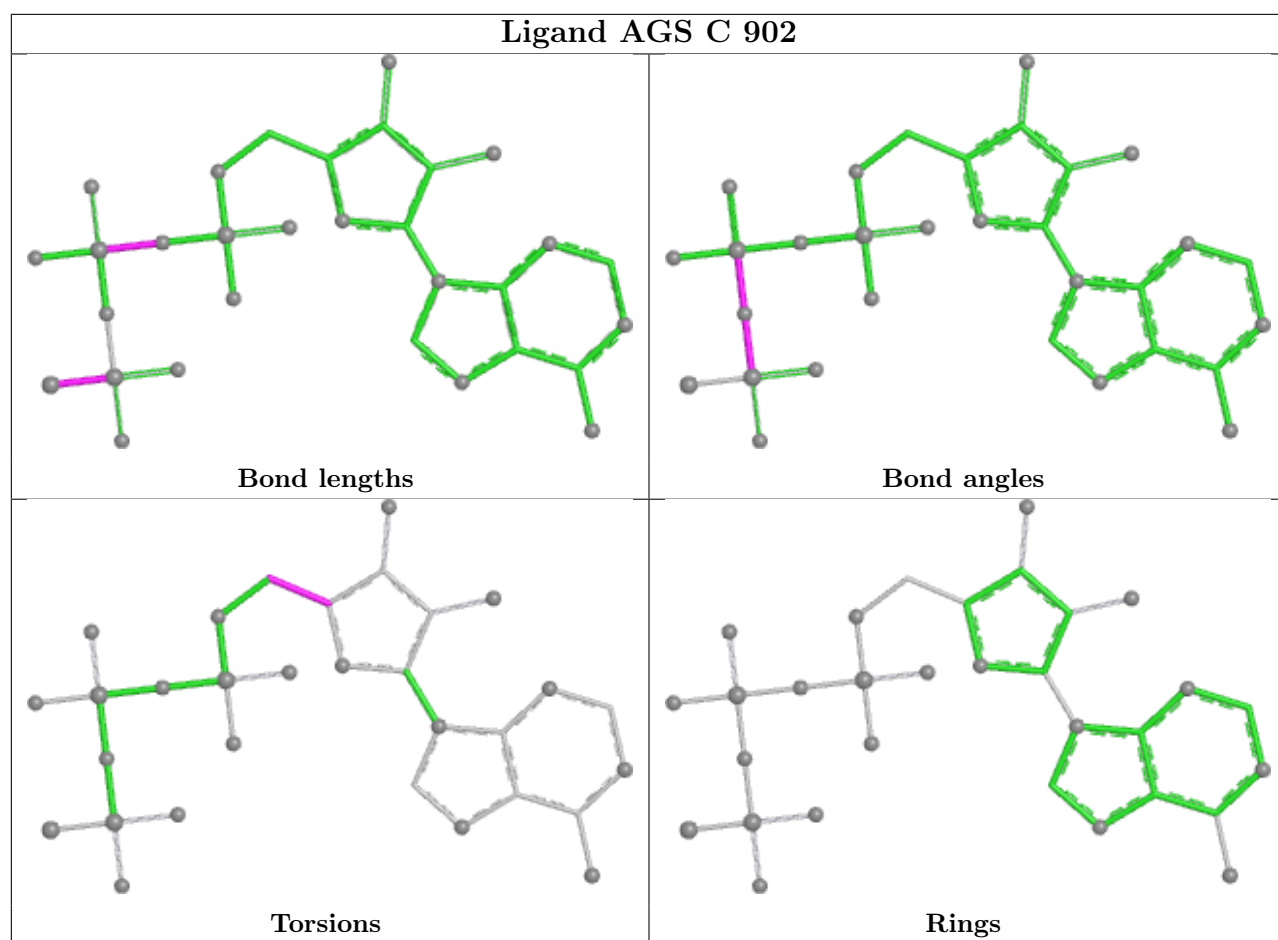
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	AGS	4	0
2	E	902	AGS	6	0
2	C	902	AGS	2	0
2	D	901	AGS	1	0
2	E	901	AGS	3	0
2	B	901	AGS	4	0
2	C	901	AGS	2	0

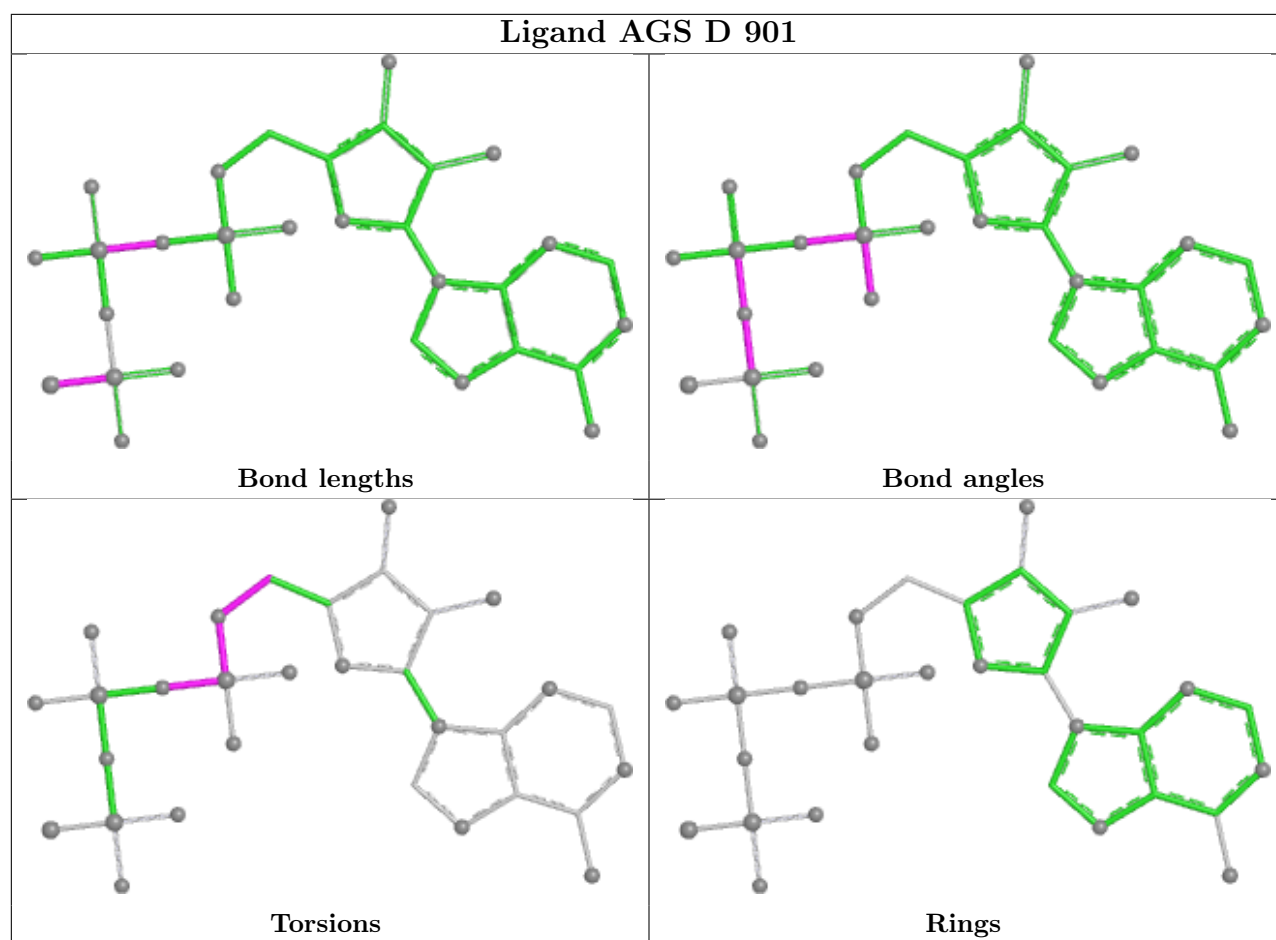
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

