



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 01:39 AM UTC

PDB ID : 8RU2 / pdb_00008ru2
EMDB ID : EMD-19503
Title : Structure of the F-actin barbed end bound by formin mDia1
Authors : Oosterheert, W.; Boiero Sanders, M.; Funk, J.; Prumbaum, D.; Raunser, S.; Bieling, P.
Deposited on : 2024-01-29
Resolution : 3.49 Å (reported)
Based on initial models : 3OBV, 8RTT

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:

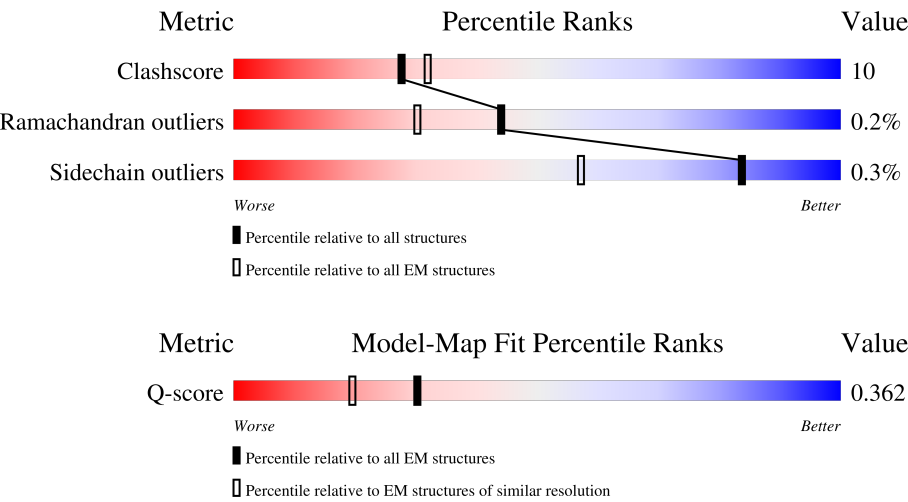
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.49 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	13600 (2.99 - 3.99)

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	B	374	<div><div></div><div>78%20%..</div></div>
1	C	374	<div><div></div><div>79%20%.</div></div>
1	D	374	<div><div></div><div>77%22%.</div></div>
2	E	783	<div><div>12%</div><div>35%12%53%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	783	<div><div><div></div><div></div><div></div></div><div>30%33%14%53%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14773 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 Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	370	Total	C	N	O	S	0	0
			2885	1828	486	550	21		
1	C	369	Total	C	N	O	S	0	0
			2873	1819	485	548	21		
1	D	370	Total	C	N	O	S	0	0
			2885	1828	486	550	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	272	ALA	CYS	engineered mutation	UNP P60709
C	272	ALA	CYS	engineered mutation	UNP P60709
D	272	ALA	CYS	engineered mutation	UNP P60709

- Molecule 2 is a protein called Methylated-DNA--protein-cysteine methyltransferase,Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	370	Total	C	N	O	S	0	0
			3023	1923	511	570	19		
2	F	370	Total	C	N	O	S	0	0
			3023	1923	511	570	19		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	479	MET	-	initiating methionine	UNP P16455
E	480	ALA	-	expression tag	UNP P16455
E	481	SER	-	expression tag	UNP P16455
E	482	THR	-	expression tag	UNP P16455
E	483	MET	-	expression tag	UNP P16455
E	484	ASP	-	expression tag	UNP P16455
E	485	ILE	-	expression tag	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
E	486	LYS	-	expression tag	UNP P16455
E	487	LEU	-	expression tag	UNP P16455
E	488	THR	-	expression tag	UNP P16455
E	489	GLY	-	expression tag	UNP P16455
E	490	GLU	-	expression tag	UNP P16455
E	491	PHE	-	expression tag	UNP P16455
E	492	ALA	-	expression tag	UNP P16455
E	554	ALA	CYS	engineered mutation	UNP P16455
E	617	ALA	LYS	engineered mutation	UNP P16455
E	619	THR	ALA	engineered mutation	UNP P16455
E	620	ALA	ARG	engineered mutation	UNP P16455
E	623	LYS	GLY	engineered mutation	UNP P16455
E	624	THR	GLY	engineered mutation	UNP P16455
E	626	LEU	MET	engineered mutation	UNP P16455
E	627	SER	ARG	engineered mutation	UNP P16455
E	642	SER	CYS	engineered mutation	UNP P16455
E	649	GLY	ASN	engineered mutation	UNP P16455
E	651	GLU	SER	engineered mutation	UNP P16455
E	675	PRO	-	linker	UNP P16455
E	676	ALA	-	linker	UNP P16455
E	677	GLY	-	linker	UNP P16455
E	678	GLY	-	linker	UNP P16455
E	679	SER	-	linker	UNP P16455
E	680	PRO	-	linker	UNP P16455
E	681	GLY	-	linker	UNP P16455
E	682	GLY	-	linker	UNP P16455
E	683	GLY	-	linker	UNP P16455
E	684	SER	-	linker	UNP P16455
E	685	GLY	-	linker	UNP P16455
E	686	GLY	-	linker	UNP P16455
E	687	SER	-	linker	UNP P16455
E	1256	HIS	-	expression tag	UNP O08808
E	1257	HIS	-	expression tag	UNP O08808
E	1258	HIS	-	expression tag	UNP O08808
E	1259	HIS	-	expression tag	UNP O08808
E	1260	HIS	-	expression tag	UNP O08808
E	1261	HIS	-	expression tag	UNP O08808
F	479	MET	-	initiating methionine	UNP P16455
F	480	ALA	-	expression tag	UNP P16455
F	481	SER	-	expression tag	UNP P16455
F	482	THR	-	expression tag	UNP P16455
F	483	MET	-	expression tag	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
F	484	ASP	-	expression tag	UNP P16455
F	485	ILE	-	expression tag	UNP P16455
F	486	LYS	-	expression tag	UNP P16455
F	487	LEU	-	expression tag	UNP P16455
F	488	THR	-	expression tag	UNP P16455
F	489	GLY	-	expression tag	UNP P16455
F	490	GLU	-	expression tag	UNP P16455
F	491	PHE	-	expression tag	UNP P16455
F	492	ALA	-	expression tag	UNP P16455
F	554	ALA	CYS	engineered mutation	UNP P16455
F	617	ALA	LYS	engineered mutation	UNP P16455
F	619	THR	ALA	engineered mutation	UNP P16455
F	620	ALA	ARG	engineered mutation	UNP P16455
F	623	LYS	GLY	engineered mutation	UNP P16455
F	624	THR	GLY	engineered mutation	UNP P16455
F	626	LEU	MET	engineered mutation	UNP P16455
F	627	SER	ARG	engineered mutation	UNP P16455
F	642	SER	CYS	engineered mutation	UNP P16455
F	649	GLY	ASN	engineered mutation	UNP P16455
F	651	GLU	SER	engineered mutation	UNP P16455
F	675	PRO	-	linker	UNP P16455
F	676	ALA	-	linker	UNP P16455
F	677	GLY	-	linker	UNP P16455
F	678	GLY	-	linker	UNP P16455
F	679	SER	-	linker	UNP P16455
F	680	PRO	-	linker	UNP P16455
F	681	GLY	-	linker	UNP P16455
F	682	GLY	-	linker	UNP P16455
F	683	GLY	-	linker	UNP P16455
F	684	SER	-	linker	UNP P16455
F	685	GLY	-	linker	UNP P16455
F	686	GLY	-	linker	UNP P16455
F	687	SER	-	linker	UNP P16455
F	1256	HIS	-	expression tag	UNP O08808
F	1257	HIS	-	expression tag	UNP O08808
F	1258	HIS	-	expression tag	UNP O08808
F	1259	HIS	-	expression tag	UNP O08808
F	1260	HIS	-	expression tag	UNP O08808
F	1261	HIS	-	expression tag	UNP O08808

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0

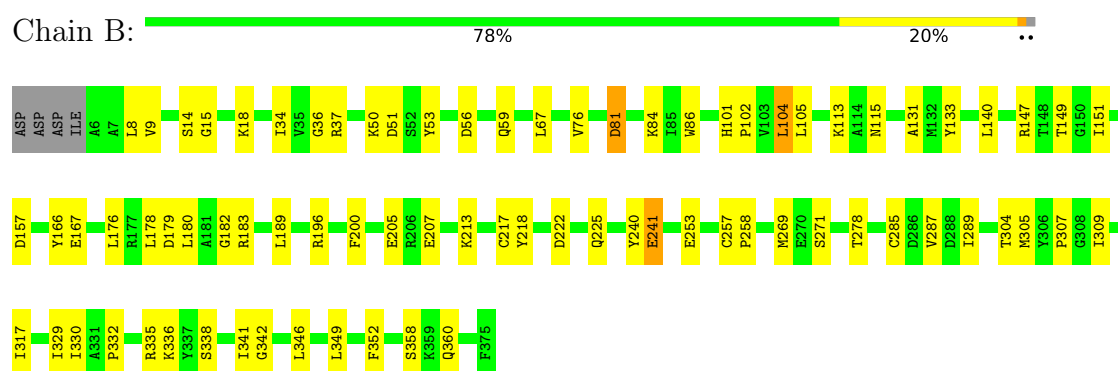
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0

