



wwPDB EM Validation Summary Report ⓘ

Sep 23, 2026 – 02:52 PM EDT

PDB ID : 9ZOE / pdb_00009zoe
EMDB ID : EMD-74486
Title : Structure of RyR1 in complex with rosuvastatin (Ca²⁺/CFF/ATP dataset; open pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-12-15
Resolution : 2.90 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:

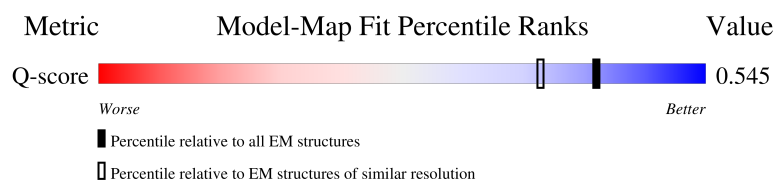
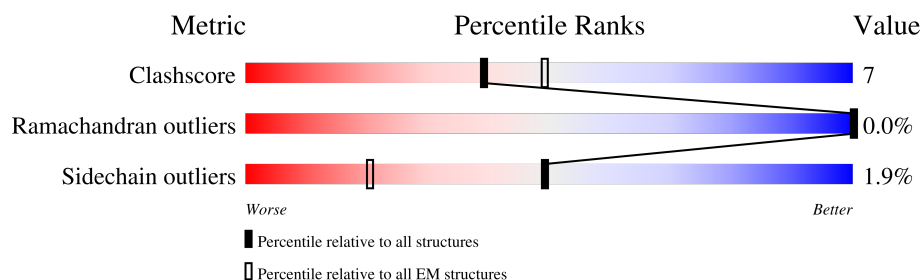
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

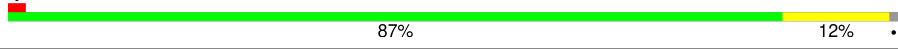
The reported resolution of this entry is 2.90 Å.

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.



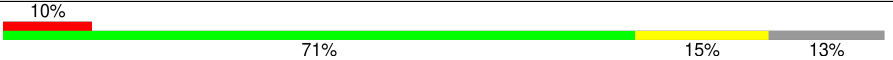
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	E	108	 85% 14% .
1	F	108	 85% 14% .
1	G	108	 86% 13% .
1	H	108	 87% 12% .

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Mol	Chain	Length	Quality of chain
2	A	5037	
2	B	5037	
2	C	5037	
2	D	5037	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 143836 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.

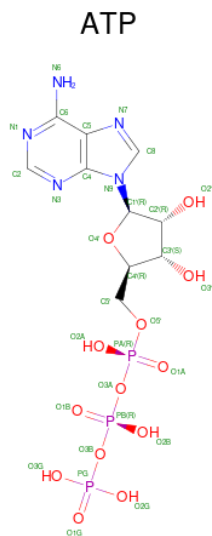
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
1	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
1	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
1	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4383	Total	C	N	O	S	5	0
			34941	22229	6018	6457	237		
2	B	4383	Total	C	N	O	S	5	0
			34941	22229	6018	6457	237		
2	D	4383	Total	C	N	O	S	5	0
			34941	22229	6018	6457	237		
2	C	4383	Total	C	N	O	S	5	0
			34941	22229	6018	6457	237		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