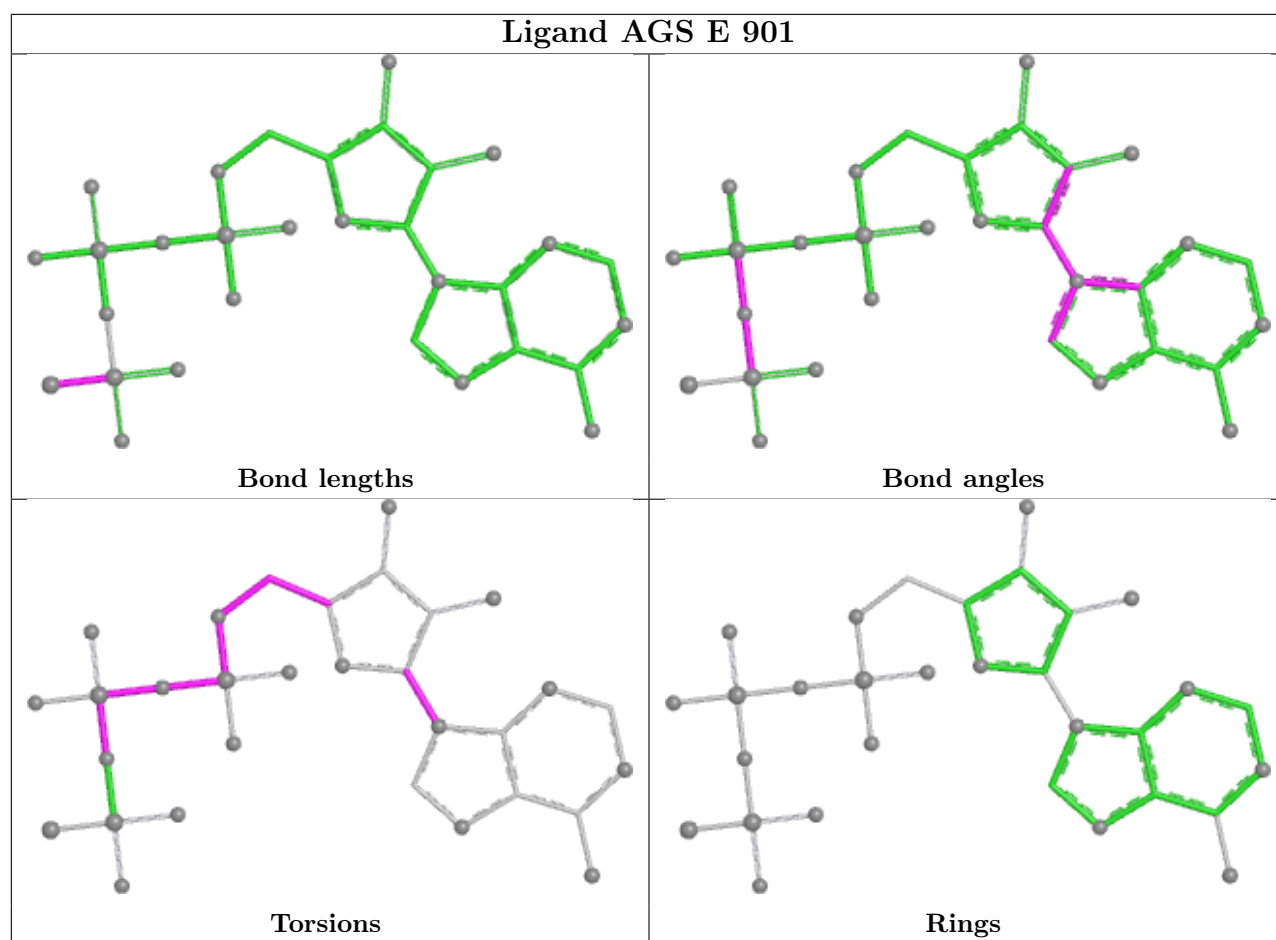
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

