



Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 03:48 PM EDT

PDB ID : 8DYV / pdb_00008dyv
EMDB ID : EMD-27783
Title : Structure of human cytoplasmic dynein-1 bound to one Lis1
Authors : Reimer, J.M.; DeSantis, M.; Reck-Peterson, S.L.; Leschziner, A.E.
Deposited on : 2022-08-05
Resolution : 3.97 Å(reported)

This is a Full wwPDB EM Validation 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

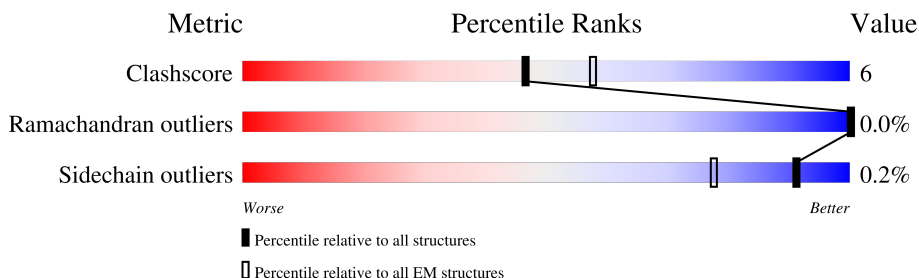
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	3328	
2	B	411	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45974 atoms, of which 22922 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2549	Total	C	H	N	O	S	0	0
			41027	13084	20519	3538	3779	107		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1319	GLY	-	expression tag	UNP Q14204

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	305	Total	C	H	N	O	S	0	0
			4787	1533	2355	428	451	20		

There are 2 discrepancies between the modelled and reference sequences:

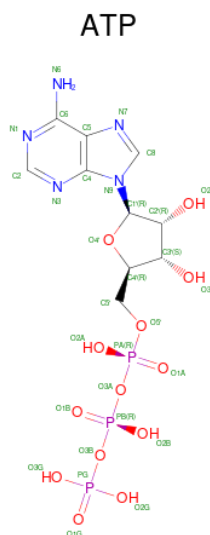
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P43034
B	1	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

ALA	GLY	SER	THR	PRO	ARG	ILE	GLN	G3926	L3938	S3939	C3940	F3944	K3945	D3946	E3967	Q3968	T3969	V3970	W3974	SER	GLU	T3978	R3989	L3990	L3991	L3992	I3993	L4002	A4003	M4004	A4005	H4006	L4013	I4020	L4042	H4043	C4044	Y4049	C4076	A4080	A4083	A4087	S4090						
V3784	E3785	E3786	T3787	D3788	I3789	V3790	M3791	Q3792	E3793	V3794	E3795	T3814	M3815	E3816	S3817	L3818	L3833	N3843	P3844	N3845	LEU	GLY	T3850	K3861	F3868	M3875	H3880	A3884	M3885	L3886	L3892	LYS	GLY	THR	VAL	GLY	GLU	L3909	R3910	G3911	N3912	ILE	GLU	VAL	LEU	SER			
F3698	V3699	N3700	L3708	N3714	D3725	E3726	K3727	R3728	L3731	L3732	K3733	L3734	E3737	F3738	Q3739	L3740	R3741	L3742	L3745	E3746	K3747	S3748	L3749	N3754	GLU	VAL	LYS	GLY	ARG	D3763	D3764	T3765	T3766	T3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	F3779	V3780	R3781	K3782	K3783
I3503	A3512	G3518	Y3519	L3528	W3532	N3540	D3546	I3547	A3548	Y3552	L3553	S3554	R3559	L3560	L3572	R3585	L3588	I3609	N3622	L3623	E3624	S3640	V3644	R3654	R3655	T3656	G3657	G3658	L3661	L3664	G3665	D3668	I3669	V3686	S3694	V3695	T3697												
ASN	TYR	GLU	ILE	VAL	ASN	ARG	ALA	ALA	TYR	GLY	GLU	TYR	ALA	ALA	GLN	ILE	ALA	GLN	ALA	VAL	GLU	LYS	VAL	ARG	ASN	GLU	LEU	GLN	LYS	LEU	GLP	ASP	ALA	ALA	LYS	ASP	ASP	ASN	GLN	GLN	LYS	ASN	ASN	VAL	GLU	GLN	MET	ILE	
LYS	LEU	ALA	THR	VAL	SER	SER	ILE	CYS	LEU	LEU	ALA	CYS	GLY	GLU	SER	ILE	ALA	THR	THR	ASP	LYS	TRP	TRP	ALA	LYS	GLN	ILE	ALA	GLN	ARG	LYS	ILE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
GLN	GLU	ILE	GLN	GLU	GLN	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN		
Y3176	R3191	L3194	M3199	H3200	L3201	R3202	K3207	I3208	K3209	E3210	Q3214	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
L3000	D3001	S3002	E3006	R3007	M3008	H3009	T3010	D3024	M3043	L3044	D3045	T3067	Q3073	D3077	R3078	L3091	N3092	W3093	F3094	G3095	D3096	W3097	S3098	T3099	E3100	E3101	L3102	Y3103	T3110	L3115	T3121	R3140	E3141	A3142	I3143	S3146	F3149	V3150	T3153	L3154	R3167	I3171							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
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R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2912	M2913	E2914	D2923	R2924	G2931	H2932	L2933	L2934	I2936	G2942	W2943	T2944	N2954	Q2960	H2964	R2965	K2966	Y2967	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	L2993							
R2869	P2870	L2871	S2874	W2875	W2876	Q2886	E2887	E2888	Y2892	R2896	L2897	E2904	L2905	L2911	F2																																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.837	Depositor
Minimum map value	-0.531	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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, 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	0.29	5/20945 (0.0%)	0.52	25/28384 (0.1%)
2	B	0.31	1/2495 (0.0%)	0.62	6/3379 (0.2%)
All	All	0.29	6/23440 (0.0%)	0.53	31/31763 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2728	LEU	C-N	-9.19	1.21	1.33
1	A	2729	ARG	C-N	7.03	1.43	1.33
1	A	2835	ASP	C-O	-6.12	1.16	1.24
1	A	4263	ARG	C-O	-5.82	1.17	1.24
1	A	2592	VAL	C-O	-5.72	1.18	1.24
2	B	95	ILE	N-CA	5.25	1.50	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4263	ARG	CA-C-O	-9.20	111.22	120.70
1	A	3782	ARG	CA-C-O	-8.30	112.10	120.82
1	A	3791	MET	N-CA-C	-7.54	103.07	111.82
1	A	4049	TYR	CA-C-O	-7.47	112.02	120.32
1	A	3769	THR	CA-C-N	7.44	130.85	120.29
1	A	3769	THR	C-N-CA	7.44	130.85	120.29
1	A	3786	GLU	CA-C-N	7.39	131.55	120.31
1	A	3786	GLU	C-N-CA	7.39	131.55	120.31
2	B	98	PRO	N-CA-C	7.38	119.70	110.70
1	A	3781	THR	N-CA-C	-7.32	103.33	111.82
2	B	96	PRO	CB-CA-C	-6.98	102.46	111.46
2	B	96	PRO	N-CA-C	6.31	120.98	111.14
2	B	95	ILE	CA-C-O	-6.09	116.77	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2728	LEU	CA-C-N	6.07	128.90	120.29
1	A	2728	LEU	C-N-CA	6.07	128.90	120.29
1	A	1938	PHE	CA-C-O	-5.86	114.34	120.55
1	A	2265	TYR	CA-C-O	-5.84	112.72	118.97
2	B	252	CYS	CA-C-O	-5.66	115.24	121.58
2	B	218	MET	CA-C-O	-5.57	114.36	120.43
1	A	3792	GLN	CA-C-O	-5.47	114.62	120.42
1	A	3552	TYR	CA-C-O	-5.43	115.30	120.90
1	A	3789	ILE	CA-C-O	-5.41	115.11	120.85
1	A	2728	LEU	O-C-N	-5.37	115.94	122.22
1	A	3777	ALA	N-CA-C	-5.34	105.53	111.36
1	A	4262	GLN	N-CA-C	-5.32	105.65	111.82
1	A	2319	LEU	N-CA-C	-5.26	106.17	112.59
1	A	2800	THR	CA-C-O	-5.21	115.03	120.55
1	A	3745	LEU	CA-C-O	-5.18	114.01	119.97
1	A	3783	LYS	CB-CA-C	-5.11	102.31	110.79
1	A	3786	GLU	CA-C-O	-5.02	114.20	119.97
1	A	3784	VAL	N-CA-C	-5.00	105.52	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20508	20519	20534	243	0
2	B	2432	2355	2355	30	0
3	A	81	36	36	4	0
4	A	31	12	12	3	0
All	All	23052	22922	22937	272	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.

