



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 06:02 AM UTC

PDB ID : 8RS0 / pdb_00008rs0
EMDB ID : EMD-19472
Title : Structure of RyR1 in detergent in primed state in complex with nanobody and FKBP
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-01-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

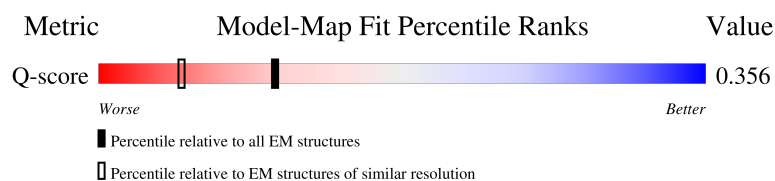
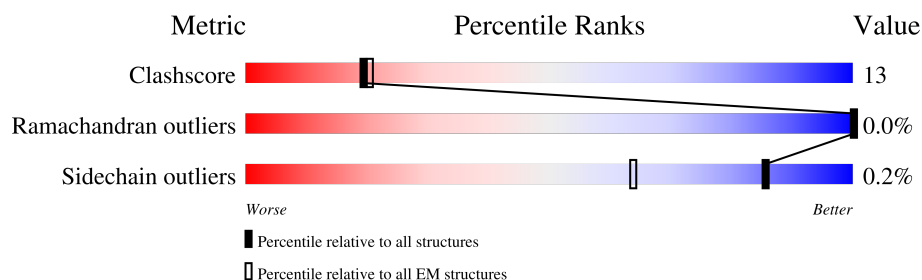
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



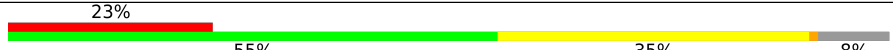
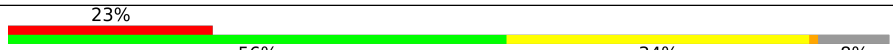
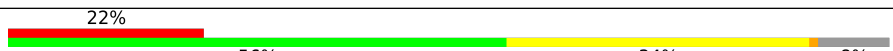
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	107	17% 63% 37%
1	D	107	18% 73% 27%
1	H	107	19% 70% 30%
1	I	107	18% 74% 26%

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Mol	Chain	Length	Quality of chain
2	B	5027	
2	E	5027	
2	G	5027	
2	J	5027	
3	C	137	
3	F	137	
3	K	137	
3	M	137	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 143570 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	D	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	I	107	Total	C	N	O	S	0	0
			816	514	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	E	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	G	4319	Total	C	N	O	S	1	0
			34149	21751	5887	6284	227		
2	J	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		

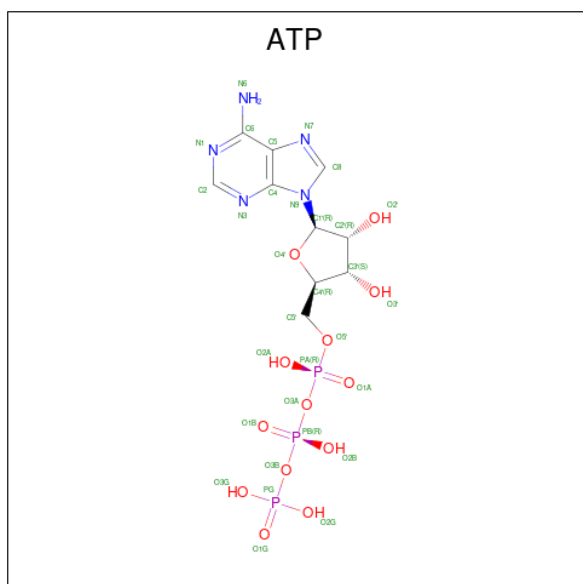
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	F	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	K	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	M	126	Total	C	N	O	S	0	0
			960	591	170	194	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



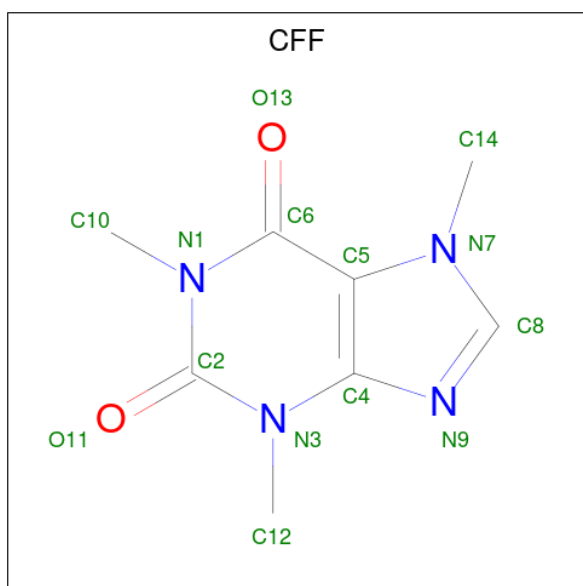
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Ca	0
			1	1	

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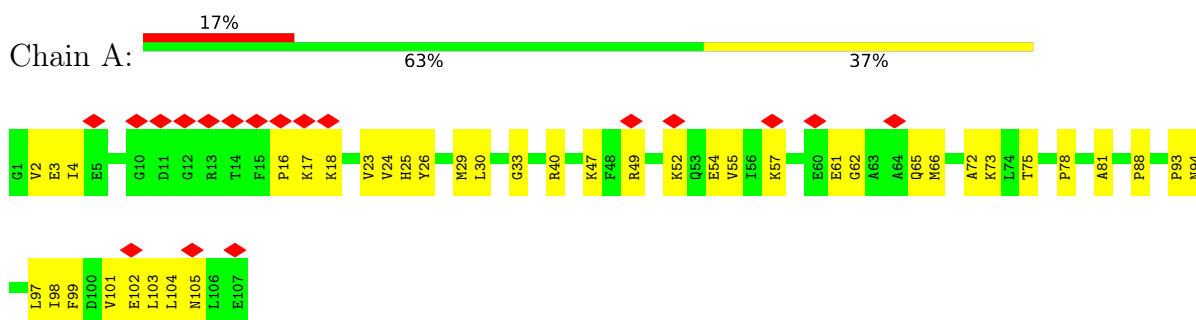
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Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

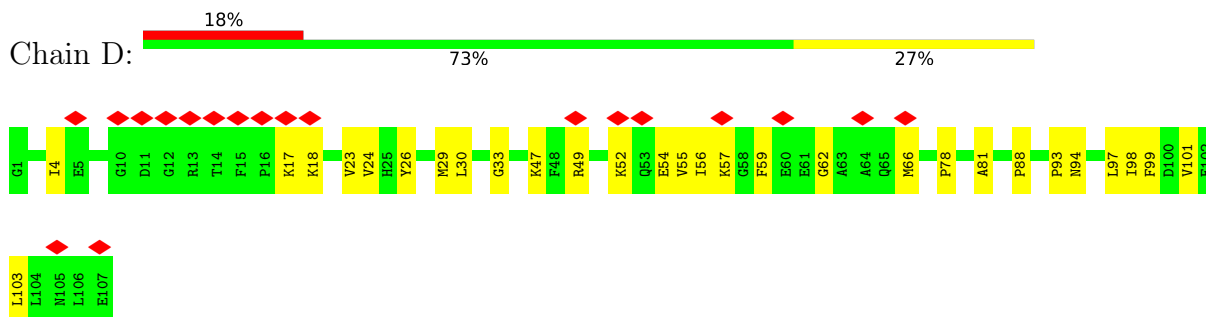
3 Residue-property plots [i](#)

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.

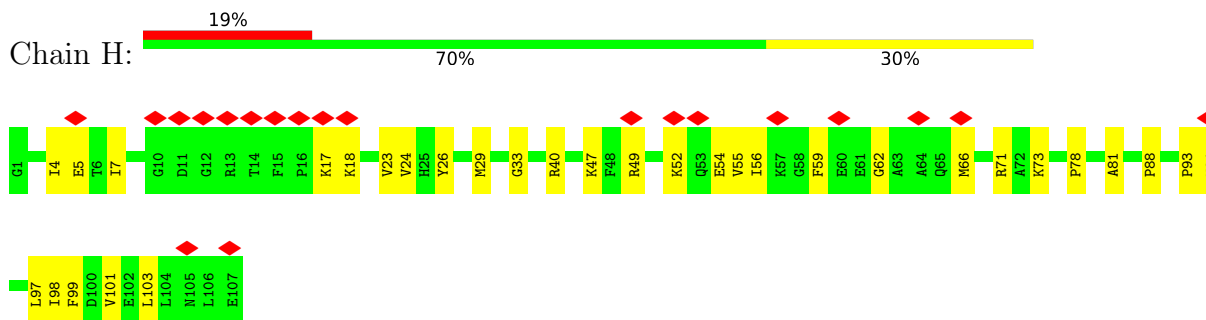
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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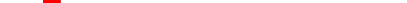
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

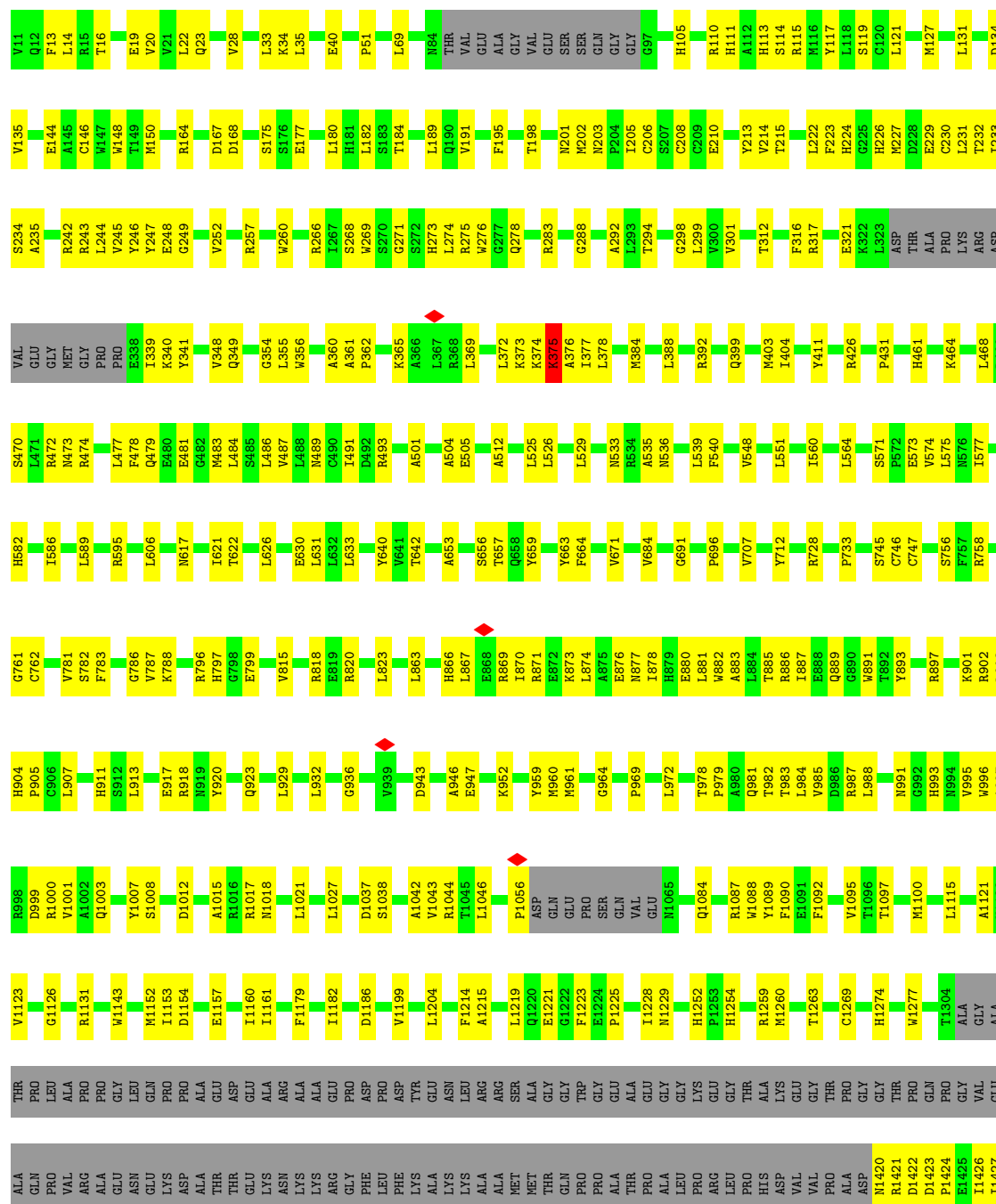


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

Chain B:  62% 23% 14%

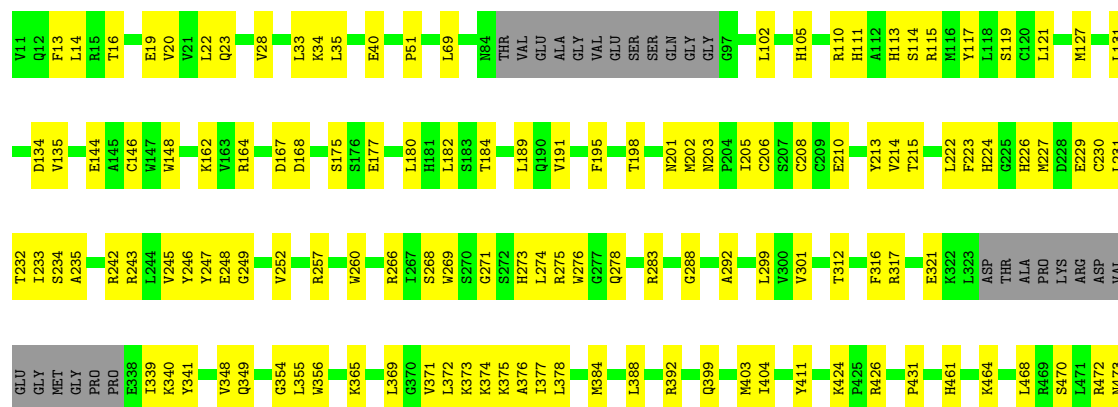


L1428	L1429	T1430	T1431	T1432	T1433	Y1434	Y1435	E1444	C1447	P1455	C1489	W1496	G1497	G1498	D1499	F1500	V1501	S1502	P1503	G1504	GLN	GLY	R1508	L1509	S1510	H1511	L1519	M1527	T1530	E1535	F1540	F1549	P1550	L1555	P1556	T1557	Q1569	I1572	A1578	L1581	L1582	R1584		