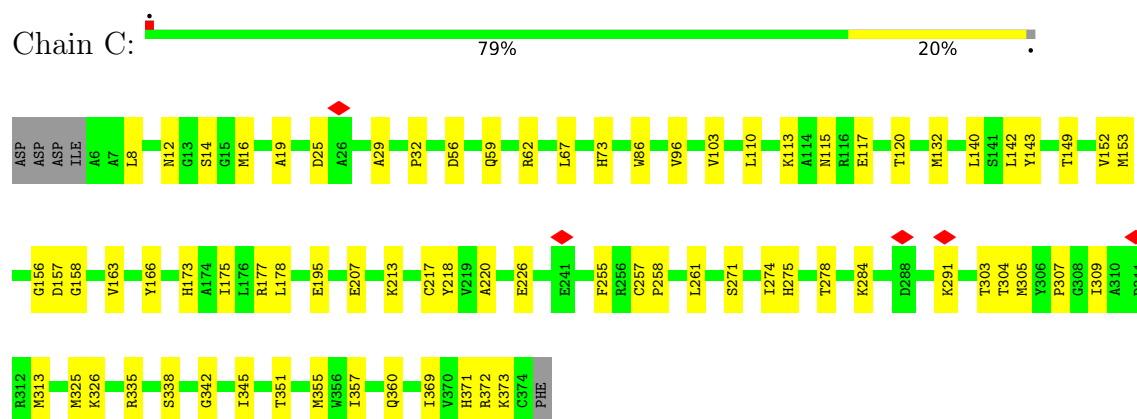
3 Residue-property plots

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

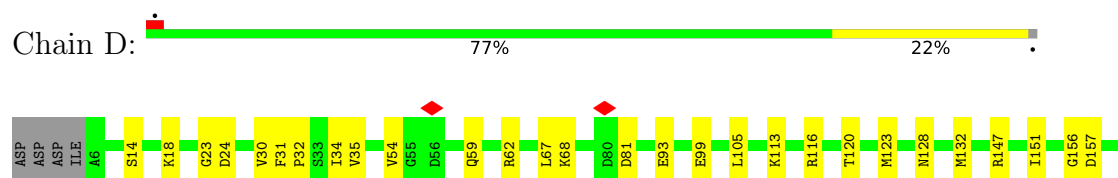
- Molecule 1: Actin, cytoplasmic 1, N-terminally processed

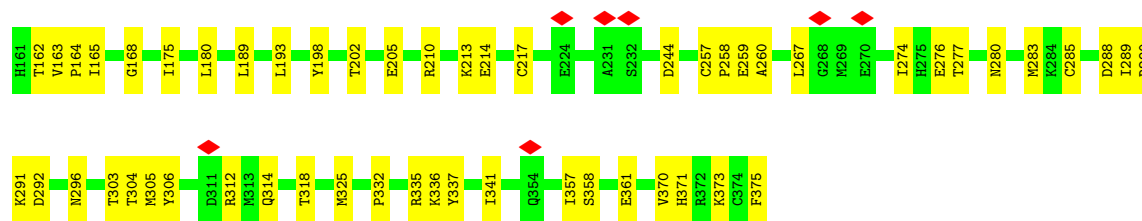


- Molecule 1: Actin, cytoplasmic 1, N-terminally processed

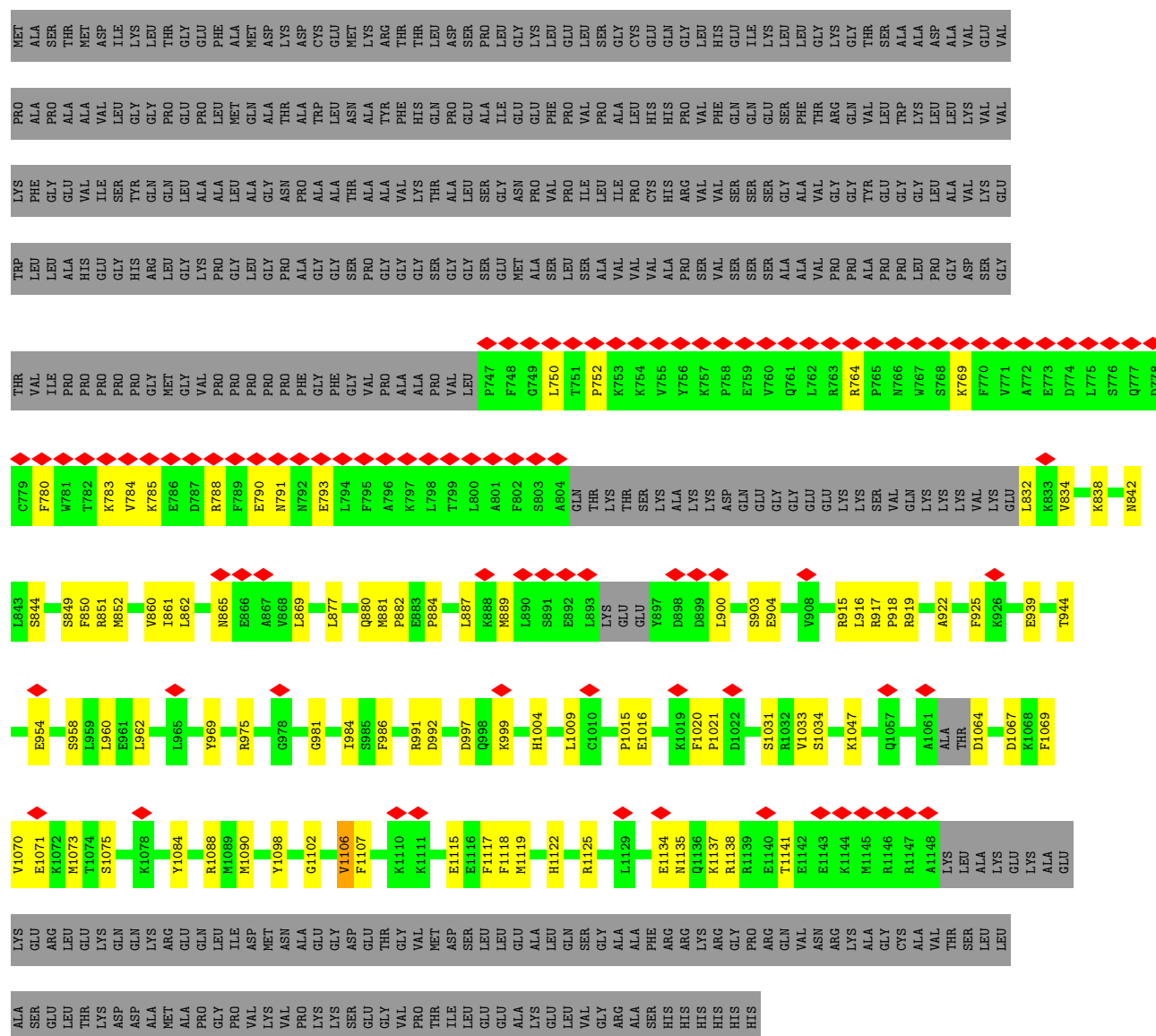
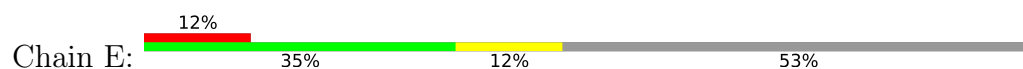


- Molecule 1: Actin, cytoplasmic 1, N-terminally processed

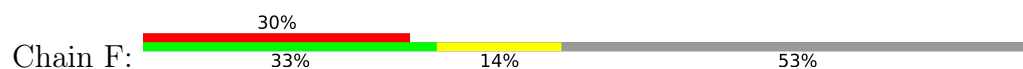




- Molecule 2: Methylated-DNA--protein-cysteine methyltransferase,Protein diaphanous homolog 1



- Molecule 2: Methylated-DNA--protein-cysteine methyltransferase,Protein diaphanous homolog 1