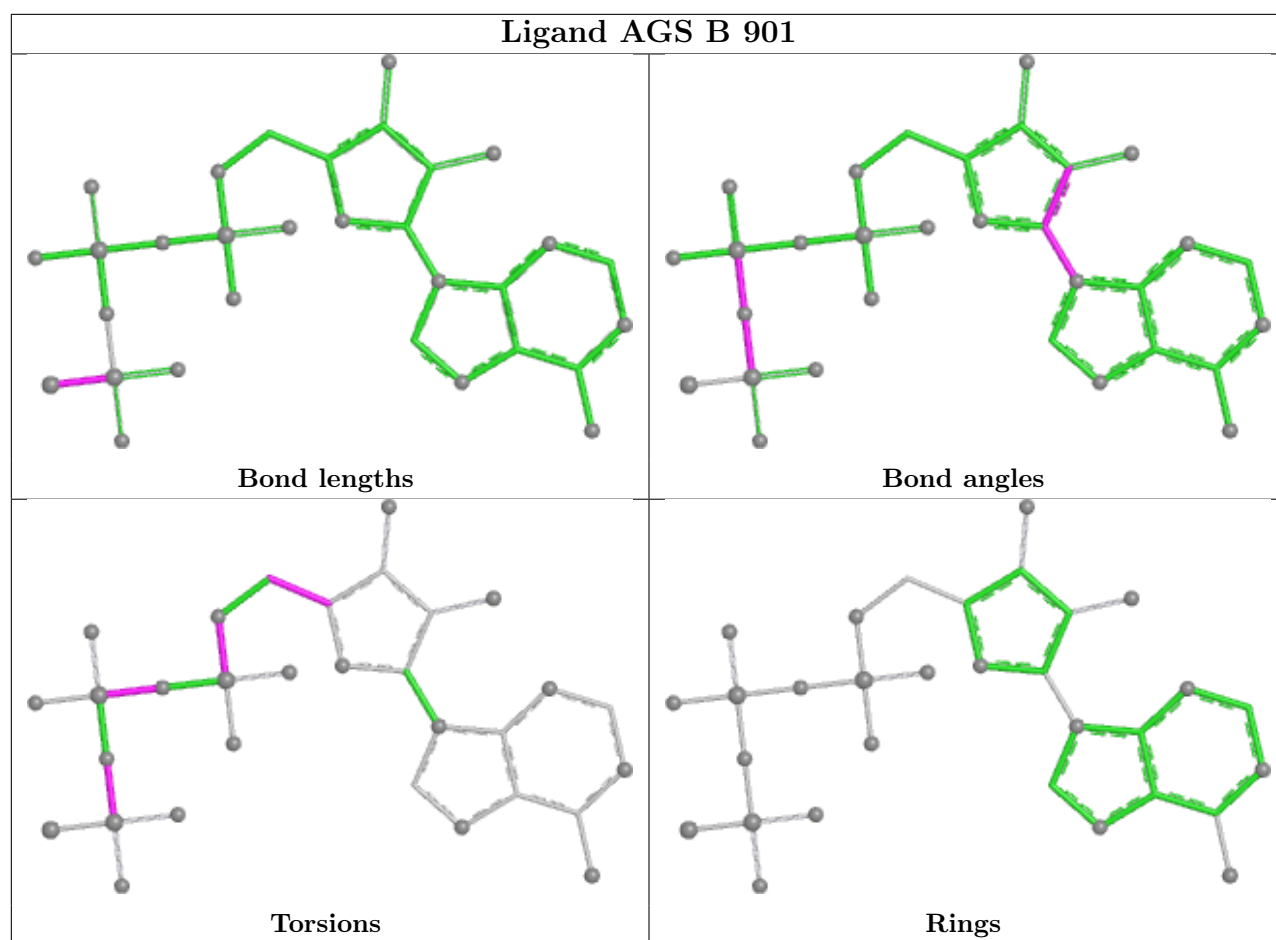


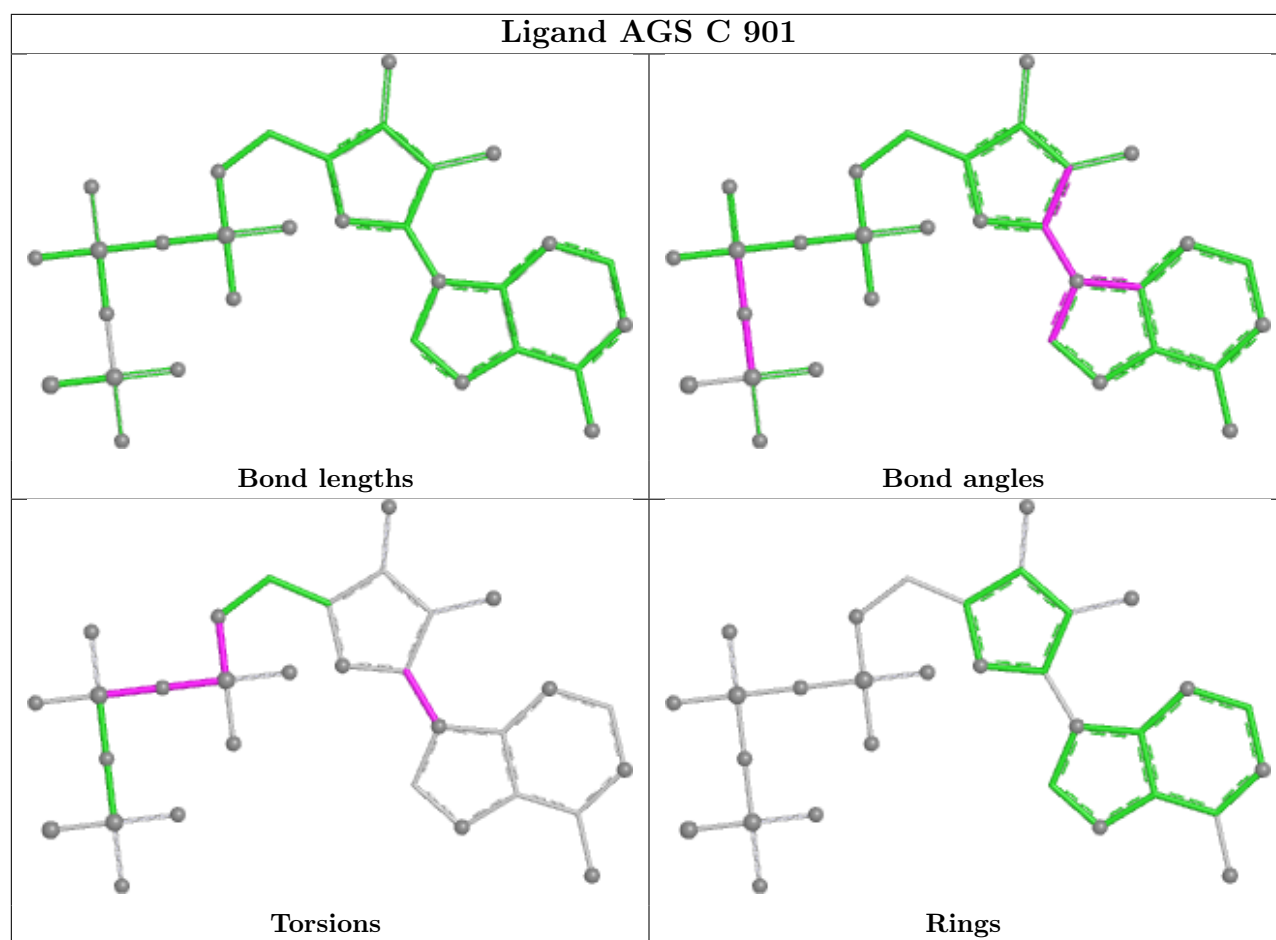












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

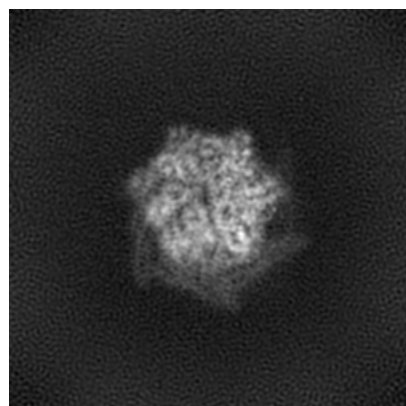
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3777. These allow visual inspection of the internal detail of the map and identification of artifacts.

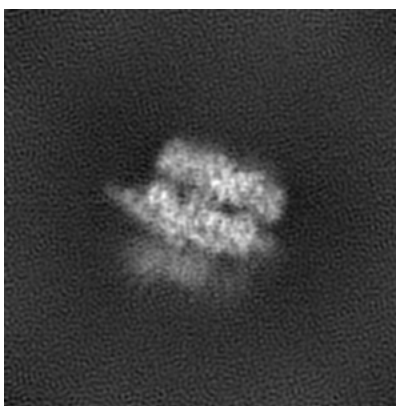
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