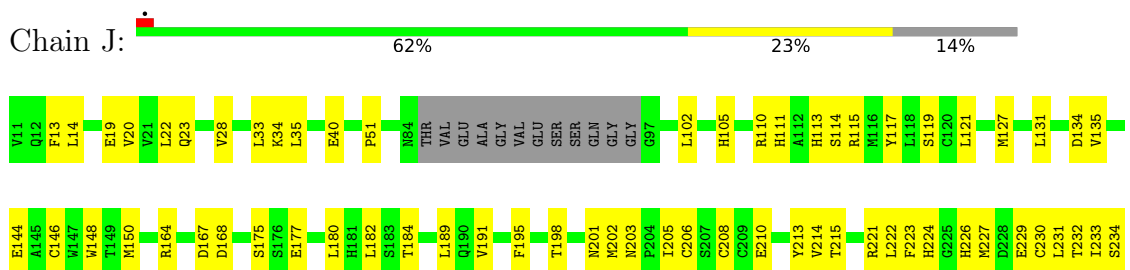








R3539	R3473	R3366	A3099	L3002	L2911	ARG	R2769	F2683	T2585	I2469	P2361
R3540	S3474	R3367	S3100	L3003	T2912	THR	K2770	D2684	T2585	I2469	P2361
R3541	R3475	R3368	D3101	P3004	A2913	GLU	I2771	S2685	R2591	L2472	F2364
R3542	Y3182	Y3182	D3102	L3005	A2917	LYS	K2772	H2688	G2592	Q2475	L2376
R3543	E3265	E3265	E3103	N3006	Q2924	LYS	N2773	Y2691	A2598	I2476	I2380
R3544	I3372	I3372	I3104	N3007	Q2924	THR	N2774	Y2696	Q2599	I2476	I2380
R3545	K3185	K3185	K3105	Q3008	Q2924	ARG	N2775	Y2696	R2600	I2476	I2380
R3546	L3186	L3186	V3107	N3012	L2927	ILE	N2776	Y2696	D2601	I2476	I2380
R3547	L3190	L3190	L3110	C3014	L2928	THR	N2777	Y2696	E2602	I2476	I2380
R3548	G3193	G3193	G3111	V3024	Q2931	GLN	N2778	Y2696	D2603	I2476	I2380
R3549	L3194	L3194	LEU	Y3024	M2932	THR	E2779	Y2696	E2604	I2476	I2380
R3550	A3195	A3195	GLY	G3029	M2933	ALA	E2780	Y2696	E2605	I2476	I2380
R3551	L3196	L3196	LYS	H3030	N2933	THR	N2781	Y2696	C2606	I2476	I2380
R3552	L3197	L3197	VAL	H3030	N2933	THR	N2782	Y2696	L2607	I2476	I2380
R3553	R3201	R3201	SER	A3031	G2934	THR	E2783	Y2696	L2610	I2476	I2380
R3554	M3202	M3202	GLN	K3034	Y2935	ASP	E2784	Y2696	L2610	I2476	I2380
R3555	V3203	V3203	ALA	E3035	A2936	PRG	E2785	Y2696	L2610	I2476	I2380
R3556	V3206	V3206	THR	K3036	V2937	ARG	E2786	Y2696	L2610	I2476	I2380
R3557	L3209	L3209	GLN	M3038	T2938	GLU	E2787	Y2696	L2610	I2476	I2380
R3558	Q3209	Q3209	LYS	I3039	R2939	GLY	E2788	Y2696	L2610	I2476	I2380
R3559	N3214	N3214	VAL	T3040	GLY	THR	E2789	Y2696	L2610	I2476	I2380
R3560	A3215	A3215	GLY	S3041	LEU	ASP	E2790	Y2696	L2610	I2476	I2380
R3561	L3312	L3312	GLY	L3042	ASP	THR	E2791	Y2696	L2610	I2476	I2380
R3562	S3313	S3313	GLY	F3043	MET	ALA	E2792	Y2696	L2610	I2476	I2380
R3563	V3218	V3218	GLN	K3044	GLU	THR	E2793	Y2696	L2610	I2476	I2380
R3564	L3315	L3315	VAL	K3045	L2946	THR	E2794	Y2696	L2610	I2476	I2380
R3565	L3316	L3316	VAL	L3046	D2947	THR	E2795	Y2696	L2610	I2476	I2380
R3566	G3317	G3317	LYS	L3049	G2958	THR	E2796	Y2696	L2610	I2476	I2380
R3567	N3318	N3318	GLY	V3050	F2959	THR	E2797	Y2696	L2610	I2476	I2380
R3568	T3221	T3221	VAL	R3051	T2960	THR	E2798	Y2696	L2610	I2476	I2380
R3569	L3319	L3319	GLY	H3052	Q2961	THR	E2799	Y2696	L2610	I2476	I2380
R3570	R3225	R3225	GLY	R3053	Q2962	THR	E2800	Y2696	L2610	I2476	I2380
R3571	E3226	E3226	GLY	V3054	L2963	THR	E2801	Y2696	L2610	I2476	I2380
R3572	R3227	R3227	GLY	L3068	L2964	THR	E2802	Y2696	L2610	I2476	I2380
R3573	A3228	A3228	GLY	I3070	R2965	THR	E2803	Y2696	L2610	I2476	I2380
R3574	I3229	I3229	VAL	L3069	R2966	THR	E2804	Y2696	L2610	I2476	I2380
R3575	F3144	F3144	GLY	I3070	M2967	THR	E2805	Y2696	L2610	I2476	I2380
R3576	I3147	I3147	GLY	S3074	S2970	THR	E2806	Y2696	L2610	I2476	I2380
R3577	F3152	F3152	GLY	L3075	Q2971	THR	E2807	Y2696	L2610	I2476	I2380
R3578	G3153	G3153	GLY	D3076	E2972	THR	E2808	Y2696	L2610	I2476	I2380
R3579	V3236	V3236	GLY	A3077	F2973	THR	E2809	Y2696	L2610	I2476	I2380
R3580	M3239	M3239	GLY	R3078	I2974	THR	E2810	Y2696	L2610	I2476	I2380
R3581	I3243	I3243	GLY	T3079	L2977	THR	E2811	Y2696	L2610	I2476	I2380
R3582	P3244	P3244	GLY	V3080	L2977	THR	E2812	Y2696	L2610	I2476	I2380
R3583	V3245	V3245	GLY	K3081	F2987	THR	E2813	Y2696	L2610	I2476	I2380
R3584	L3246	L3246	GLY	Q3162	E2987	THR	E2814	Y2696	L2610	I2476	I2380
R3585	D3247	D3247	GLY	C3165	H2991	THR	E2815	Y2696	L2610	I2476	I2380
R3586	R3248	R3248	GLY	L3092	E2992	THR	E2816	Y2696	L2610	I2476	I2380
R3587	S3249	S3249	GLY	R3093	E2992	THR	E2817	Y2696	L2610	I2476	I2380
R3588	M3250	M3250	GLY	F3095	I2995	THR	E2818	Y2696	L2610	I2476	I2380
R3589	I3172	I3172	GLY	F3096	K2996	THR	E2819	Y2696	L2610	I2476	I2380
R3590	F3173	F3173	GLY	E3097	F2997	THR	E2820	Y2696	L2610	I2476	I2380
R3591	S3174	S3174	GLY	F2998	F2998	THR	E2821	Y2696	L2610	I2476	I2380
R3592	G3363	G3363	GLY	A2999	A2999	THR	E2822	Y2696	L2610	I2476	I2380
R3593	A3257	A3257	GLY	K3000	T2910	THR	E2823	Y2696	L2610	I2476	I2380
R3594				Y2908	D2908	THR	E2824	Y2696	L2610	I2476	I2380
R3595				T2910	T2910	THR	E2825	Y2696	L2610	I2476	I2380
R3596						THR	E2826	Y2696	L2610	I2476	I2380
R3597						THR	E2827	Y2696	L2610	I2476	I2380
R3598						THR	E2828	Y2696	L2610	I2476	I2380
R3599						THR	E2829	Y2696	L2610	I2476	I2380
R3600						THR	E2830	Y2696	L2610	I2476	I2380
R3601						THR	GLU	Y2696	L2610	I2476	I2380
R3602						THR	GLU	Y2696	L2610	I2476	I2380
R3603						THR	GLU	Y2696	L2610	I2476	I2380
R3604						THR	GLU	Y2696	L2610	I2476	I2380
R3605						THR	GLU	Y2696	L2610	I2476	I2380
R3606						THR	GLU	Y2696	L2610	I2476	I2380
R3607						THR	GLU	Y2696	L2610	I2476	I2380
R3608						THR	GLU	Y2696	L2610	I2476	I2380
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R3610						THR	GLU	Y2696	L2610	I2476	I2380
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R3613						THR	GLU	Y2696	L2610	I2476	I2380
R3614						THR	GLU	Y2696	L2610	I2476	I2380
R3615						THR	GLU	Y2696	L2610	I2476	I2380
R3616						THR	GLU	Y2696	L2610	I2476	I2380
R3617						THR	GLU	Y2696	L2610	I2476	I2380
R3618						THR	GLU	Y2696	L2610	I2476	I2380
R3619						THR	GLU	Y2696	L2610	I2476	I2380
R3620						THR	GLU	Y2696	L2610	I2476	I2380
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R3624						THR	GLU	Y2696	L2610	I2476	I2380
R3625						THR	GLU	Y2696	L2610	I2476	I2380
R3626						THR	GLU	Y2696	L2610	I2476	I2380
R3627						THR	GLU	Y2696	L2610	I2476	I2380
R3628						THR	GLU	Y2696	L2610	I2476	I2380
R3629						THR	GLU	Y2696	L2610	I2476	I2380
R3630						THR	GLU	Y2696	L2610	I2476	I2380
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R3632						THR	GLU	Y2696	L2610	I2476	I2380
R3633						THR	GLU	Y2696	L2610	I2476	I2380
R3634						THR	GLU	Y2696	L2610	I2476	I2380
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R3639						THR	GLU	Y2696	L2610	I2476	I2380
R3640						THR	GLU	Y2696	L2610	I2476	I2380
R3641						THR	GLU	Y2696	L2610	I2476	I2380
R3642						THR	GLU	Y2696	L2610	I2476	I2380
R3643						THR	GLU	Y2696	L2610	I2476	I2380
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R3645						THR	GLU	Y2696	L2610	I2476	I2380
R3646						THR	GLU	Y2696	L2610	I2476	I2380
R3647						THR	GLU	Y2696	L2610	I2476	I2380
R3648						THR	GLU	Y2696	L2610	I2476	I2380
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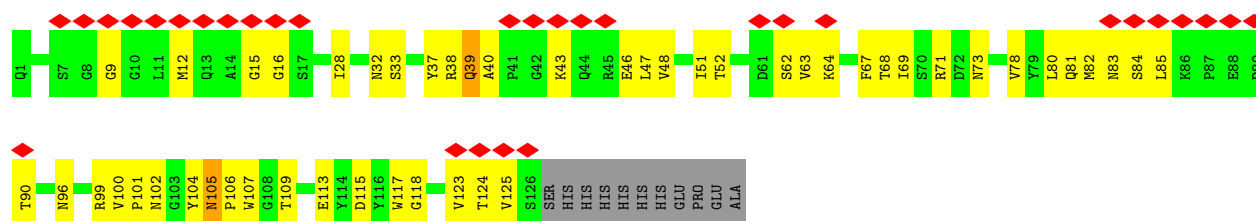