All (272) 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:3938:LEU:HD13	1:A:3991:LEU:HD22	1.67	0.76
1:A:3738:PHE:CG	1:A:3783:LYS:HB2	2.22	0.74
1:A:4319:SER:N	1:A:4325:ASN:OD1	2.23	0.71
1:A:4264:LEU:HD12	1:A:4264:LEU:O	1.93	0.69
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.25	0.69
1:A:1879:LEU:O	1:A:1881:GLN:NE2	2.25	0.69
1:A:2284:LEU:O	1:A:2288:ILE:HD12	1.93	0.69
1:A:1853:VAL:HG12	1:A:1853:VAL:O	1.92	0.68
1:A:4149:PRO:O	1:A:4195:ARG:NH2	2.26	0.68
1:A:4505:LYS:HD2	1:A:4527:TYR:HE2	1.57	0.68
1:A:3742:LEU:HD13	1:A:3780:VAL:HG21	1.74	0.68
1:A:4215:ALA:HB1	1:A:4247:MET:HE1	1.76	0.68
1:A:2220:LEU:HD12	1:A:2221:MET:H	1.60	0.67
1:A:2664:ASP:OD1	1:A:2665:GLU:OE2	2.13	0.67
1:A:3738:PHE:CD2	1:A:3783:LYS:HB2	2.30	0.67
1:A:3149:PHE:O	1:A:3153:THR:HG23	1.95	0.67
1:A:2220:LEU:HD11	1:A:2362:VAL:HG23	1.76	0.66
1:A:2484:GLU:O	1:A:2488:ARG:NH1	2.30	0.65
1:A:4193:ARG:NH1	1:A:4321:LEU:O	2.30	0.65
1:A:4090:SER:O	1:A:4092:ARG:NH1	2.30	0.64
1:A:2217:ASN:HD22	1:A:2360:GLY:HA3	1.62	0.64
1:A:2904:GLU:O	1:A:3654:ARG:NH1	2.31	0.63
1:A:2319:LEU:HD22	1:A:2359:CYS:SG	2.38	0.63
1:A:2507:ARG:NH1	1:A:2735:TYR:OH	2.31	0.62
1:A:4203:LYS:NZ	1:A:4616:ALA:O	2.32	0.62
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.33	0.62
1:A:2506:SER:O	1:A:2511:ARG:NH1	2.33	0.61
1:A:2230:LYS:N	4:A:4703:ATP:O1B	2.34	0.61
1:A:4129:GLU:O	1:A:4131:ASN:ND2	2.32	0.61
1:A:4206:GLU:N	1:A:4206:GLU:OE1	2.33	0.61
1:A:4263:ARG:HD2	1:A:4636:TYR:CE1	2.36	0.61
1:A:2592:VAL:HG12	1:A:2592:VAL:O	2.01	0.60
1:A:3146:SER:O	1:A:3150:VAL:HG13	2.00	0.60
2:B:324:ASP:OD2	2:B:327:THR:HG22	2.02	0.60
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.83	0.60
1:A:3006:GLU:O	1:A:3010:THR:HG23	2.01	0.60
1:A:4307:GLN:N	1:A:4307:GLN:OE1	2.36	0.59
1:A:2600:GLY:N	3:A:4702:ADP:O2A	2.35	0.59
1:A:2888:GLU:N	1:A:2888:GLU:OE2	2.34	0.58
2:B:123:MET:HE2	2:B:137:TYR:HB3	1.86	0.58
1:A:3518:GLY:O	1:A:3700:ASN:N	2.35	0.58
1:A:3790:VAL:HG22	1:A:3790:VAL:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2960:GLN:HB3	1:A:2993:ILE:HD12	1.85	0.58
1:A:1814:GLU:OE2	1:A:1818:GLN:NE2	2.37	0.57
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.36	0.57
2:B:169:SER:OG	2:B:171:ASP:OD1	2.21	0.57
1:A:4328:GLU:OE1	1:A:4328:GLU:N	2.37	0.57
1:A:2222:MET:N	1:A:2222:MET:SD	2.78	0.57
1:A:3741:ARG:O	1:A:3745:LEU:HG	2.05	0.57
1:A:1896:LEU:O	1:A:1899:ARG:NH2	2.37	0.57
1:A:1766:LEU:HD12	1:A:1778:LEU:HD11	1.87	0.56
1:A:3191:ARG:NE	1:A:3500:MET:SD	2.78	0.56
1:A:3073:GLU:N	1:A:3073:GLU:OE1	2.38	0.56
2:B:248:LEU:HD13	2:B:261:TRP:O	2.05	0.56
1:A:2897:LEU:HD11	1:A:2911:LEU:HD13	1.86	0.56
1:A:1853:VAL:O	1:A:1853:VAL:CG1	2.54	0.56
1:A:2781:GLN:NE2	1:A:2794:TYR:O	2.39	0.55
1:A:2621:ASN:ND2	1:A:3010:THR:HG22	2.21	0.55
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.39	0.55
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.40	0.55
1:A:3868:PHE:CE1	1:A:3884:ALA:HB2	2.42	0.55
1:A:4509:VAL:HG13	1:A:4560:VAL:HG23	1.88	0.55
1:A:4263:ARG:HD2	1:A:4636:TYR:CZ	2.43	0.54
1:A:3814:THR:HG23	1:A:3886:LEU:HD13	1.88	0.54
1:A:2452:LEU:HD11	4:A:4703:ATP:H4'	1.89	0.54
1:A:3121:ILE:O	1:A:3540:ASN:ND2	2.40	0.54
1:A:3519:TYR:CD1	1:A:3519:TYR:O	2.60	0.54
2:B:271:GLU:C	2:B:272:LEU:HD12	2.32	0.54
1:A:4434:VAL:HG21	1:A:4451:LEU:HD22	1.90	0.54
1:A:3102:LEU:HD11	1:A:3176:TYR:CG	2.42	0.54
1:A:2296:GLN:N	1:A:2296:GLN:OE1	2.41	0.54
1:A:4577:LEU:O	1:A:4638:ARG:NH2	2.41	0.54
1:A:1939:GLN:N	1:A:1939:GLN:OE1	2.41	0.54
1:A:3100:GLU:N	1:A:3100:GLU:OE1	2.41	0.54
1:A:3772:ASN:O	1:A:3775:ARG:HB2	2.07	0.54
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.44	0.53
1:A:2461:MET:HE2	1:A:2497:ALA:HB2	1.89	0.53
1:A:3154:LEU:HB3	1:A:3171:ILE:HG21	1.89	0.53
1:A:2687:VAL:HG11	1:A:2730:HIS:HB3	1.91	0.53
1:A:4306:VAL:HG12	1:A:4310:GLU:OE2	2.09	0.53
1:A:2075:LEU:HD23	1:A:4522:THR:HG23	1.91	0.53
1:A:2480:PRO:O	1:A:2482:GLN:NE2	2.40	0.53
1:A:3102:LEU:HD11	1:A:3176:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4208:GLY:N	1:A:4211:ASP:OD2	2.42	0.53
2:B:252:CYS:HB2	2:B:282:ILE:HG12	1.91	0.52
1:A:2143:GLU:OE1	1:A:2212:GLN:NE2	2.42	0.52
1:A:2892:TYR:OH	1:A:2896:ARG:NH2	2.41	0.52
1:A:3482:LEU:HD21	1:A:3770:LEU:HD21	1.91	0.52
2:B:287:GLU:N	2:B:287:GLU:OE1	2.43	0.52
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	1.91	0.52
1:A:2666:ILE:HG12	1:A:2712:CYS:HB3	1.91	0.52
1:A:2886:GLN:NE2	1:A:2913:ASN:OD1	2.40	0.52
2:B:155:ASP:OD1	2:B:156:ILE:N	2.43	0.52
1:A:1938:PHE:O	1:A:1938:PHE:CD1	2.63	0.52
1:A:3875:MET:O	1:A:3880:HIS:NE2	2.44	0.52
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.91	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:4463:SER:HG	1:A:4464:TRP:CD1	2.29	0.51
1:A:1931:ASN:ND2	1:A:2314:ASN:O	2.43	0.51
1:A:2220:LEU:HD12	1:A:2221:MET:N	2.25	0.51
1:A:2305:GLY:O	1:A:2726:ARG:NH1	2.43	0.51
1:A:2500:TRP:CE2	1:A:2580:LEU:HD13	2.45	0.51
1:A:3843:ASN:ND2	1:A:3845:ASN:O	2.44	0.50
2:B:210:ALA:HB1	2:B:237:VAL:CG2	2.41	0.50
2:B:256:GLN:OE1	2:B:256:GLN:N	2.44	0.50
1:A:2039:LEU:HD23	1:A:2040:ALA:N	2.26	0.50
1:A:3478:LEU:HD21	1:A:3770:LEU:HD13	1.93	0.50
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.92	0.50
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.43	0.50
1:A:4215:ALA:CB	1:A:4247:MET:HE1	2.42	0.50
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.44	0.50
1:A:3818:LEU:HD12	1:A:4346:MET:SD	2.52	0.50
1:A:4505:LYS:HD2	1:A:4527:TYR:CE2	2.43	0.49
1:A:3478:LEU:HG	1:A:3770:LEU:HD22	1.93	0.49
1:A:2776:PHE:O	1:A:2780:SER:N	2.44	0.49
1:A:3008:MET:HA	1:A:3008:MET:HE2	1.94	0.49
1:A:2593:LEU:HD12	1:A:2593:LEU:H	1.77	0.49
1:A:3528:LEU:HD11	1:A:3532:TRP:CZ2	2.48	0.49
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.45	0.49
1:A:3194:LEU:HD12	1:A:3503:ILE:HD11	1.93	0.49
1:A:4481:ASP:OD1	1:A:4485:ARG:NE	2.45	0.49
1:A:4566:GLN:OE1	1:A:4615:ARG:NH2	2.43	0.49
1:A:2137:LEU:HD22	1:A:2165:PHE:CZ	2.48	0.49
1:A:2936:ILE:O	1:A:3094:PHE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2500:TRP:CH2	1:A:2734:VAL:HG23	2.48	0.49
1:A:3077:ASP:OD2	1:A:3078:ARG:NH2	2.46	0.49
1:A:2580:LEU:O	1:A:2584:TRP:CD1	2.66	0.48
1:A:4020:ILE:HD12	1:A:4020:ILE:H	1.78	0.48
1:A:1965:GLU:N	1:A:1965:GLU:OE1	2.45	0.48
1:A:2226:SER:OG	4:A:4703:ATP:O2G	2.20	0.48
1:A:2507:ARG:HB2	1:A:2510:MET:HE2	1.94	0.48
1:A:3554:SER:O	1:A:3559:ARG:NH1	2.47	0.48
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.44	0.48
1:A:2570:PRO:O	1:A:2746:GLN:NE2	2.47	0.48
1:A:2748:TYR:O	1:A:2752:ASN:ND2	2.47	0.48
1:A:2942:GLY:N	3:A:4704:ADP:O2B	2.46	0.48
1:A:3528:LEU:HD11	1:A:3532:TRP:CE2	2.48	0.48
1:A:1912:LYS:N	3:A:4701:ADP:O2A	2.47	0.48
1:A:2500:TRP:HH2	1:A:2734:VAL:HG23	1.79	0.48
1:A:3043:MET:N	1:A:3043:MET:HE2	2.28	0.48
1:A:2358:ARG:NH2	3:A:4701:ADP:O1B	2.47	0.48
1:A:2288:ILE:HD12	1:A:2288:ILE:H	1.78	0.48
1:A:3500:MET:SD	1:A:3503:ILE:HD12	2.54	0.48
1:A:2876:TRP:O	2:B:339:ASN:ND2	2.46	0.48
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.31	0.47
1:A:2643:ARG:HG2	1:A:2648:VAL:HG22	1.96	0.47
2:B:312:LEU:HD23	2:B:344:VAL:HB	1.96	0.47
1:A:1892:MET:HG2	1:A:1919:LEU:HD23	1.96	0.47
1:A:2075:LEU:CD2	1:A:4522:THR:HG23	2.44	0.47
1:A:3771:GLU:O	1:A:3775:ARG:HG3	2.13	0.47
1:A:3909:LEU:HD21	1:A:4343:MET:SD	2.55	0.47
1:A:3103:TYR:OH	1:A:3141:GLU:OE1	2.31	0.47
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.44	0.47
1:A:2457:SER:CB	1:A:2501:SER:HG	2.26	0.47
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.47	0.47
1:A:1813:THR:HG22	1:A:2052:VAL:CG1	2.44	0.47
1:A:2731:VAL:O	1:A:2731:VAL:HG13	2.14	0.47
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.50	0.47
1:A:2874:SER:HB2	1:A:2876:TRP:CD1	2.50	0.47
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.45	0.46
1:A:2970:GLU:OE1	1:A:2971:ASP:N	2.48	0.46
1:A:3167:ARG:NH2	1:A:3686:VAL:O	2.49	0.46
1:A:3885:MET:HE3	1:A:3990:LEU:HD21	1.98	0.46
1:A:4042:LEU:HD21	1:A:4044:CYS:HB2	1.98	0.46
1:A:4087:ALA:O	1:A:4091:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2078:GLU:OE1	1:A:4522:THR:OG1	2.34	0.46
1:A:3167:ARG:O	1:A:3519:TYR:OH	2.32	0.46
1:A:2933:LEU:HD21	1:A:2935:LEU:HD21	1.97	0.46
1:A:3770:LEU:C	1:A:3770:LEU:HD23	2.41	0.46
1:A:3727:LYS:O	1:A:3731:LEU:HG	2.16	0.46
1:A:2552:VAL:HG13	1:A:2552:VAL:O	2.16	0.45
2:B:210:ALA:HB1	2:B:237:VAL:HG23	1.97	0.45
1:A:1958:ASP:OD1	1:A:1959:GLU:N	2.49	0.45
1:A:2752:ASN:ND2	1:A:2770:THR:OG1	2.49	0.45
1:A:2203:TRP:CZ2	1:A:2236:VAL:HG11	2.51	0.45
1:A:2614:ASP:C	1:A:2615:MET:HE2	2.42	0.45
2:B:165:LEU:HD11	2:B:179:PHE:HD1	1.82	0.45
1:A:2549:GLN:HA	1:A:2552:VAL:HG12	1.98	0.45
1:A:3733:LYS:NZ	1:A:3737:GLU:OE2	2.49	0.45
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.46	0.45
1:A:2064:VAL:HG12	1:A:2068:LYS:HD3	1.99	0.44
2:B:257:THR:HG22	2:B:273:ARG:HB2	1.99	0.44
1:A:1806:ARG:NH2	1:A:1809:GLU:OE1	2.50	0.44
1:A:2784:PHE:CD2	1:A:2837:LEU:HD21	2.52	0.44
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.47	0.44
1:A:3970:VAL:HG21	1:A:3989:ARG:HG2	1.99	0.44
2:B:162:GLY:O	2:B:163:LYS:C	2.61	0.44
1:A:4572:ASN:OD1	1:A:4572:ASN:N	2.48	0.44
2:B:150:THR:OG1	2:B:171:ASP:OD2	2.36	0.44
1:A:2510:MET:SD	1:A:2510:MET:N	2.90	0.44
2:B:324:ASP:HB2	2:B:331:LEU:HD11	1.99	0.44
1:A:1877:ASP:OD1	1:A:1878:LYS:N	2.50	0.44
1:A:2869:ARG:O	1:A:2871:ILE:N	2.51	0.44
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.53	0.44
1:A:4339:MET:C	1:A:4339:MET:HE3	2.43	0.44
1:A:2965:ARG:NH1	1:A:3640:SER:OG	2.51	0.44
1:A:2012:MET:SD	1:A:2013:ALA:N	2.91	0.43
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.51	0.43
1:A:1913:THR:HG23	1:A:1956:CYS:SG	2.58	0.43
1:A:3967:GLU:OE1	1:A:3967:GLU:N	2.43	0.43
1:A:2621:ASN:OD1	1:A:2621:ASN:N	2.51	0.43
1:A:3938:LEU:HD11	1:A:3944:PHE:CD2	2.52	0.43
1:A:3989:ARG:NH2	1:A:4004:MET:SD	2.91	0.43
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.51	0.43
2:B:134:VAL:HG11	2:B:179:PHE:CE1	2.54	0.43
1:A:3770:LEU:HD23	1:A:3770:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2914:GLU:N	1:A:2914:GLU:OE1	2.51	0.43
1:A:3714:ASN:OD1	1:A:3728:ARG:NH1	2.51	0.43
1:A:4264:LEU:O	1:A:4264:LEU:CD1	2.65	0.43
1:A:2446:ILE:HG23	1:A:2447:MET:HG3	2.00	0.43
2:B:149:HIS:CG	2:B:169:SER:HG	2.33	0.43
1:A:3194:LEU:CD1	1:A:3503:ILE:HD11	2.49	0.43
1:A:3814:THR:CG2	1:A:3886:LEU:HD13	2.48	0.43
1:A:3969:THR:HG23	1:A:3969:THR:O	2.19	0.43
1:A:1948:LEU:O	1:A:1952:GLY:N	2.50	0.42
1:A:2198:GLU:OE1	1:A:2198:GLU:N	2.46	0.42
1:A:2221:MET:HE1	1:A:2348:LEU:HD11	2.00	0.42
1:A:3861:LYS:NZ	1:A:4013:LEU:O	2.52	0.42
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	2.00	0.42
1:A:2138:ILE:HD13	1:A:2161:LEU:HD22	2.01	0.42
1:A:2272:THR:OG1	1:A:2273:ARG:N	2.51	0.42
1:A:3482:LEU:CD2	1:A:3770:LEU:HD21	2.49	0.42
1:A:4264:LEU:HD13	1:A:4636:TYR:C	2.44	0.42
1:A:2935:LEU:HD12	1:A:3067:THR:HG22	2.01	0.42
1:A:3512:ALA:HB1	1:A:3532:TRP:CZ2	2.55	0.42
1:A:2320:ASP:O	1:A:2321:ASP:C	2.61	0.42
1:A:2944:THR:HG23	1:A:2993:ILE:HG21	2.01	0.42
1:A:2559:THR:HG22	1:A:2754:ALA:O	2.19	0.42
1:A:2644:THR:OG1	1:A:2646:ASN:OD1	2.34	0.42
1:A:3885:MET:HE3	1:A:3990:LEU:CD2	2.50	0.42
2:B:252:CYS:SG	2:B:281:CYS:N	2.92	0.42
2:B:344:VAL:O	2:B:345:LEU:HD22	2.19	0.42
1:A:1802:PRO:O	1:A:1804:ARG:NH1	2.50	0.42
1:A:2217:ASN:ND2	1:A:2360:GLY:HA3	2.33	0.42
1:A:4509:VAL:HG22	1:A:4510:CYS:H	1.85	0.42
1:A:3790:VAL:O	1:A:3790:VAL:CG2	2.66	0.42
2:B:312:LEU:HD21	2:B:353:ILE:CG2	2.50	0.42
1:A:4124:LEU:HD21	1:A:4126:LEU:HD21	2.01	0.41
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.61	0.41
1:A:2791:HIS:CD2	1:A:3091:LEU:HD22	2.55	0.41
1:A:4521:ILE:O	1:A:4524:THR:OG1	2.37	0.41
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.56	0.41
1:A:2254:ILE:HG23	1:A:2279:LEU:CD2	2.50	0.41
2:B:233:HIS:CE1	2:B:237:VAL:HG12	2.55	0.41
1:A:2664:ASP:CG	1:A:2665:GLU:OE2	2.63	0.41
1:A:1710:ARG:NH1	1:A:1871:GLU:OE2	2.47	0.41
1:A:3548:ALA:O	1:A:3552:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3738:PHE:CB	1:A:3783:LYS:HB2	2.50	0.41
1:A:3099:THR:OG1	1:A:3100:GLU:OE1	2.39	0.41
1:A:2593:LEU:HD12	1:A:2710:GLY:O	2.20	0.41
1:A:2828:GLU:OE2	1:A:2924:ARG:NH1	2.47	0.41
1:A:3993:ILE:HD13	1:A:4004:MET:HB3	2.03	0.41
1:A:4388:LEU:HA	1:A:4391:ILE:HD12	2.03	0.41
2:B:114:VAL:HG11	2:B:404:VAL:HG13	2.03	0.41
1:A:2825:TRP:CZ3	1:A:2854:ALA:HB2	2.56	0.41
2:B:123:MET:HE3	2:B:135:TRP:NE1	2.35	0.41
1:A:3585:ARG:NH1	1:A:3696:VAL:O	2.54	0.40
1:A:2838:VAL:HG12	1:A:3093:TRP:CH2	2.56	0.40
1:A:3745:LEU:O	1:A:3749:LEU:HG	2.21	0.40
1:A:3794:VAL:O	1:A:3794:VAL:CG1	2.69	0.40
2:B:236:TRP:O	2:B:254:ASN:ND2	2.47	0.40
1:A:1758:TRP:HH2	1:A:1821:VAL:HG11	1.87	0.40
1:A:2869:ARG:O	1:A:2869:ARG:NE	2.54	0.40
2:B:197:SER:OG	2:B:239:MET:HA	2.21	0.40
1:A:1806:ARG:NH1	1:A:1877:ASP:OD2	2.50	0.40
1:A:2155:PRO:O	1:A:4411:ARG:NH1	2.55	0.40
1:A:2728:LEU:O	1:A:2728:LEU:HD12	2.21	0.40
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	2.03	0.40
1:A:3661:LEU:N	1:A:3661:LEU:HD12	2.36	0.40
1:A:4509:VAL:CG1	1:A:4560:VAL:HG23	2.51	0.40
2:B:164:LEU:HB3	2:B:176:LEU:HD21	2.03	0.40
2:B:164:LEU:HD22	2:B:164:LEU:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2511/3328 (76%)	2434 (97%)	77 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	299/411 (73%)	273 (91%)	25 (8%)	1 (0%)	37	70
All	All	2810/3739 (75%)	2707 (96%)	102 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	PRO