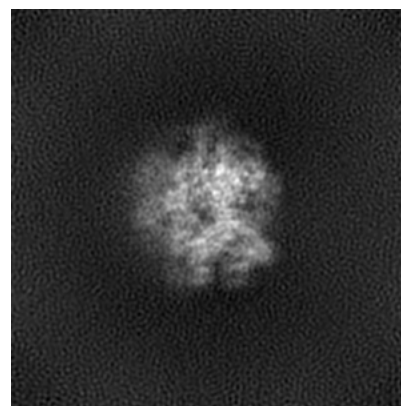
6.1.1 Primary map



X

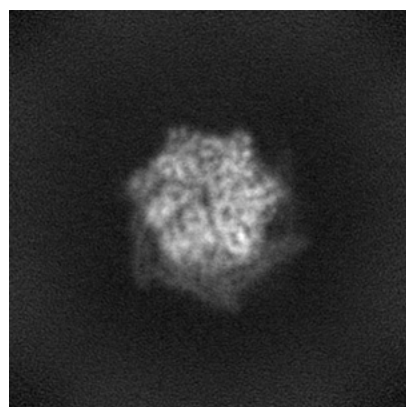


Y

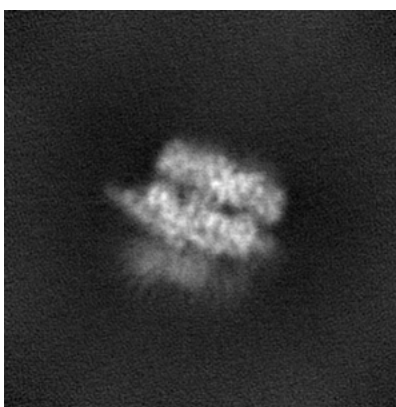


Z

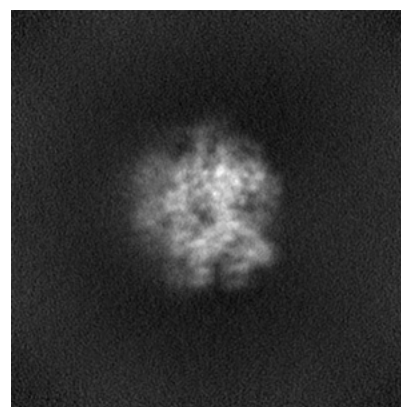
6.1.2 Raw map



X



Y

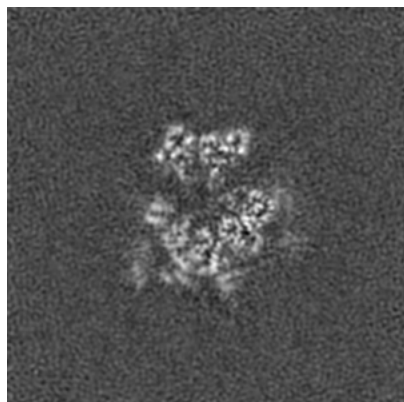


Z

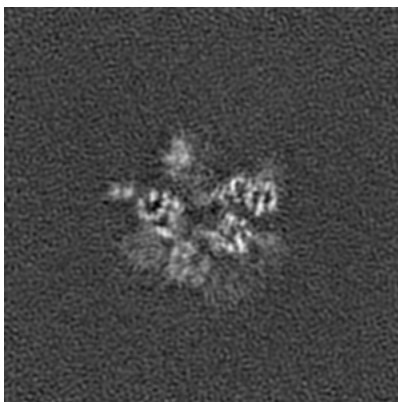
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

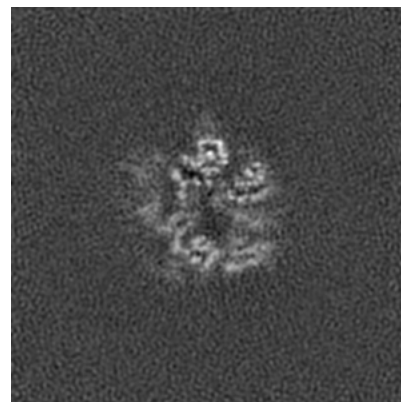
6.2.1 Primary map



X Index: 128

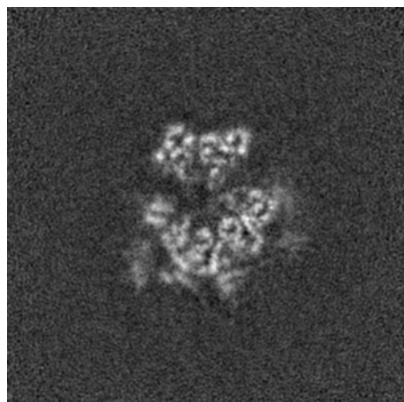


Y Index: 128

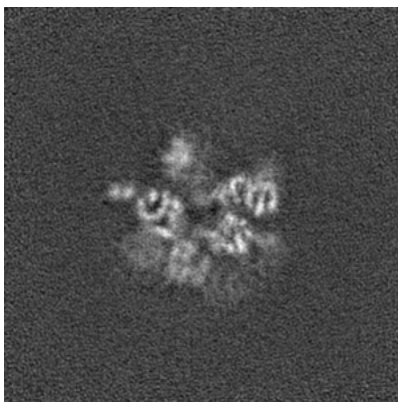


Z Index: 128

6.2.2 Raw map



X Index: 128



Y Index: 128

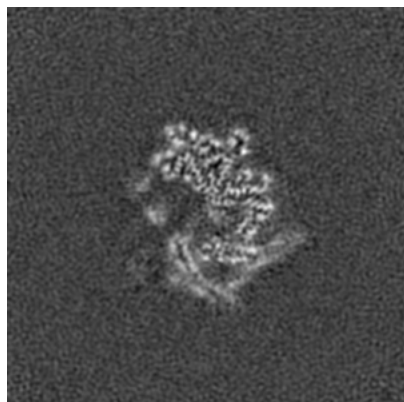


Z Index: 128

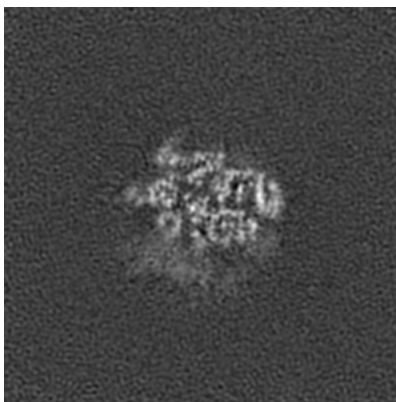
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

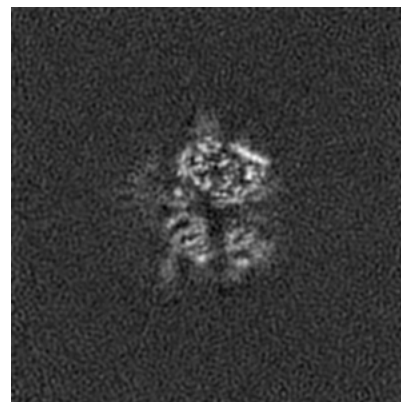
6.3.1 Primary map



X Index: 134

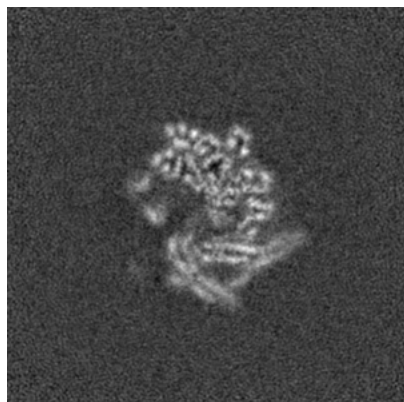


Y Index: 151

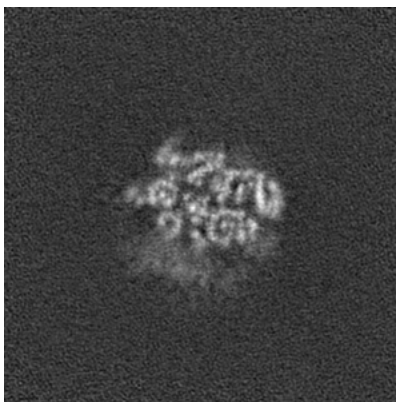


Z Index: 132

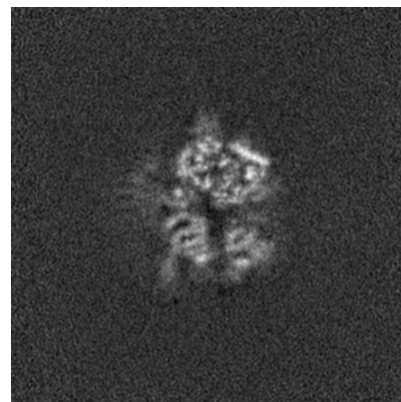
6.3.2 Raw map



X Index: 135



Y Index: 151

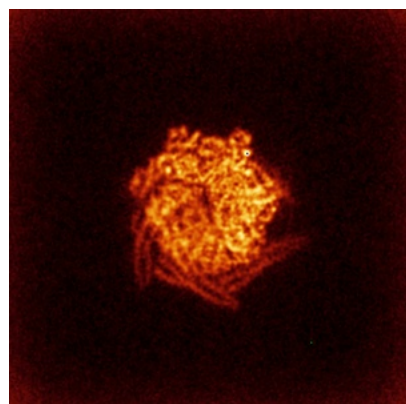


Z Index: 132

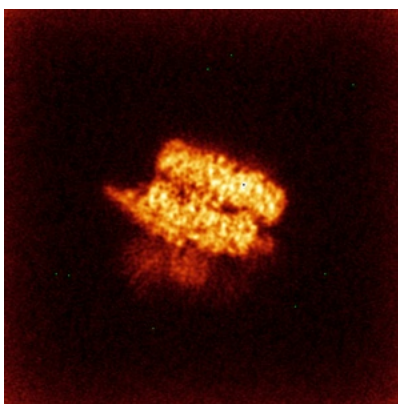
The images above show the largest variance slices of the map in three orthogonal directions.