ARG	SER	GLY	R1827	M1637	V1496	LYS	ALA	L1021	L929	V815	L606	L477	A235
LEU	LEU	GLY	F1836	A1638	G1497	LYS	ALA	L1027	L932	R818	T622	F478	R242
LEU	LEU	GLY	F1836	L1639	D1499	ARG	PRO	A1042	G936	R820	L626	Q479	R243
THR	THR	ASP	V1845	E1643	F1500	PHE	ASP	V1043	C937	L823	E630	G482	V245
VAL	VAL	ASP	V1845	L1669	S1502	PHE	ASP	R1044	D943	L863	L631	M483	Y246
ARG	ARG	LYS	L1949	V1673	G1503	LYS	TYR	T1045	E947	H866	L633	L484	Y247
LEU	LEU	ALA	F1854	R1680	G1504	ALA	GLN	L1046	E947	H866	L633	L486	E248
LYS	LYS	LYS	R1680	R1680	F1214	ASN	ASN	T1053	A946	H866	L633	L486	G249
LYS	LYS	ALA	L1684	L1684	L1219	ARG	ARG	P1056	K952	L867	Y640	L488	V252
GLY	GLY	ALA	L1684	L1684	Q1220	SER	SER	ASP	K952	E868	Y640	M489	G354
GLY	GLY	MET	L1684	L1684	G1220	GLN	GLN	GLN	Y959	R869	T642	C490	R257
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GLY	GLY	THR	L1684	L1684	G1220	GLN	GLN	GLN	Y959	R869	T642	C490	L259
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GLY	GLY	PRO	L1684	L1684	G1220	GLN	GLN	GLN	Y959	R869	T642	C490	ARG
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GLY	GLY	PRO	L1684	L1684	G1220	GLN	GLN	GLN	Y959	R869	T642	C490	VAL
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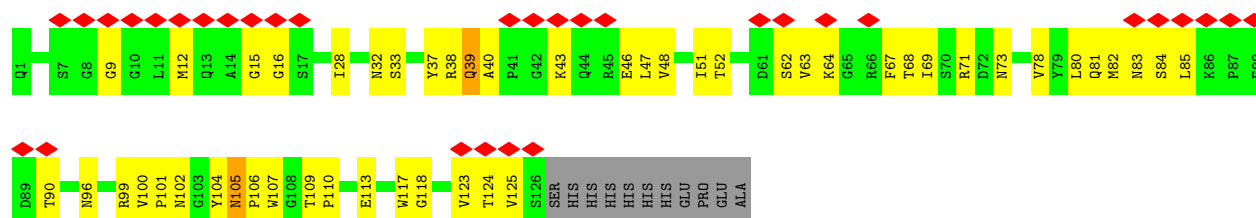
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V3394	W3285	M3201	LEU	C3014		SER	G2778	Y2696	G2592	Q2475	L2380	M2250	R2162
E3397	E3286	V3202	GLY	V3024		THR	E2779			I2476	E2381	Y2256	S2164
V3400	R3287	V3203	VAL	G3029		ALA	V2780			L2479	E2382	G2262	L2165
	L3296	L3206	SER	H3030		GLN	V2781			L2496	E2383	G2263	W2170
	C3304	Q3209	ALA	A3031		THR	E2783			P2496	E2384	G2264	Q2173
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L3413	G3317	T3221	GLY	S3041		THR	R2792			L2506	ASP	E2292	K2189
N3414	N3318	K3222	GLY	L3042		VAL	P2793			L2506	ASP	Q2293	Y2192
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	N3325	A3228	P3138	L3049		GLY	F2797			L2519	PHE	C2310	L2201
	W3334	I3229	V3139	V3050		THR	S2798			L2522	GLY	P2311	T2206
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R3435	P3345	L3263	L3147	R2869		ALA	E2803			R2531	N2414	L2321	M2211
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V3438	S3347	A3239	L3172	L2876		THR	K2806			L2550	N2416	Y2331	W2213
G3439	R3348	M3239	L3175	A2875		GLY	L2809			R2552	H2418	L2332	W2214
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Y3444	L3353	P3244	Q3162	S3074		ALA	E2811			R2567	M2435	F2334	THR
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F3451	H3355	D3247	C3165	A3077		VAL	L2817			A2566	E2449	R2336	GLU
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M3250	H3357	L3249	L3173	T3079		THR	V2819			R2576	L2430	L2336	R2224
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A3472	K3367	Y3263	T3181	S3094		GLY	F2826				L2356		R2234
S3474	R3368	T3264	Y3182	F3095		THR	L2827				Y2357		F2235
K3475	E3265	E3265	E3184	E3097		ALA	A2828				L2357		C2237
SER	K3371	I3272	K3185	S3098		THR	R2827				L2358		Y2238
LYS	Y3372	T3273	L3186	E3101		GLY	F2828				L2359		C2240
LYS	E3376	L3274	L3186	L3102		THR	G2829				M2578		R2241
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D4744	R4892	GLU	GLU	GLY	GLU	PHE	LEU	LEU	ALA	M4231	K4090	E3968	V3812	R3648	P3567	ARG
S4747	I4897	GLU	GLY	GLY	VAL	GLY	GLY	GLY	ARG	E4232	K4091	E3969	M3816	N3651	L3568	THR
L4748	L4748	GLU	LEU	GLY	GLY	GLY	GLY	GLY	ARG	C4238	A4096	C3971	M3816	E3655	R3570	LYS
E4749	I4901	VAL	GLU	HIS	GLY	LEU	GLY	LEU	GLY	E4238	M4097	P3972	L3820	E3655	W3571	LYS
H4753	F4916	PRO	GLY	GLY	GLY	VAL	GLY	VAL	ARG	E4239	Q4100	R3984	E3825	K3658	Q3572	ARG
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P4762	L4943	PRO	GLY	GLY	GLY	LYS	GLY	LYS	SER	E4244	G4105	A3988	M3836	Q3683	R3577	ASP
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V4853	F5022	GLY	GLY	PRO	GLY	GLY	ALA	GLY	GLY	ALA	Y4194	V4055	L3903	VAL	ALA	
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															MET	
															T3639	

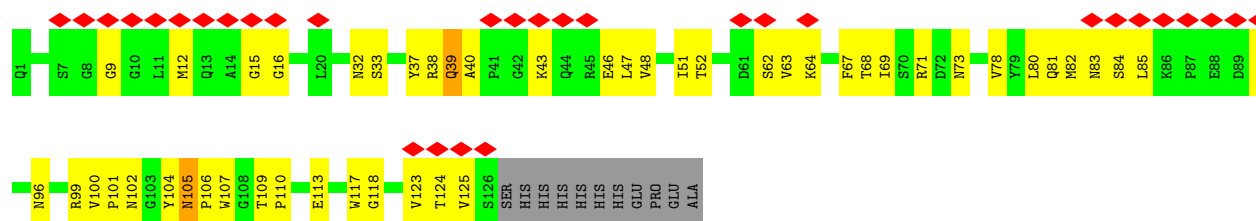
• Molecule 3: Nanobody 9657



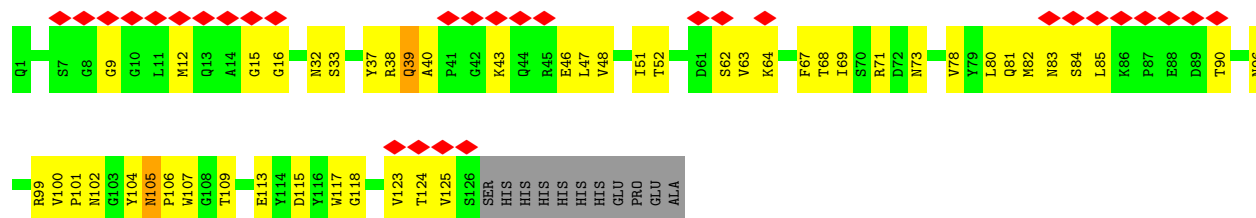
• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.519	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.057	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	500.64, 500.64, 500.64	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ATP, CA, ZN

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	0.17	0/831	0.54	0/1118
1	D	0.18	0/831	0.56	0/1118
1	H	0.18	0/831	0.56	0/1118
1	I	0.18	0/831	0.56	0/1118
2	B	0.14	0/34814	0.33	3/47183 (0.0%)
2	E	0.14	0/34814	0.33	1/47183 (0.0%)
2	G	0.14	0/34921	0.33	1/47329 (0.0%)
2	J	0.13	0/34814	0.33	1/47183 (0.0%)
3	C	0.17	0/979	0.41	0/1329
3	F	0.16	0/979	0.41	0/1329
3	K	0.17	0/979	0.41	0/1329
3	M	0.16	0/979	0.41	0/1329
All	All	0.14	0/146603	0.34	6/198666 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1503	PRO	N-CA-CB	6.24	110.19	103.33
2	J	1503	PRO	N-CA-CB	6.20	110.15	103.33
2	B	1503	PRO	N-CA-CB	6.16	110.11	103.33
2	G	1503	PRO	N-CA-CB	6.15	110.09	103.33
2	B	3247	ASP	N-CA-C	5.65	122.83	110.80

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	816	0	818	30	0
1	D	816	0	818	23	0
1	H	816	0	818	25	0
1	I	816	0	818	24	0
2	B	34043	0	33446	841	0
2	E	34043	0	33446	846	0
2	G	34149	0	33547	853	0
2	J	34043	0	33446	836	0
3	C	960	0	909	38	0
3	F	960	0	909	42	0
3	K	960	0	909	41	0
3	M	960	0	909	41	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	0	0
5	E	31	0	12	0	0
5	G	31	0	12	0	0
5	J	31	0	12	0	0
6	B	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143570	0	140881	3586	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 13.

The worst 5 of 3586 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)
2:B:4961:CYS:SG	2:B:4983:HIS:CE1	2.61	0.94
2:G:4961:CYS:SG	2:G:4983:HIS:CE1	2.60	0.93
2:E:4961:CYS:SG	2:E:4983:HIS:CE1	2.60	0.93
3:K:100:VAL:HG22	3:K:105:ASN:HD22	1.34	0.92
2:J:4961:CYS:SG	2:J:4983:HIS:CE1	2.60	0.92

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	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	I	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	B	4264/5027 (85%)	4160 (98%)	103 (2%)	1 (0%)	100	100
2	E	4264/5027 (85%)	4162 (98%)	102 (2%)	0	100	100
2	G	4280/5027 (85%)	4175 (98%)	105 (2%)	0	100	100
2	J	4264/5027 (85%)	4161 (98%)	103 (2%)	0	100	100
3	C	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	F	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	K	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	M	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
All	All	17988/21084 (85%)	17529 (97%)	458 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	LYS

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	87/88 (99%)	86 (99%)	1 (1%)	65	76
1	D	87/88 (99%)	87 (100%)	0	100	100
1	H	87/88 (99%)	87 (100%)	0	100	100
1	I	87/88 (99%)	87 (100%)	0	100	100
2	B	3662/4270 (86%)	3658 (100%)	4 (0%)	88	90
2	E	3662/4270 (86%)	3656 (100%)	6 (0%)	87	88
2	G	3674/4270 (86%)	3670 (100%)	4 (0%)	88	90
2	J	3662/4270 (86%)	3658 (100%)	4 (0%)	88	90
3	C	103/114 (90%)	101 (98%)	2 (2%)	50	68
3	F	103/114 (90%)	101 (98%)	2 (2%)	50	68
3	K	103/114 (90%)	101 (98%)	2 (2%)	50	68
3	M	103/114 (90%)	101 (98%)	2 (2%)	50	68
All	All	15420/17888 (86%)	15393 (100%)	27 (0%)	85	88

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	4720	VAL
2	J	4720	VAL
3	K	105	ASN
2	J	4080	TYR
2	J	5014	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	2574	HIS
2	G	4133	GLN
3	K	105	ASN
2	G	2881	ASN
2	G	3449	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	ATP	B	5102	-	32,33,33	0.28	0	48,52,52	0.37	0
5	ATP	G	5102	-	32,33,33	0.28	0	48,52,52	0.37	0
6	CFF	B	5103	-	15,15,15	1.66	4 (26%)	23,23,23	1.75	6 (26%)
5	ATP	E	5102	-	32,33,33	0.28	0	48,52,52	0.37	0
6	CFF	E	5103	-	15,15,15	1.66	4 (26%)	23,23,23	1.78	6 (26%)
6	CFF	J	5103	-	15,15,15	1.66	4 (26%)	23,23,23	1.78	6 (26%)
6	CFF	G	5103	-	15,15,15	1.66	4 (26%)	23,23,23	1.79	8 (34%)
5	ATP	J	5102	-	32,33,33	0.28	0	48,52,52	0.37	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
5	ATP	B	5102	-	-	8/22/38/38	0/3/3/3
5	ATP	G	5102	-	-	8/22/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
5	ATP	E	5102	-	-	8/22/38/38	0/3/3/3
6	CFF	E	5103	-	-	-	0/2/2/2
6	CFF	J	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
5	ATP	J	5102	-	-	8/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5103	CFF	C4-N3	-2.95	1.33	1.38
6	E	5103	CFF	C4-N3	-2.94	1.33	1.38
6	G	5103	CFF	C4-N3	-2.92	1.33	1.38
6	E	5103	CFF	C5-N7	-2.92	1.33	1.38
6	G	5103	CFF	C5-N7	-2.92	1.33	1.38

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5103	CFF	N3-C2-N1	4.27	122.48	117.14
6	J	5103	CFF	N3-C2-N1	4.23	122.43	117.14
6	E	5103	CFF	N3-C2-N1	4.22	122.41	117.14
6	B	5103	CFF	N3-C2-N1	4.12	122.29	117.14
6	G	5103	CFF	C6-N1-C2	-3.03	120.73	125.66

There are no chirality outliers.

