



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:21 PM UTC

PDB ID : 8RV2 / pdb_00008rv2
EMDB ID : EMD-19522
Title : Structure of the formin INF2 bound to the barbed end of F-actin.
Authors : Oosterheert, W.; Boiero Sanders, M.; Funk, J.; Prumbaum, D.; Raunser, S.; Bieling, P.
Deposited on : 2024-01-31
Resolution : 3.41 Å(reported)
Based on initial models : 8A2S, .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

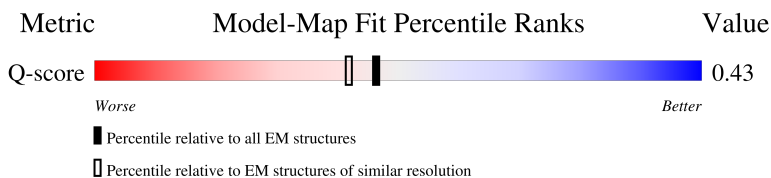
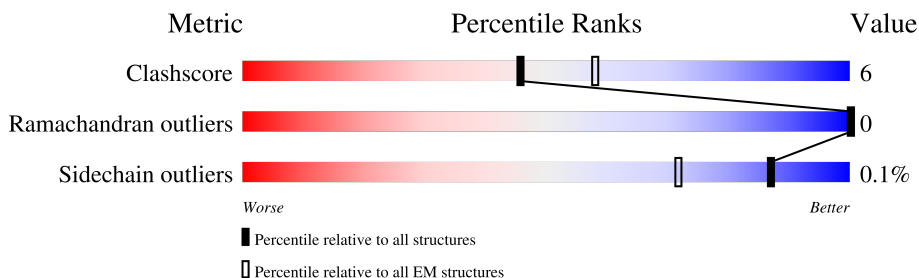
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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	13997 (2.91 - 3.91)

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	375	10% 81% 18%
1	B	375	84% 15%
1	C	375	81% 17%
1	D	375	83% 15%

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Mol	Chain	Length	Quality of chain
2	E	777	16% 40% 5% 55%
2	F	777	40% 38% 7% 55%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17248 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2899	1837	489	552	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	370	Total	C	N	O	S	0	0
			2888	1828	488	551	21		
1	D	370	Total	C	N	O	S	0	0
			2888	1828	488	551	21		

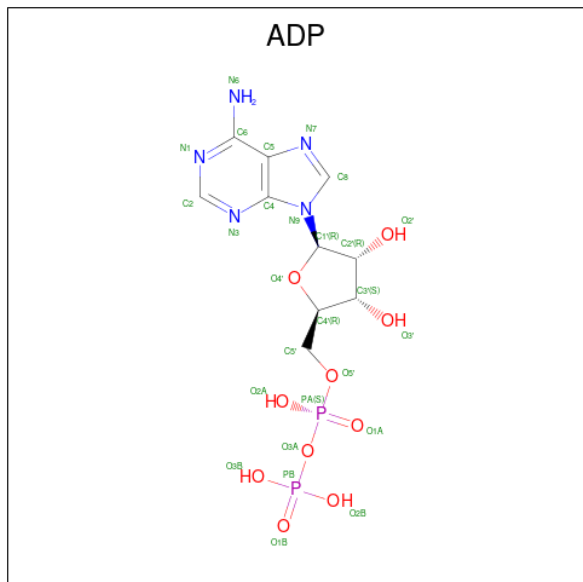
- Molecule 2 is a protein called Isoform 2 of Inverted formin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	348	Total	C	N	O	S	0	0
			2776	1757	479	527	13		
2	F	348	Total	C	N	O	S	0	0
			2776	1757	479	527	13		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	464	GLY	-	expression tag	UNP Q27J81
E	465	GLY	-	expression tag	UNP Q27J81
E	466	GLY	-	expression tag	UNP Q27J81
E	467	GLY	-	expression tag	UNP Q27J81
E	468	GLY	-	expression tag	UNP Q27J81
E	488	SER	PRO	conflict	UNP Q27J81
F	464	GLY	-	expression tag	UNP Q27J81
F	465	GLY	-	expression tag	UNP Q27J81
F	466	GLY	-	expression tag	UNP Q27J81
F	467	GLY	-	expression tag	UNP Q27J81
F	468	GLY	-	expression tag	UNP Q27J81
F	488	SER	PRO	conflict	UNP Q27J81

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

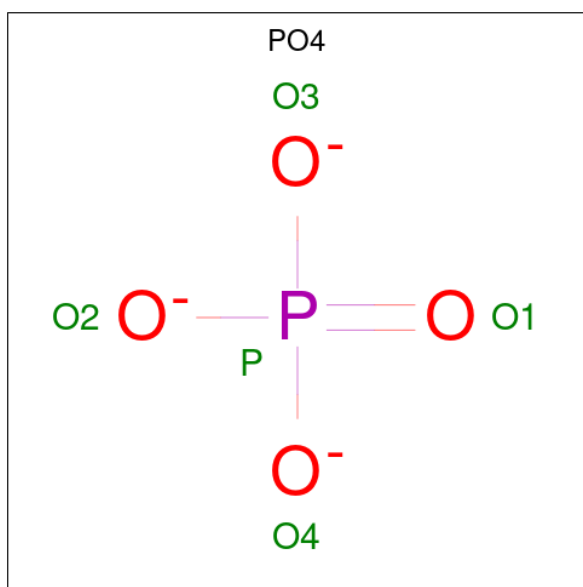


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

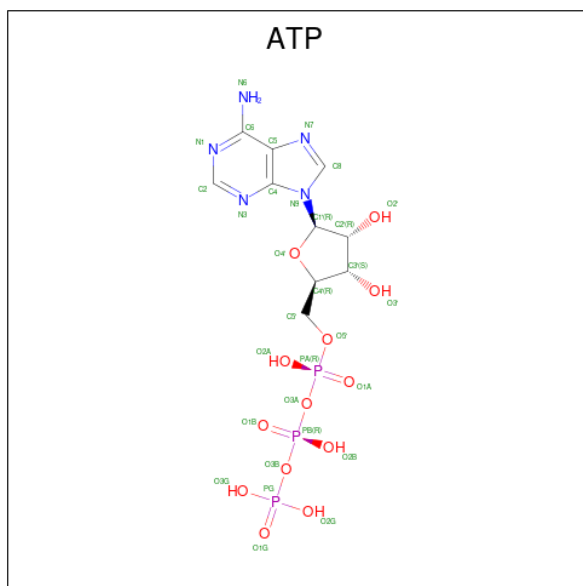
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	O	P	0
			5	4	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

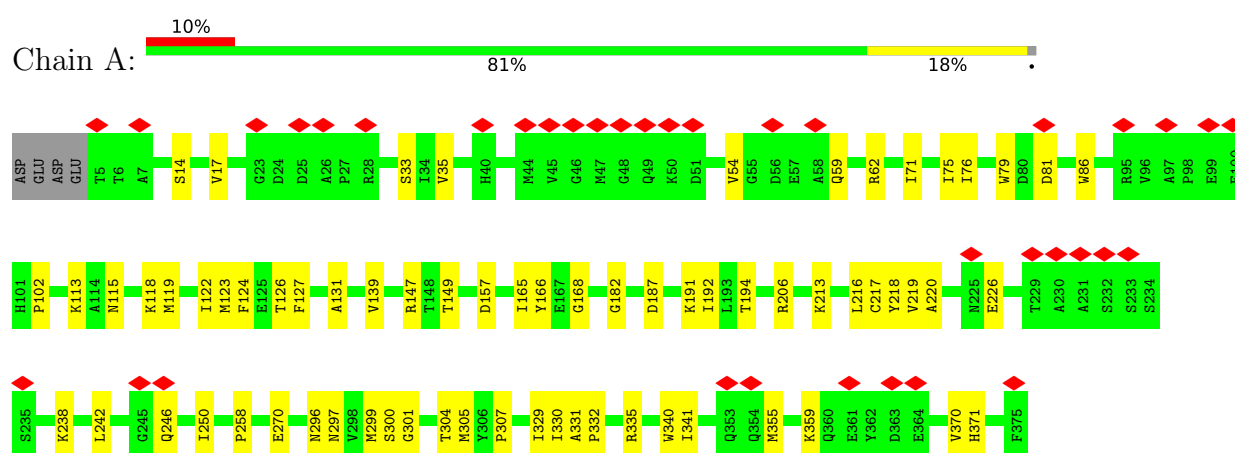


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

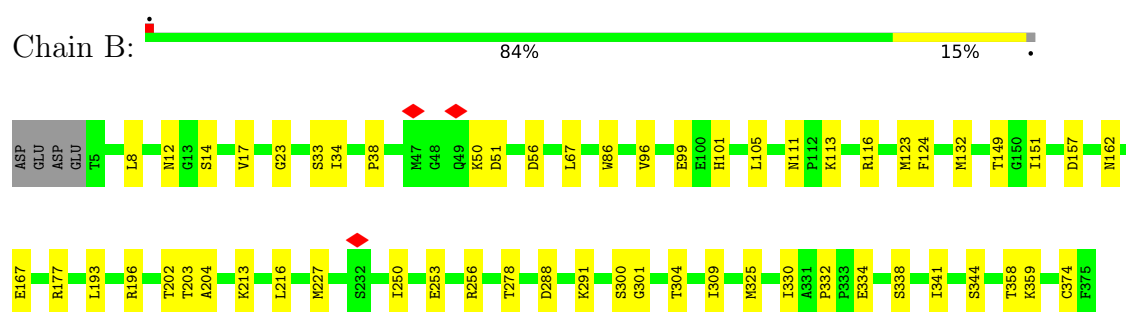
3 Residue-property plots [i](#)

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.