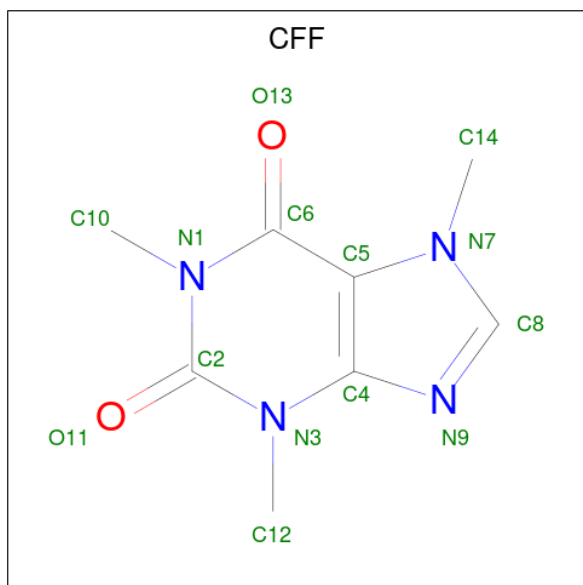
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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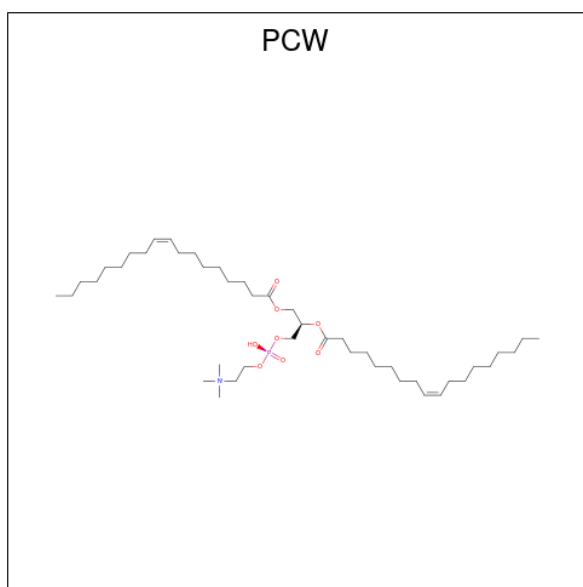
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



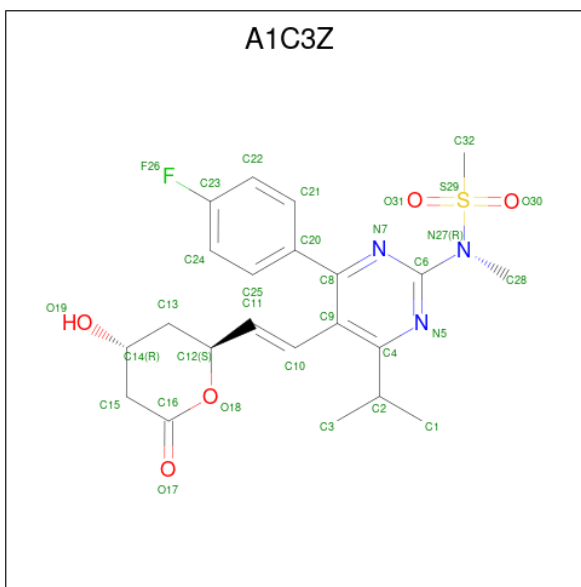
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	D	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is rosuvastatin lactone (CCD ID: A1C3Z) (formula: $C_{22}H_{26}FN_3O_5S$) (labeled as "Ligand of Interest" by depositor).

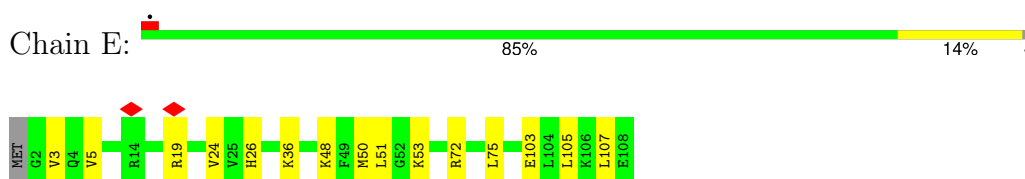


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
8	A	1	32	22	1	3	5	1	0
8	B	1	32	22	1	3	5	1	0
8	D	1	32	22	1	3	5	1	0
8	C	1	32	22	1	3	5	1	0

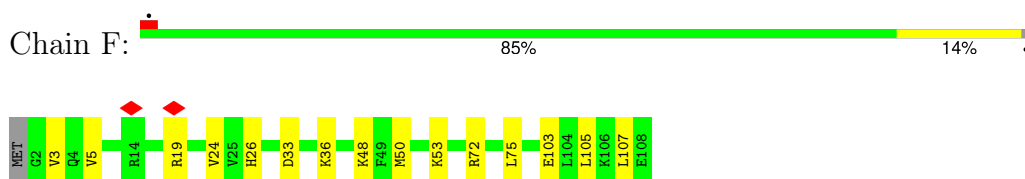
3 Residue-property plots

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

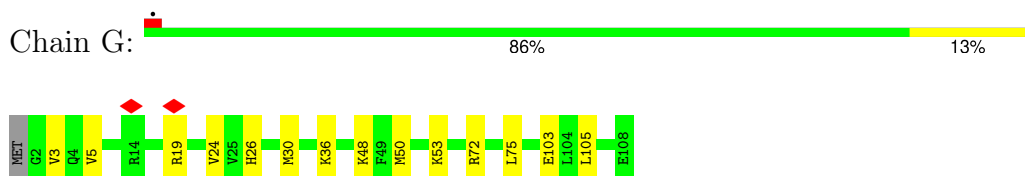
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