ASP	ALA	GLN	Y1104	Q1039	A979	R917	M852	T782	LYS	TRP	LYS	PRO	ALA	MET
ALA	GLN	LYS	F1105	K1040	F980	G917	P853	K783	ALA	ALA	PHE	ALA	ALA	ALA
MET	ARG	ARG	V1106	S1041	G981	L920	Y854	V784	PRO	PRO	GLY	PRO	ALA	THR
PRO	GLN	GLN	F1107	D1042	F982	N921	Q855	K785	VAL	VAL	VAL	ALA	ALA	THR
GLY	LEU	LEU	D1108	L1043	F983	A922	E856	R788	GLU	GLU	ILE	VAL	ASP	ASP
PRO	ILE	ASP	P1109	Q1044	I984	I923	I857	F789	PRO	PRO	THR	LEU	ILE	ILE
VAL	ASP	ASP	K1110	M1045	S985	F925	V860	E790	LYS	LYS	THR	GLY	LYS	LYS
LYS	MET	ASP	K1111	K1046	F986	Q928	I861	N791	GLU	GLU	THR	GLY	GLY	GLY
VAL	ASN	ASN	L1112	Q1048	L987	F929	L862	M792	PRO	PRO	ALA	GLY	GLY	THR
PRO	ALA	ALA	S1113	I1049	C988	S930	E863	E793	GLY	GLY	ALA	PRO	GLY	GLY
LYS	GLY	GLY	V1114	A1050	X989	E931	V864	L794	LYS	LYS	ALA	PRO	ALA	PHE
SER	ASP	ASP	E1115	V1052	L990	Q932	N865	F795	GLY	GLY	LEU	LEU	ALA	ALA
GLU	GLU	GLU	E1116	E1053	R991	V933	E866	T799	PRO	PRO	ALA	MET	GLN	MET
VAL	THR	THR	F1117	R1054	D992	E934	A867	F802	GLY	GLY	ALA	GLN	ALA	ASP
THR	MET	ASP	F1118	E1054	T993	N935	V868	S803	ALA	ALA	PRO	ALA	TRP	ASP
ILE	ASP	ASP	M1119	Q1057	K994	I936	L869	A804	GLY	GLY	ALA	TRP	ALA	CYS
LEU	SER	SER	D1120	N1058	S995	K937	T870	E802	GLY	GLY	ALA	ALA	ALA	GLY
LEU	LEU	LEU	L1121	F1059	A996	P938	E871	A804	THR	THR	ALA	ASN	GLY	MET
GLU	GLU	GLU	H1122	P1060	D997	E939	S872	T870	GLY	GLY	VAL	ALA	ALA	LYS
ALA	ALA	ALA	H1123	A1061	Q998	I940	Q875	ALA	GLY	GLY	ALA	THR	ALA	THR
GLU	LEU	LEU	M1124	THR	Q999	V941	N876	PRO	SER	SER	THR	THR	GLN	LEU
LEU	GLN	GLN	F1125	E1064	M1000	S942	L877	VAL	LYS	LYS	ALA	ALA	PRO	ASP
VAL	SER	SER	M1126	E1065	T1001	V943	K879	LEU	LYS	LYS	GLY	GLY	GLY	SER
ARG	ALA	ALA	M1127	ALA	L1002	E944	Q880	F748	ILE	ILE	ALA	ILE	ALA	PRO
ALA	ALA	ALA				T944	M881	G749	GLY	GLY	GLY	GLY	ALA	LEU
ALA	ALA	ALA				A945	P882	L750	GLY	GLY	PRO	PRO	GLY	LYS
SER	PHE	PHE	F1128	K1068	L1003	A946	E883	L751	VAL	VAL	VAL	PHE	PHE	LEU
HIS	ARG	ARG	L1129	F1069	H1004	C947	P884	P752	PRO	PRO	VAL	PRO	GLY	GLY
HIS	ARG	ARG	Q1130	E1070	F1005	E948	E885	K753	LEU	LEU	VAL	VAL	ILE	LEU
HIS	LYS	LYS	A1131	E1071	L1006	E948	Q886	K754	PRO	PRO	ALA	ALA	ILE	SER
HIS	GLY	GLY	V1132	M1072	A1007	E949	L887	V755	LEU	LEU	ALA	ALA	ILE	GLY
PRO	PRO	PRO	K1133	M1073	E1008	L950	K888	Y756	VAL	VAL	PRO	PRO	PRO	CYS
ARG	ARG	ARG	E1134	T1074	L1009	R951	M889	Y757	VAL	VAL	CYS	HIS	HIS	GLY
VAL	GLN	GLN	M1135	S1075	C1010	K952	L890	K757	ALA	ALA	GLN	HIS	HIS	GLN
ASN	ASN	ASN	Q1136	F1076	E1011	S953	S891	P758	VAL	VAL	ARG	PRO	ARG	GLY
ARG	LYS	LYS	K1137	V1077	N1012	E954	E892	E759	VAL	VAL	VAL	VAL	VAL	LEU
LYS	ALA	ALA	R1138	D1079	D1013	N955	L893	V760	THR	THR	PHE	PHE	PHE	GLY
PRO	PRO	PRO	R1139	A1080	H1014	F956	L932	Q761	GLY	GLY	GLN	GLN	GLN	ILE
GLY	CYS	CYS	R1140	Q1081	H1015	S957	GLY	R763	SER	SER	SER	SER	SER	LYS
ALA	ALA	ALA	E1141	E1082	P1015	S958	GLU	R764	ALA	ALA	ALA	ALA	ALA	LEU
VAL	VAL	VAL	T1141	E1082	E1016	S958	Y897	F765	VAL	VAL	VAL	VAL	VAL	GLY
THR	THR	THR	E1142	L1087	V1017	L959	D898	W766	THR	THR	THR	THR	THR	GLY
SER	SER	SER	E1143	R1088	L1018	L960	D899	W834	GLY	GLY	GLY	GLY	GLY	LYS
LEU	LEU	LEU	F1143	M1089	K1019	E961	L900	S768	ALA	ALA	ALA	ALA	ALA	THR
LEU	LEU	LEU	K1144	M1090	F1020	L962	A901	K769	PRO	PRO	PRO	PRO	PRO	GLY
ALA	ALA	ALA	M1145	H1091	P1021	T963	E904	F770	LYS	LYS	LYS	LYS	LYS	ALA
SER	SER	SER	R1146	M1090	D1022	T963	G907	D774	GLY	GLY	GLY	GLY	GLY	ASP
GLU	GLU	GLU	R1147	S1092	E1023	L964	V909	L775	LEU	LEU	LEU	LEU	LEU	ALA
LEU	LEU	LEU	A1148	N1093	E1024	L965	M910	Q777	VAL	VAL	VAL	VAL	VAL	VAL
THR	THR	THR	LYS	M1094	L1024	V966	G907	D778	GLY	GLY	GLY	GLY	GLY	VAL
LYS	LYS	LYS	ALA	E1095	A1025	G967	V909	L778	ASP	ASP	ASP	ASP	ASP	GLY
ASP	ASP	ASP	LEU	T1096	H1026	N968	G911	F846	GLY	GLY	GLY	GLY	GLY	VAL
			LYS	L1097	E1027	Y969	M910	R851	VAL	VAL	VAL	VAL	VAL	VAL
			GLY	Y1098	V1028	M970	T912		GLY	GLY	GLY	GLY	GLY	GLY
			LYS	K1099	E1029	N971	R915		GLY	GLY	GLY	GLY	GLY	GLY
			ALA	E1100	A1030	A972	L916		GLY	GLY	GLY	GLY	GLY	GLY
			GLU	L1101	S1031	G973			GLY	GLY	GLY	GLY	GLY	GLY
			LYS	D1102	R1032	S974			GLY	GLY	GLY	GLY	GLY	GLY
			ARG	G1102	V1033	R975			GLY	GLY	GLY	GLY	GLY	GLY
			LEU	D1103	S1034	N976			GLY	GLY	GLY	GLY	GLY	GLY
			LYS		A1035	N976			GLY	GLY	GLY	GLY	GLY	GLY
			GLN		E1036	G978			GLY	GLY	GLY	GLY	GLY	GLY
					N1037				GLY	GLY	GLY	GLY	GLY	GLY
					L1038				GLY	GLY	GLY	GLY	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150807	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 ($e^-/\text{\AA}^2$)	67.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.553	Depositor
Minimum map value	-1.222	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.367	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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: ADP, HIC, MG

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	B	0.11	0/2935	0.26	0/3972
1	C	0.11	0/2922	0.27	0/3956
1	D	0.11	0/2935	0.24	0/3972
2	E	0.10	0/3075	0.29	0/4126
2	F	0.11	0/3075	0.30	0/4126
All	All	0.11	0/14942	0.27	0/20152

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	B	2885	0	2857	50	0
1	C	2873	0	2848	45	0
1	D	2885	0	2857	55	0
2	E	3023	0	3028	65	0
2	F	3023	0	3028	87	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	14773	0	14654	286	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 10.

The worst 5 of 286 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:14:SER:HB2	1:D:157:ASP:HB3	1.69	0.74
1:C:304:THR:O	1:C:335:ARG:NH1	2.23	0.71
2:F:924:LEU:HD12	2:F:928:GLN:HE22	1.56	0.70
1:D:304:THR:O	1:D:335:ARG:NH1	2.25	0.70
1:C:14:SER:HB2	1:C:157:ASP:HB2	1.74	0.70

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	B	367/374 (98%)	357 (97%)	10 (3%)	0	100	100
1	C	366/374 (98%)	355 (97%)	11 (3%)	0	100	100
1	D	367/374 (98%)	358 (98%)	9 (2%)	0	100	100
2	E	362/783 (46%)	345 (95%)	15 (4%)	2 (1%)	21	54
2	F	362/783 (46%)	343 (95%)	18 (5%)	1 (0%)	36	67
All	All	1824/2688 (68%)	1758 (96%)	63 (4%)	3 (0%)	44	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1070	VAL
2	F	1070	VAL
2	E	1106	VAL

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	B	311/315 (99%)	308 (99%)	3 (1%)	68	75
1	C	310/315 (98%)	310 (100%)	0	100	100
1	D	311/315 (99%)	311 (100%)	0	100	100
2	E	338/660 (51%)	338 (100%)	0	100	100
2	F	338/660 (51%)	336 (99%)	2 (1%)	78	79
All	All	1608/2265 (71%)	1603 (100%)	5 (0%)	84	83

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

Mol	Chain	Res	Type
1	B	81	ASP
1	B	104	LEU
1	B	241	GLU
2	F	770	PHE
2	F	1017	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	761	GLN
2	F	905	GLN
2	F	880	GLN
1	D	246	GLN
2	E	1130	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	HIC	C	73	1	10,11,12	0.46	0	9,14,16	0.55	0
1	HIC	D	73	1	10,11,12	0.48	0	9,14,16	0.55	0
1	HIC	B	73	1	10,11,12	0.47	0	9,14,16	0.56	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
1	HIC	C	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	73	HIC	CA-CB-CG-ND1
1	C	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	401	4	28,29,29	1.39	4 (14%)	43,45,45	1.80	10 (23%)
3	ADP	D	401	4	28,29,29	1.40	4 (14%)	43,45,45	1.82	8 (18%)
3	ADP	B	401	4	28,29,29	1.41	4 (14%)	43,45,45	1.78	9 (20%)

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	ADP	C	401	4	-	5/16/32/32	0/3/3/3
3	ADP	D	401	4	-	4/16/32/32	0/3/3/3
3	ADP	B	401	4	-	3/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C4	4.64	1.47	1.39
3	D	401	ADP	C5-C4	4.64	1.47	1.39
3	C	401	ADP	C5-C4	4.61	1.47	1.39
3	D	401	ADP	C5-C6	2.69	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C6	2.64	1.48	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C5-C4-N3	-5.88	118.62	126.72
3	B	401	ADP	C5-C4-N3	-5.64	118.95	126.72
3	C	401	ADP	C5-C4-N3	-5.63	118.97	126.72
3	D	401	ADP	N3-C4-N9	4.66	135.09	127.17
3	C	401	ADP	N3-C4-N9	4.48	134.79	127.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