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	2269/2953 (77%)	2264 (100%)	5 (0%)	92	94
2	B	273/364 (75%)	273 (100%)	0	100	100
All	All	2542/3317 (77%)	2537 (100%)	5 (0%)	91	94

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

Mol	Chain	Res	Type
1	A	1967	MET
1	A	2592	VAL
1	A	2773	MET
1	A	3782	ARG
1	A	3886	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1850	GLN
1	A	1921	HIS
1	A	1985	HIS
1	A	2079	GLN
1	A	2139	GLN

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Mol	Chain	Res	Type
1	A	2171	HIS
1	A	2217	ASN
1	A	2577	HIS
1	A	2730	HIS
1	A	2752	ASN
1	A	2827	HIS
1	A	2960	GLN
1	A	3069	ASN
1	A	3499	GLN
1	A	3792	GLN
1	A	3800	GLN
1	A	3843	ASN
1	A	4098	ASN
1	A	4249	GLN
2	B	222	GLN
2	B	381	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.28	2 (6%)
4	ATP	A	4703	-	28,33,33	0.64	0	34,52,52	0.87	1 (2%)
3	ADP	A	4701	-	24,29,29	0.93	0	29,45,45	1.24	2 (6%)
3	ADP	A	4702	-	24,29,29	0.87	0	29,45,45	1.26	2 (6%)