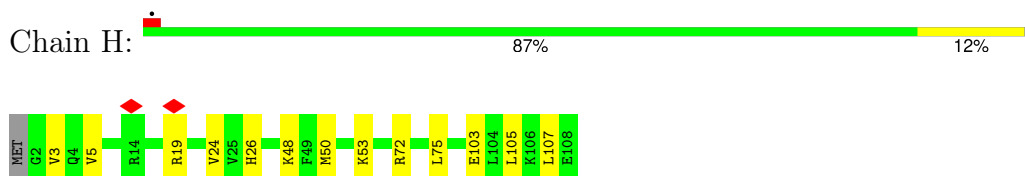
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



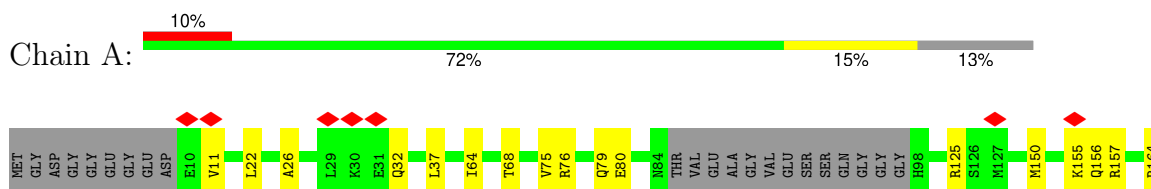
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