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

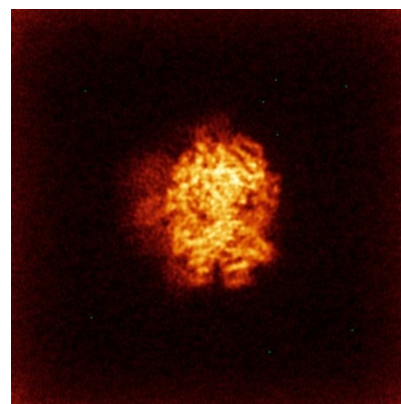
6.4.1 Primary map



X

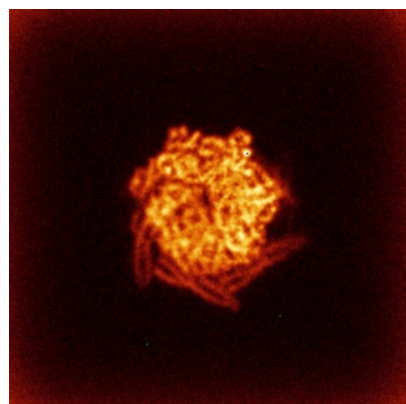


Y

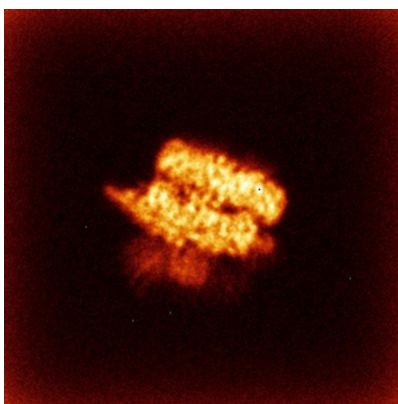


Z

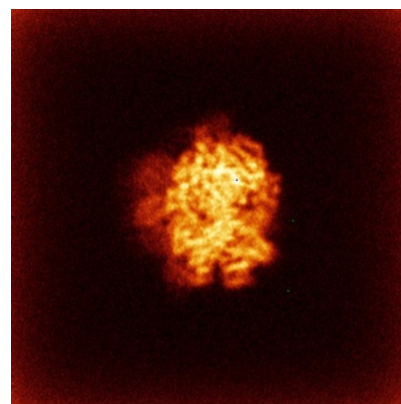
6.4.2 Raw map



X



Y

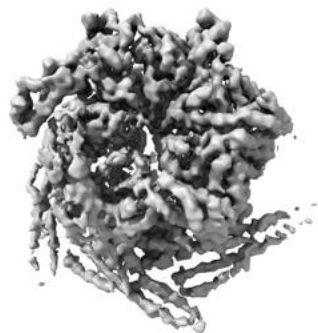


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. 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



X



Y



Z

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.

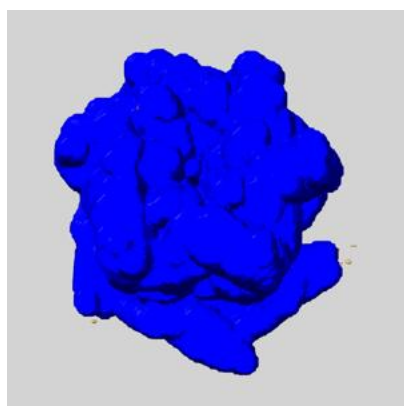
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

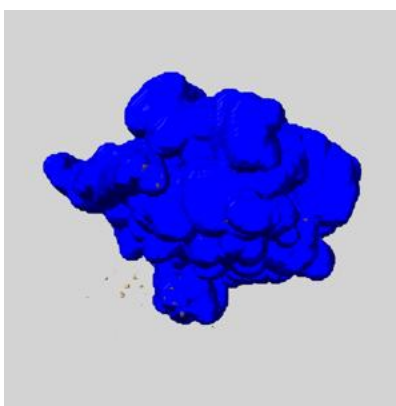
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

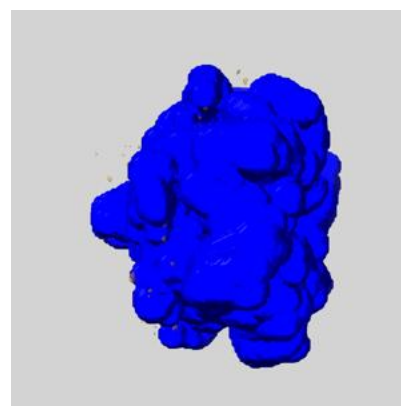
6.6.1 emd_3777_msk_1.map [i](#)