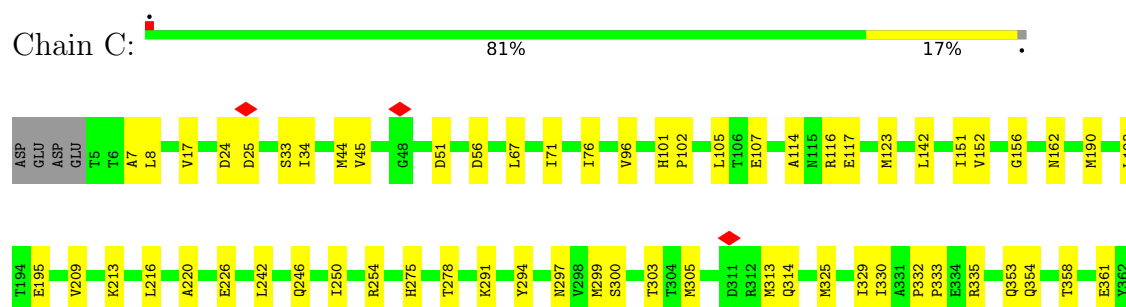
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

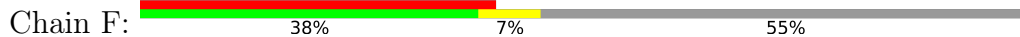


- Molecule 1: Actin, alpha skeletal muscle



SER
LYS
GLY
THR
GLY
LYS
ARG
ARG
LYS
LYS
ARG
PRO
SER
SER
SER
GLN
GLU
GLY
LEU
ARG
PRO
ARG
PRO
LYS
ALA
LYS

- Molecule 2: Isoform 2 of Inverted formin-2



GLY	GLY	GLY	GLY	GLY	MET	ALA	PRO	PRO	ALA	ALA	PRO	PRO	PRO	LEU	LEU	PRO	PRO	GLY	SER	CYS	GLU	PHE	LEU	LEU	SER	PRO	PRO	PRO	PRO	PRO	PRO	LEU	LEU	GLY	GLY	CYS	PRO	PRO	PRO	PRO	PRO	PRO	GLY	TRP	GLY	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	LEU	LEU	LEU	PRO
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CYS	THR	CYS	SER	PRO	PRO	VAL	GLY	GLY	MET	GLU	GLU	VAL	ILE	VAL	ALA	GLN	VAL	ASP	HIS	GLY	LEU	GLY	SER	ALA	TRP	VAL	PRO	SER	HIS	ARG	ARG	VAL	ASN	P560	P569	T561	L562	R563	N564	Q570	K571	L572	P573	S574	N575	V576	A577	R578	E579	H580	N581	S582	N583	N584	A585	S586	L587
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\$588	\$589	\$590	\$591	\$592	\$593	\$594	\$595	\$596	\$597	\$598	\$599	\$600	\$601	\$602	\$603	\$604	\$605	\$606	\$607	\$608	\$609	\$610	\$611	\$612	\$613	\$614	\$615	\$616	\$617	\$618	\$619	\$620	\$621	\$622	\$623	\$624	\$625	\$626	\$627	\$628	\$629	\$630	\$631	\$632	\$633	\$634	\$635	\$636	\$637	\$638	\$639	\$640	\$641	\$642	\$643	\$644	\$645	\$646	\$647	\$648	\$649	\$650	\$651	\$652	\$653	\$654	\$655	\$656	\$657	\$658	\$659	\$660	\$661	\$662	\$663	\$664	\$665	\$666	\$667	\$668	\$669	\$670	\$671	\$672	\$673	\$674	\$675	\$676	\$677	\$678	\$679	\$680	\$681	\$682	\$683	\$684	\$685	\$686	\$687	\$688	\$689	\$690	\$691	\$692	\$693	\$694	\$695	\$696	\$697	\$698	\$699	\$700	\$701	\$702	\$703	\$704	\$705	\$706	\$707	\$708	\$709	\$710	\$711	\$712	\$713	\$714	\$715	\$716	\$717	\$718	\$719	\$720	\$721	\$722	\$723	\$724	\$725	\$726	\$727	\$728	\$729	\$730	\$731	\$732	\$733	\$734	\$735	\$736	\$737	\$738	\$739	\$740	\$741	\$742	\$743	\$744	\$745	\$746	\$747	\$748	\$749	\$750	\$751	\$752	\$753	\$754	\$755	\$756	\$757	\$758	\$759	\$760	\$761	\$762	\$763	\$764	\$765	\$766	\$767	\$768	\$769	\$770	\$771	\$772	\$773	\$774	\$775	\$776	\$777	\$778	\$779	\$780	\$781	\$782	\$783	\$784	\$785	\$786	\$787	\$788	\$789	\$790	\$791	\$792	\$793	\$794	\$795	\$796	\$797	\$798	\$799	\$800	\$801	\$802	\$803	\$804	\$805	\$806	\$807	\$808	\$809	\$810	\$811	\$812	\$813	\$814	\$815	\$816	\$817	\$818	\$819	\$820	\$821	\$822	\$823	\$824	\$825	\$826	\$827	\$828	\$829	\$830	\$831	\$832	\$833	\$834	\$835	\$836	\$837	\$838	\$839	\$840	\$841	\$842	\$843	\$844	\$845	\$846	\$847	\$848	\$849	\$850	\$851	\$852	\$853	\$854	\$855	\$856	\$857	\$858	\$859	\$860	\$861	\$862	\$863	\$864	\$865	\$866	\$867	\$868	\$869	\$870	\$871	\$872	\$873	\$874	\$875	\$876	\$877	\$878	\$879	\$880	\$881	\$882	\$883	\$884	\$885	\$886	\$887	\$888	\$889	\$890	\$891	\$892	\$893	\$894	\$895	\$896	\$897	\$898	\$899	\$900	\$901	\$902	\$903	\$904	\$905	\$906	\$907	\$908	\$909	\$910	\$911	\$912	\$913	\$914	\$915	\$916	\$917	\$918	\$919	\$920	\$921	\$922	\$923	\$924	\$925	\$926	\$927	\$928	\$929	\$930	\$931	\$932	\$933	\$934	\$935	\$936	\$937	\$938	\$939	\$940	\$941	\$942	\$943	\$944	\$945	\$946	\$947	\$948	\$949	\$950	\$951	\$952	\$953	\$954	\$955	\$956	\$957	\$958	\$959	\$960	\$961	\$962	\$963	\$964	\$965	\$966	\$967	\$968	\$969	\$970	\$971	\$972	\$973	\$974	\$975	\$976	\$977	\$978	\$979	\$980	\$981	\$982	\$983	\$984	\$985	\$986	\$987	\$988	\$989	\$990	\$991	\$992	\$993	\$994	\$995	\$996	\$997	\$998	\$999	\$1000
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[illegible]

E719	C720	M721	L722	L723	C724	E725	G726	A727	A728	A729	V730	L731	D732	M733	V734	R735	P736	K737	A738	A739	L740	V741	L742	A743	A744	G745	E746	S747	L748	L749	T750	S751	R752	G753	L754	P755	L756	F757	G758	C759	L760	L761	L762	R763	L764	G765	M766	F767	L768	M769	V770	G771	S772	H773	T774	G775	D776	A777	T778
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G779	F780	K781	T782	S783	T784	L785	L786	K787	L788	T789	E790	T791	K792	S793	T794	Q795	N796	K797	T798	T799	L800	L801	H802	H803	H804	L805	E806	E807	A808	E809	K810	S811	H812	P813	D814	L815	L816	Q817	L818	P819	R820	D821	L822	S823	E824	P825	S826	Q827	A828	A829	G830	L831	H832	L833	E834	L835	L836	R837	S838
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E839	A840	S841	S842	N843	L844	K845	K846	L847	L848	E849	T850	E851	R852	K853	V854	S855	A856	S857	V858	A859	E860	V861	K862	S863	K864	V865	T866	E867	R868	L869	K870	K871	S872	L873	S874	A875	F876	R877	A878	L879	D880	E881	L882	L883	E884	A885	T886	E887	Q888	K889	Q890	R891	E892	L893	A894	D895	V896	L897	V898
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E899
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F910
S911
T912
M913
K914
A915
A916
R917
D918
L919
F920
L921
R922
A923
L924
K925
E926
N927
K928
D929
H930
X931
E932
Q933
ALA
ALA
LYS
ALA
GLU
ARG
ARG
LYS
GLN
GLN
LEU
ALA
GLU
GLU
GLU
ALA
ALA
ARG
ARG
PRO
ARG
GLY
ASP
PHE
CYS

PRO	VAL	ARG	LYS	GLY	PRO	GLY	LYS	GLN	GLU	GLU	VAL	CYS	VAL	ILE	ASP	ALA	LEU	LEU	ALA	ASP	ILE	ARG	LYS	GLY	PHE	GLN	LEU	ARG	LYS	THR	ALA	ALA	ARG	GLY	GLY	GLY	SER	LYS	ALA	ALA	SER	MET	ASP	PRO	PRO	PRO	ARG	ALA	ALA	THR	ALA	THR	SER	ASN
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PRO	ALA	GLY	ASP	PRO	VAL	GLY	SER	THR	ARG	CYS	PRO	ALA	SER	GLU	PRO	GLY	LEU	ASP	ALA	ALA	THR	THR	ALA	SER	SER	GLU	ARG	SER	GLY	TRP	TRP	ASP	VAL	LEU	VAL	ASP	ALA	ALA	VAL	THR	THR	PRO	PRO	GLY	GLN	PRO	PRO	THR	LEU	GLU	GLN	LEU	GLY	GLU	GLY	PRO	PRO	ARG	ARG	LEU	SER	SER	PER
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TTR	VAL	ASP	ALA	SER	ASP	VAL	LEU	THR	THR	GLU	ASP	PRO	GLN	CYS	PRO	GLN	PRO	LEU	GLU	GLY	ALA	GLY	TRP	PRO	VAL	THR	THR	LEU	GLY	ASP	ALA	GLN	ALA	LEU	LEU	PRO	PRO	LYS	LEU	LEU	LYS	PHE	SER	SER	ASN	GLN	PRO	PRO	ALA	ALA	GLY	SER	SER	ARG	GLN	ASP	ALA	LYS	ASP	PRO	THR	THR	SER	SER	LEU	LEU
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GLY	VAL	LEU	GLN	ALA	GLU	ALA	ASP	SER	THR	SER	SER	GLY	LEU	GLU	ASP	ALA	ALA	VAL	HIS	SER	ARG	GLY	GLY	PRO	GLY	GLY	ASP	ASP	ASP	ASP	GLU	GLU	GLU	GLU	ASP	THR	ALA	ALA	PRO	PRO	GLU	LEU	ASP	LYS	SER	PHE	SER	GLU	ASP	ALA	VAL
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THR	ASP	SER	SER	GLY	SER	GLY	THR	LEU	PRO	ARG	ALA	ARG	GLY	ARG	ALA	SER	LYS	GLY	THR	GLY	LYS	ARG	ARG	LYS	LYS	ARG	PRO	SER	SER	ARG	GLN	GLU	GLY	GLY	LEU	ARG	PRO	ARG	PRO	LYS	ALA	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142549	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 ($e^-/\text{\AA}^2$)	60.6	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	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, PO4, MG, HIC, ATP