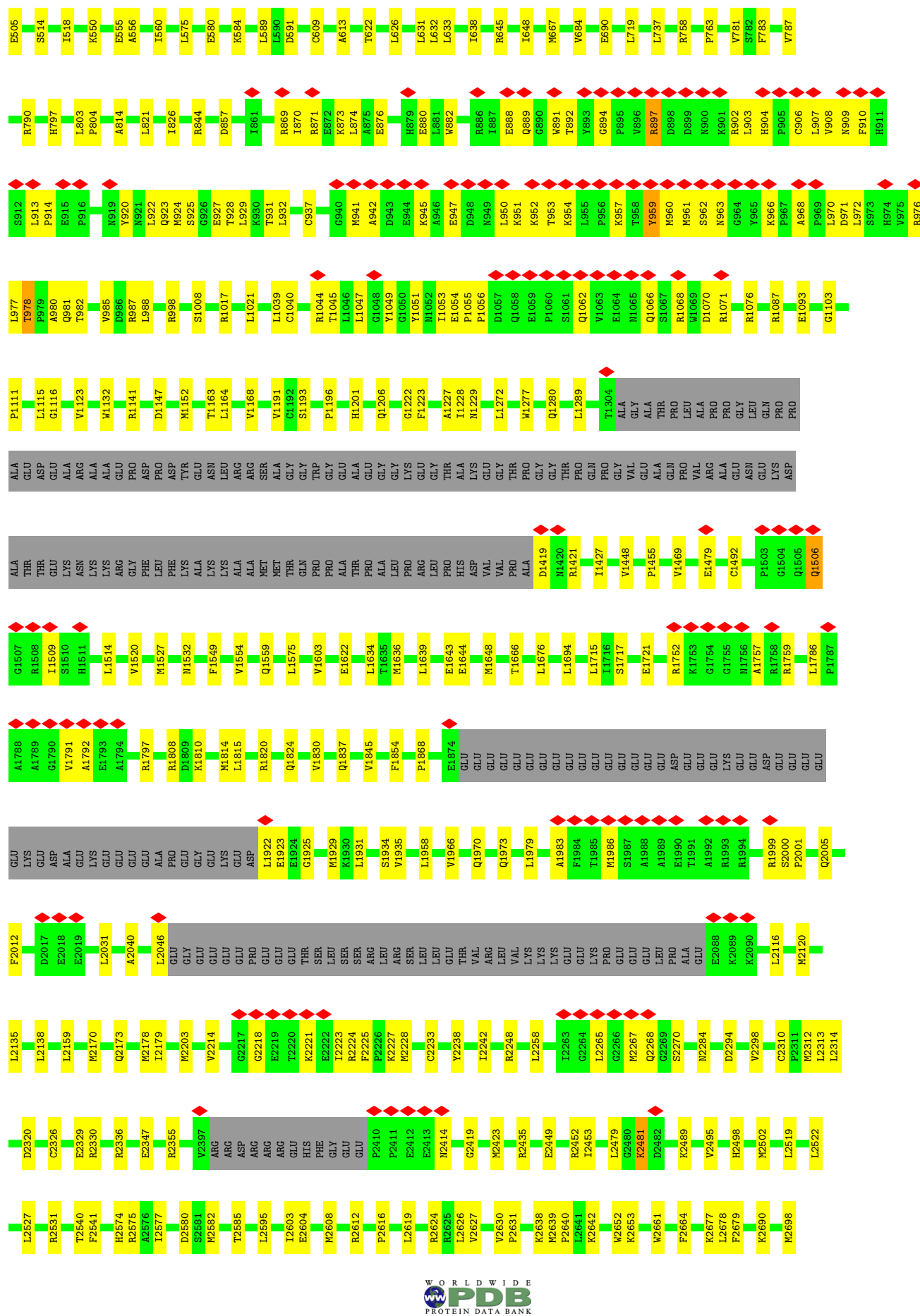
- Molecule 2: Ryanodine receptor 1



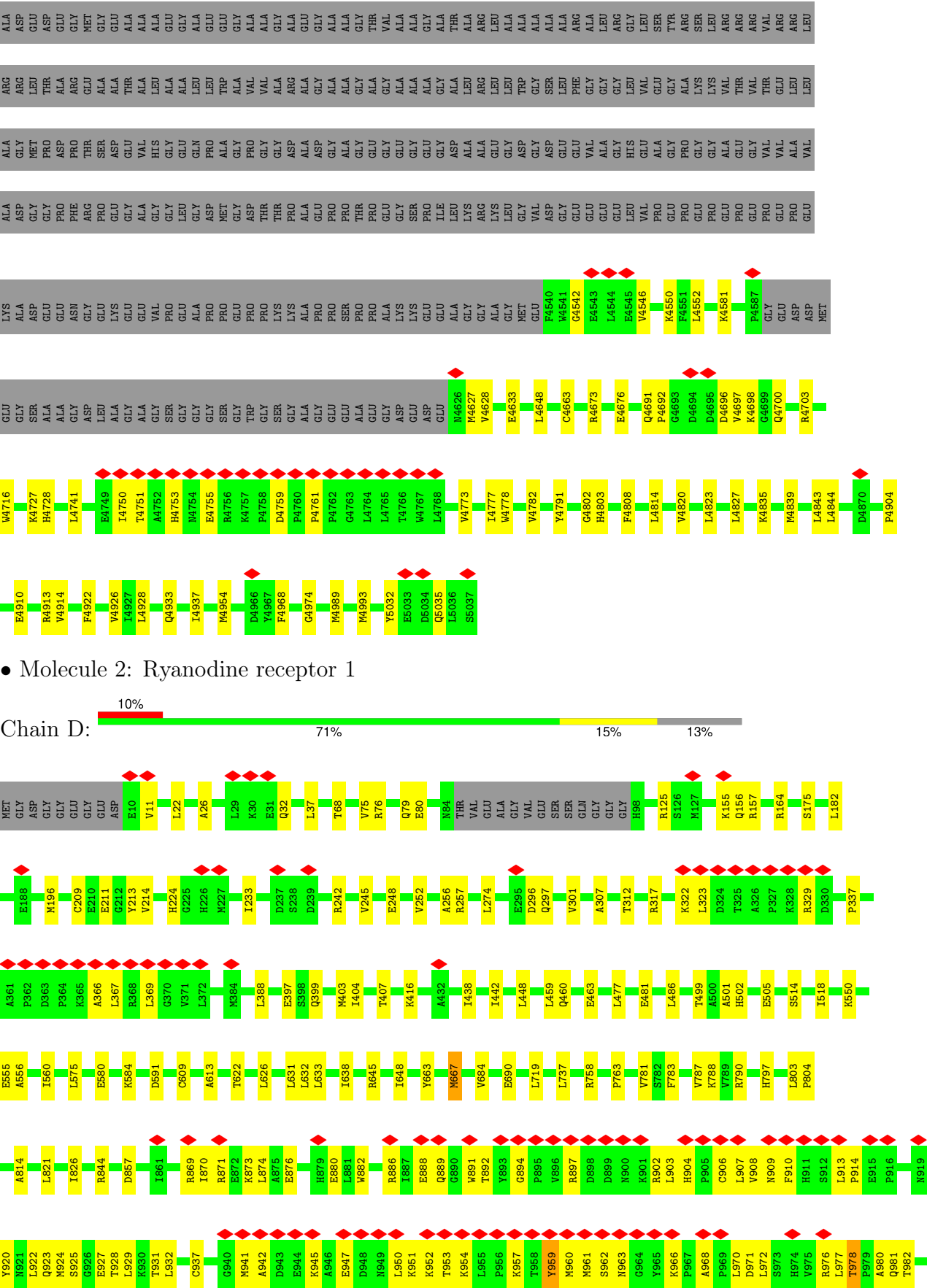


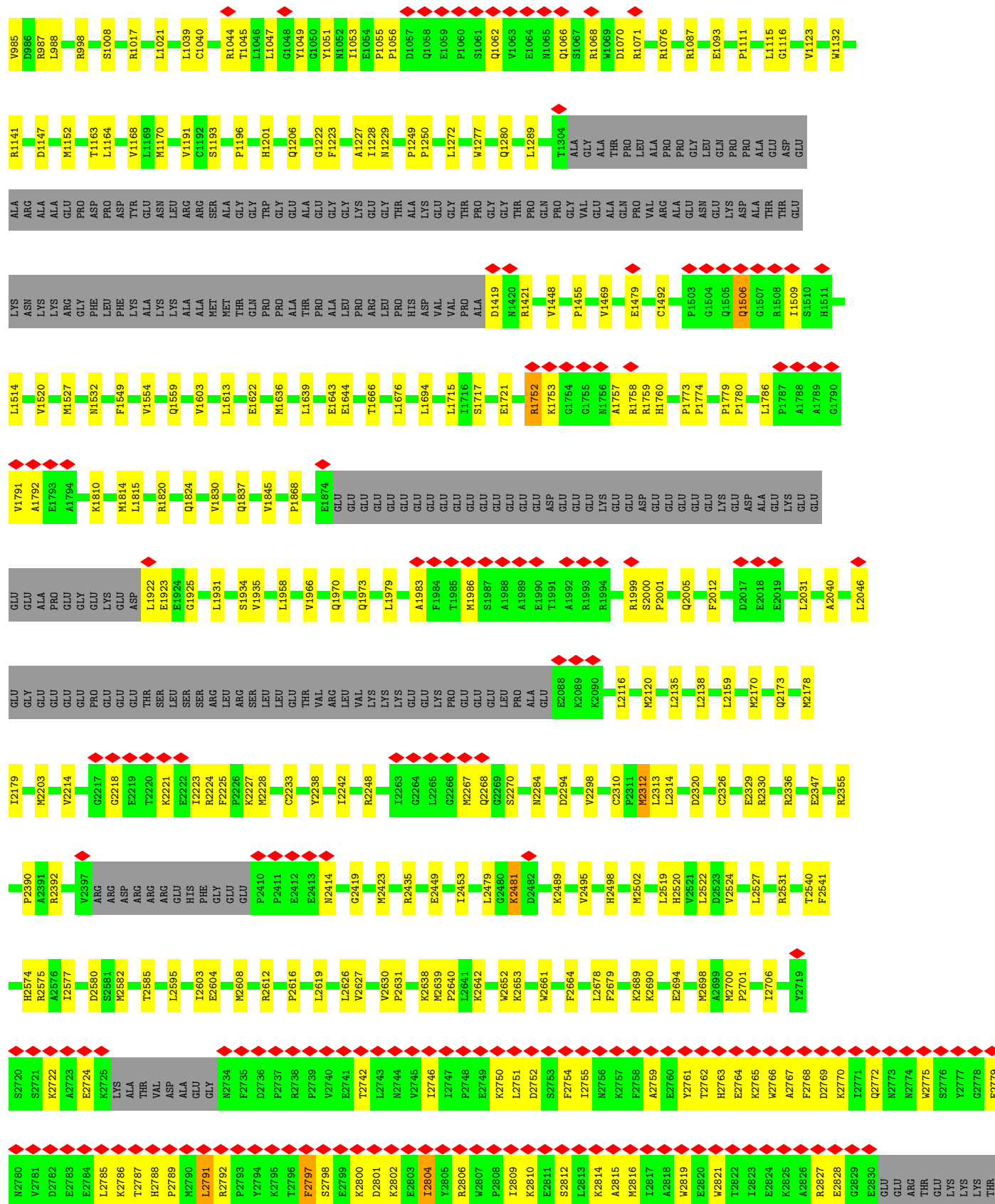






V4072	E3685	I3592	R3499	R3395	F2973	E2893	ARG	N2773	K2699
G4086	E3686	V3593	G3500	D3396	I2974	L2894	THR	N2774	K2700
L4087	E3687	E3594	D3501	L3405	H2975	E2895	GLU	W2775	P2701
I4088	E3688	R3595	R3502	L3406	H2976	A2896	LYS	S2776	
E4107	E3689	Q3597	Y3503	Y3409	L2977	K2897	LYS	G2777	I2706
L4112	E3690	Q3598	S3504	R3414	A2978	G2898	THR	G2778	V2719
E4119	E3691	V3599	V3505	Y3415	A2979	G2899	ARG	E2779	S2720
N4124	E3692	V3602	Q3506	V3416	V2980	G2900	LYS	N2780	S2721
F4125	H3704	L3603	P3519	R3420	V2981	G2901	SER	V2781	K2722
F4128	T3708	H3604	L3522	E3432	S2983	H2902	GLN	D2782	A2723
A4129	T3711	H3605	N3523	E3454	G2984	P2903	ALA	E2783	E2724
F4132	E3712	L3606	M3524	E3455	R2985	L2904	GLN	K2784	K2725
Q4133	K3713	L3607	M3531	Q3456	V2986	L2905	THR	LYS	
Q3889	I3728	E3611	D3531	Q3457	E2987	V2906	TYR	ALA	