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	A	4704	-	-	2/12/32/32	0/3/3/3
4	ATP	A	4703	-	-	2/18/38/38	0/3/3/3
3	ADP	A	4701	-	-	8/12/32/32	0/3/3/3
3	ADP	A	4702	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	N3-C2-N1	-4.37	122.74	128.67
3	A	4704	ADP	N3-C2-N1	-3.89	123.39	128.67
3	A	4701	ADP	N3-C2-N1	-3.85	123.45	128.67
3	A	4704	ADP	C4-C5-N7	-2.72	106.47	109.34
3	A	4702	ADP	C4-C5-N7	-2.43	106.77	109.34
3	A	4701	ADP	C4-C5-N7	-2.29	106.92	109.34
4	A	4703	ATP	C5-C6-N6	2.26	123.76	120.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4701	ADP	PA-O3A-PB-O3B
3	A	4701	ADP	C5'-O5'-PA-O1A
3	A	4701	ADP	C5'-O5'-PA-O2A
3	A	4701	ADP	C5'-O5'-PA-O3A
3	A	4702	ADP	PA-O3A-PB-O2B
3	A	4702	ADP	C5'-O5'-PA-O1A
3	A	4704	ADP	O4'-C4'-C5'-O5'

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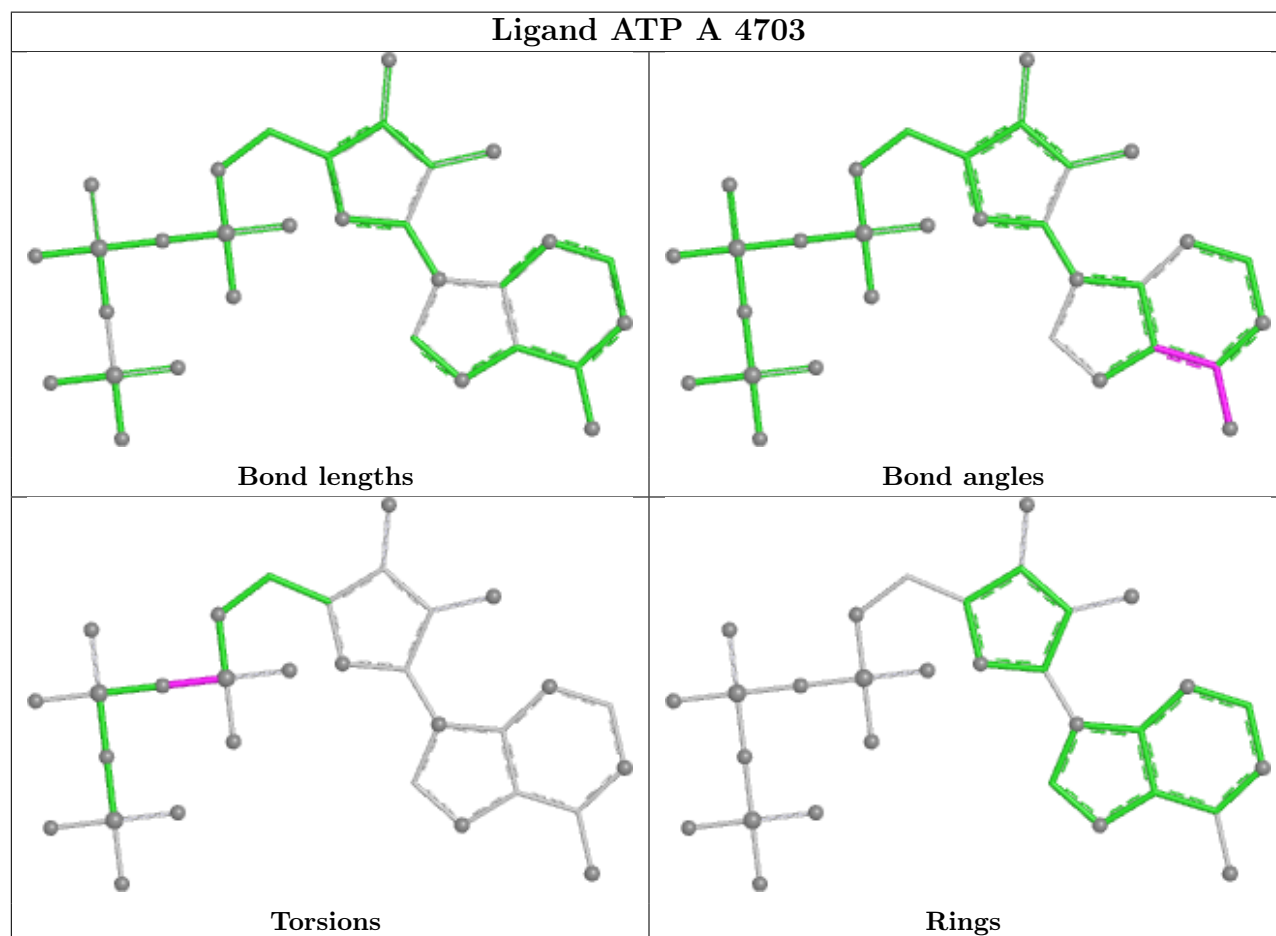
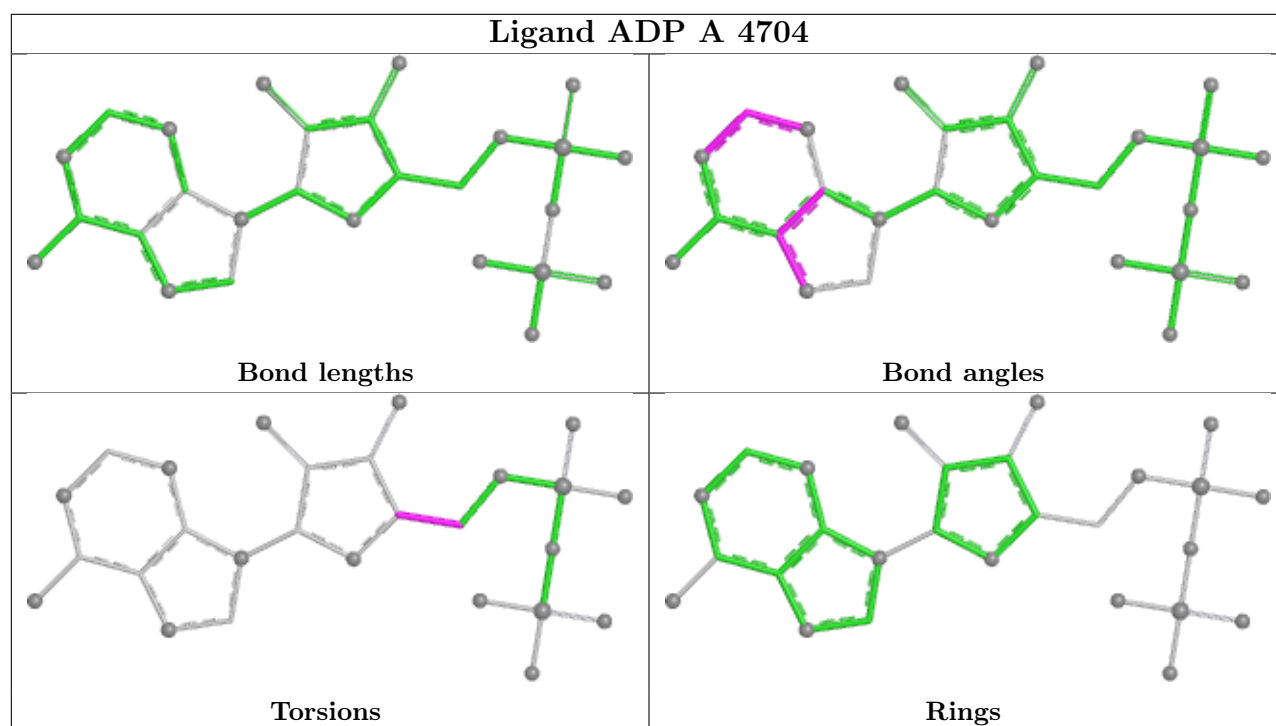
Mol	Chain	Res	Type	Atoms
3	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4701	ADP	C3'-C4'-C5'-O5'
3	A	4701	ADP	PA-O3A-PB-O2B
4	A	4703	ATP	PB-O3A-PA-O1A
3	A	4701	ADP	PA-O3A-PB-O1B
3	A	4702	ADP	PA-O3A-PB-O3B
4	A	4703	ATP	PB-O3A-PA-O2A

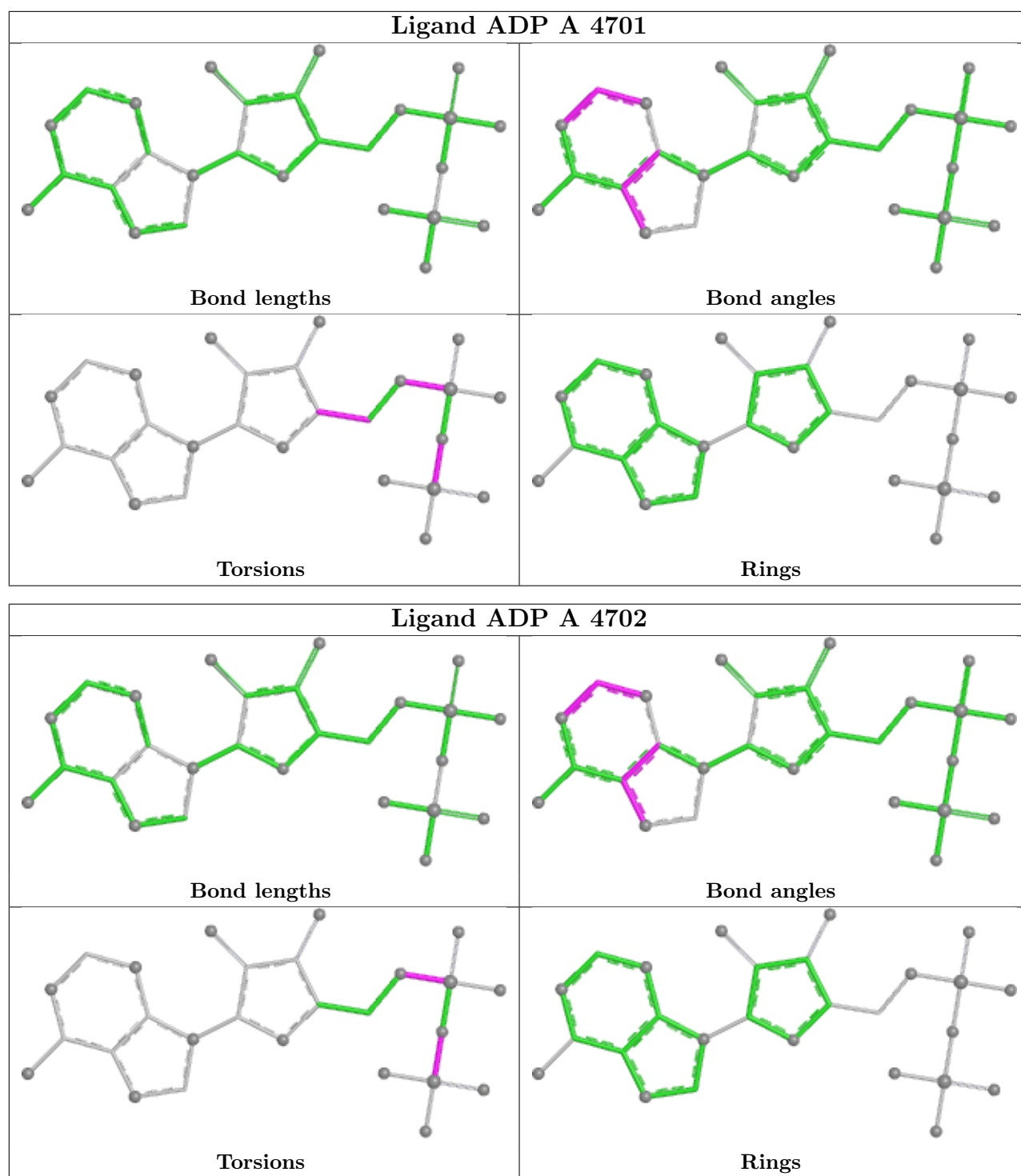
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4704	ADP	1	0
4	A	4703	ATP	3	0
3	A	4701	ADP	2	0
3	A	4702	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