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	0.07	0/2949	0.20	0/3994
1	B	0.09	0/2950	0.24	0/3994
1	C	0.10	0/2937	0.24	0/3978
1	D	0.09	0/2937	0.24	0/3978
2	E	0.07	0/2817	0.21	0/3794
2	F	0.08	0/2817	0.22	0/3794
All	All	0.08	0/17407	0.23	0/23532

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	2899	0	2872	45	0
1	B	2900	0	2872	36	0
1	C	2888	0	2863	43	0
1	D	2888	0	2863	35	0
2	E	2776	0	2827	29	0
2	F	2776	0	2827	40	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	1	0
3	C	27	0	12	0	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
5	B	5	0	0	0	0
6	D	31	0	12	2	0
All	All	17248	0	17172	214	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 6.

The worst 5 of 214 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:HG23	1:A:166:TYR:HA	1.66	0.76
1:B:291:LYS:HD3	1:B:325:MET:HE1	1.69	0.75
1:A:305:MET:HA	1:A:335:ARG:HH21	1.52	0.74
1:C:314:GLN:HG2	1:C:329:ILE:HD12	1.73	0.71
1:B:17:VAL:HG23	1:B:33:SER:HB2	1.75	0.68

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	368/375 (98%)	363 (99%)	5 (1%)	0	100	100
1	B	368/375 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	367/375 (98%)	365 (100%)	2 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	367/375 (98%)	360 (98%)	7 (2%)	0	100	100
2	E	342/777 (44%)	334 (98%)	8 (2%)	0	100	100
2	F	342/777 (44%)	335 (98%)	7 (2%)	0	100	100
All	All	2154/3054 (70%)	2116 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/317 (99%)	313 (100%)	0	100	100
1	B	313/317 (99%)	313 (100%)	0	100	100
1	C	312/317 (98%)	311 (100%)	1 (0%)	86	84
1	D	312/317 (98%)	312 (100%)	0	100	100
2	E	307/645 (48%)	307 (100%)	0	100	100
2	F	307/645 (48%)	307 (100%)	0	100	100
All	All	1864/2558 (73%)	1863 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	ASN
2	F	864	GLN
2	E	739	GLN
2	F	903	GLN

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Mol	Chain	Res	Type
2	F	703	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	0.48	0	9,14,16	0.55	0
1	HIC	B	73	1	10,11,12	0.47	0	9,14,16	0.53	0
1	HIC	D	73	1	10,11,12	0.48	0	9,14,16	0.60	0
1	HIC	A	73	1	10,11,12	0.47	0	9,14,16	0.50	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	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	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 (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	B	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)
6	ATP	D	401	4	32,33,33	0.30	0	48,52,52	0.36	0
3	ADP	C	401	4	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
3	ADP	A	401	4	28,29,29	1.44	5 (17%)	43,45,45	1.79	9 (20%)
5	PO4	B	403	4	4,4,4	1.55	1 (25%)	6,6,6	0.51	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	ADP	C	401	4	-	5/16/32/32	0/3/3/3
3	ADP	A	401	4	-	1/16/32/32	0/3/3/3
6	ATP	D	401	4	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	401	-	-	7/16/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C5-C4	4.69	1.47	1.39
3	C	401	ADP	C5-C4	4.61	1.47	1.39
3	B	401	ADP	C5-C4	4.60	1.47	1.39
5	B	403	PO4	P-O1	2.73	1.57	1.50
3	A	401	ADP	C5-C6	2.72	1.48	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ADP	C5-C4-N3	-5.88	118.62	126.72
3	A	401	ADP	C5-C4-N3	-5.75	118.80	126.72
3	B	401	ADP	C5-C4-N3	-5.74	118.81	126.72
3	C	401	ADP	N3-C4-N9	4.60	134.98	127.17
3	A	401	ADP	N3-C4-N9	4.57	134.94	127.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	ADP	C5'-O5'-PA-O1A
3	B	401	ADP	C5'-O5'-PA-O2A
3	B	401	ADP	O4'-C4'-C5'-O5'
3	B	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	C5'-O5'-PA-O1A

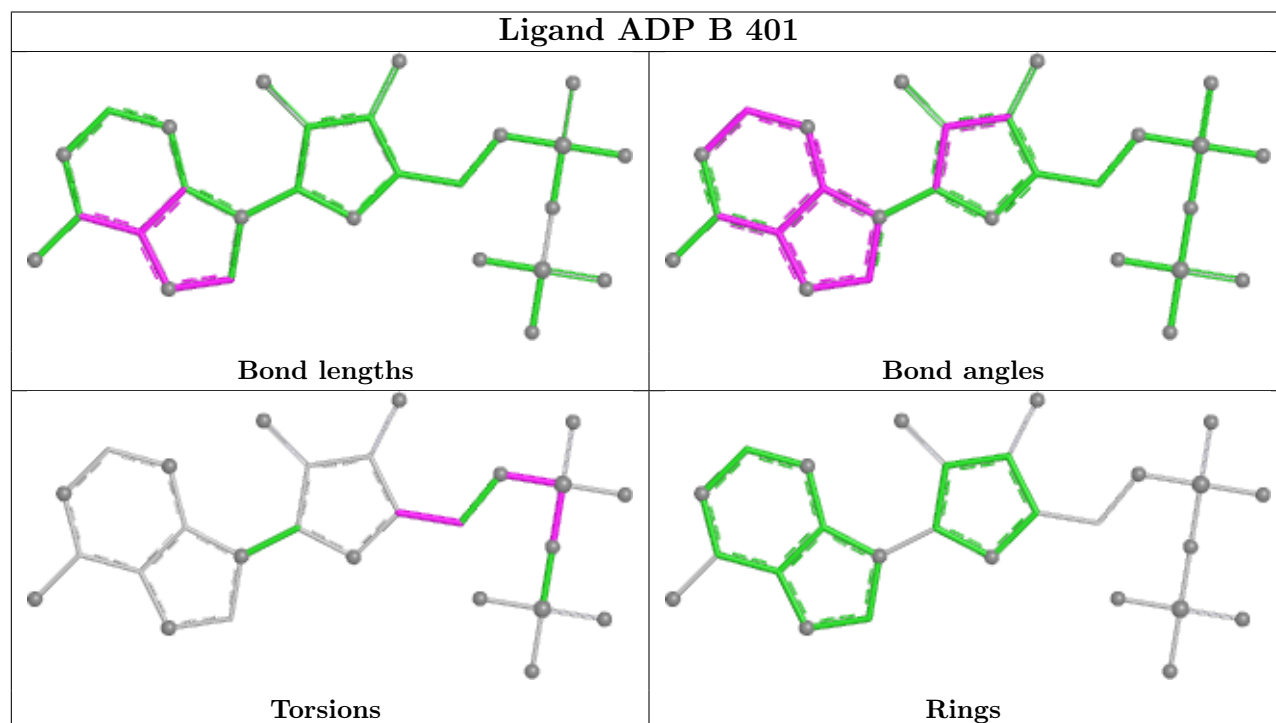
There are no ring outliers.