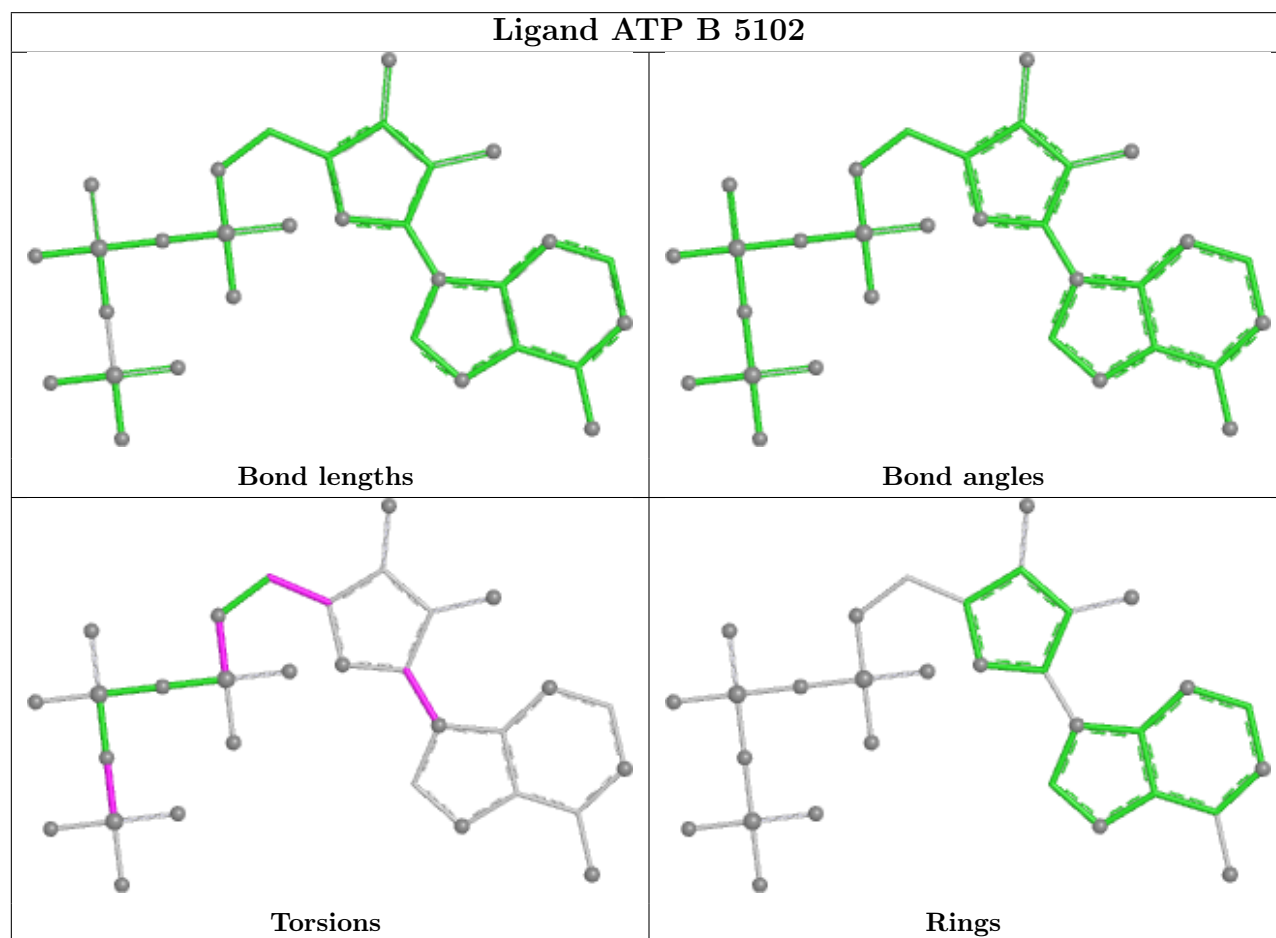
5 of 32 torsion outliers are listed below:

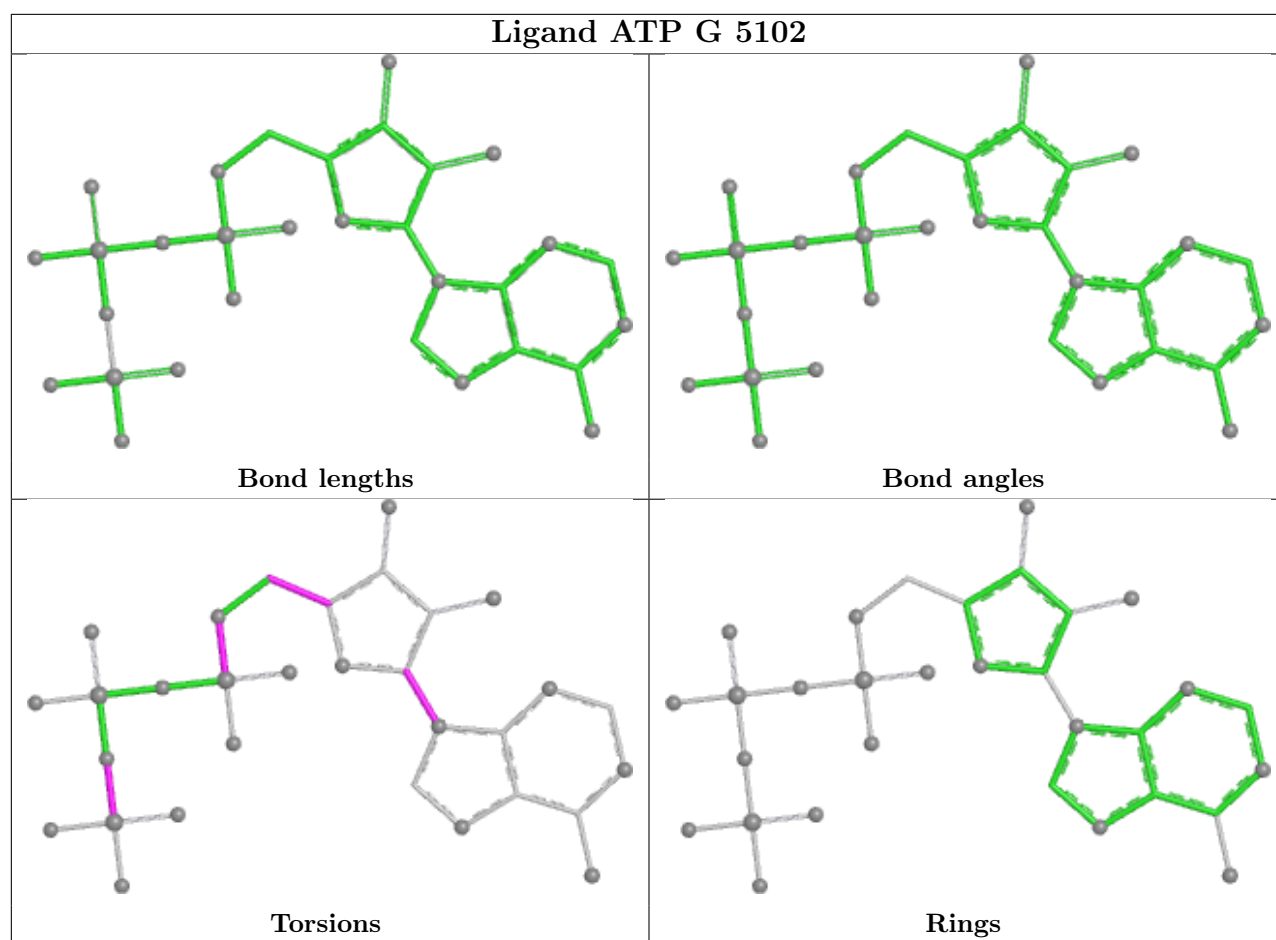
Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	PB-O3B-PG-O2G
5	B	5102	ATP	C5'-O5'-PA-O3A
5	E	5102	ATP	PB-O3B-PG-O2G
5	E	5102	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	PB-O3B-PG-O2G

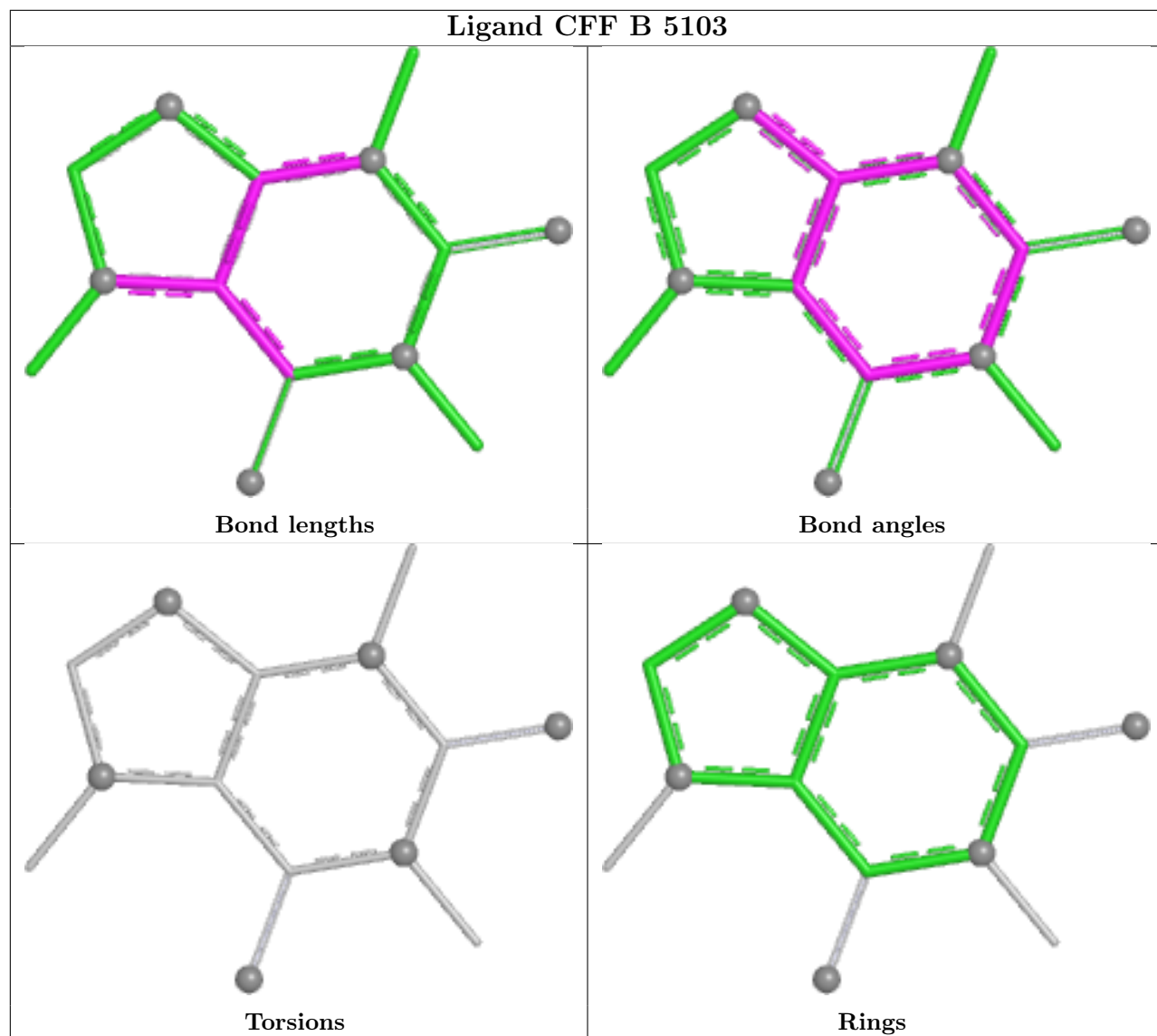
There are no ring outliers.