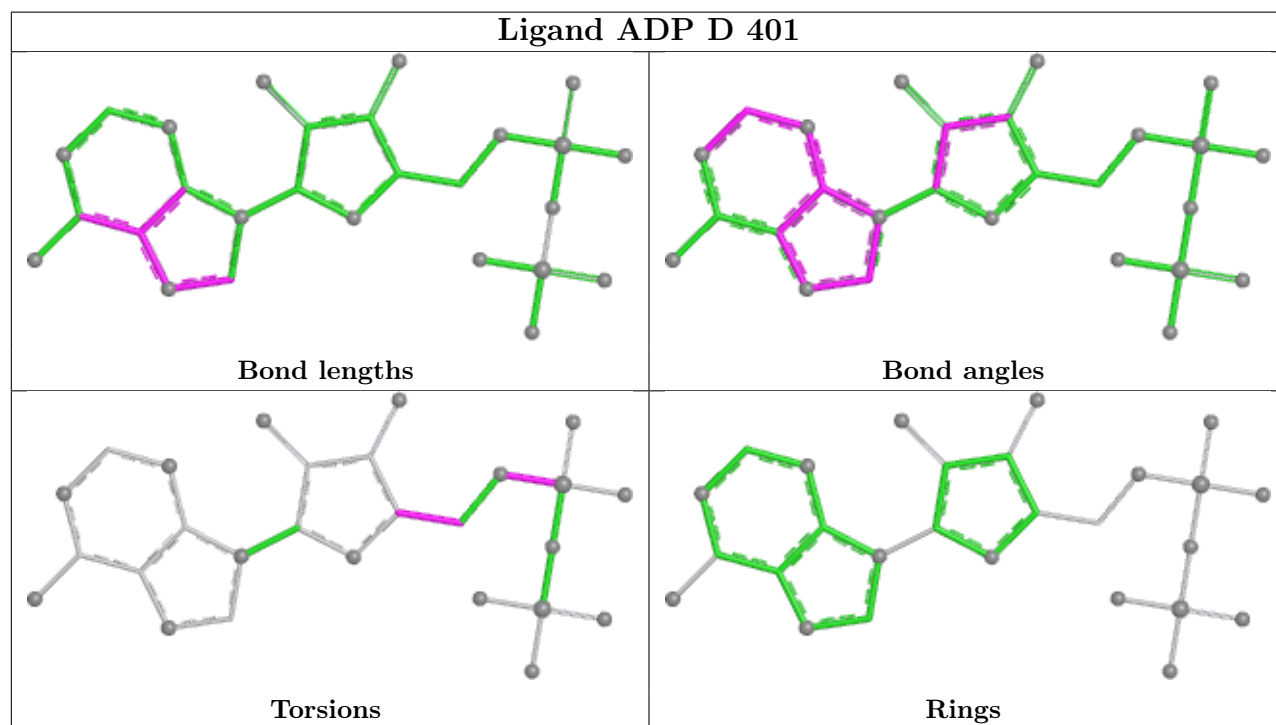
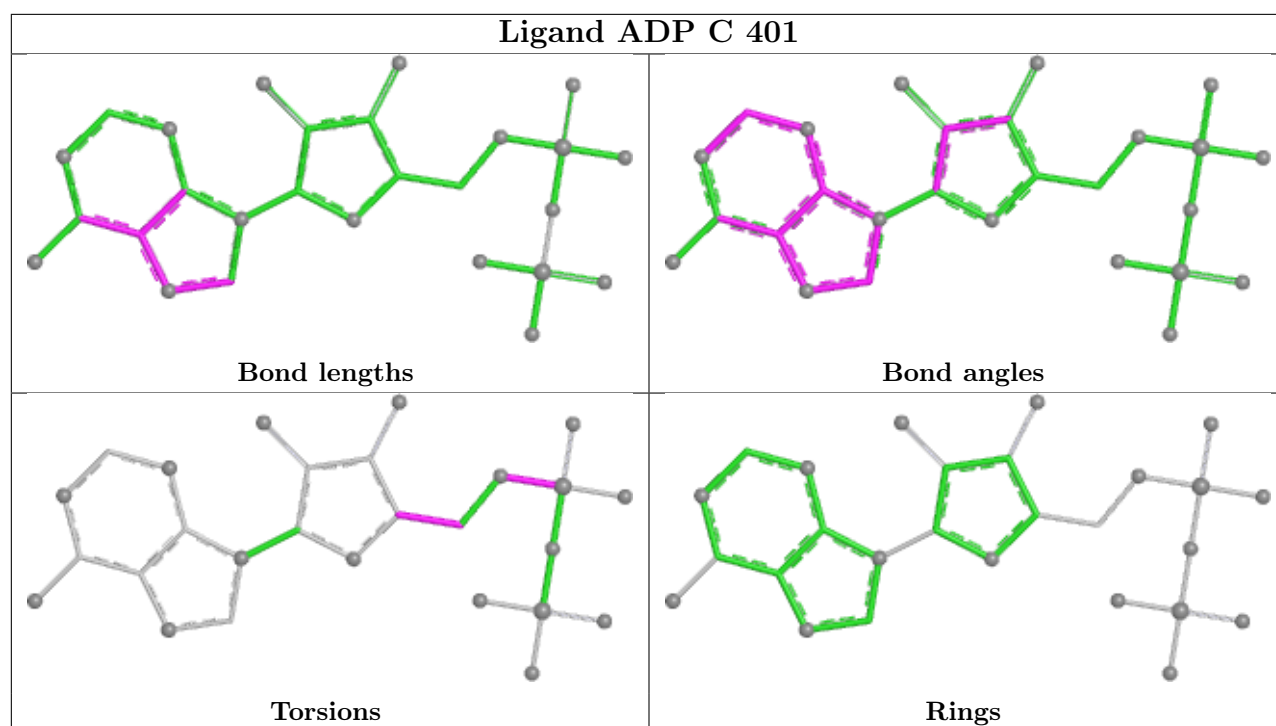
Mol	Chain	Res	Type	Atoms
3	B	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	O4'-C4'-C5'-O5'
3	C	401	ADP	C5'-O5'-PA-O1A
3	C	401	ADP	C5'-O5'-PA-O2A
3	C	401	ADP	C5'-O5'-PA-O3A

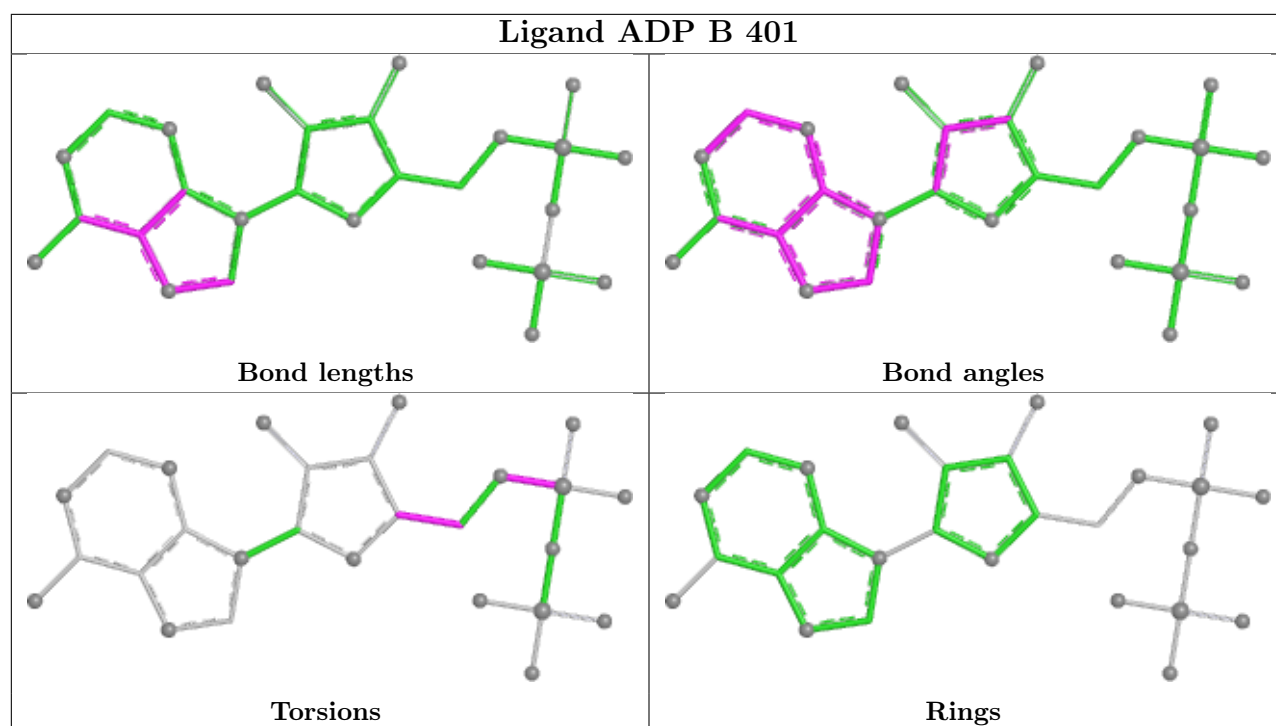
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	1	0
3	B	401	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

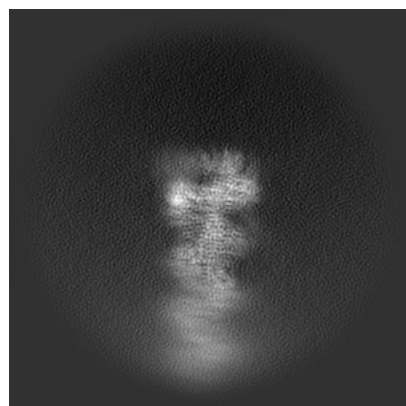
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19503. These allow visual inspection of the internal detail of the map and identification of artifacts.

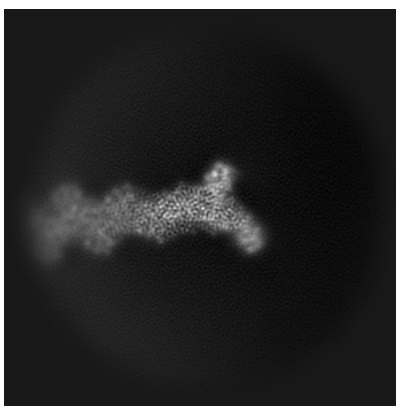
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