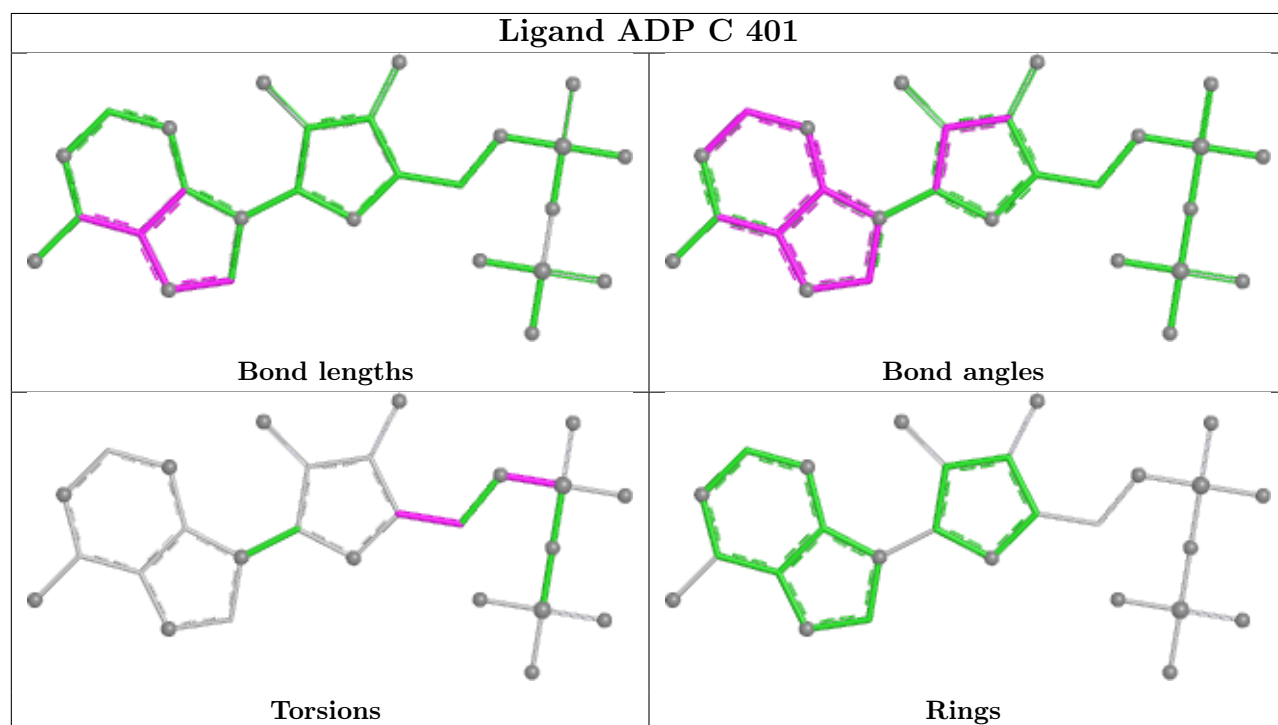
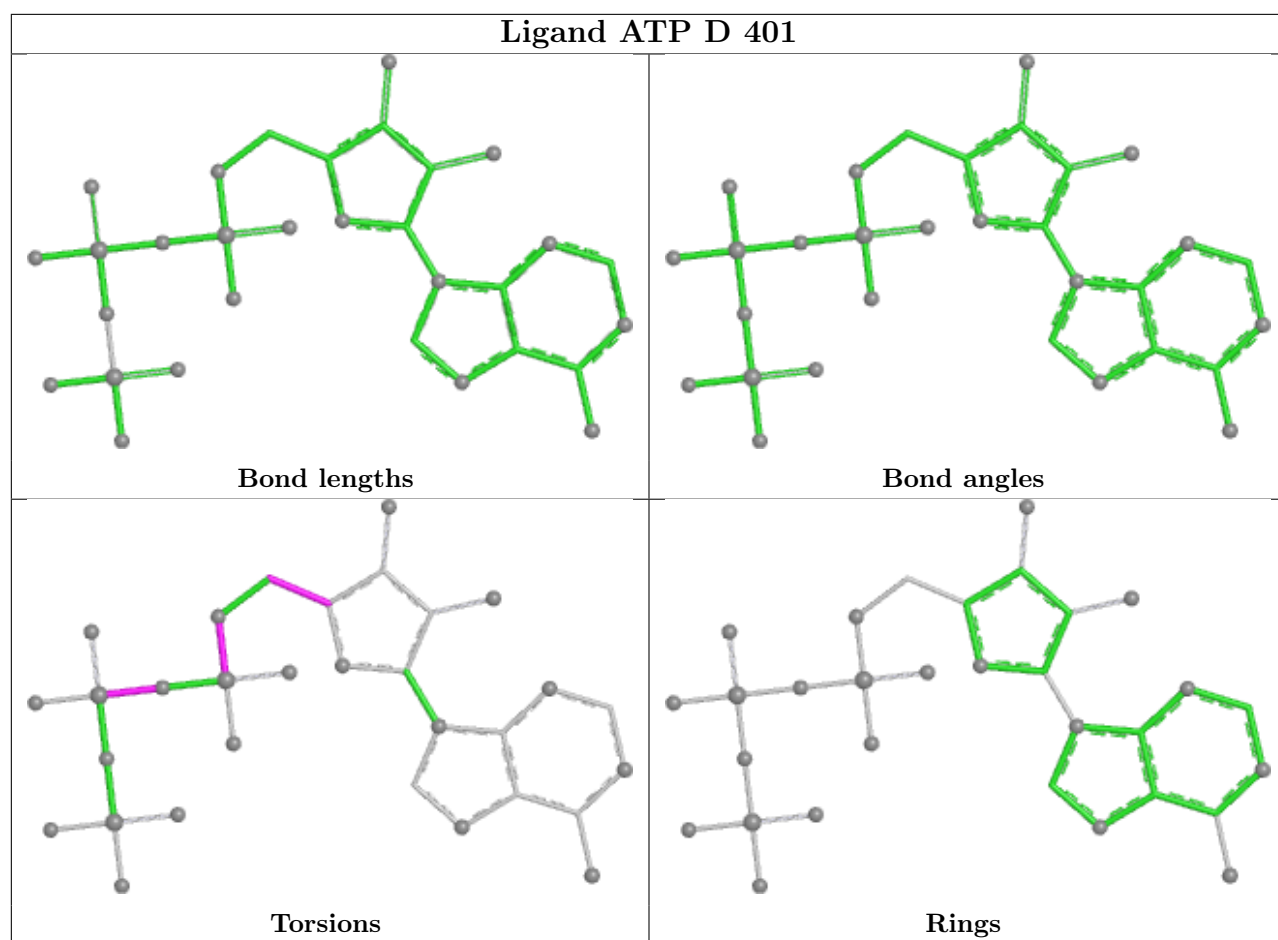
2 monomers are involved in 3 short contacts:

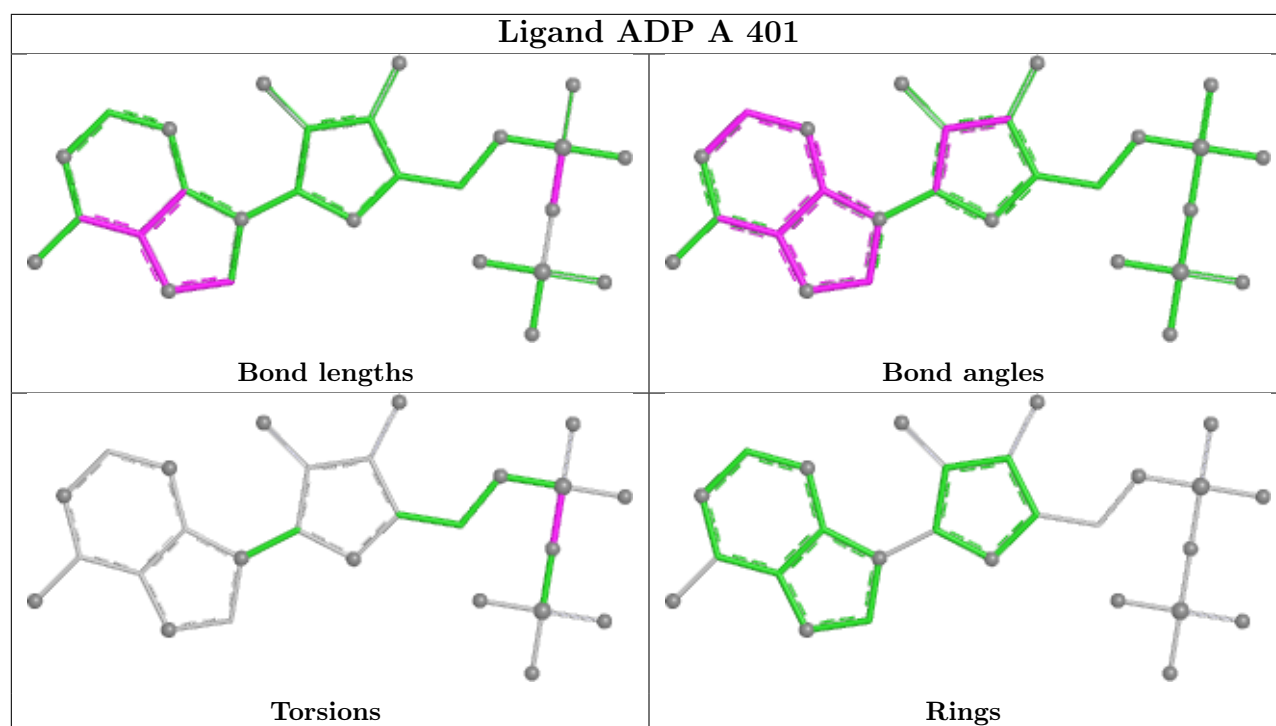
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ADP	1	0
6	D	401	ATP	2	0

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.

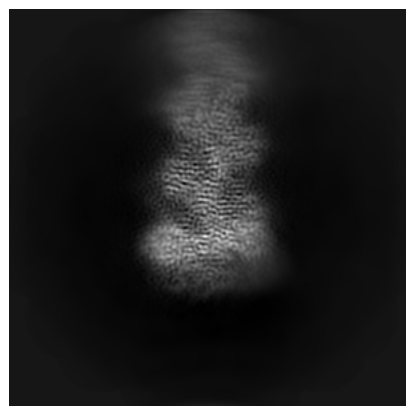
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19522. These allow visual inspection of the internal detail of the map and identification of artifacts.