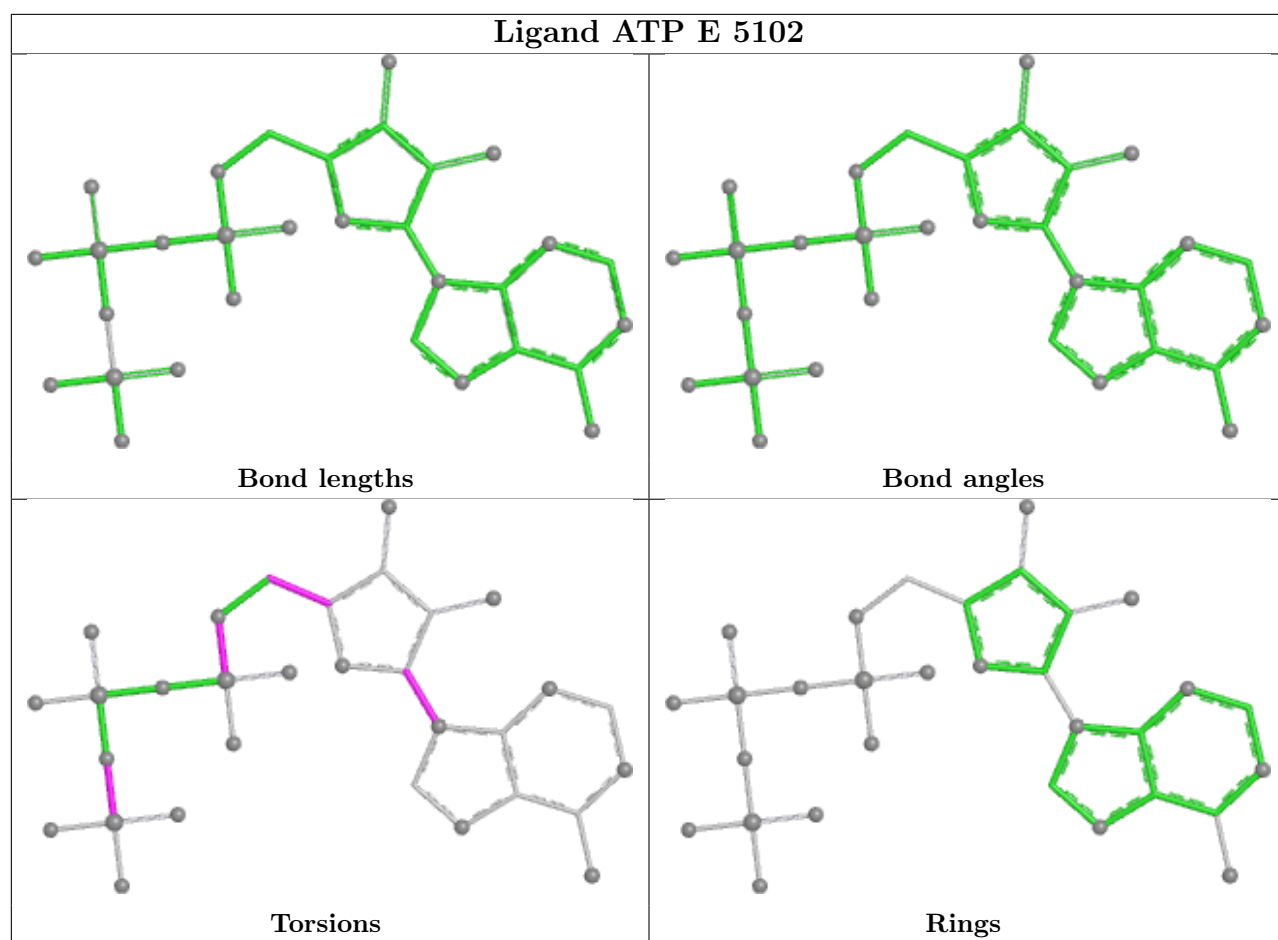
No monomer is involved in short contacts.

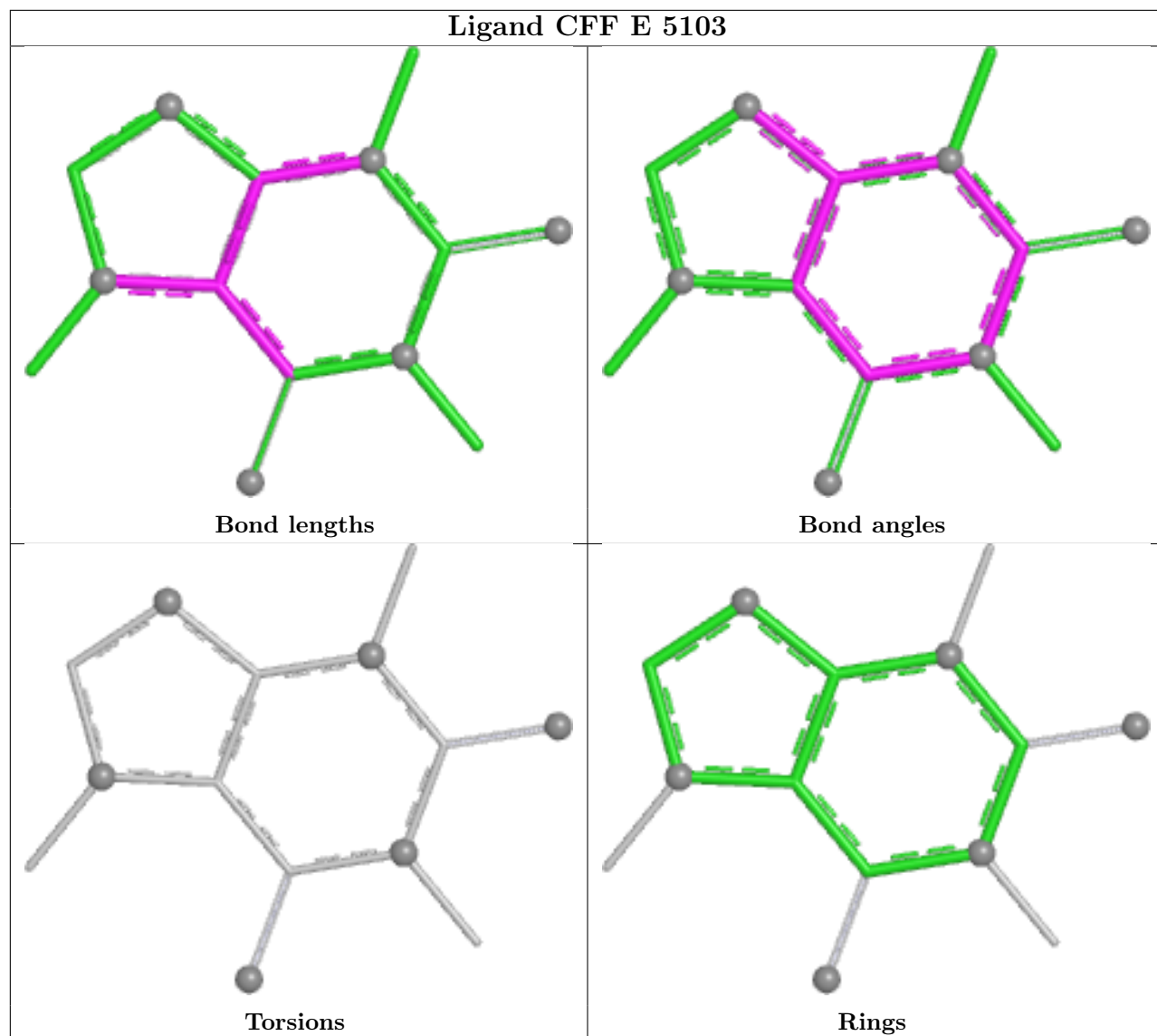
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