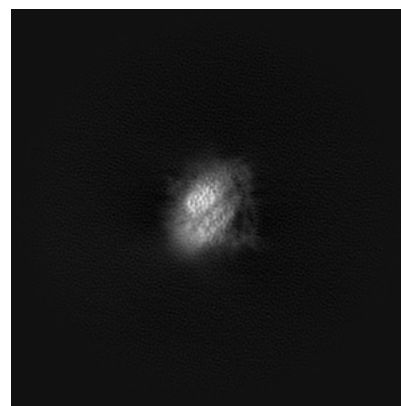
6.1.1 Primary map



X

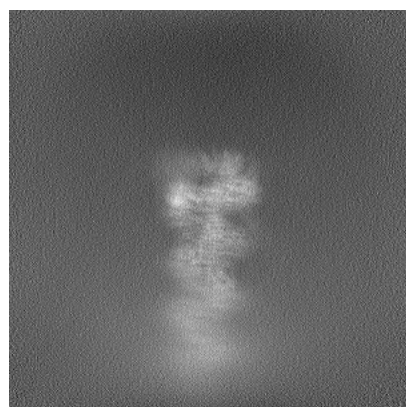


Y

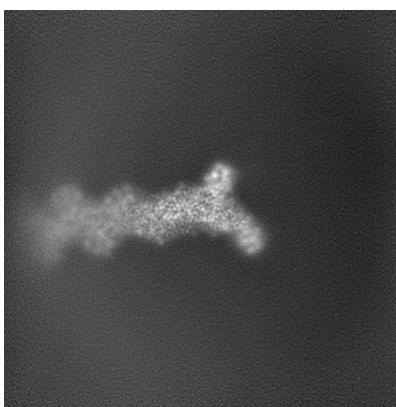


Z

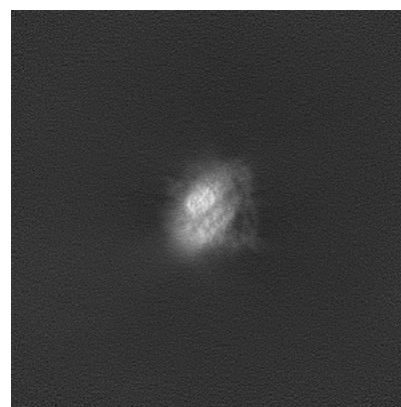
6.1.2 Raw map



X



Y

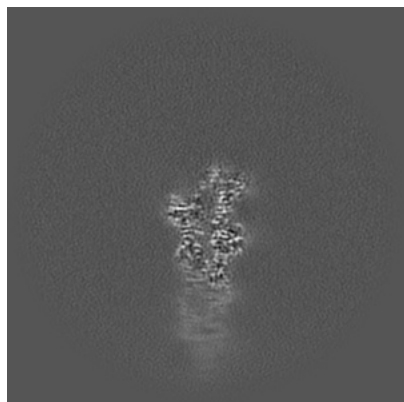


Z

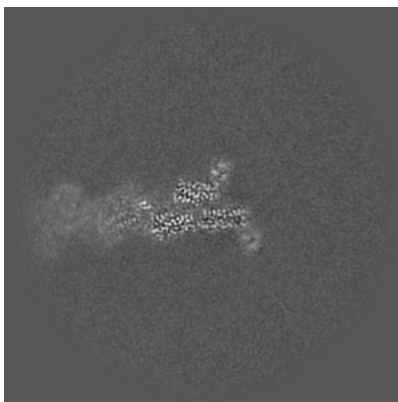
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

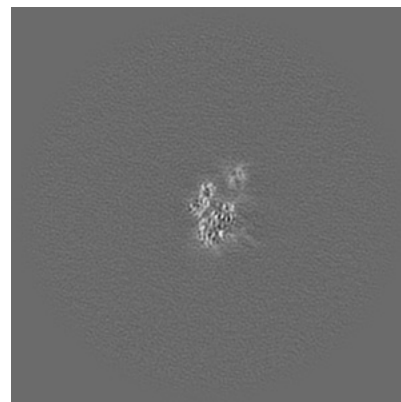
6.2.1 Primary map



X Index: 240

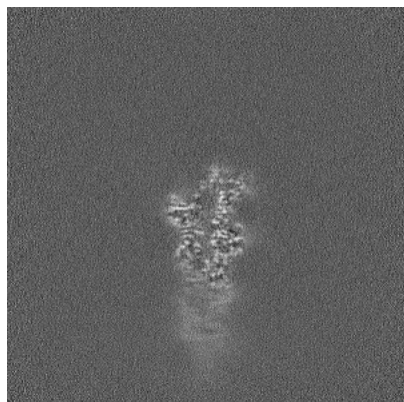


Y Index: 240

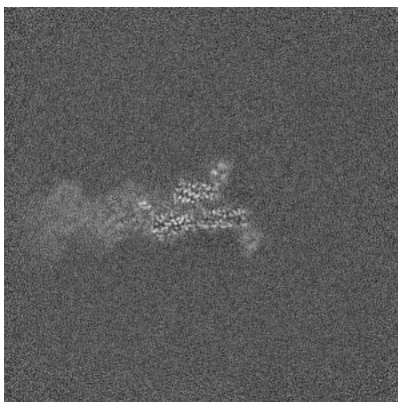


Z Index: 240

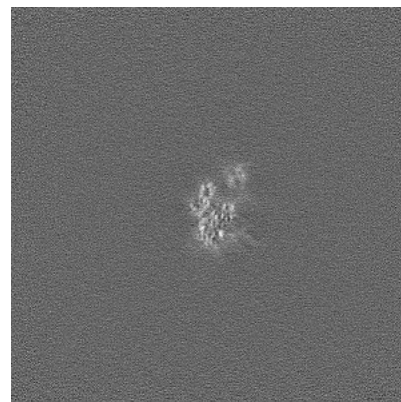
6.2.2 Raw map



X Index: 240



Y Index: 240

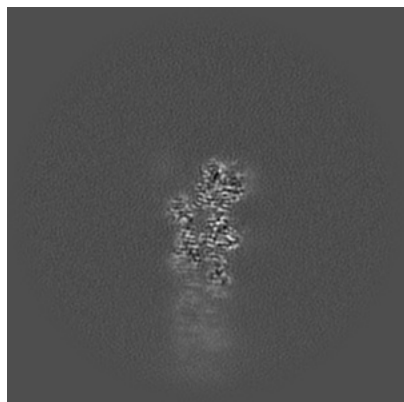


Z Index: 240

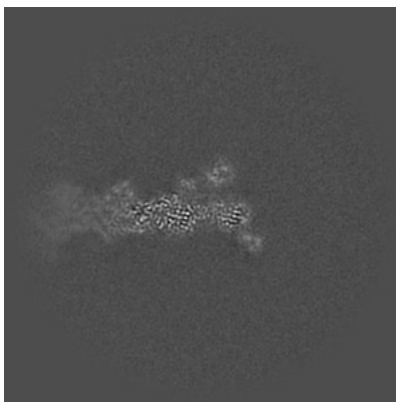
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

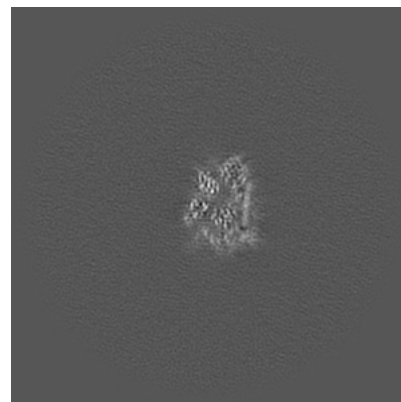
6.3.1 Primary map



X Index: 231

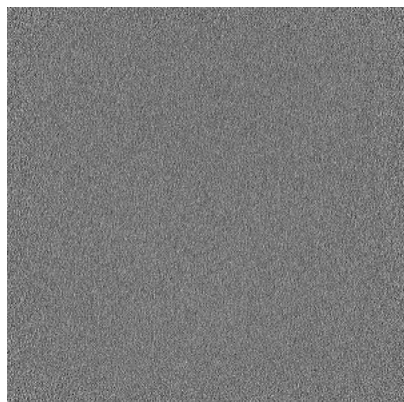


Y Index: 252

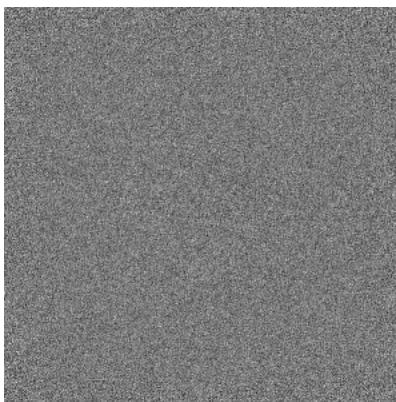


Z Index: 252

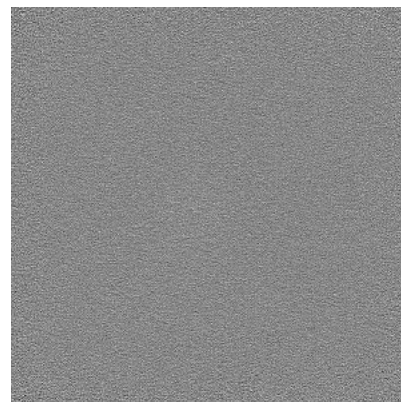
6.3.2 Raw map



X Index: 0



Y Index: 0

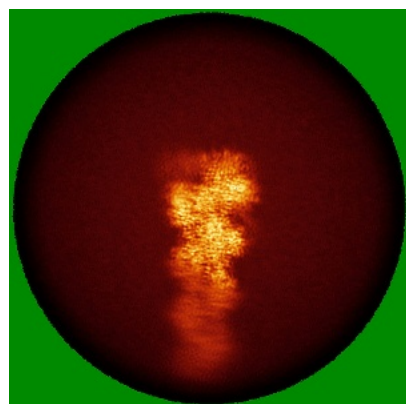


Z Index: 0

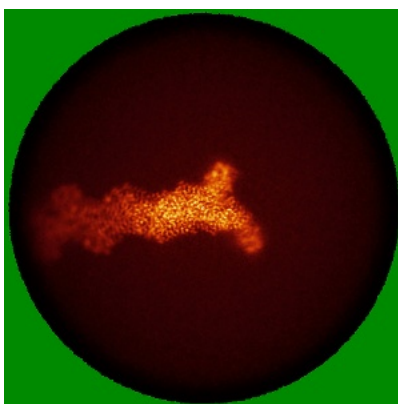
The images above show the largest variance slices of the map in three orthogonal directions.