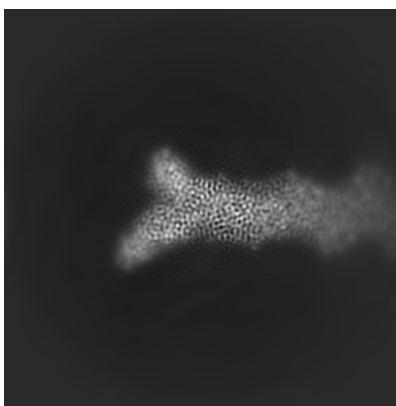
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

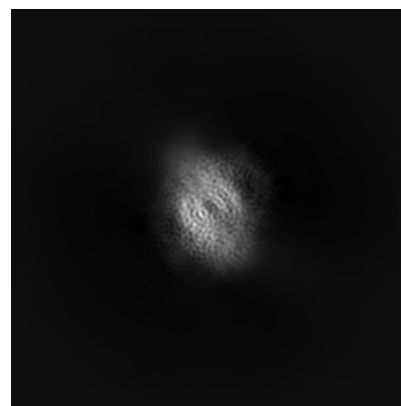
6.1.1 Primary map



X

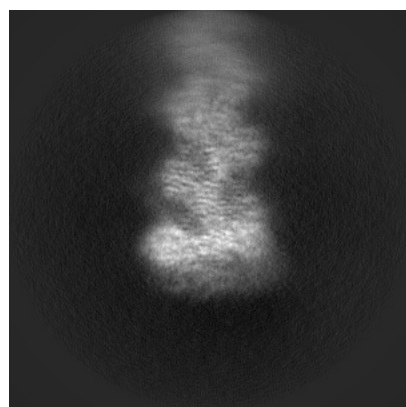


Y

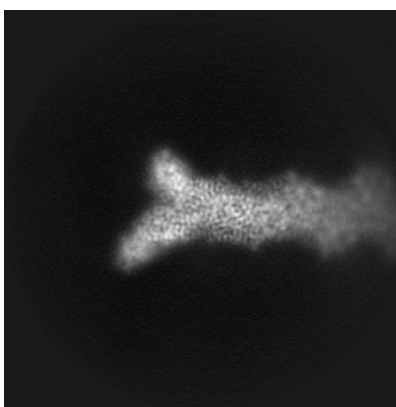


Z

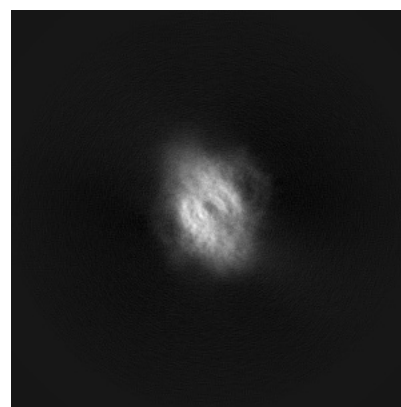
6.1.2 Raw map



X



Y

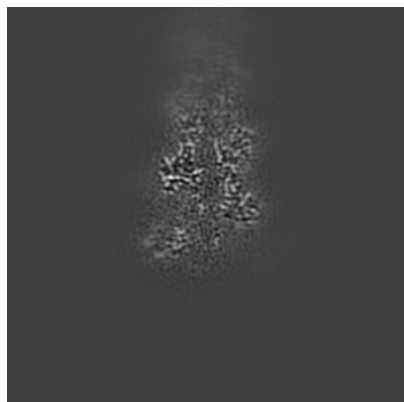


Z

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

6.2 Central slices [i](#)

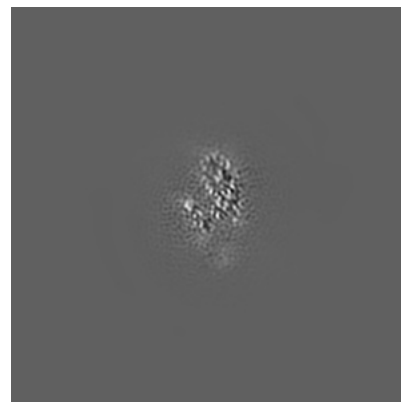
6.2.1 Primary map



X Index: 180

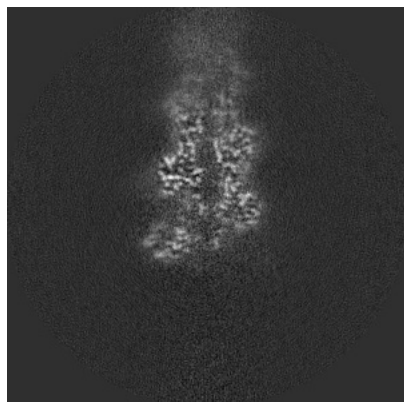


Y Index: 180

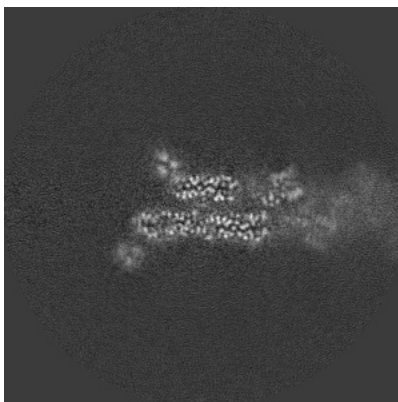


Z Index: 180

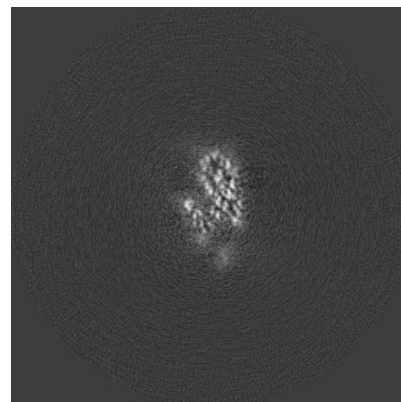
6.2.2 Raw map



X Index: 180



Y Index: 180

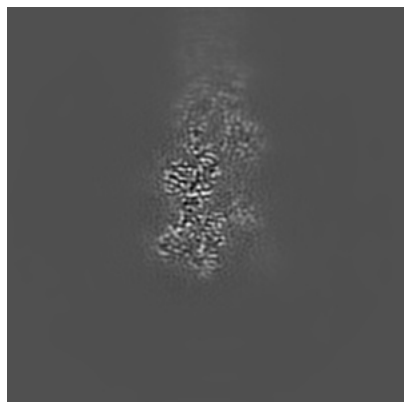


Z Index: 180

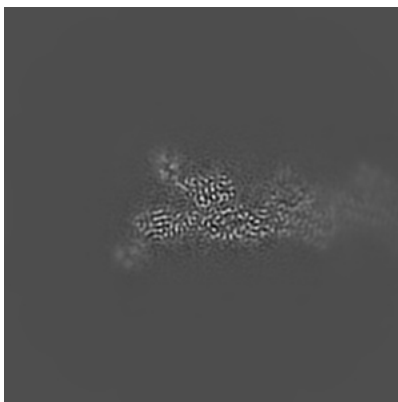
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

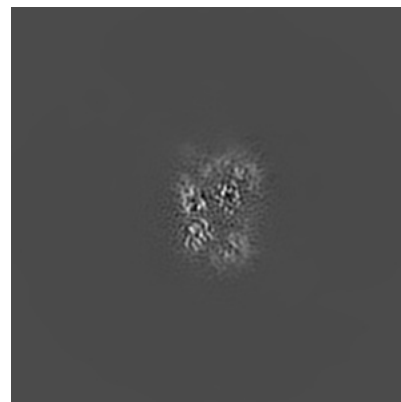
6.3.1 Primary map



X Index: 170

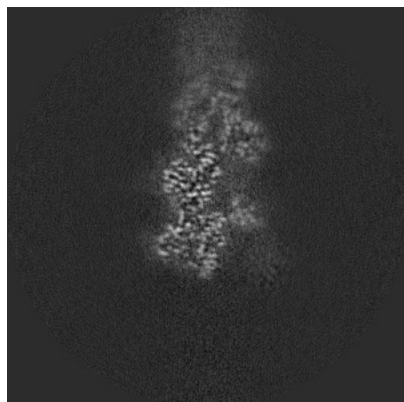


Y Index: 175

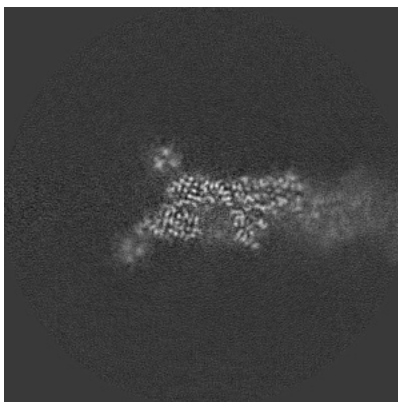


Z Index: 160

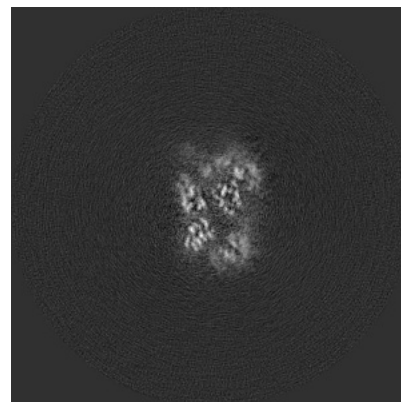
6.3.2 Raw map



X Index: 170



Y Index: 189

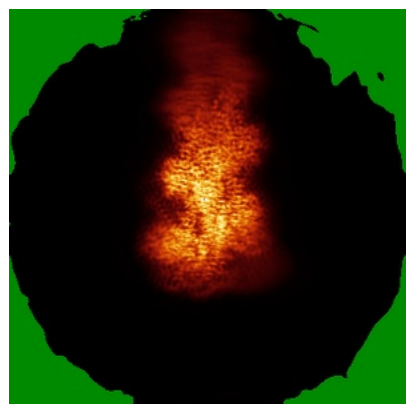


Z Index: 160

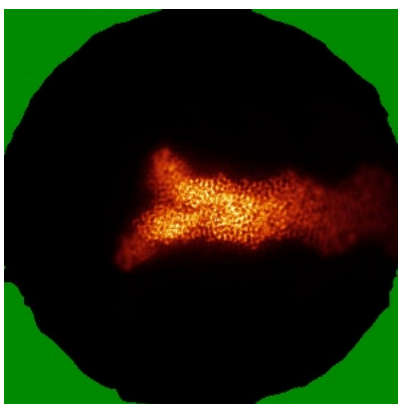
The images above show the largest variance slices of the map in three orthogonal directions.