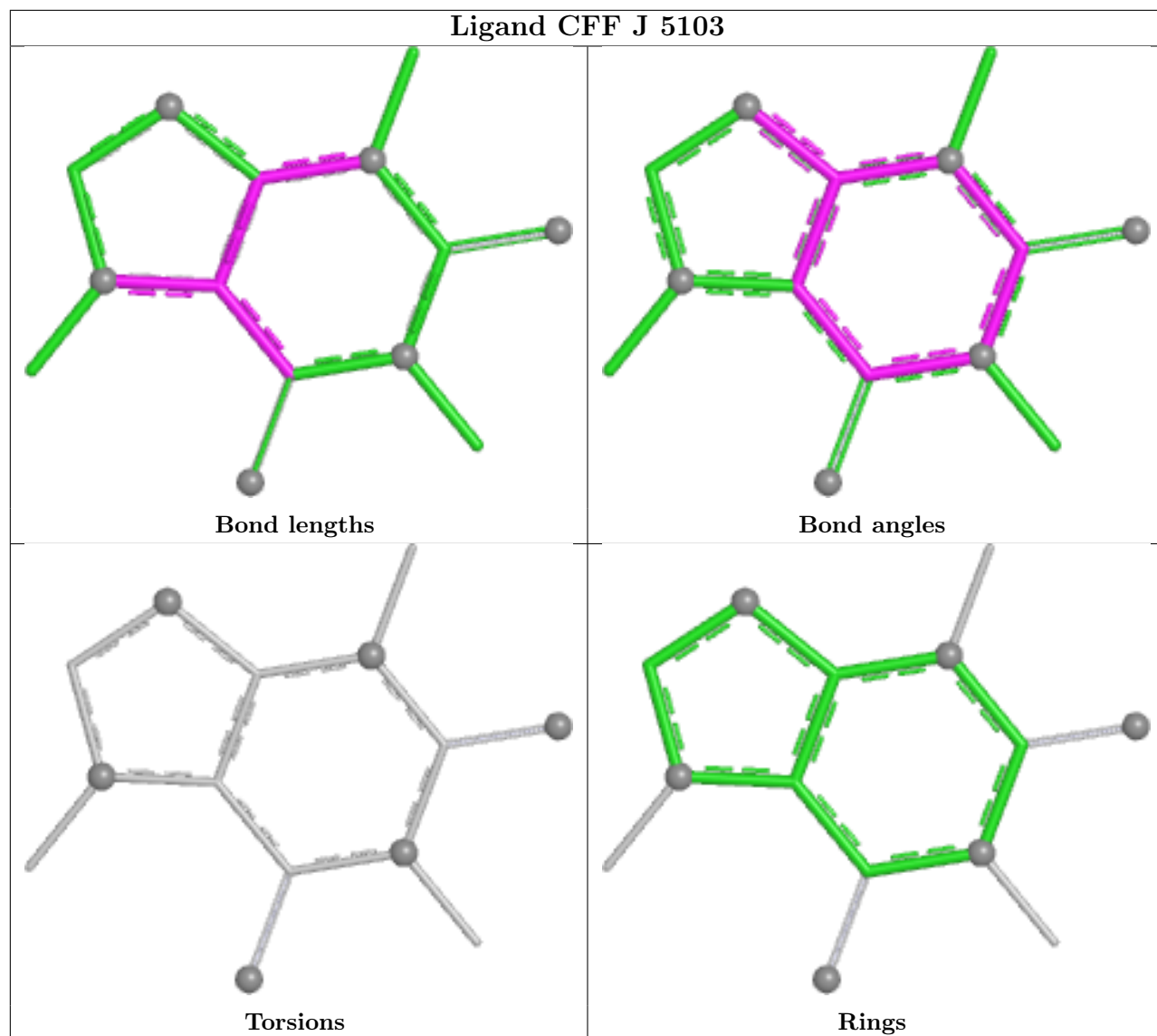


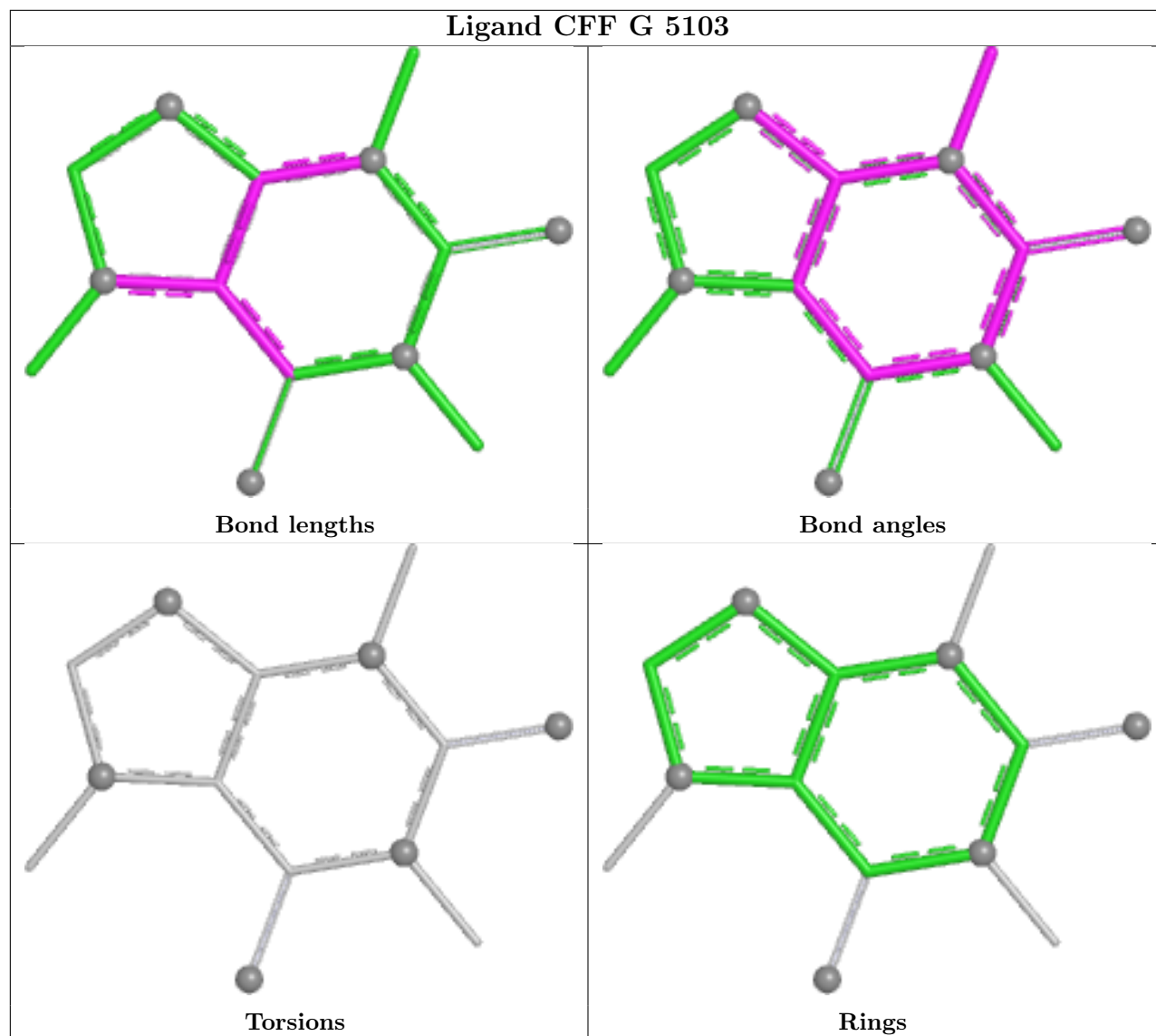


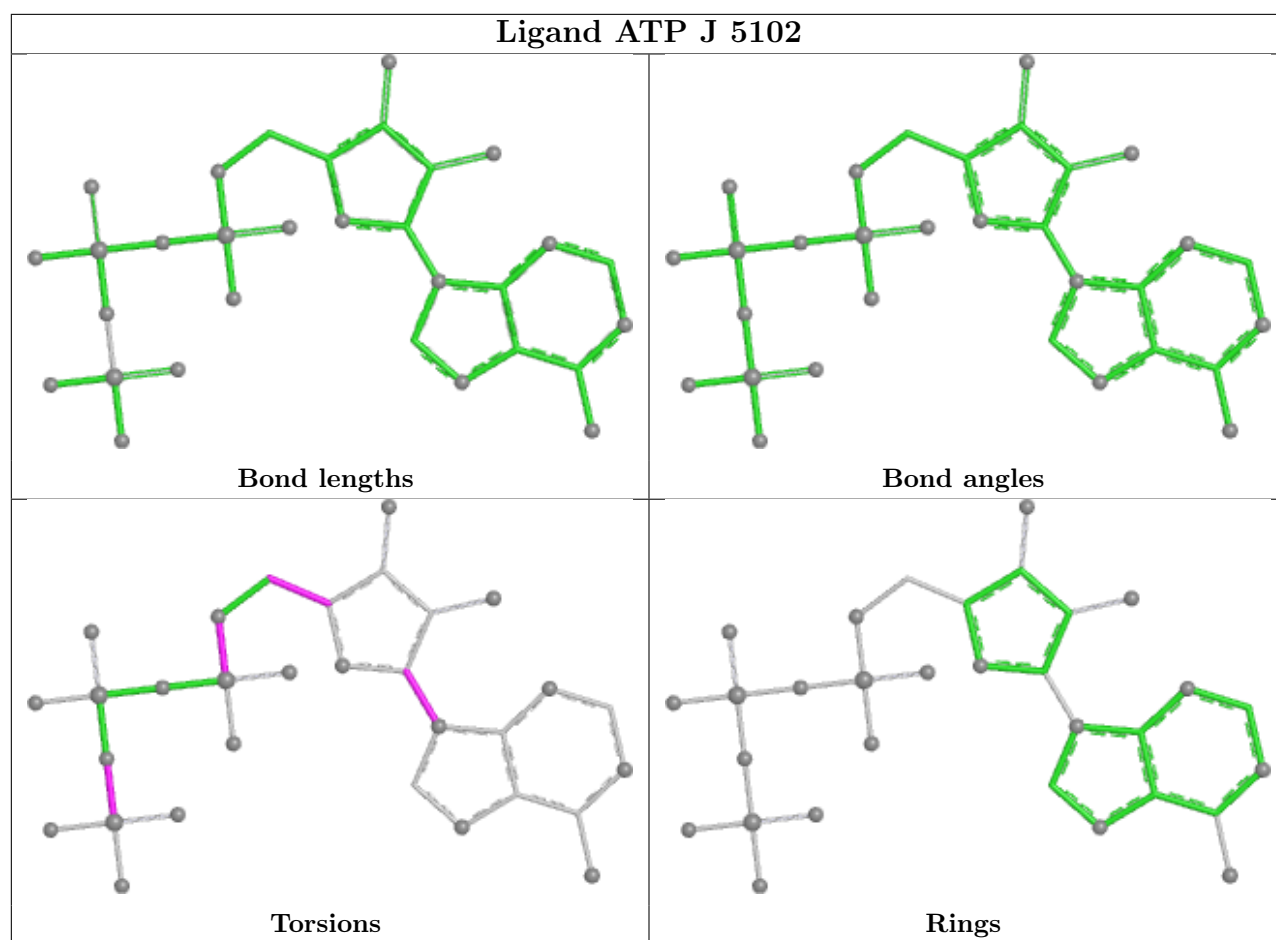












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

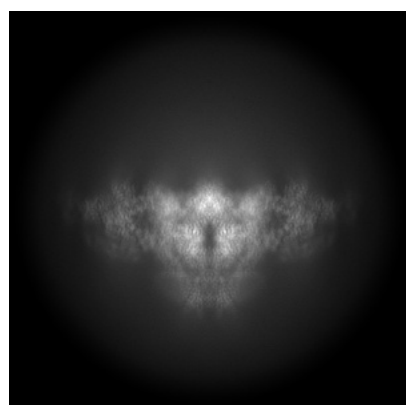
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19472. These allow visual inspection of the internal detail of the map and identification of artifacts.

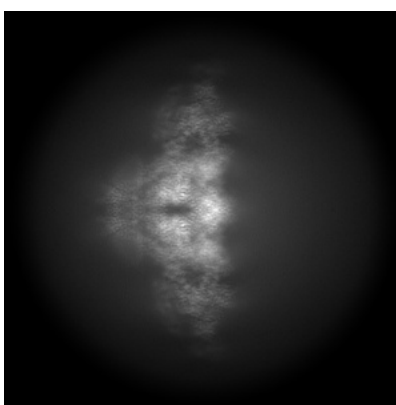
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

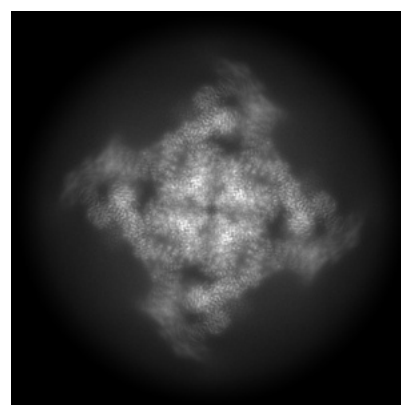
6.1.1 Primary map



X



Y

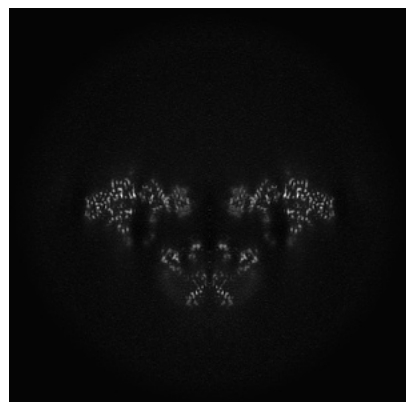


Z

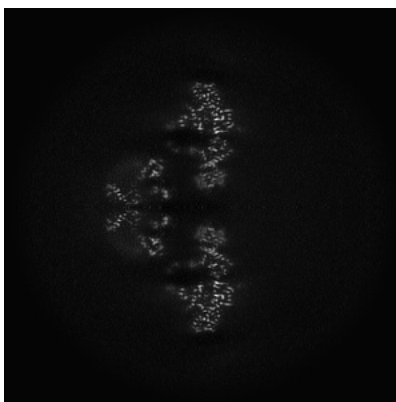
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

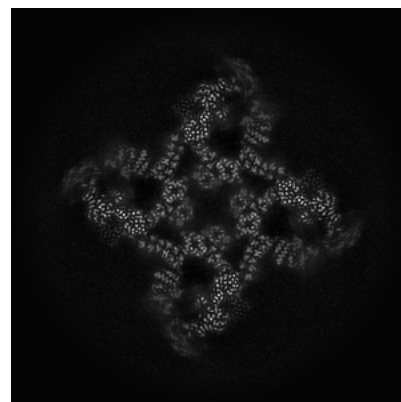
6.2.1 Primary map



X Index: 168



Y Index: 168

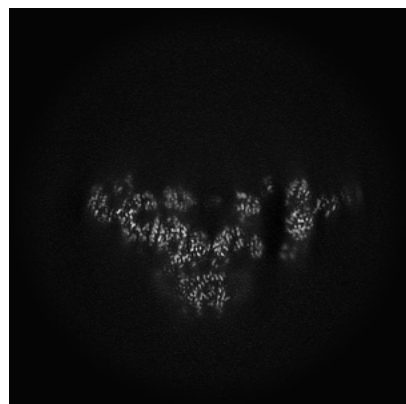


Z Index: 168

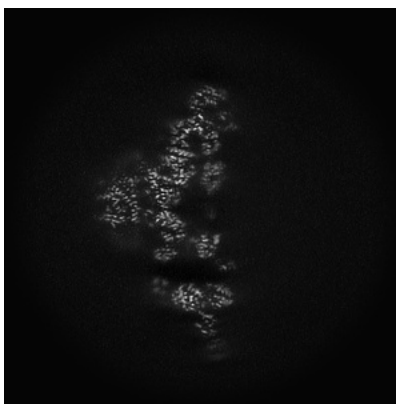
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

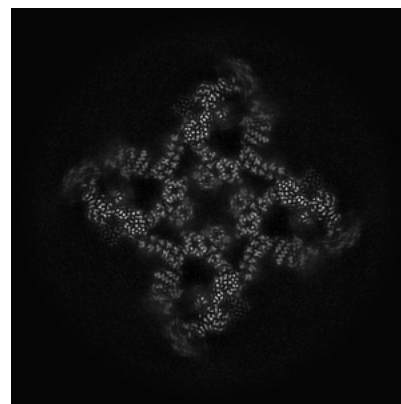
6.3.1 Primary map



X Index: 178



Y Index: 178

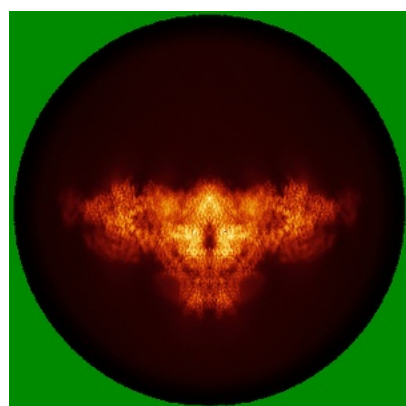


Z Index: 168

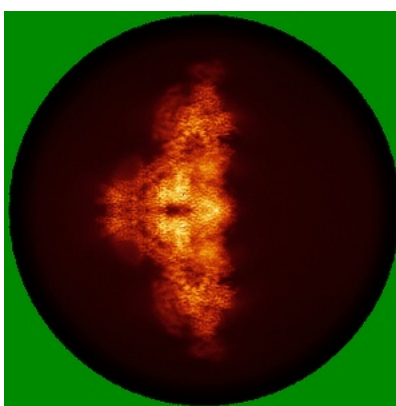
The images above show the largest variance slices of the map in three orthogonal directions.