I3915	L3735	H3612	L3532	F3458	K2988	P2907	ASP	THR	
I3916	H3734	TYR	M3533	V3459	S2989	D2909	PRO	VAL	
Y3934	L3736	LYS	M3534	Q3461	E2992	T2910	ARG	ASP	
K3959	E3736	LYS	A3536	M3462	Q2993	T2911	GLU	ALA	
S3964	GLU	LYS	K3537	E3463	E2994	T2912	GLY	GLY	
Q3971	GLY	ALA	T3538	I3464	K2995	A2913		N2794	N2734
P3972	GLY	ALA	R3539	I3465	K2996	K2914		R2792	F2735
L3980	GLY	TRP	Y3540	M3465	F2997	E2915		P2793	D2736
F3996	ASN	LYS	A3541	N3466	F2998	K2916		Y2794	P2737
M3999	GLY	LYS	L3542	M3467		P2917		K2795	K2738
M4000	ALA	LEU	K3543	S3468	L3002	A2918		T2796	P2739
M4001	ALA	LEU	E3547	F3469	L3003	K2919		F2797	V2740
A4004	GLU	LYS	E3548	L3470	P3004	D2919		S2798	E2741
I4010	GLU	LYS	E3551	T3471	I3006	R2920		E2799	T2742
K4014	GLU	ARG	E3552	A3472	F3010	E2921		K2800	L2743
I4017	GLU	ARG	L3553	D3473	S3027	K2922		D2801	N2744
Q4020	VAL	ALA	G3561	S3474	K3034	A2923		K2802	V2745
K4021	VAL	VAL	K3562	K3475	M3038	Q2924		E2803	I2746
M4057	A3634	A3635	V3563	S3476		E2925		I2804	I2747