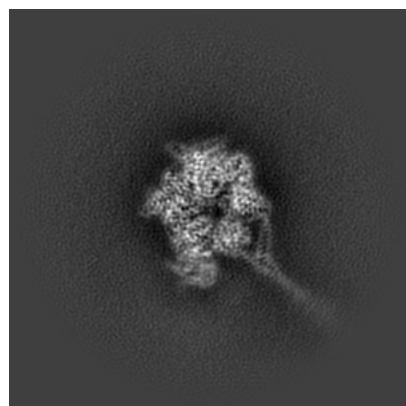
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27783. These allow visual inspection of the internal detail of the map and identification of artifacts.

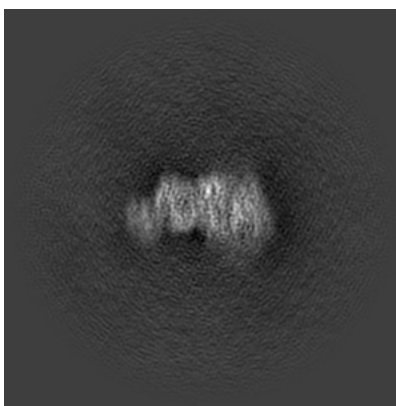
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

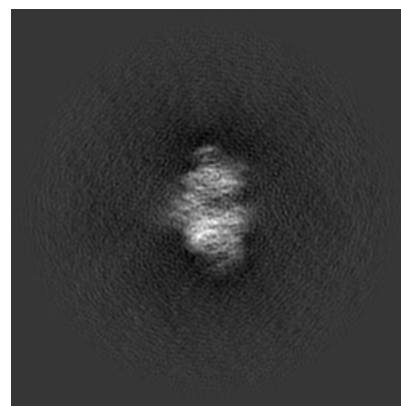
6.1.1 Primary map



X

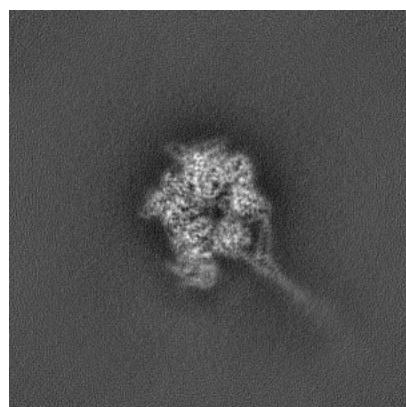


Y

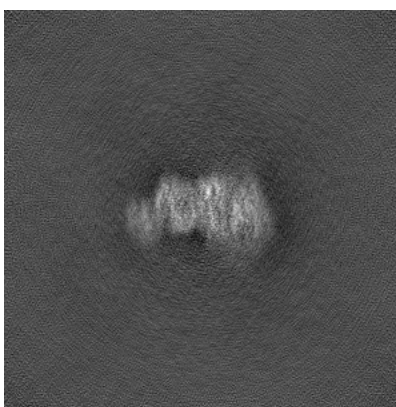


Z

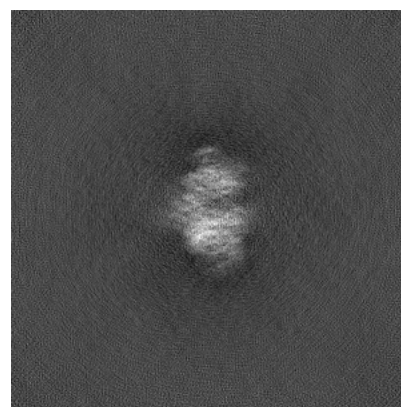
6.1.2 Raw map



X



Y

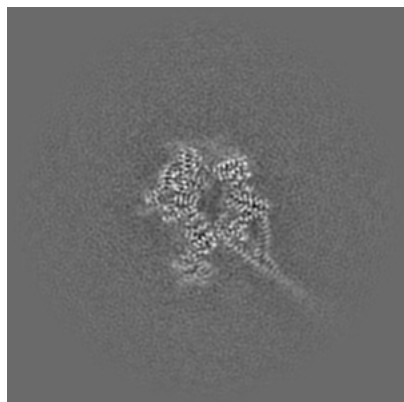


Z

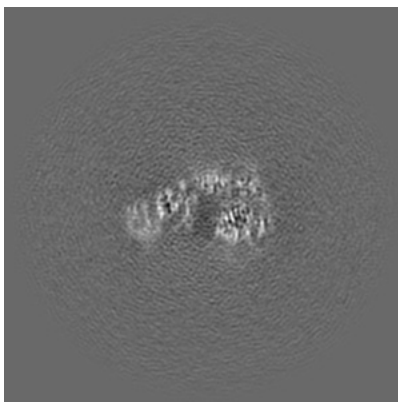
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

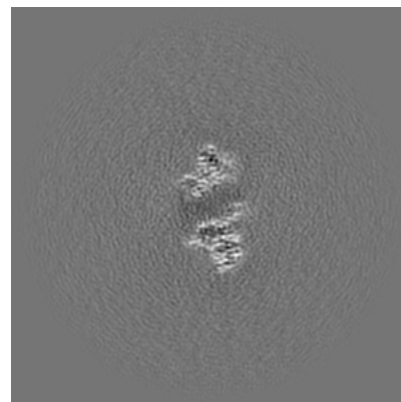
6.2.1 Primary map



X Index: 176

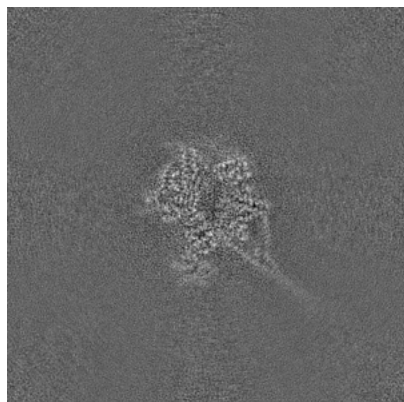


Y Index: 176

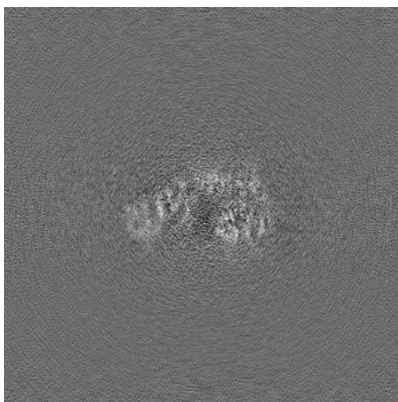


Z Index: 176

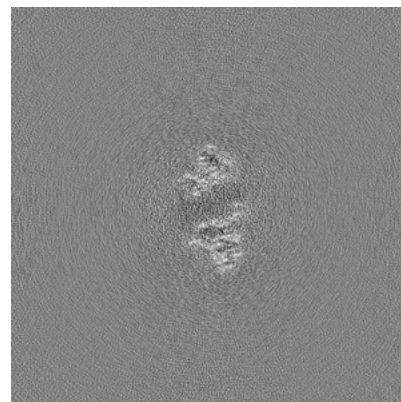
6.2.2 Raw map



X Index: 176



Y Index: 176

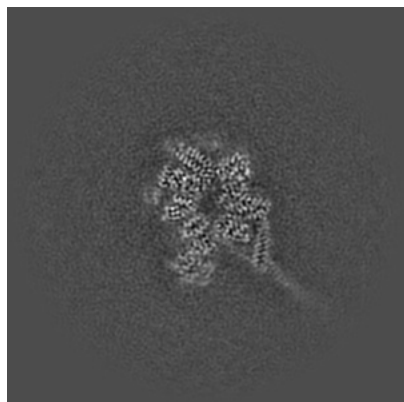


Z Index: 176

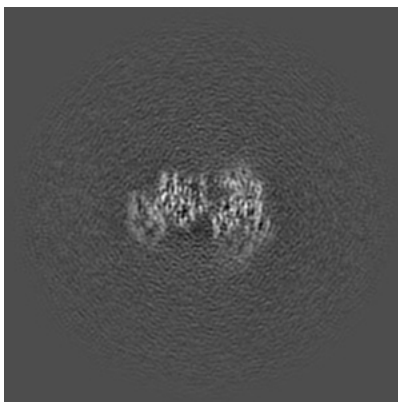
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