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

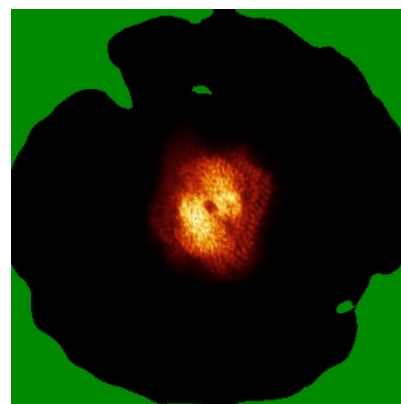
6.4.1 Primary map



X

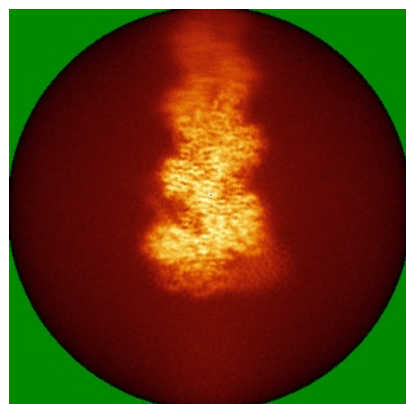


Y

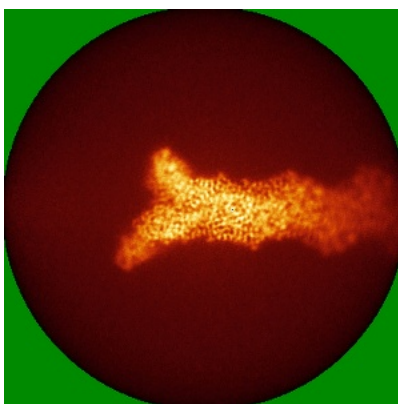


Z

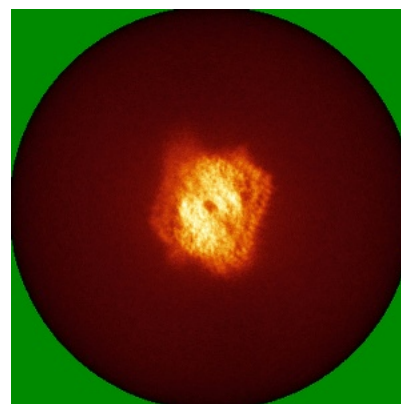
6.4.2 Raw map



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 0.03. 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.

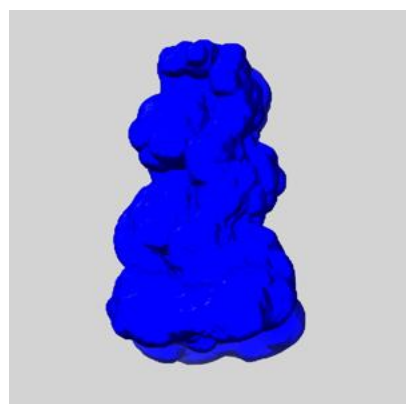
6.6 Mask visualisation [i](#)

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

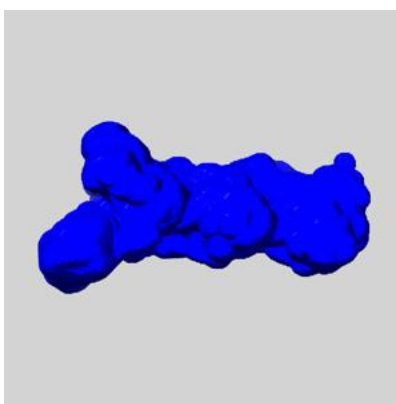
A mask typically either:

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

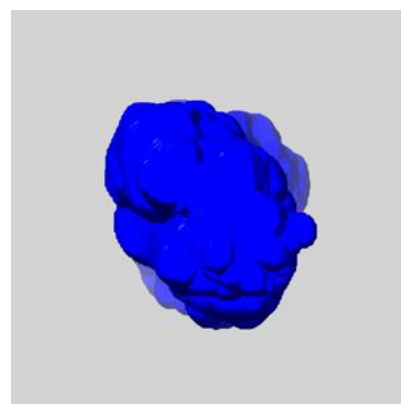
6.6.1 emd_19522_msk_1.map [i](#)



X

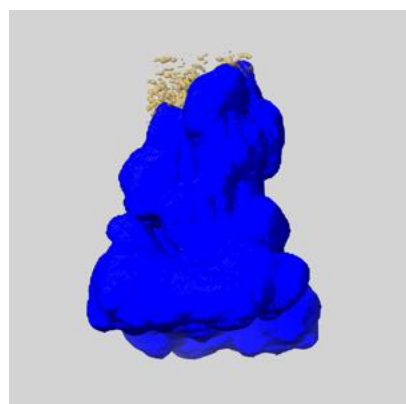


Y

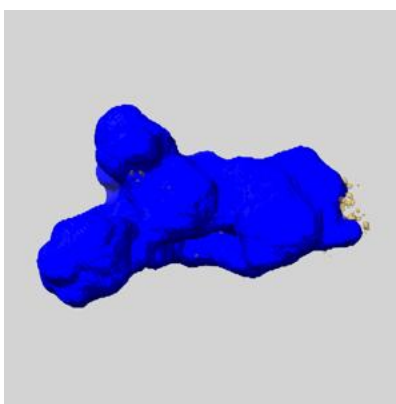


Z

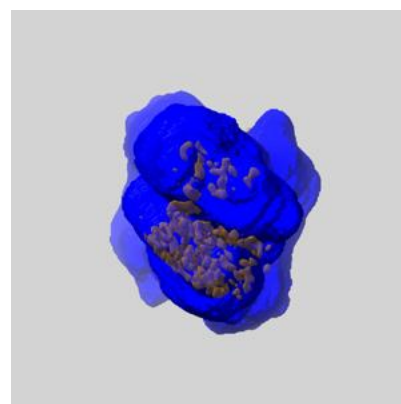
6.6.2 emd_19522_msk_2.map [i](#)