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

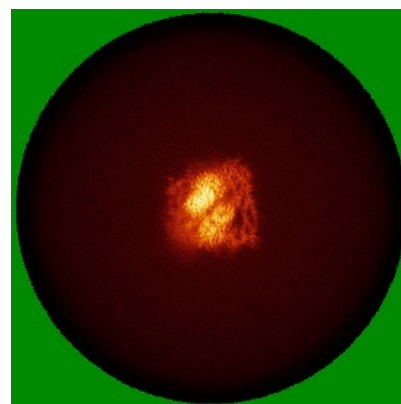
6.4.1 Primary map



X

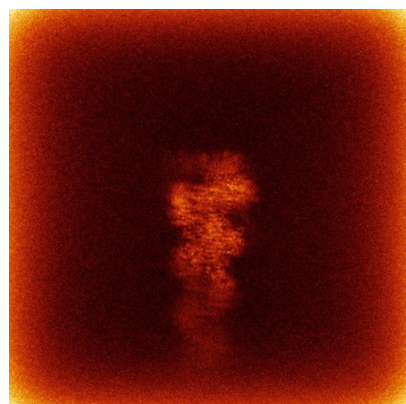


Y

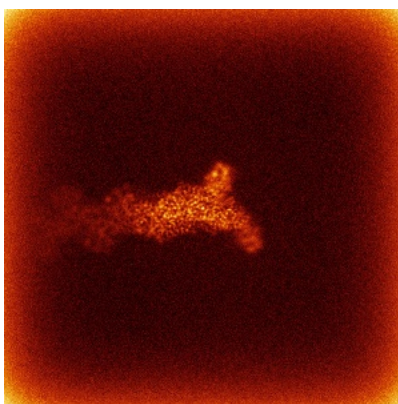


Z

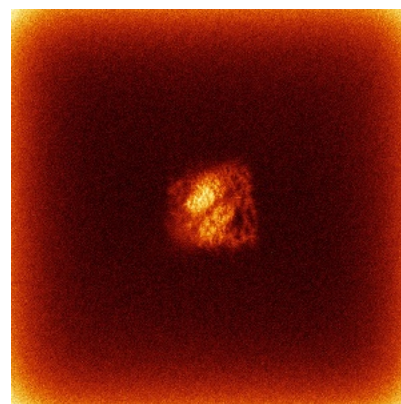
6.4.2 Raw map



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.

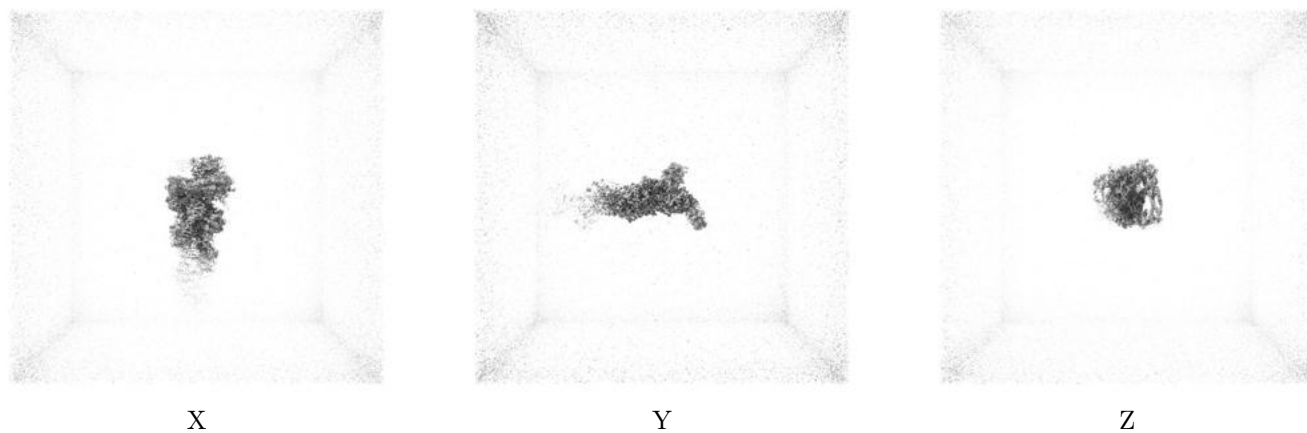
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.367. 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.

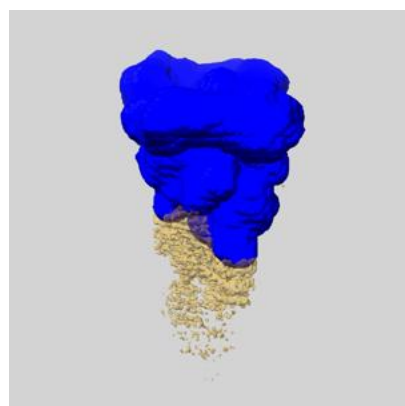
6.6 Mask visualisation [i](#)

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

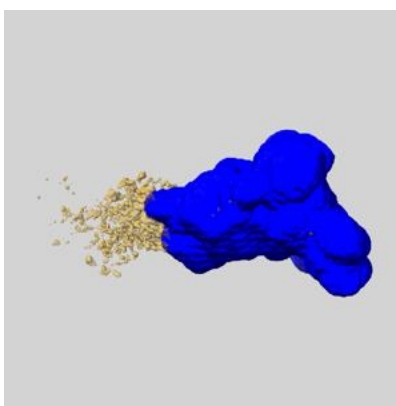
A mask typically either:

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

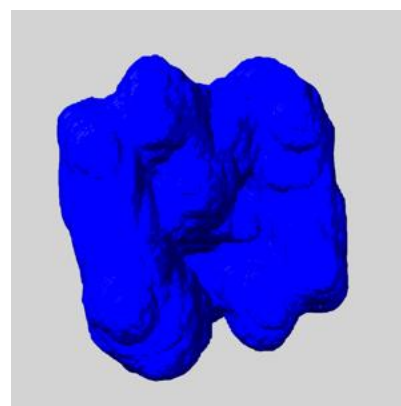
6.6.1 emd_19503_msk_1.map [i](#)