X



Y

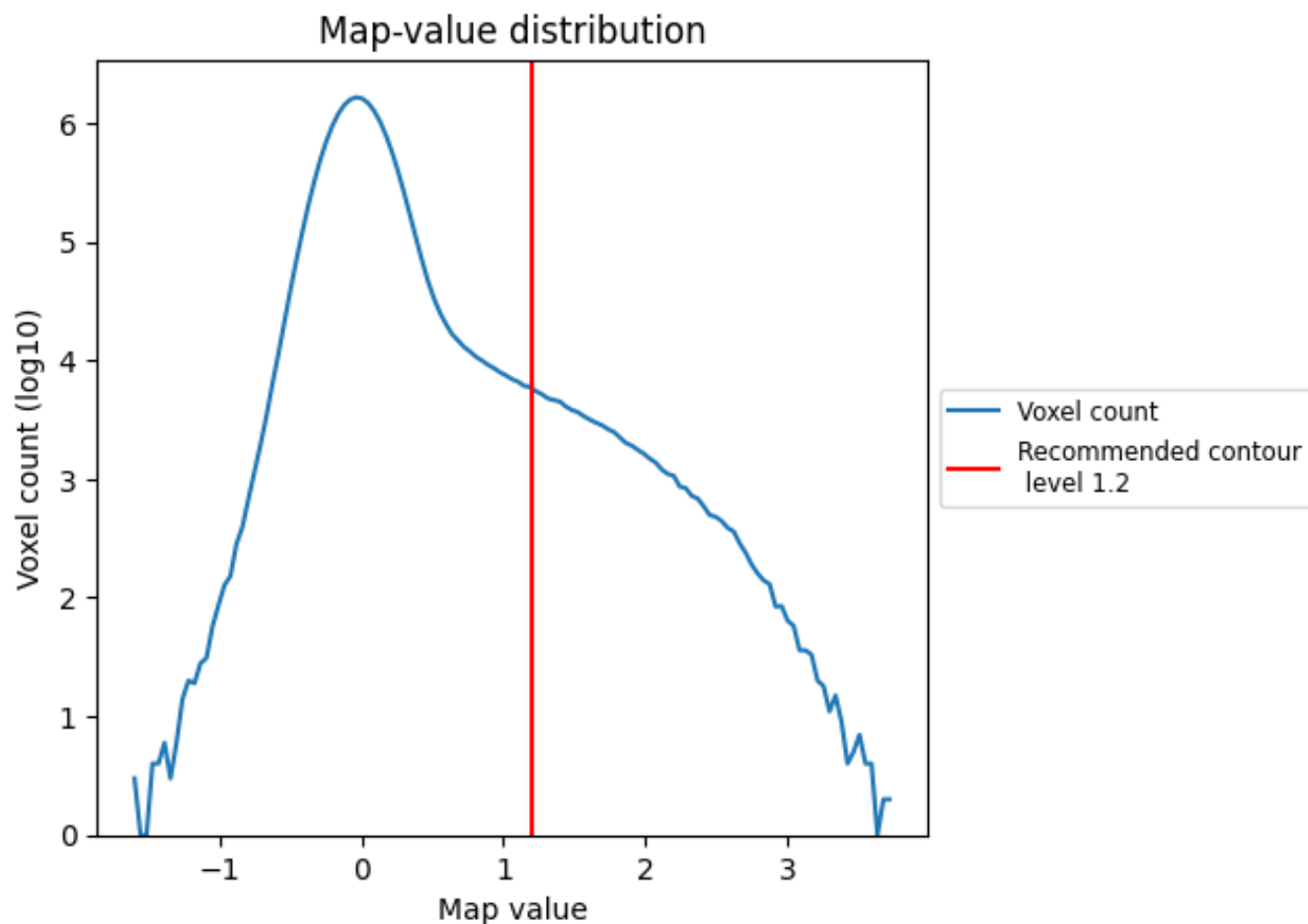


Z

7 Map analysis [i](#)

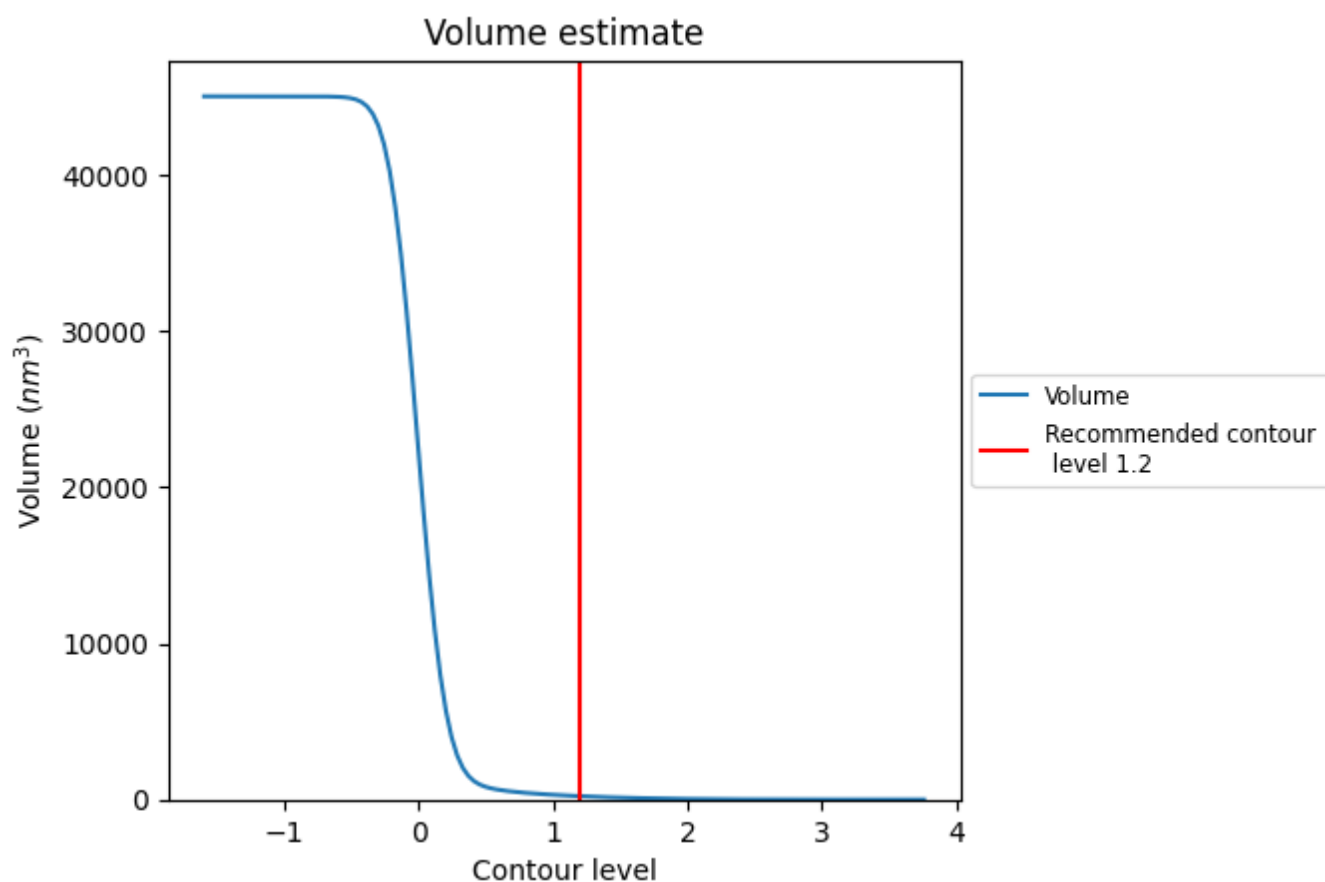
This section contains the results of statistical analysis of the map.

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.

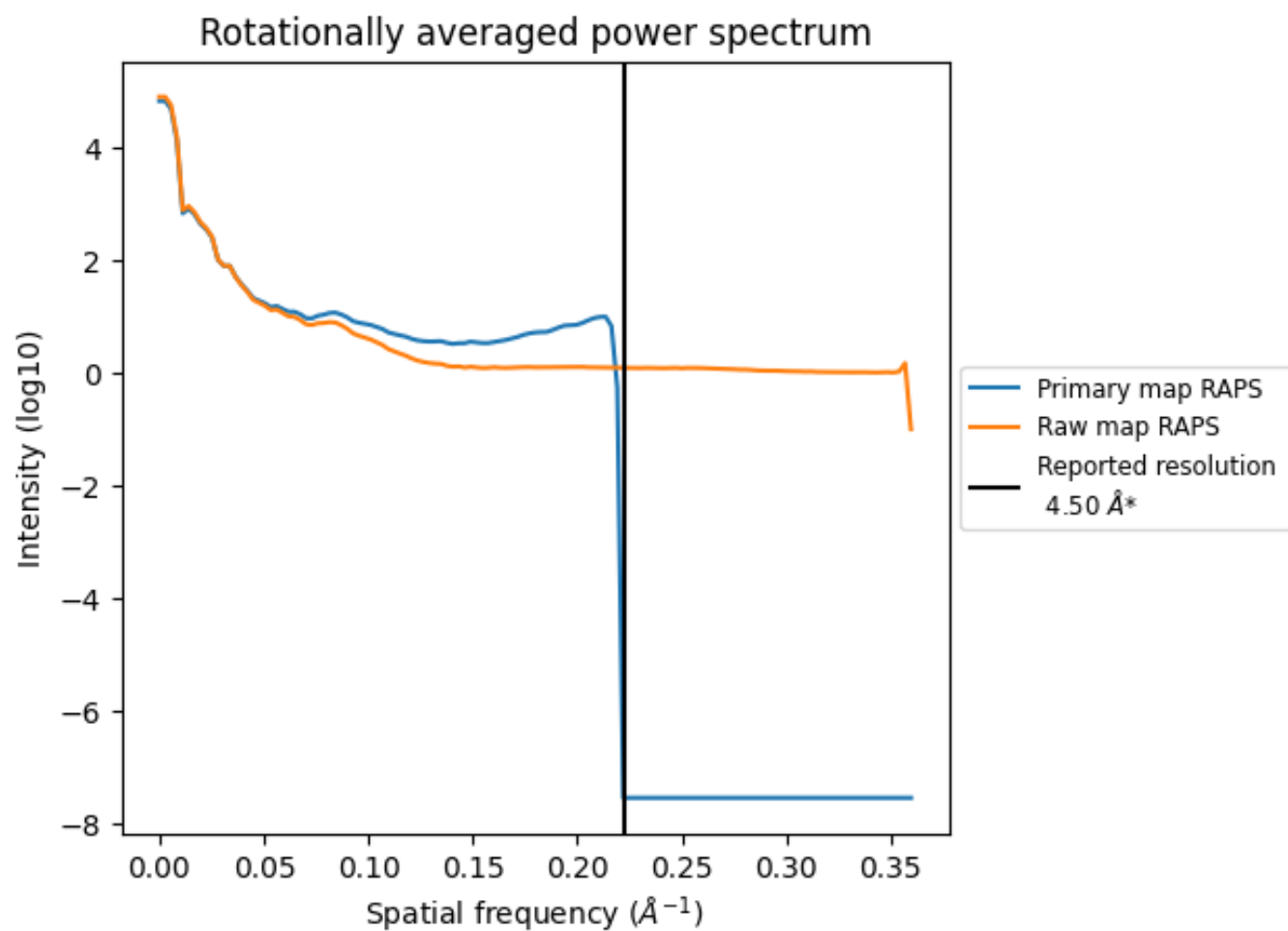
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217 nm³; this corresponds to an approximate mass of 196 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 ⓘ