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

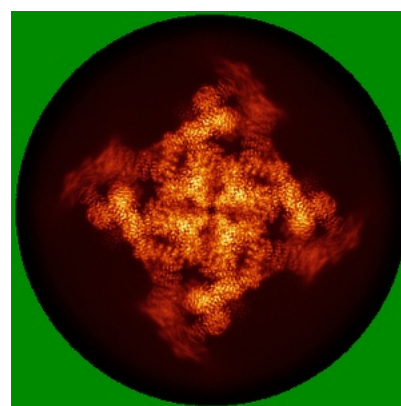
6.4.1 Primary map



X



Y

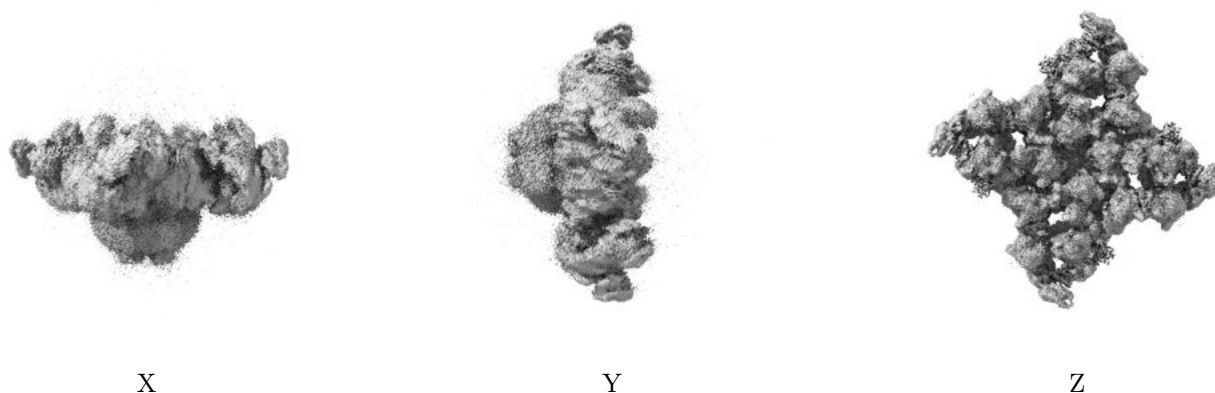


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

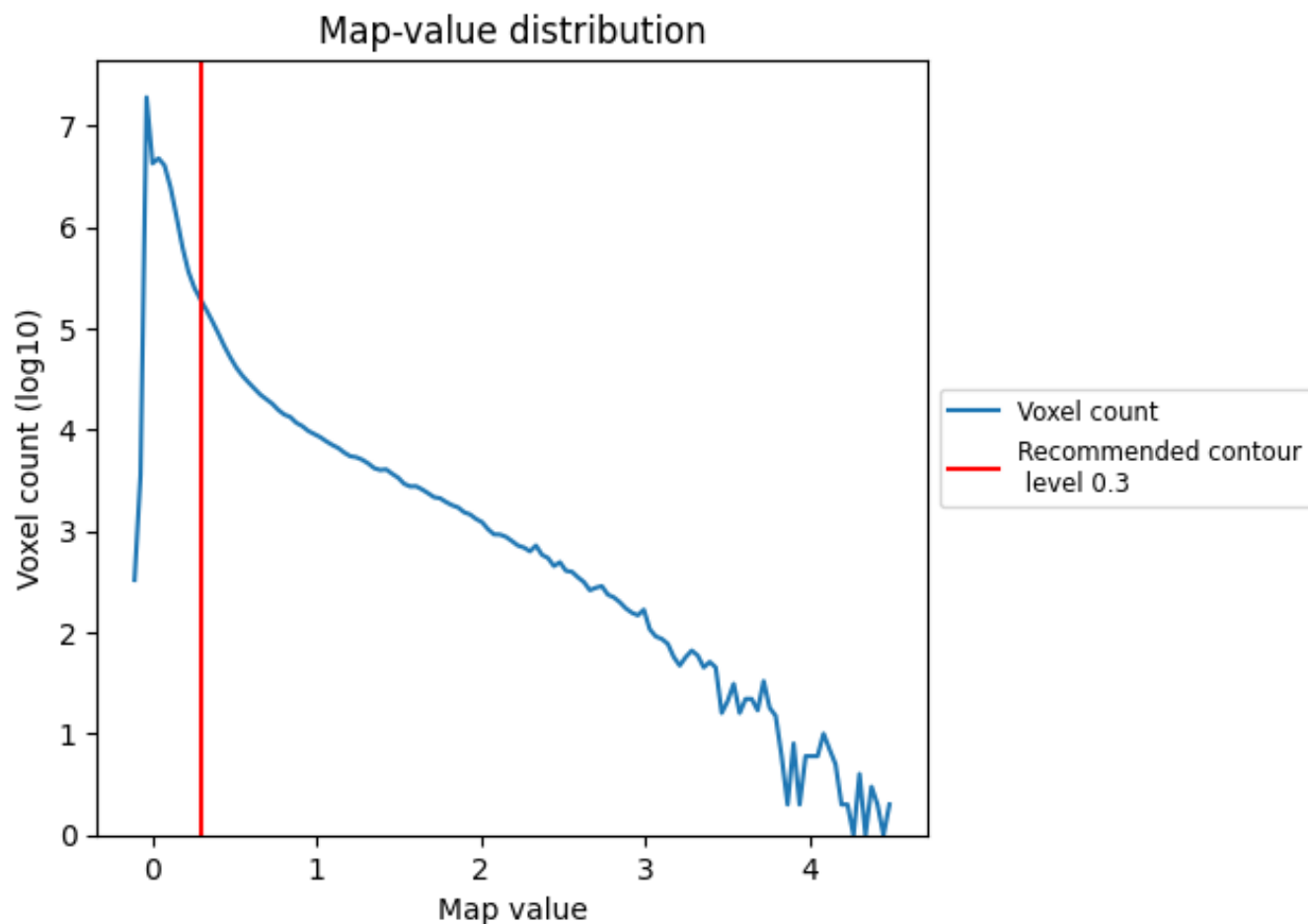
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

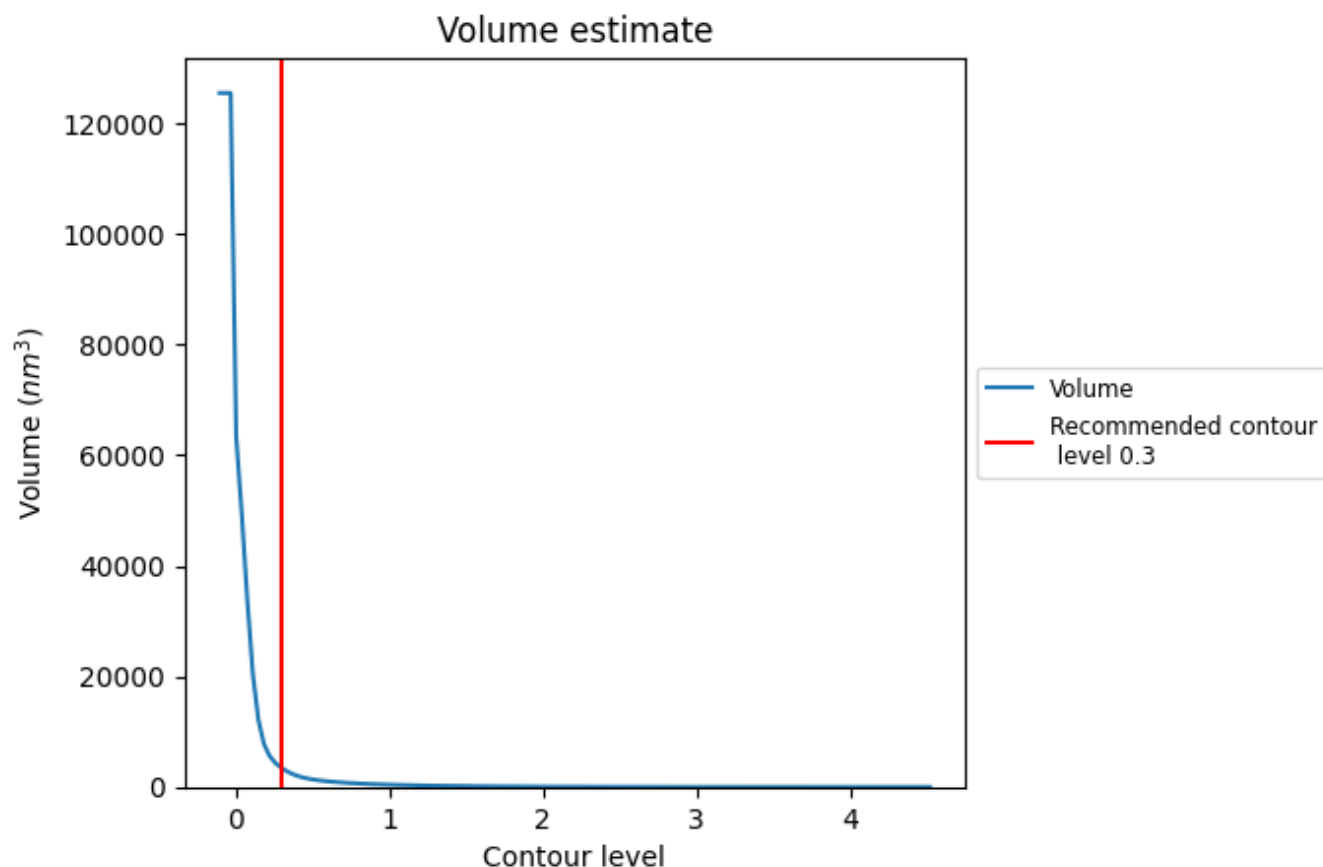
This section contains the results of statistical analysis of the map.

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.

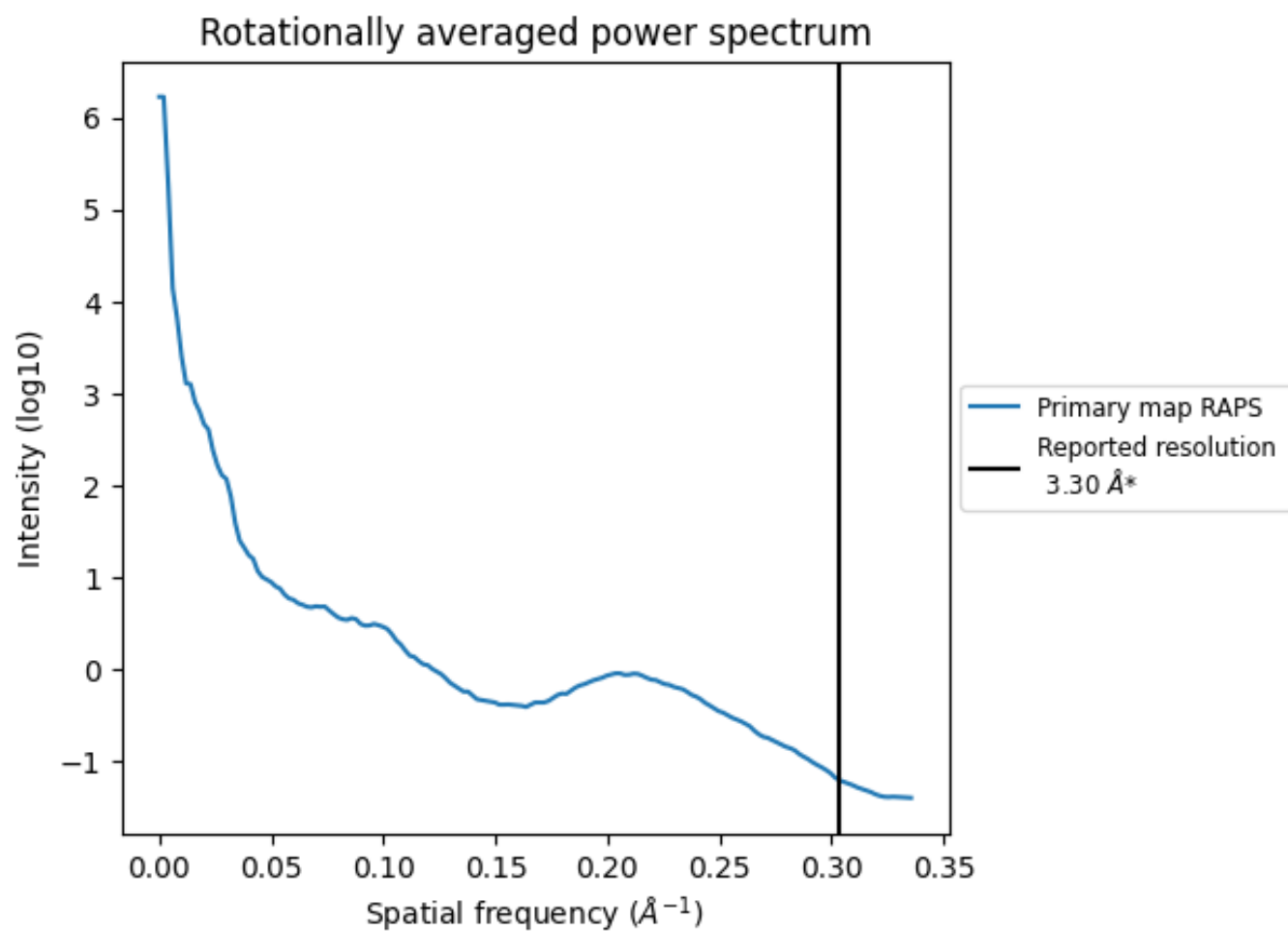
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3395 nm^3 ; this corresponds to an approximate mass of 3067 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 ⓘ