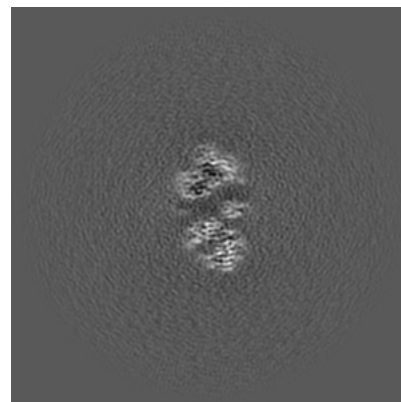
6.3.1 Primary map



X Index: 172

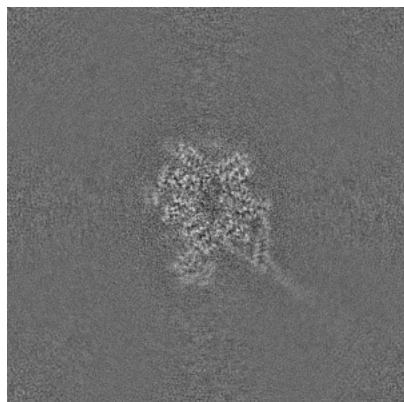


Y Index: 164

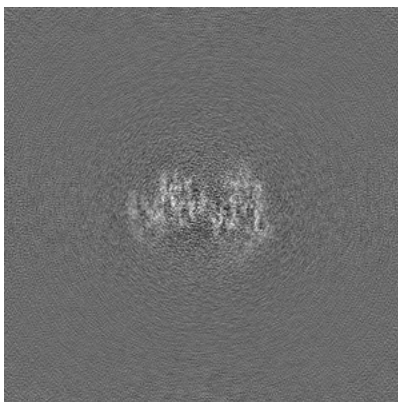


Z Index: 180

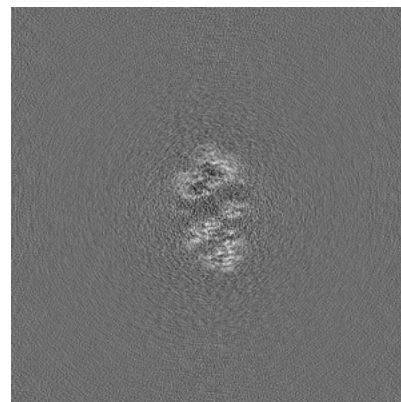
6.3.2 Raw map



X Index: 173



Y Index: 163

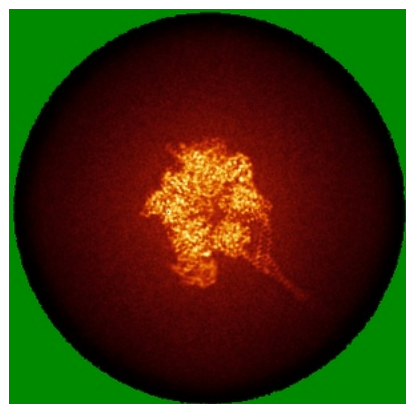


Z Index: 180

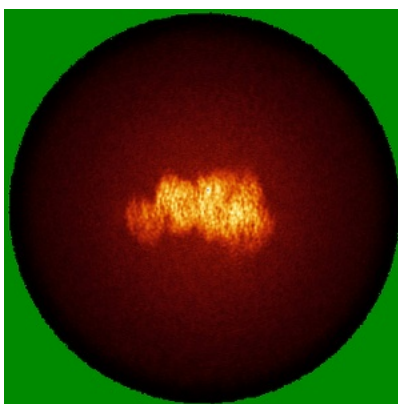
The images above show the largest variance slices of the map in three orthogonal directions.

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

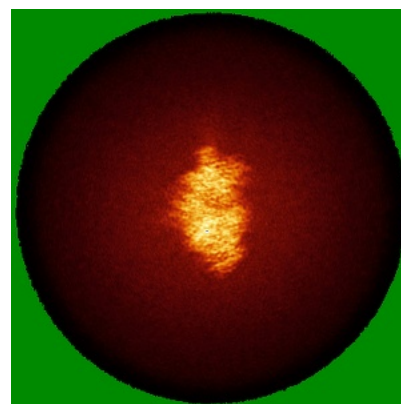
6.4.1 Primary map



X

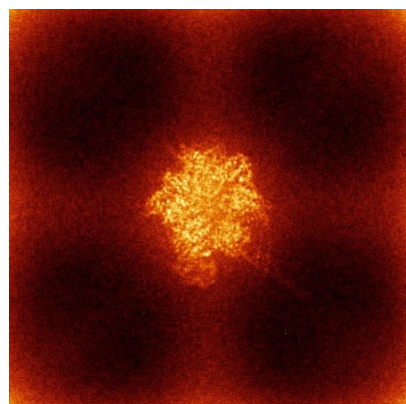


Y

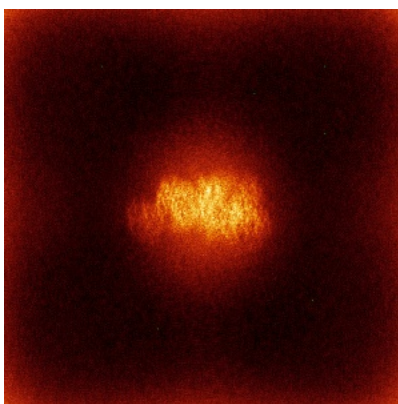


Z

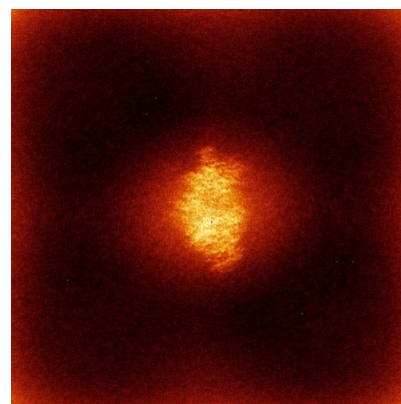
6.4.2 Raw map



X



Y

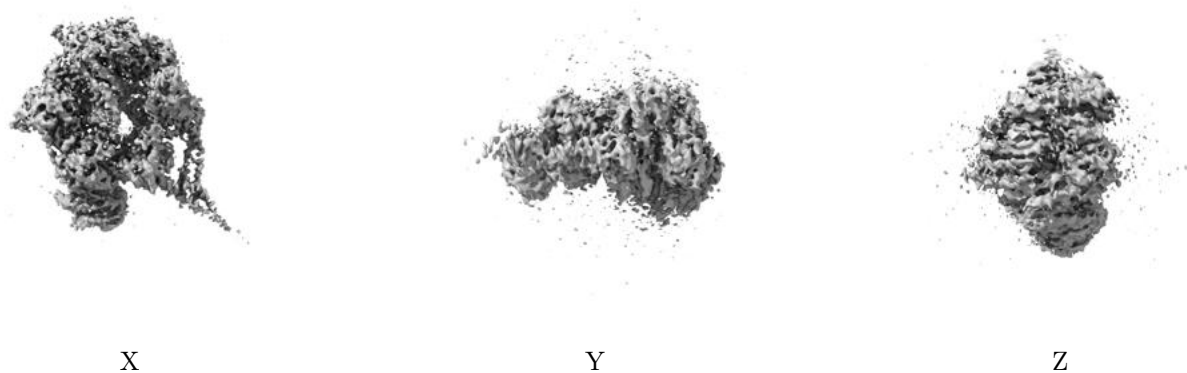


Z

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.

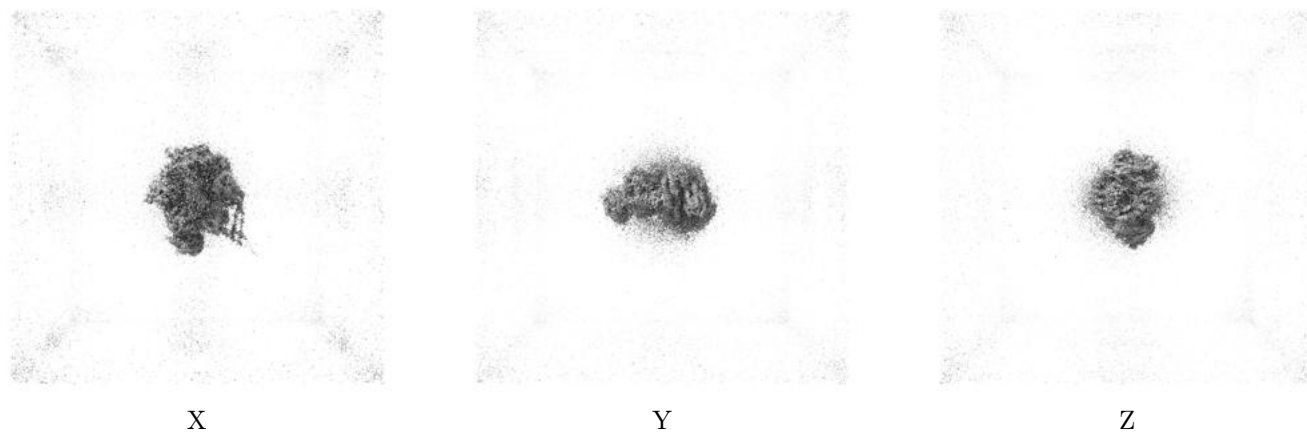
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

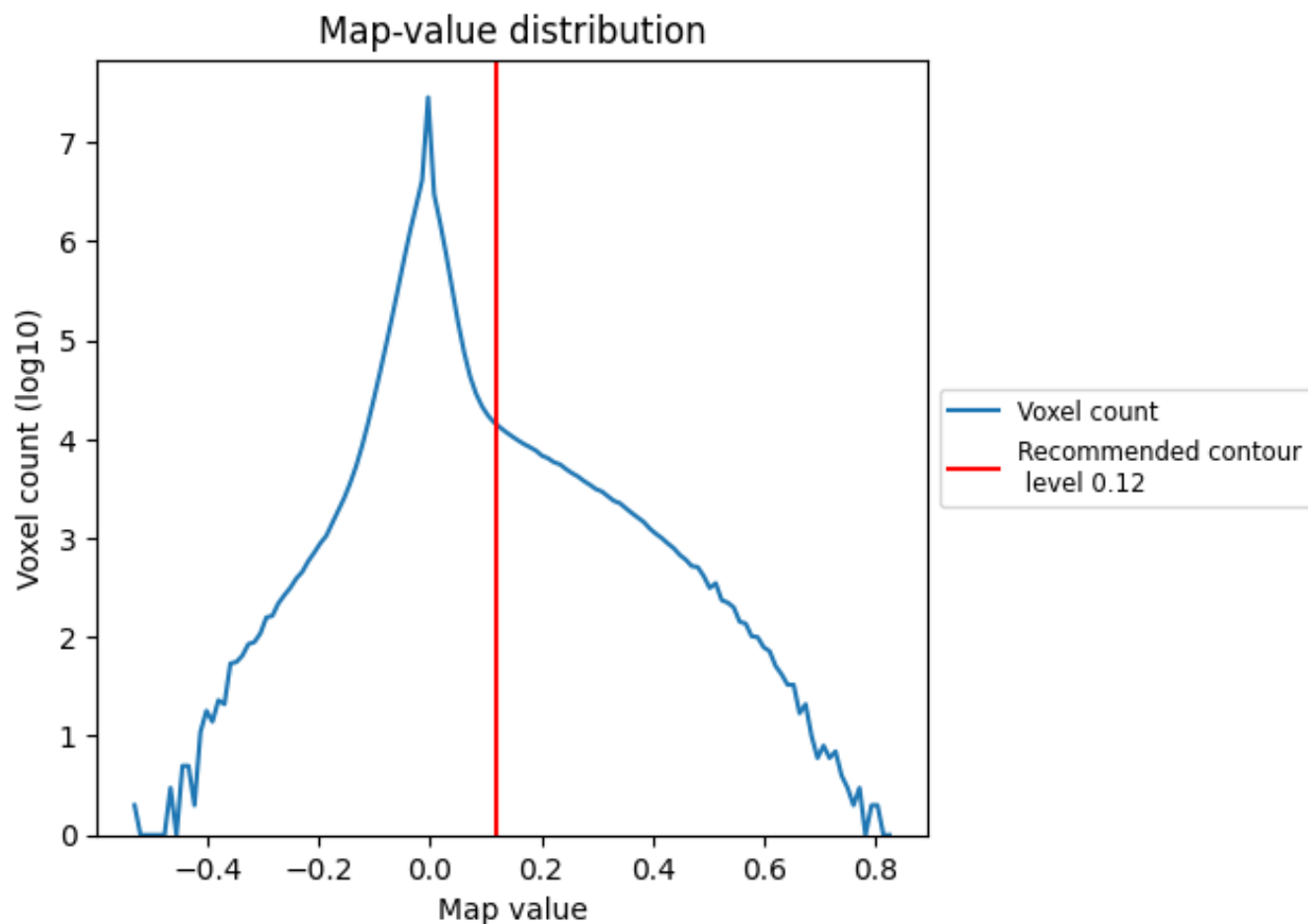
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