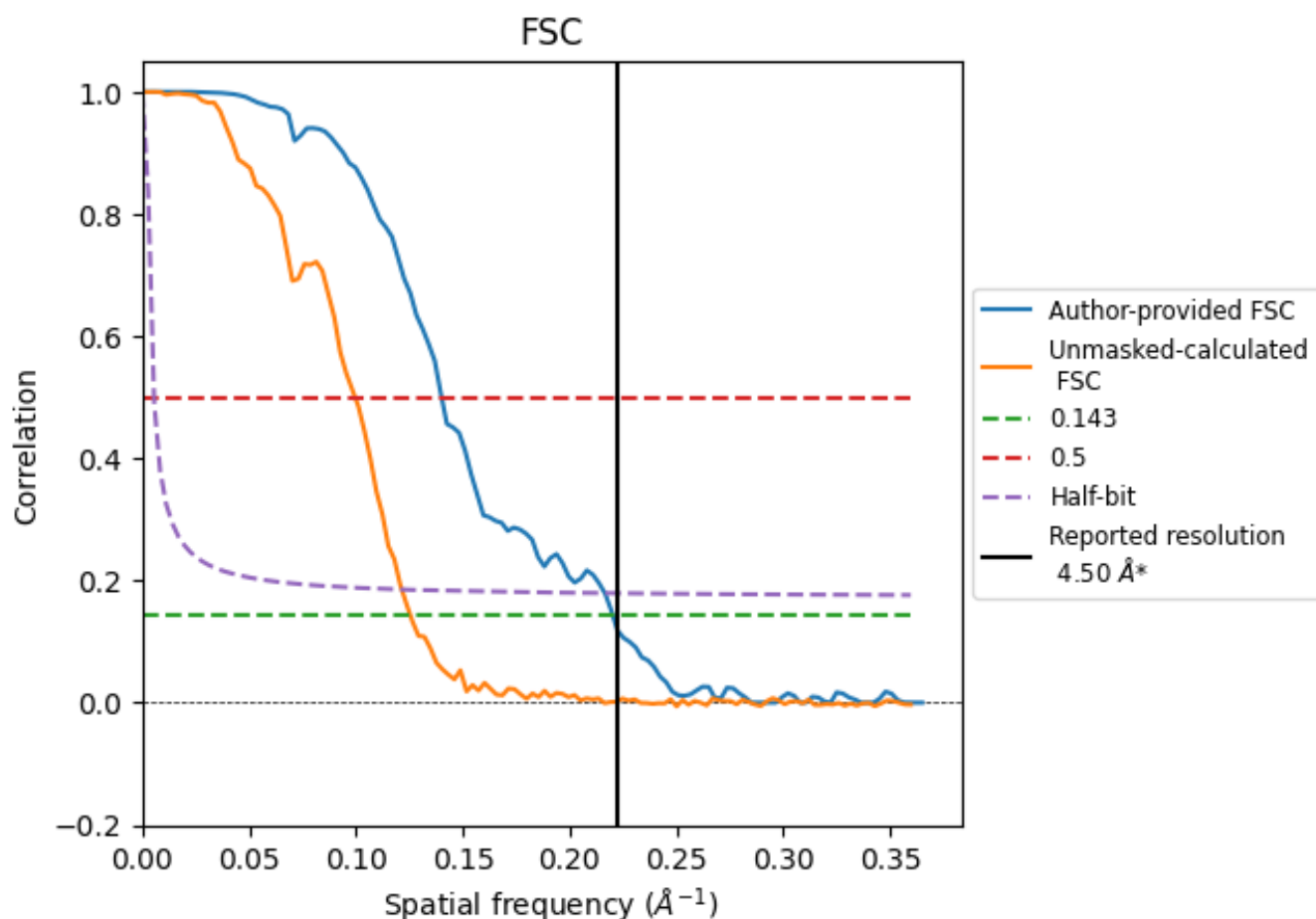


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 $0.222 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

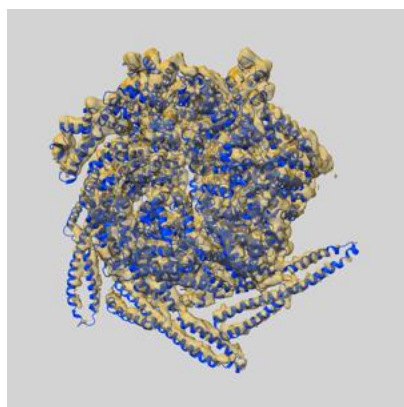
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	7.14	4.62
Unmasked-calculated*	7.97	10.04	8.23

*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 7.97 differs from the reported value 4.5 by more than 10 %

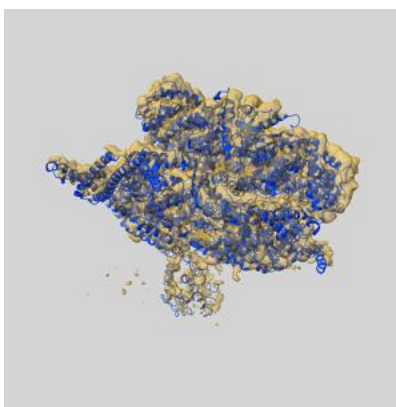
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3777 and PDB model 5OG1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

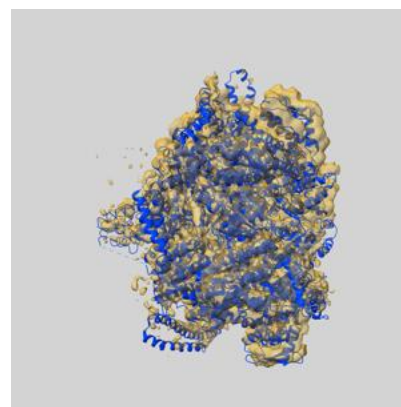
9.1 Map-model overlay [i](#)