K4060	F3635	F3636	E3564	K3477		L2926		Y2805	P2748
M4064	R3637	R3638	G3565	M3478		L2927		R2806	E2749
K4067	L3641	L3642	S3568	A3479		K2928		W2807	K2750
L4069	L3641	Y3642	L3569	LYS		F2929		P2808	L2751
I4071	L3642	L3663	R3571	ALA		L2930		L2809	D2752
	M3816	L3666	R3577	GLY		Q2931		K2810	S2753
	L3835	D3666	G3581	ASP		M2932		E2811	F2754
	M3836	L3666	R3582	ALA		N2933		S2812	I2755
	L3844	D3666	E3583	SER		G2934		L2813	N2756
	E3848	E3670	E3584	GLY		V2935		K2814	K2757
	L3856	D3671	D3585	SER		A2936		A2815	F2758
	M3857	A3680	A3586	ASP		V2937		M2816	A2759
	M3858	Q3683	D3587	GLN		T2938		I2817	E2760
	V3859	E3684	E3588	GLU		R2939		M2883	V2761
			P3589	ARG		GLY		N2884	V2762
			K3591	THR		LEU		W2819	T2763
				LYS		LYS		E2820	H2763
				LYS		ASP		W2821	E2764
				LYS		GLU		T2822	K2765
						L2946		I2823	K2766
						D2947		E2824	A2767
								K2825	F2768
								D2769	D2769
								A2826	K2770
								R2827	I2771
								E2828	Q2772
								G2829	
								GLU	
								GLU	