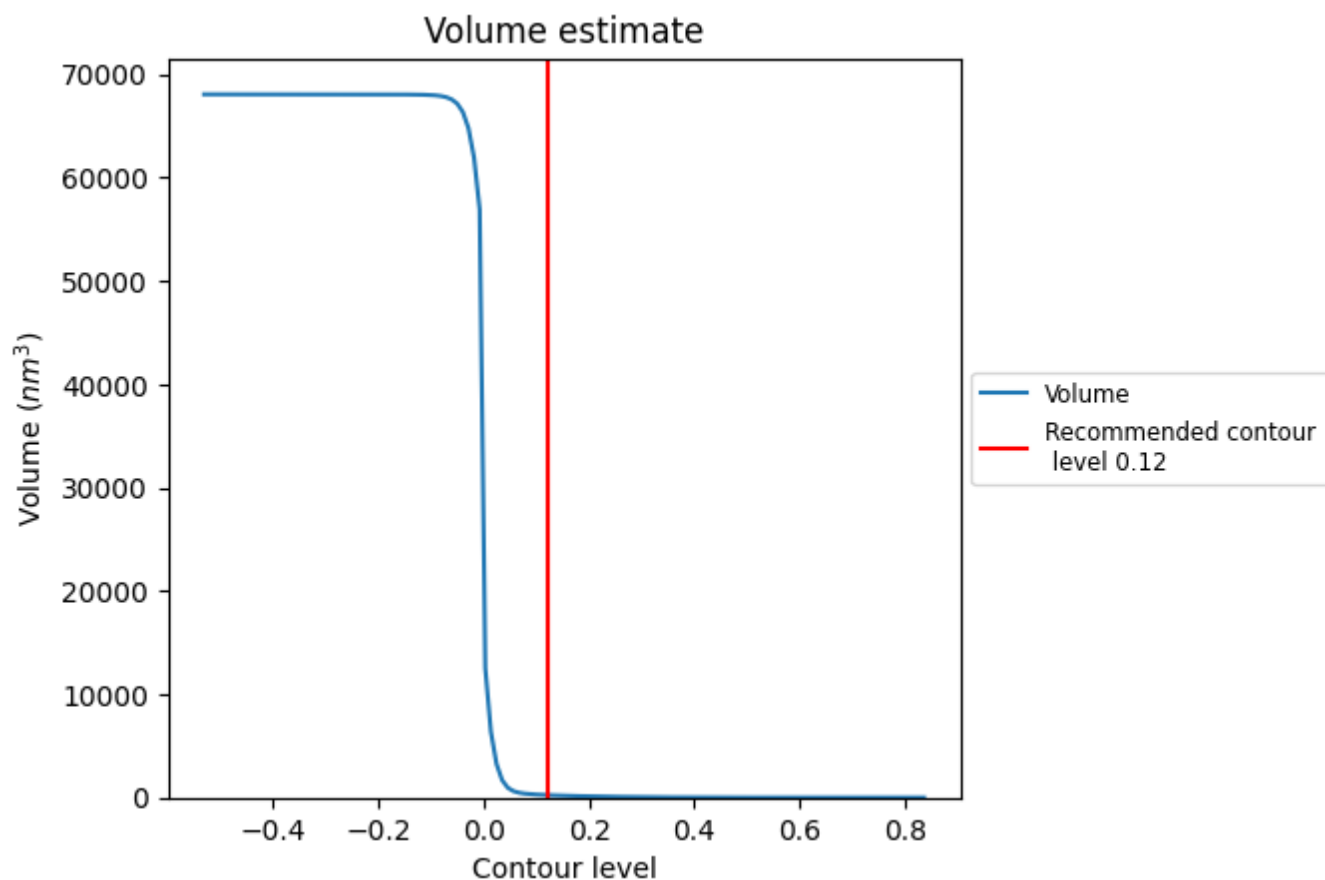
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

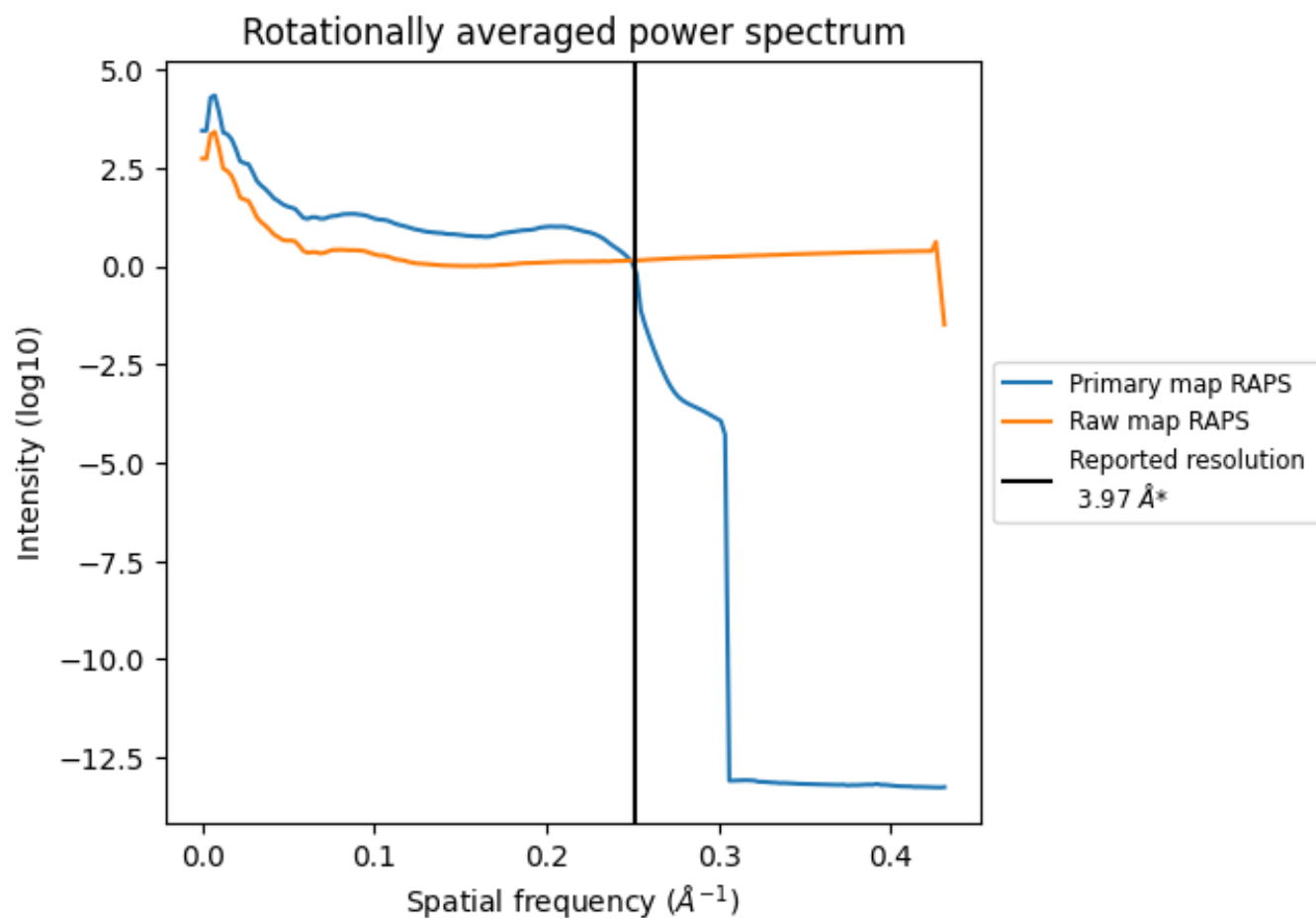
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 217 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 ⓘ