X



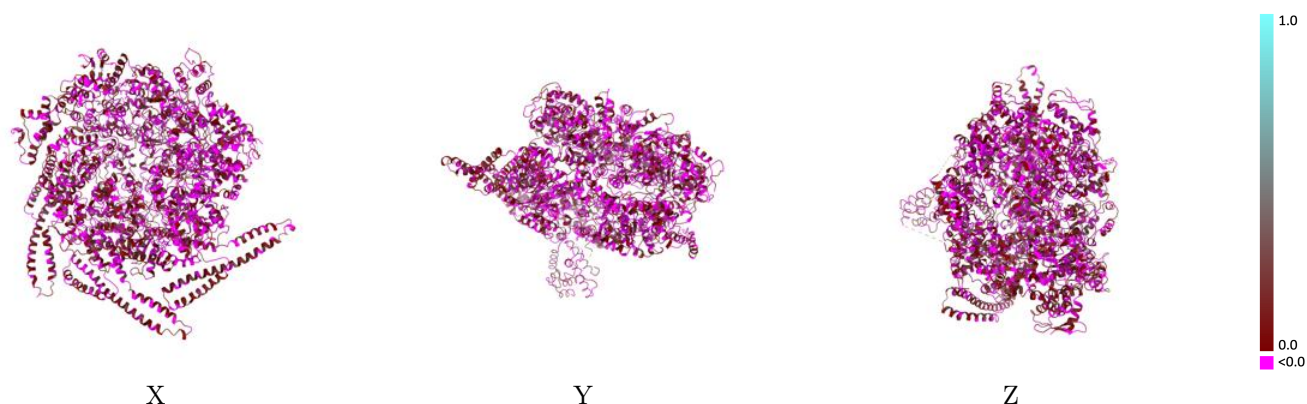
Y



Z

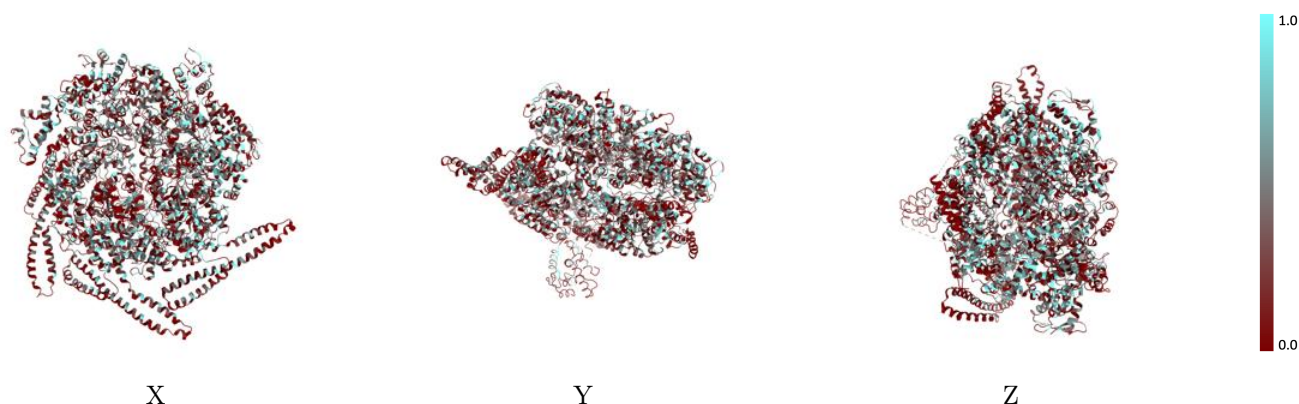
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



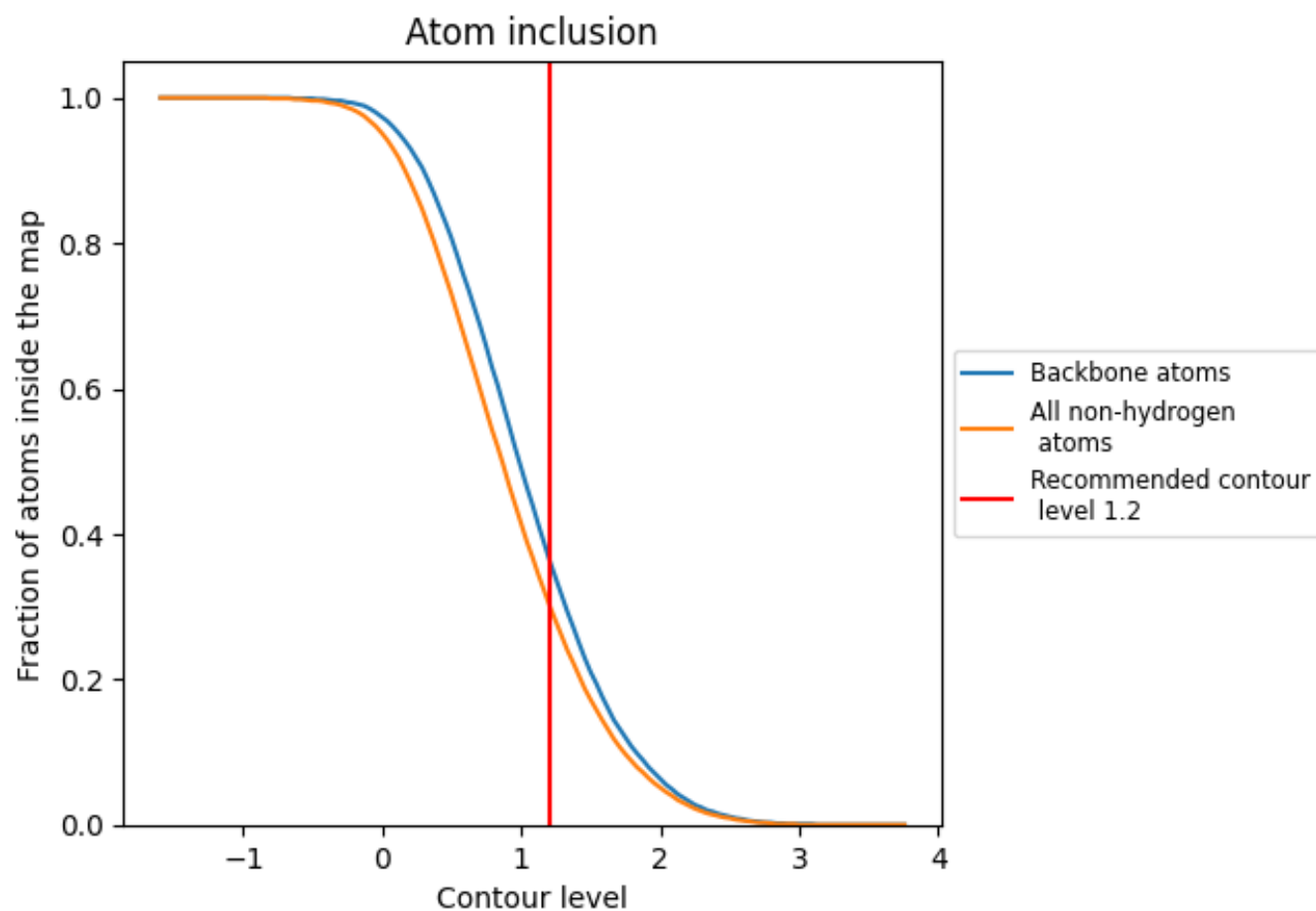
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 30% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3030	0.0230
A	0.2710	0.0440
B	0.3240	0.0230
C	0.3200	0.0170
D	0.3160	-0.0010
E	0.3160	0.0170
F	0.2800	0.0330

1.0

0.0

<0.0