X



Y

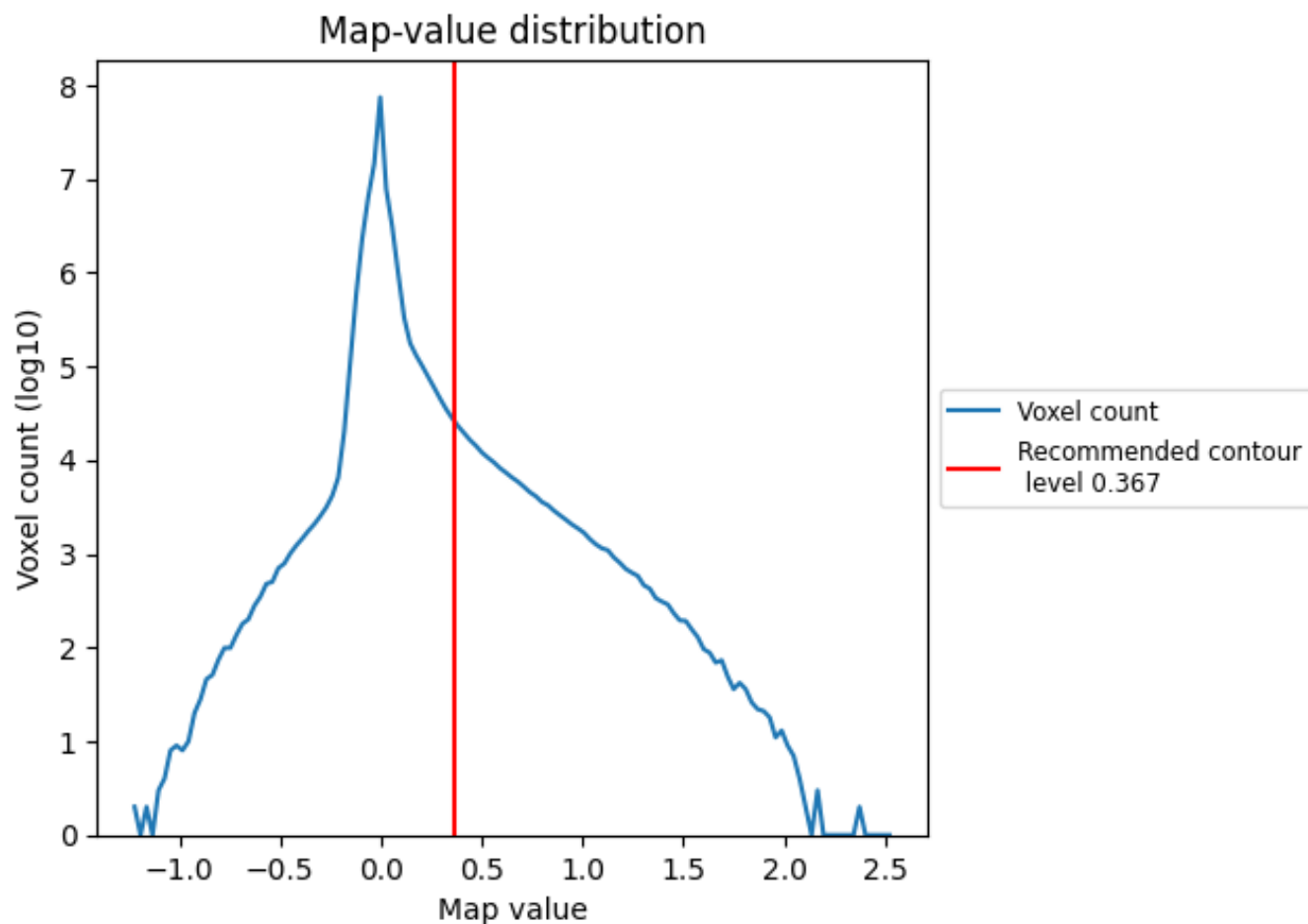


Z

7 Map analysis [i](#)

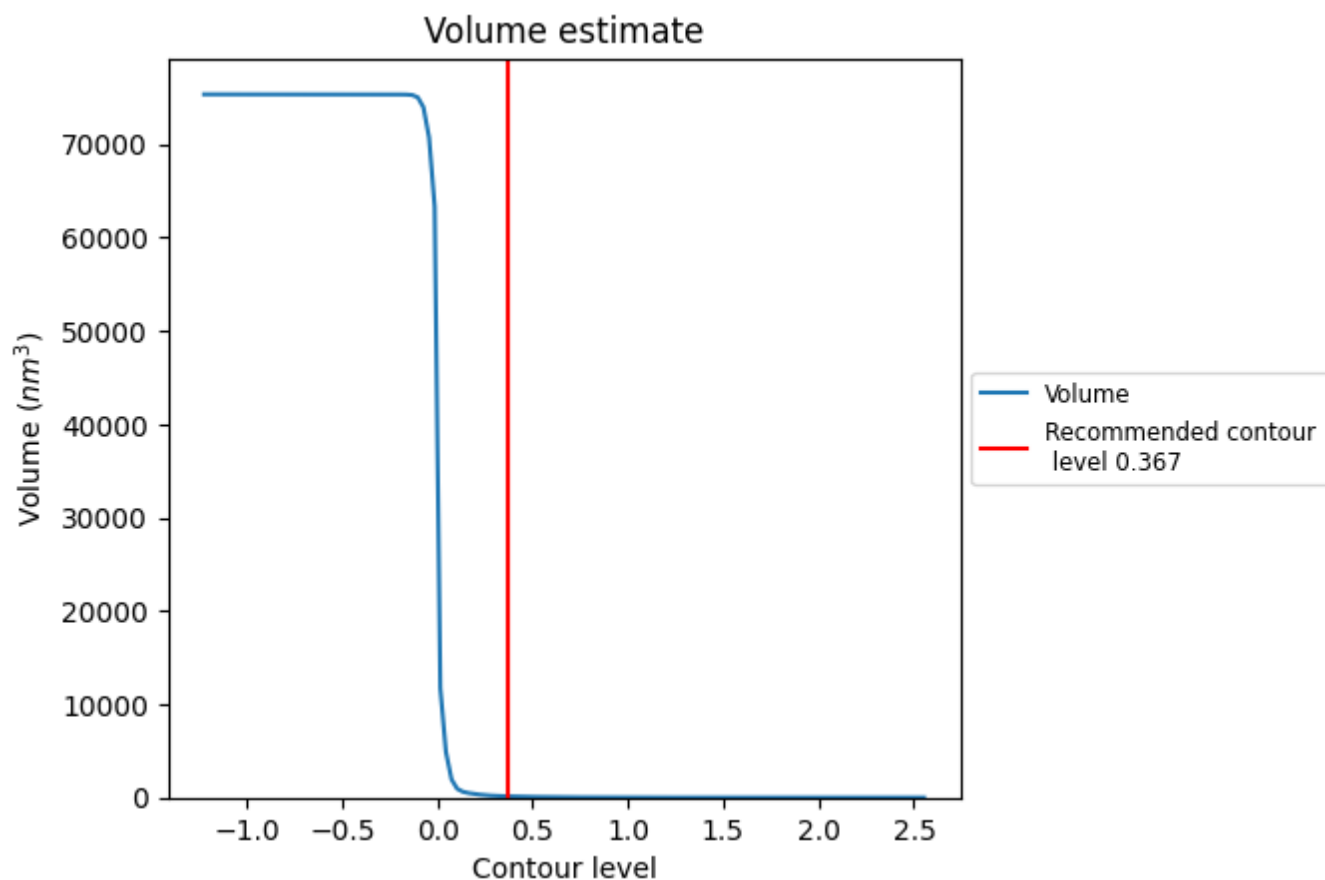
This section contains the results of statistical analysis of the map.

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.

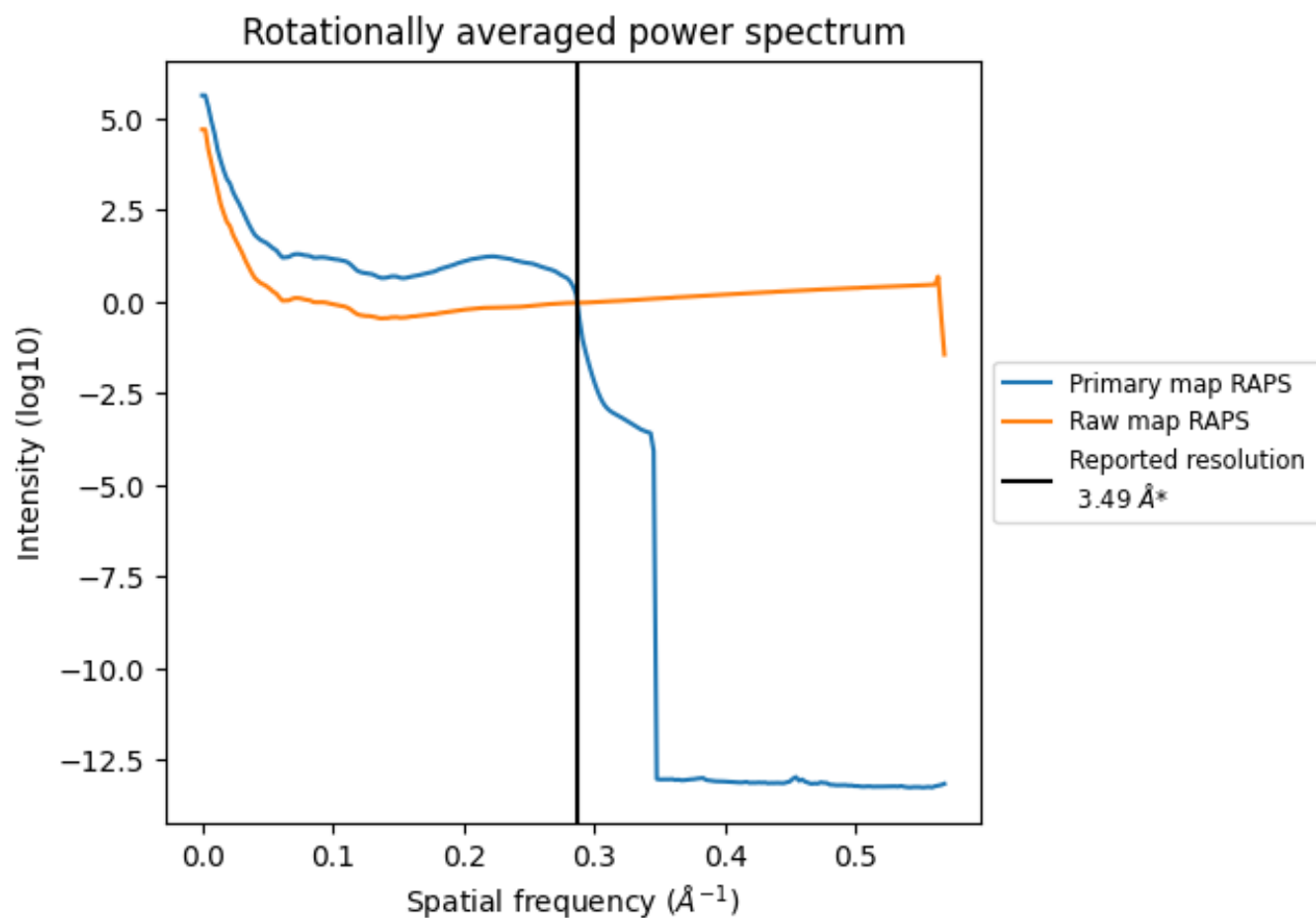
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 ⓘ