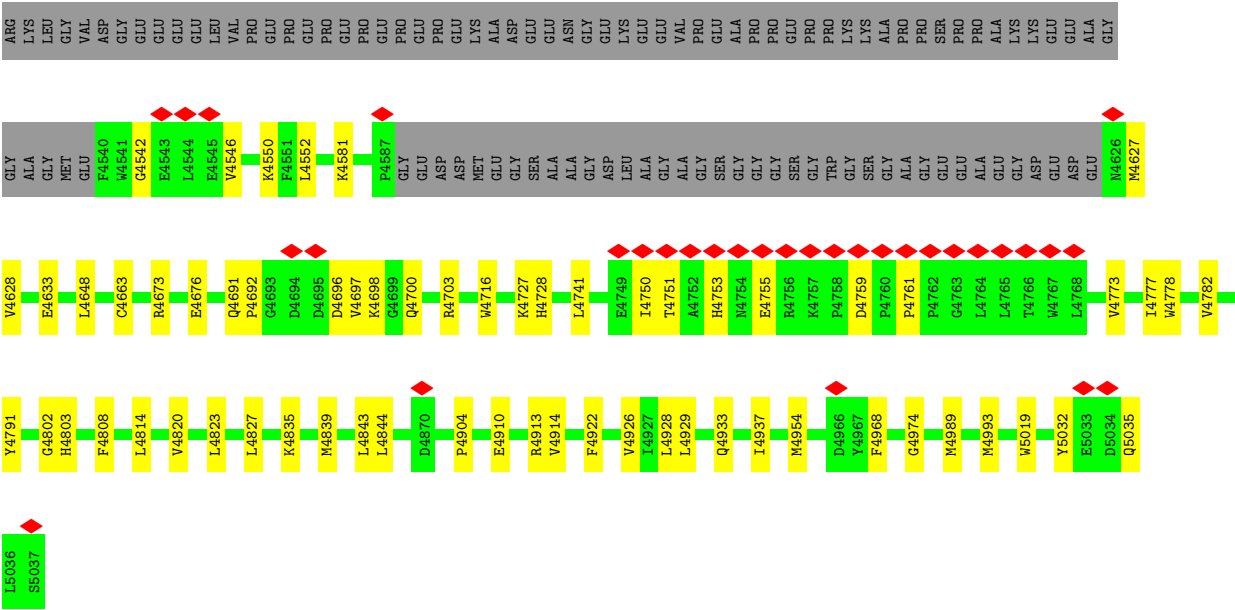












ARG
LYS
LEU
GLY
MET
VAL
ASP
GLY
GLU
GLU
GLU
LEU
VAL
PRO
GLU
PRO
GLU
PRO
GLY
LYS
ALA
GLY
SER
GLU
ALA
ASN
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LYS
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GLY
ALA
MET
GLU
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W4541
G4542
E4543
L4544
E4545
V4546
K4550
F4551
L4552
K4581
P4587
GLY
GLU
ASP
ASP
MET
GLY
GLY
SER
ALA
ALA
GLY
ASP
LEU
ALA
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ALA
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GLY
ALA
GLY
GLY
GLU
GLU
ALA
ALA
GLY
ASP
ASP
GLY
M4626
M4627

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101680	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.632	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1C3Z, ATP, PCW, CA, CFF, 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	E	0.10	0/850	0.30	0/1146
1	F	0.11	0/850	0.30	0/1146
1	G	0.11	0/850	0.30	0/1146
1	H	0.11	0/850	0.30	0/1146
2	A	0.13	0/35750	0.35	2/48423 (0.0%)
2	B	0.14	0/35750	0.35	2/48423 (0.0%)
2	C	0.14	0/35750	0.35	2/48423 (0.0%)
2	D	0.14	0/35750	0.35	2/48423 (0.0%)
All	All	0.14	0/146400	0.34	8/198276 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2481	LYS	CA-C-N	5.79	132.33	123.47
2	A	2481	LYS	C-N-CA	5.79	132.33	123.47
2	C	2481	LYS	CA-C-N	5.79	132.33	123.47
2	C	2481	LYS	C-N-CA	5.79	132.33	123.47
2	B	2481	LYS	CA-C-N	5.77	132.29	123.47