X



Y

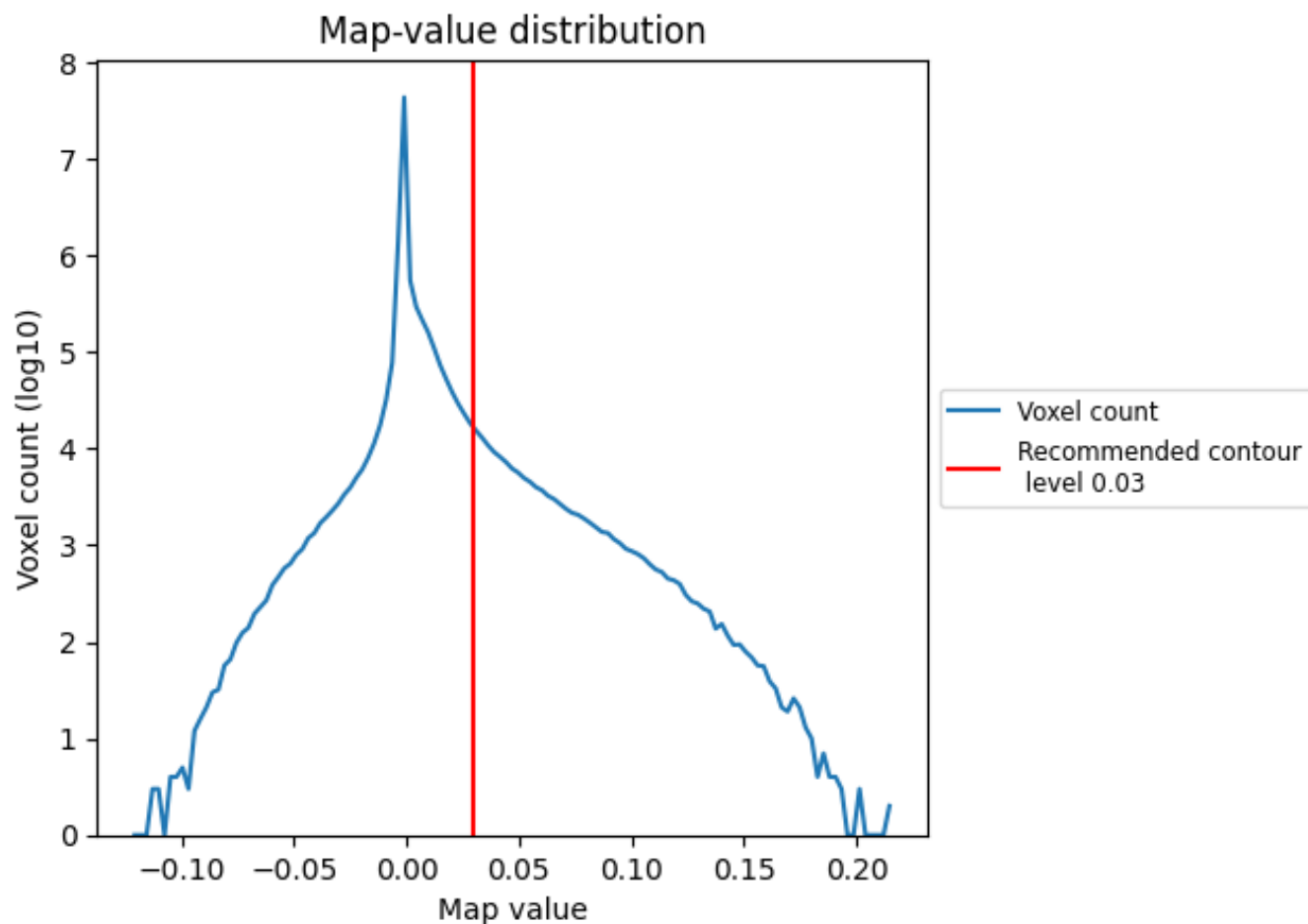


Z

7 Map analysis [i](#)

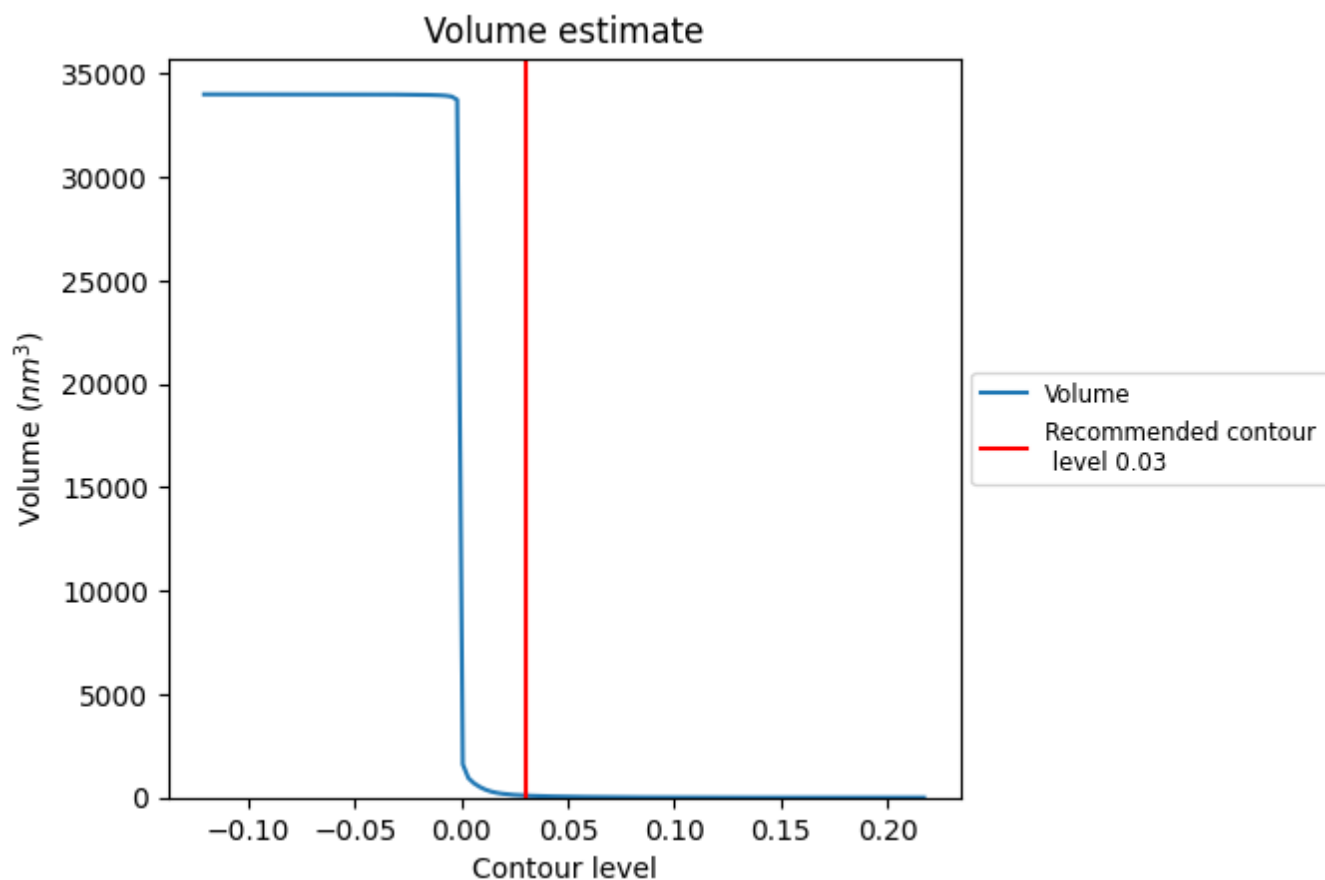
This section contains the results of statistical analysis of the map.

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.

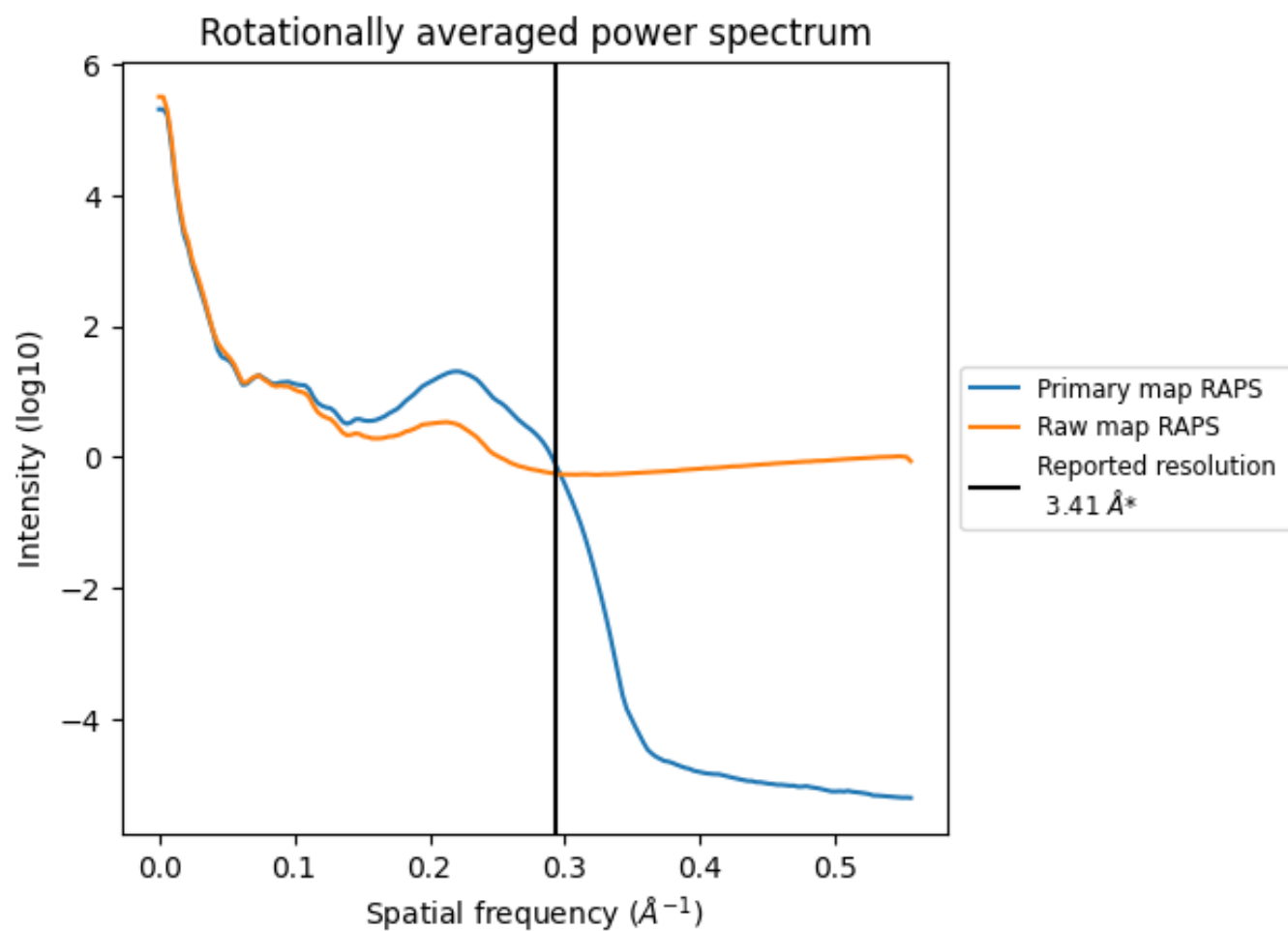
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

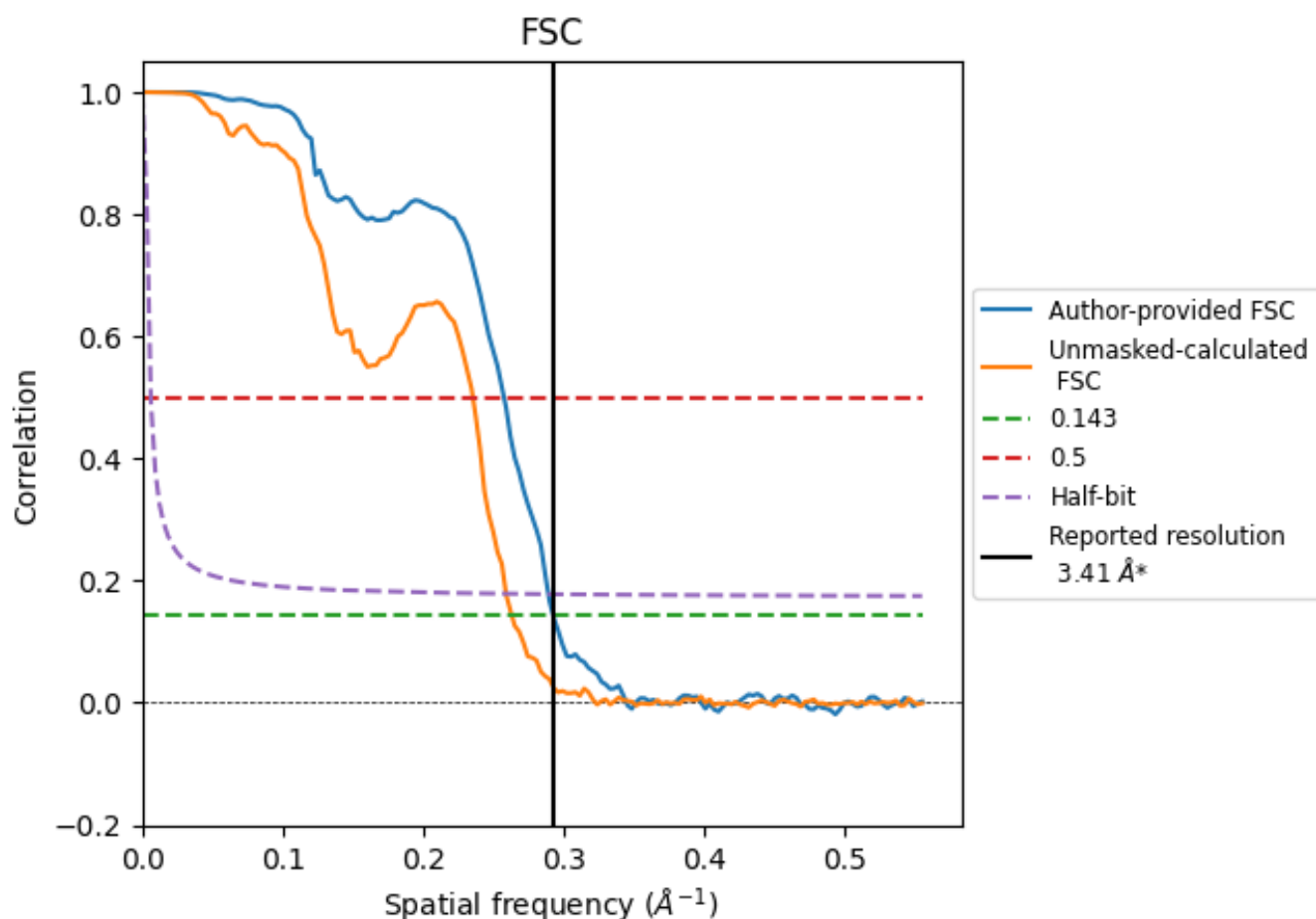


*Reported resolution corresponds to spatial frequency of 0.293 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.293 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