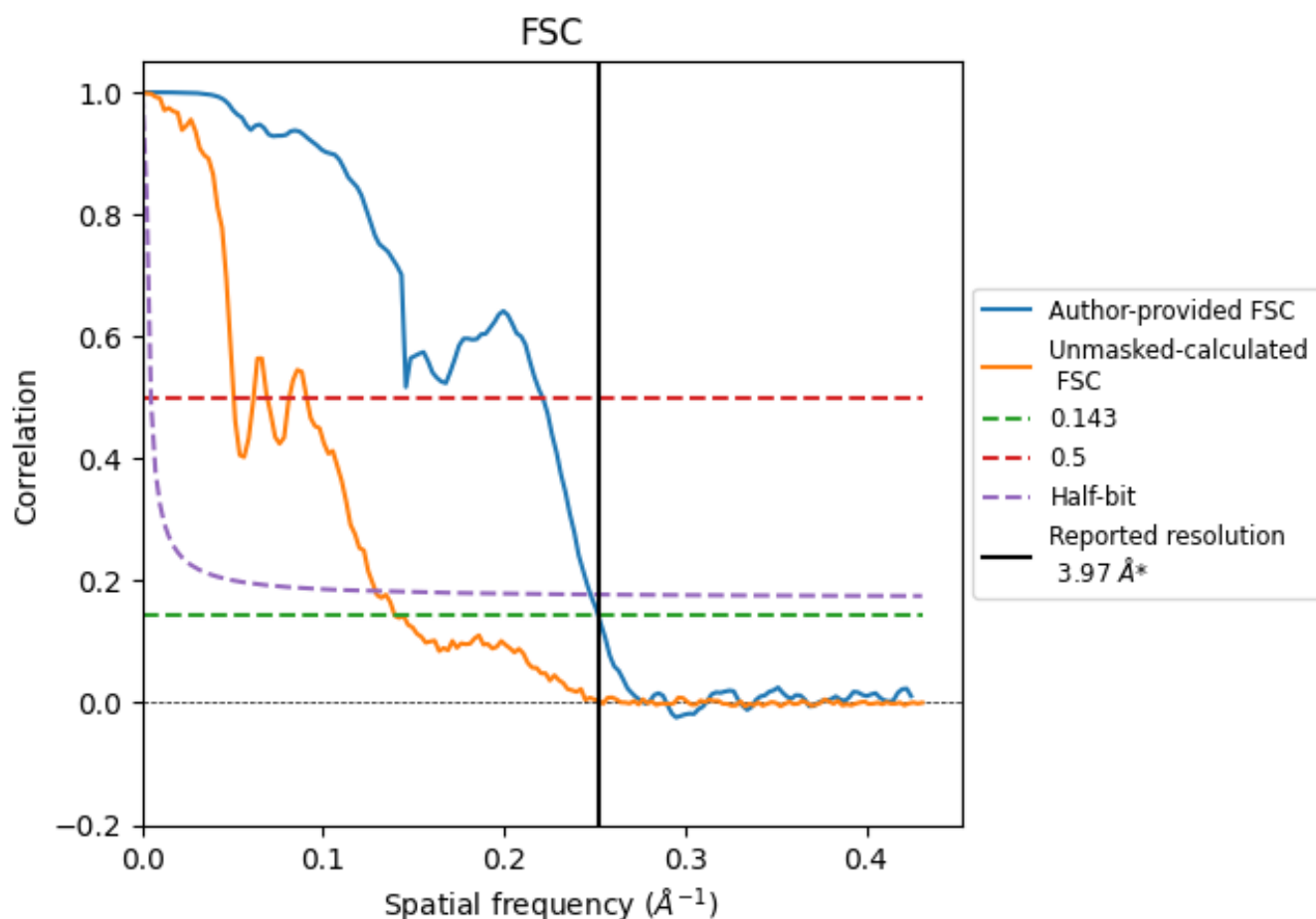


*Reported resolution corresponds to spatial frequency of 0.252 Å⁻¹

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 0.252 \AA^{-1}

8.2 Resolution estimates [i](#)

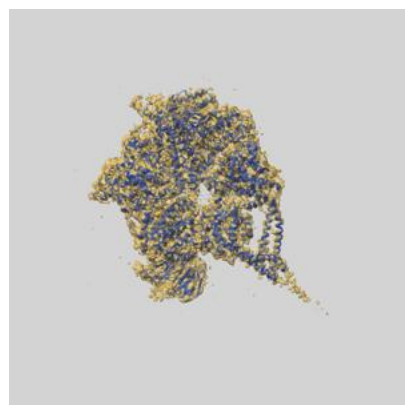
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.97	4.52	4.04
Unmasked-calculated*	7.17	19.76	7.75

*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 7.17 differs from the reported value 3.97 by more than 10 %

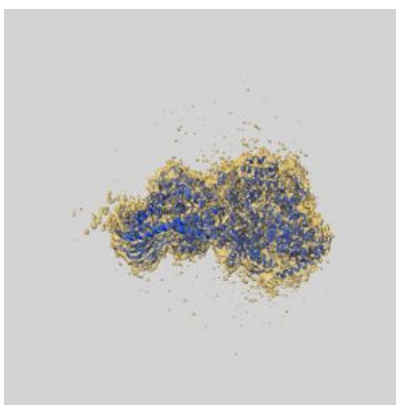
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27783 and PDB model 8DYV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

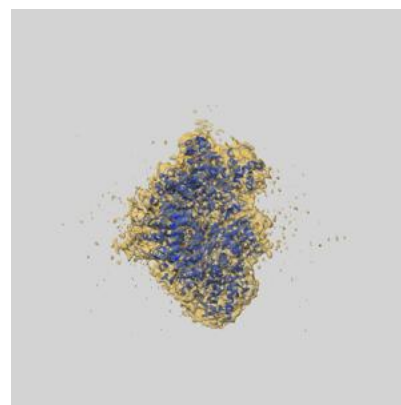
9.1 Map-model overlay [i](#)



X



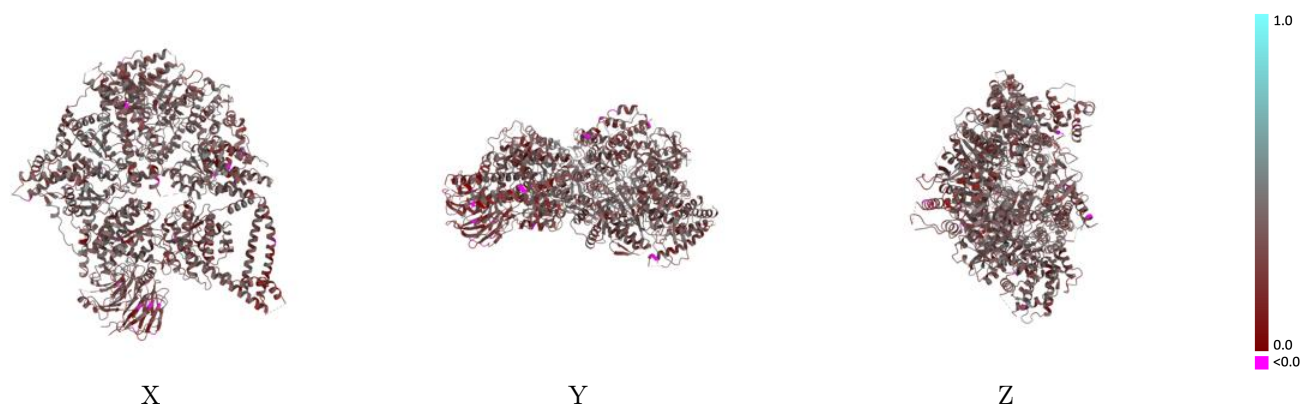
Y



Z

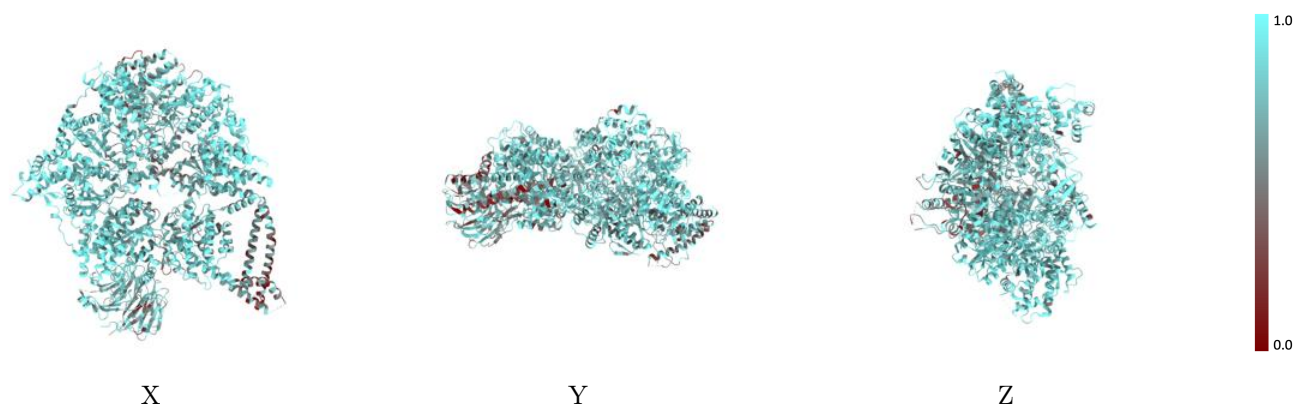
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



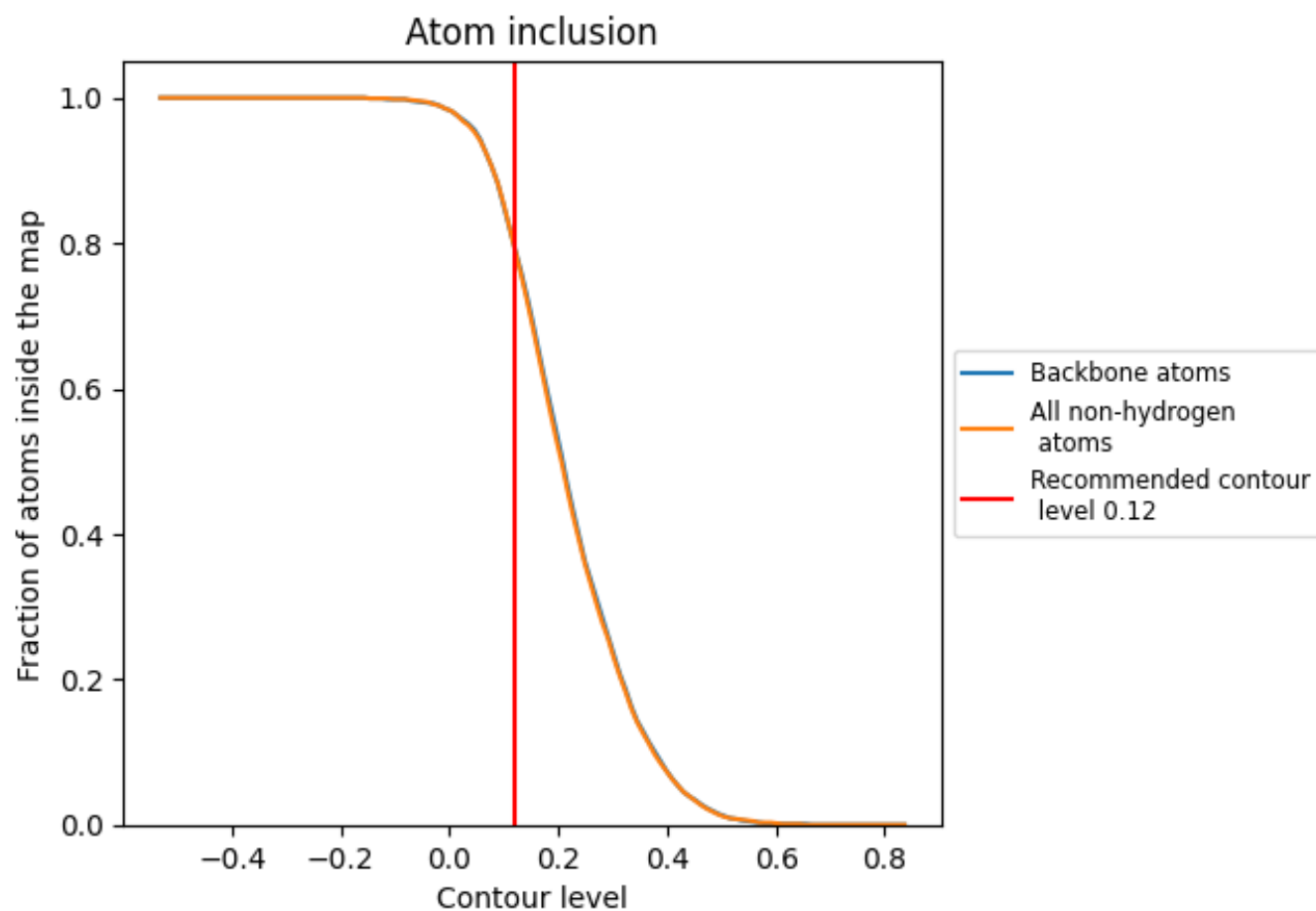
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7920	<div></div> 0.3400
A	<div></div> 0.8050	<div></div> 0.3480
B	<div></div> 0.7230	<div></div> 0.2690