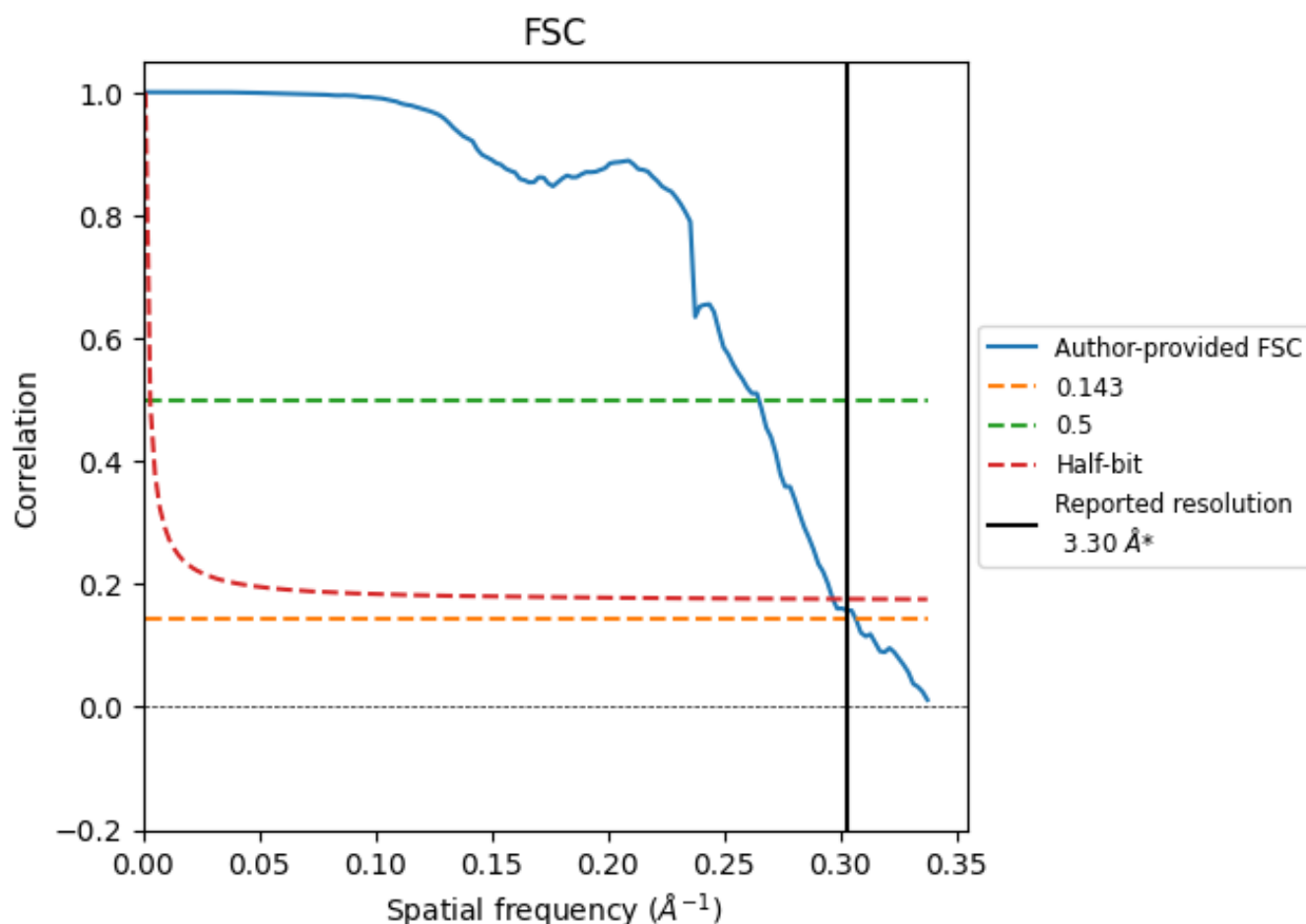


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

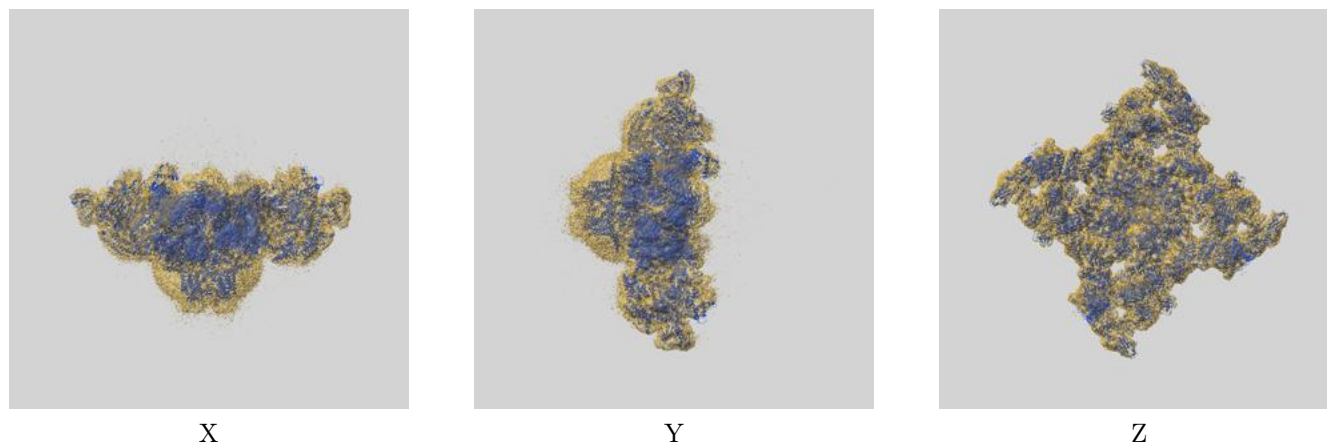
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.78	3.37
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

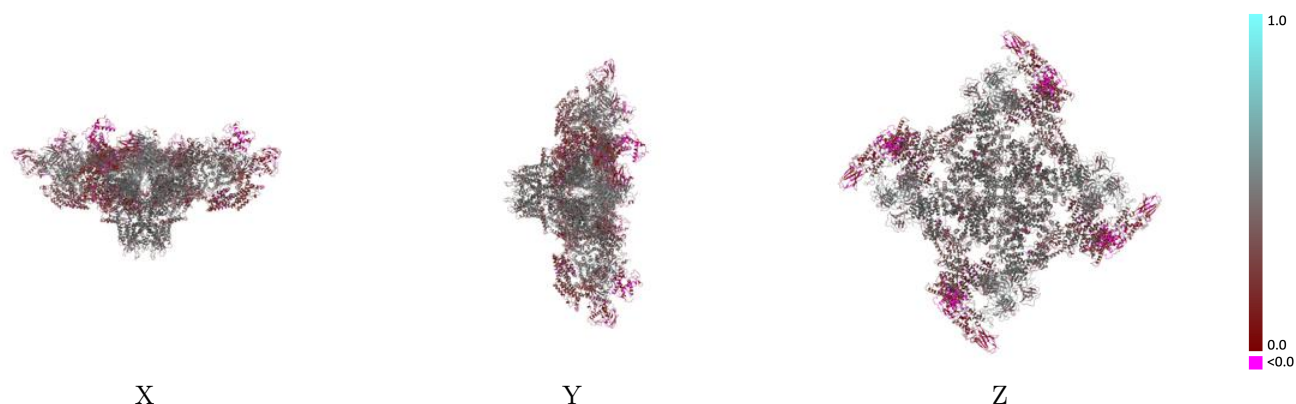
This section contains information regarding the fit between EMDB map EMD-19472 and PDB model 8RS0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



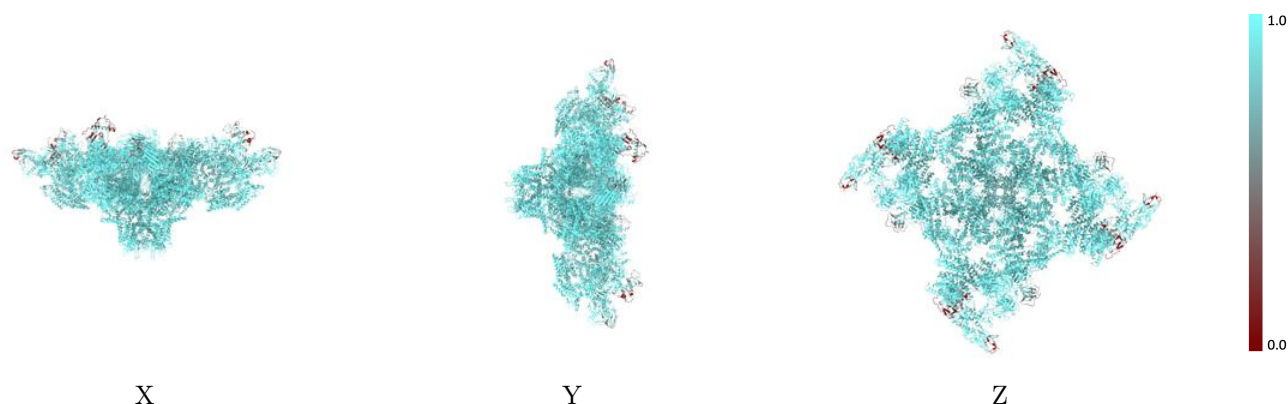
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



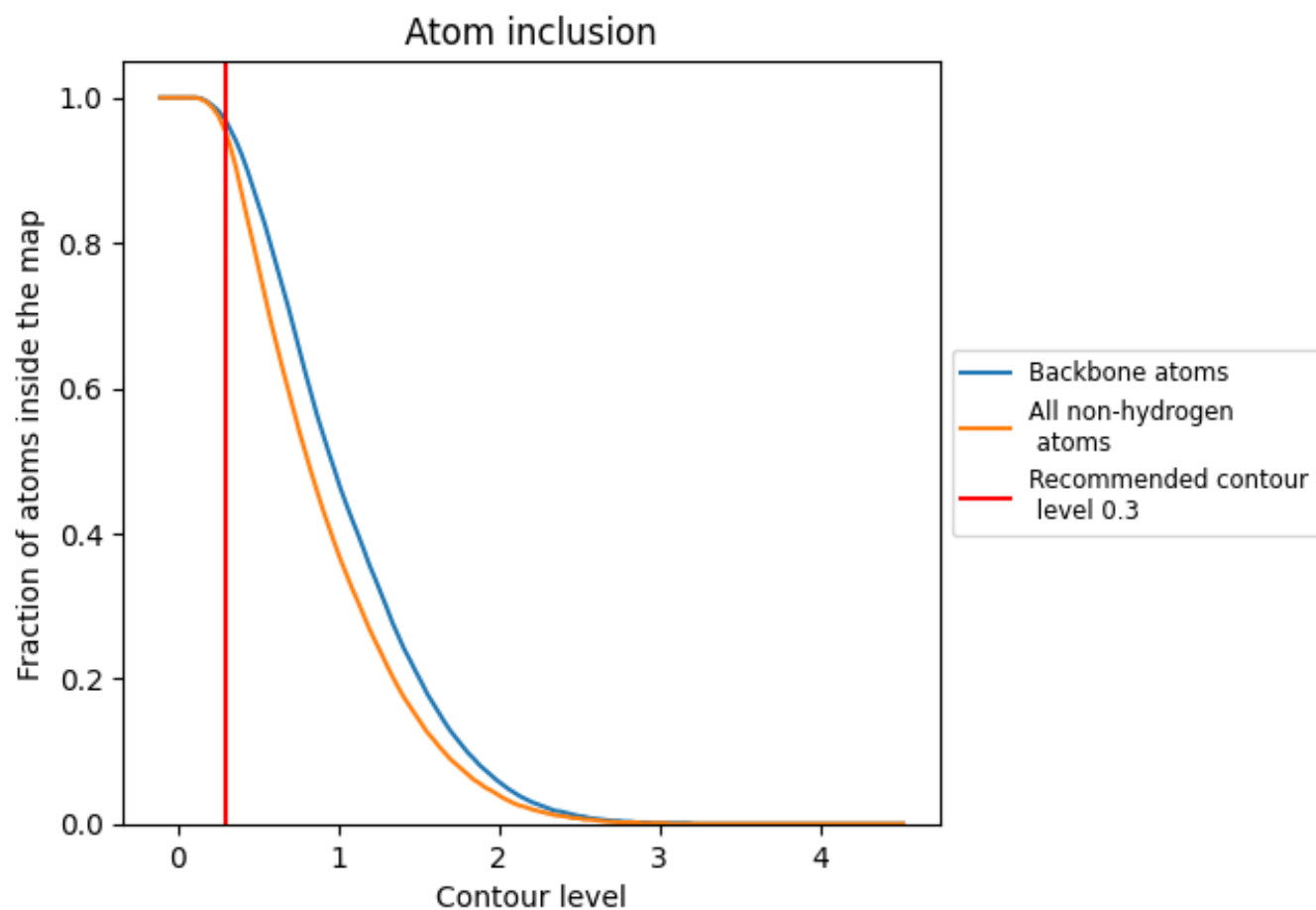
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.3560
A	0.6870	0.3860
B	0.9670	0.3620
C	0.6930	0.1320
D	0.6890	0.3950
E	0.9670	0.3620
F	0.6880	0.1320
G	0.9670	0.3610
H	0.6880	0.3920
I	0.6850	0.3940
J	0.9670	0.3620
K	0.6880	0.1340
M	0.6910	0.1310

1.0

0.0

<0.0