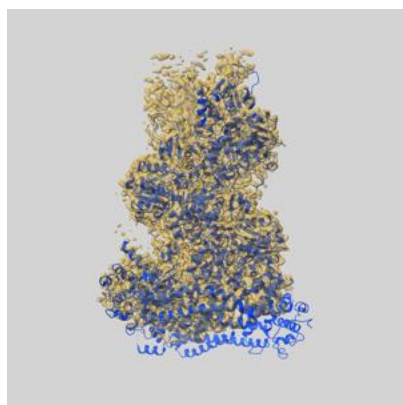
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.42	3.88	3.46
Unmasked-calculated*	3.80	4.25	3.86

*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 3.80 differs from the reported value 3.41 by more than 10 %

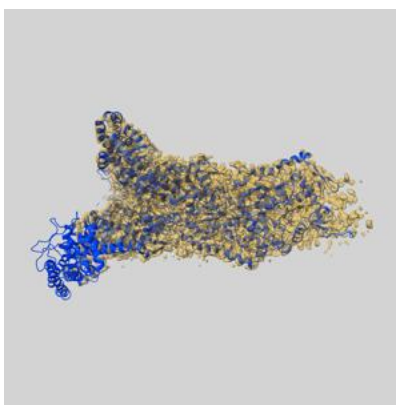
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19522 and PDB model 8RV2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

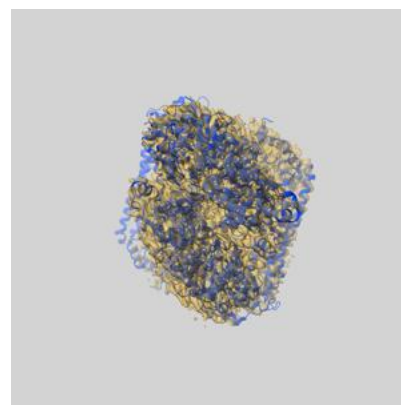
9.1 Map-model overlay [i](#)



X



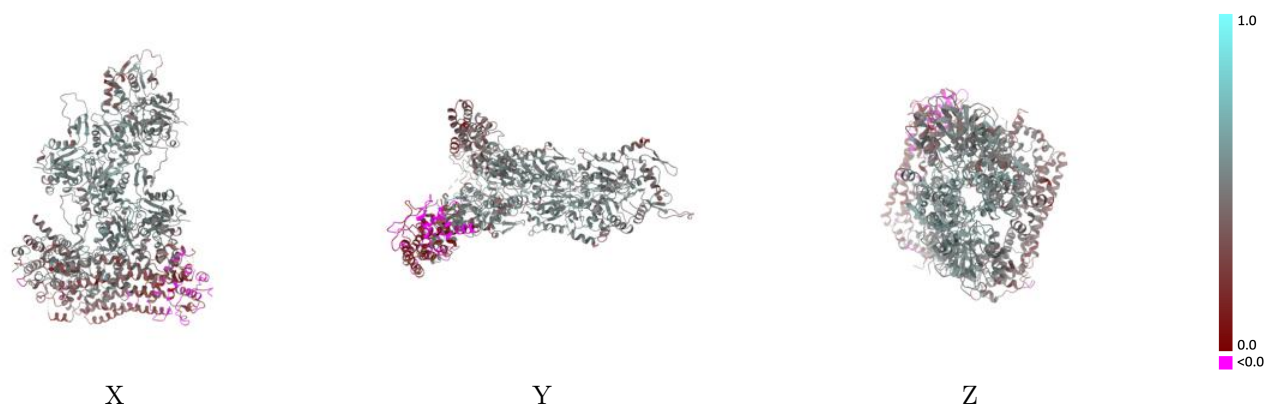
Y



Z

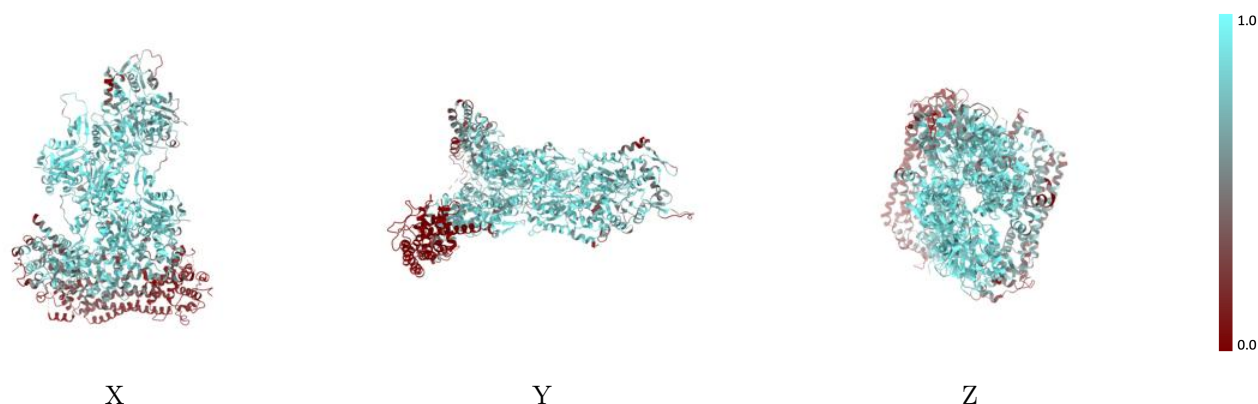
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



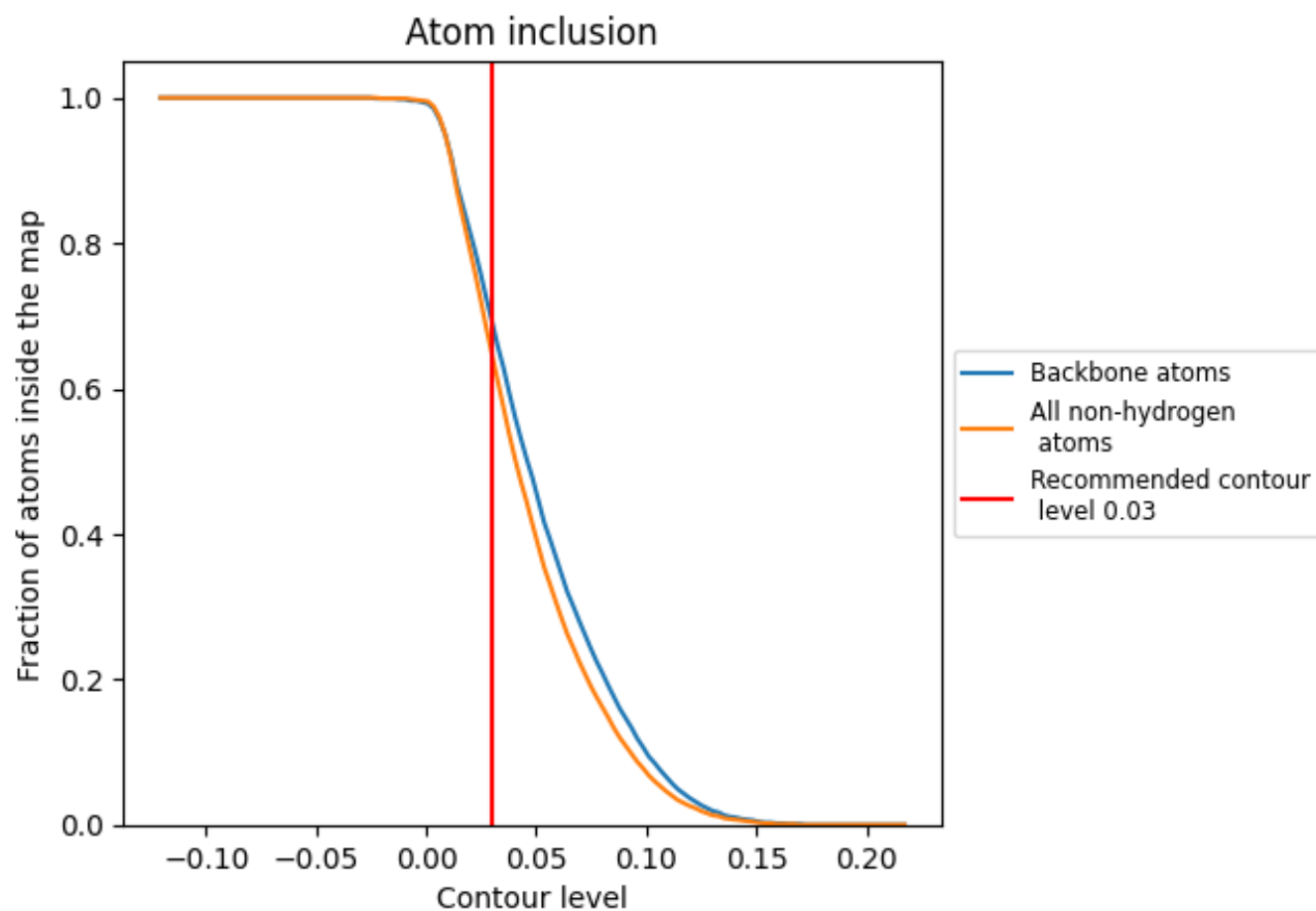
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 64% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.4300
A	0.7020	0.4800
B	0.8640	0.5290
C	0.8530	0.5150
D	0.8050	0.5050
E	0.5010	0.3440
F	0.1110	0.1900

1.0

0.0

<0.0