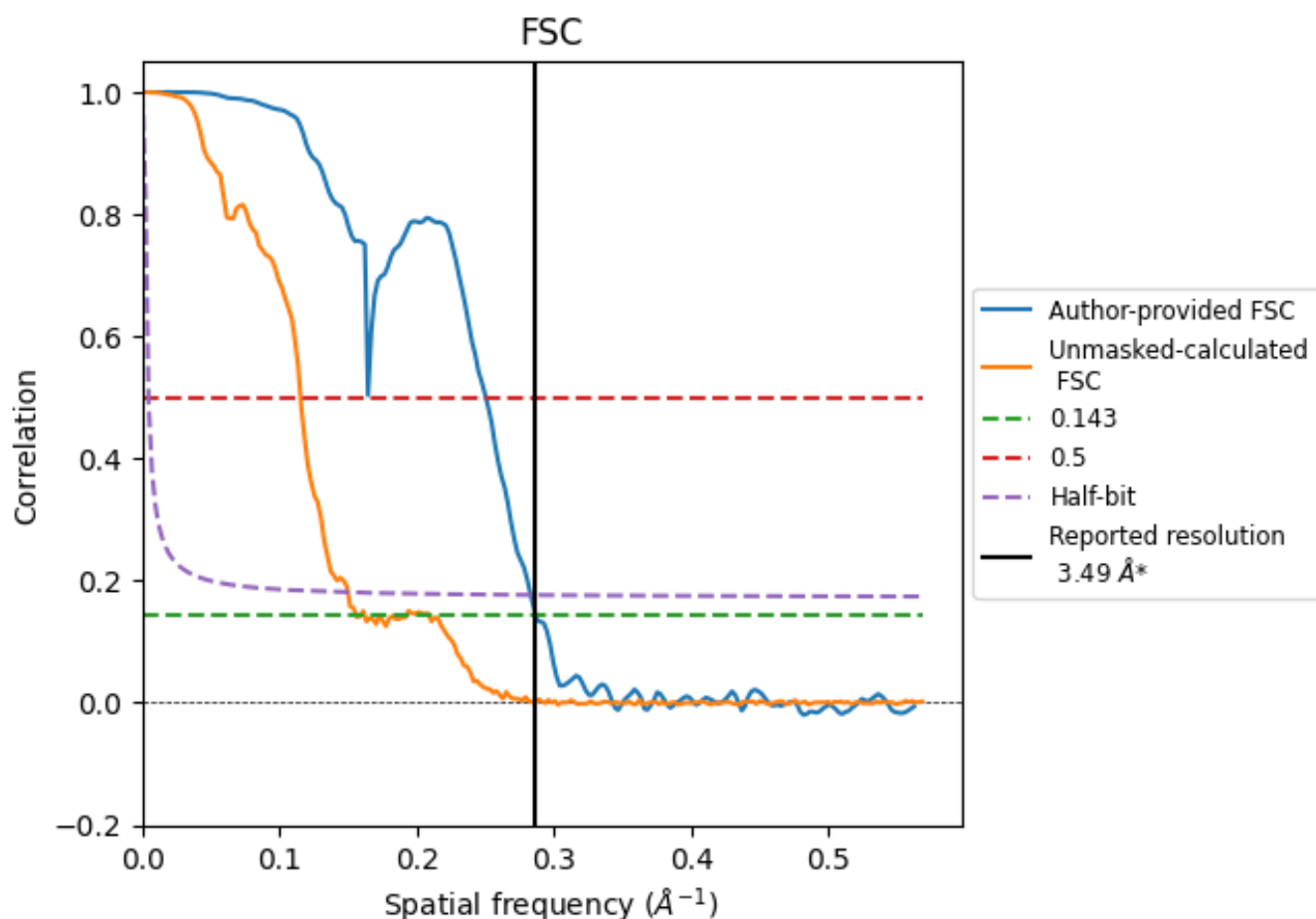


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

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 0.287 \AA^{-1}

8.2 Resolution estimates [i](#)

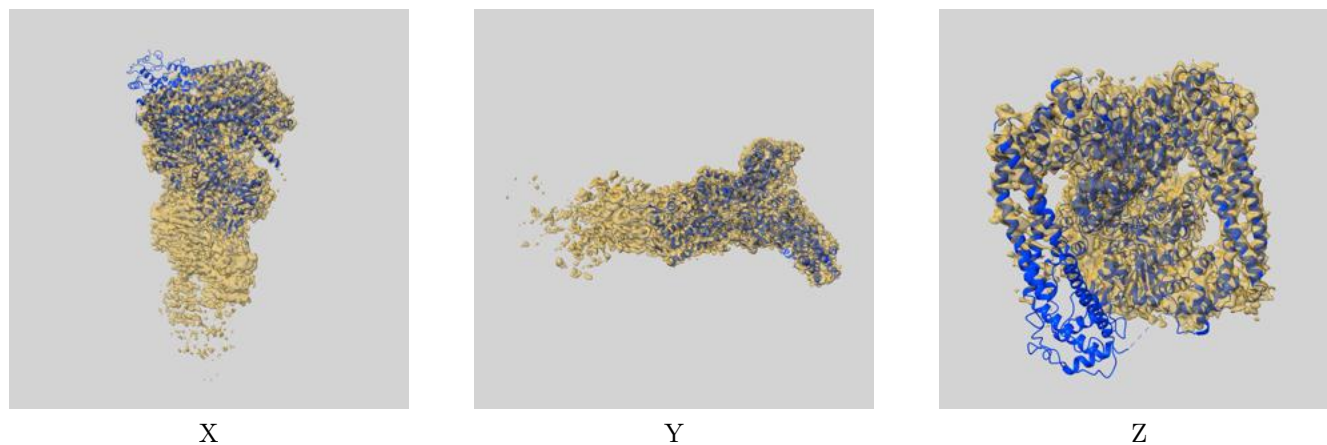
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.00	3.53
Unmasked-calculated*	6.42	8.67	6.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.42 differs from the reported value 3.49 by more than 10 %

9 Map-model fit [i](#)

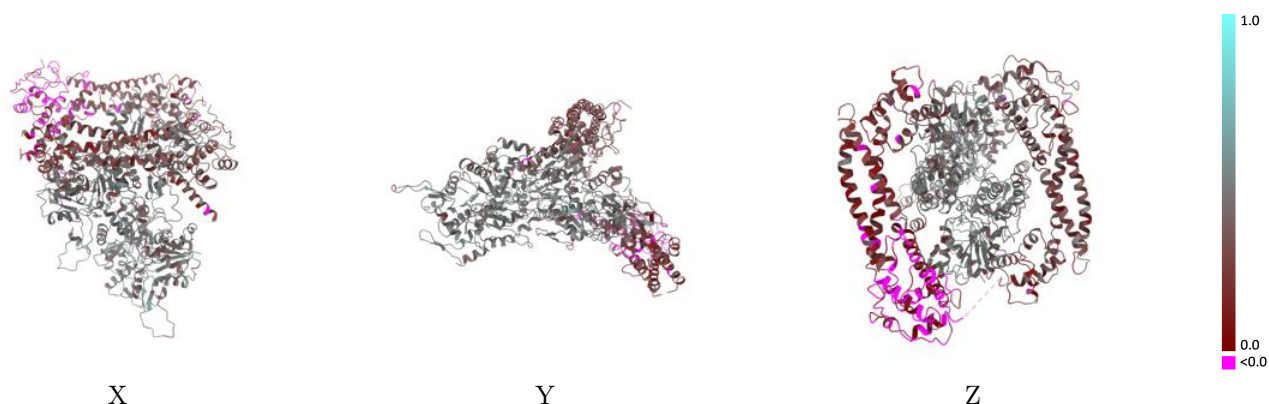
This section contains information regarding the fit between EMDB map EMD-19503 and PDB model 8RU2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



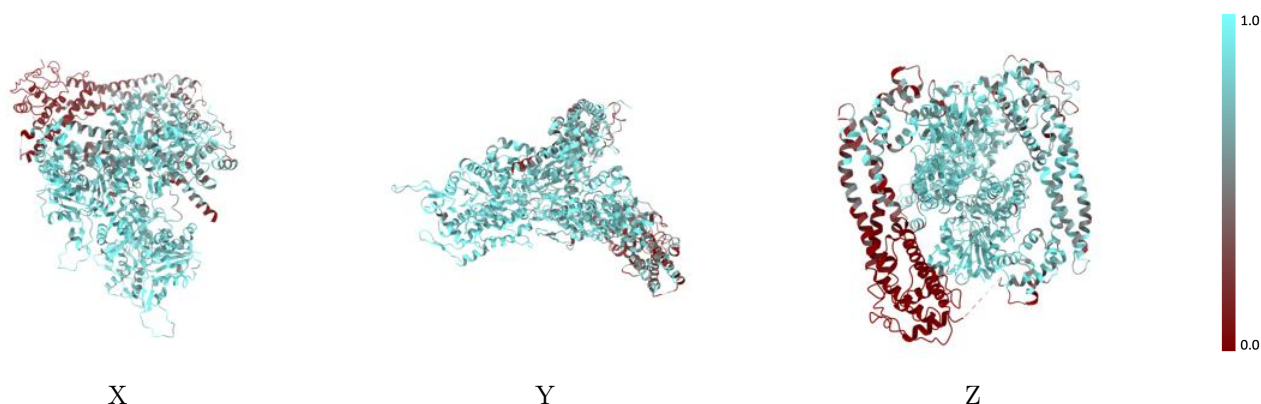
The images above show the 3D surface view of the map at the recommended contour level 0.367 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



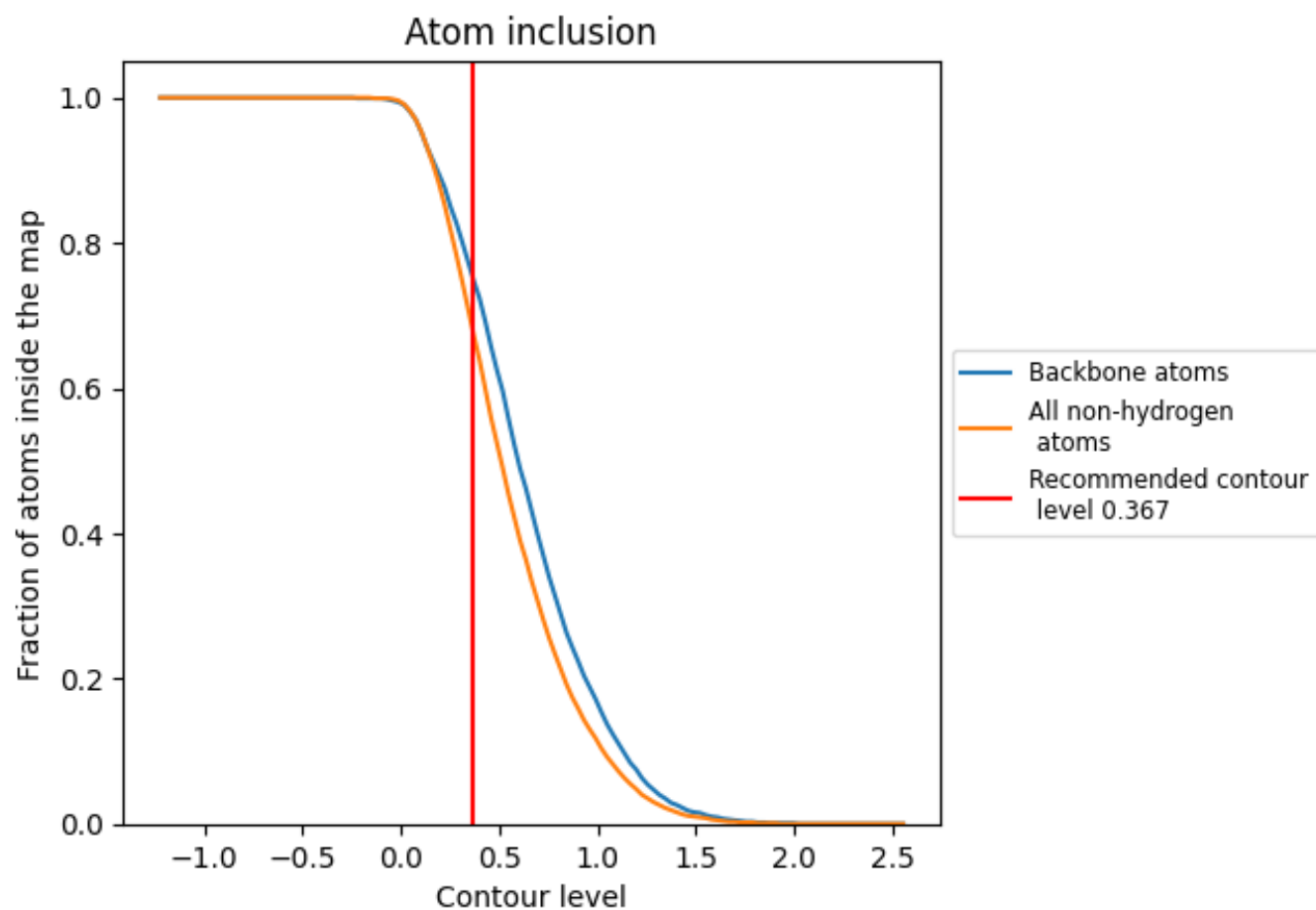
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.367).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.367) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6770	<div></div> 0.3620
B	<div></div> 0.8590	<div></div> 0.4670
C	<div></div> 0.8550	<div></div> 0.4630
D	<div></div> 0.8140	<div></div> 0.4540
E	<div></div> 0.5690	<div></div> 0.2670
F	<div></div> 0.3070	<div></div> 0.1700