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	E	831	0	828	10	0
1	F	831	0	828	10	0
1	G	831	0	828	9	0
1	H	831	0	828	7	0
2	A	34941	0	34555	501	0
2	B	34941	0	34555	502	0
2	C	34941	0	34555	516	0
2	D	34941	0	34555	510	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	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	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	14	0	10	0	0
6	B	14	0	10	0	0
6	C	14	0	10	0	0
6	D	14	0	10	0	0
7	A	108	0	168	10	0
7	B	108	0	168	9	0
7	C	108	0	168	10	0
7	D	108	0	168	10	0
8	A	32	0	0	5	0
8	B	32	0	0	5	0
8	C	32	0	0	5	0
8	D	32	0	0	5	0
All	All	143836	0	142292	2063	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 7.

The worst 5 of 2063 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:972:LEU:HD23	2:B:1044:ARG:HB3	1.62	0.82
2:D:972:LEU:HD23	2:D:1044:ARG:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2767:ALA:HA	2:D:2770:LYS:HG2	1.62	0.82
2:A:972:LEU:HD23	2:A:1044:ARG:HB3	1.62	0.81
2:A:2767:ALA:HA	2:A:2770:LYS:HG2	1.62	0.81

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	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4358/5037 (86%)	4249 (98%)	107 (2%)	2 (0%)	100	100
2	B	4358/5037 (86%)	4249 (98%)	107 (2%)	2 (0%)	100	100
2	C	4358/5037 (86%)	4249 (98%)	107 (2%)	2 (0%)	100	100
2	D	4358/5037 (86%)	4250 (98%)	106 (2%)	2 (0%)	100	100
All	All	17852/20580 (87%)	17405 (98%)	439 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2752	ASP
2	B	2752	ASP
2	D	2752	ASP
2	C	2752	ASP
2	A	3300	ALA

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	E	89/90 (99%)	88 (99%)	1 (1%)	65	88
1	F	89/90 (99%)	88 (99%)	1 (1%)	65	88
1	G	89/90 (99%)	88 (99%)	1 (1%)	65	88
1	H	89/90 (99%)	88 (99%)	1 (1%)	65	88
2	A	3813/4276 (89%)	3738 (98%)	75 (2%)	48	78
2	B	3813/4276 (89%)	3743 (98%)	70 (2%)	51	80
2	C	3813/4276 (89%)	3737 (98%)	76 (2%)	48	78
2	D	3813/4276 (89%)	3736 (98%)	77 (2%)	48	78
All	All	15608/17464 (89%)	15306 (98%)	302 (2%)	49	79

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	245	VAL
2	C	3324	VAL
2	C	959	TYR
2	C	2724	GLU
2	C	4628	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	3814	GLN
2	C	1760	HIS
2	D	4005	GLN
2	D	4946	GLN
2	C	2924	GLN

5.3.3 RNA ⓘ

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 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z > 2$
7	PCW	A	5306	-	53,53,53	0.49	0	59,61,61	0.48	0
7	PCW	B	5305	-	53,53,53	0.49	0	59,61,61	0.46	0
3	ATP	D	5301	-	32,33,33	0.29	0	48,52,52	0.37	0
7	PCW	C	5305	-	53,53,53	0.49	0	59,61,61	0.46	0
7	PCW	A	5305	-	53,53,53	0.49	0	59,61,61	0.46	0
6	CFF	A	5304	-	15,15,15	0.53	0	23,23,23	0.80	1 (4%)
3	ATP	C	5301	-	32,33,33	0.29	0	48,52,52	0.37	0
6	CFF	C	5304	-	15,15,15	0.53	0	23,23,23	0.79	1 (4%)
8	A1C3Z	B	5307	-	33,34,34	0.19	0	40,50,50	0.33	0
7	PCW	D	5306	-	53,53,53	0.49	0	59,61,61	0.48	0
8	A1C3Z	A	5307	-	33,34,34	0.19	0	40,50,50	0.33	0
6	CFF	D	5304	-	15,15,15	0.53	0	23,23,23	0.79	1 (4%)
3	ATP	A	5301	-	32,33,33	0.29	0	48,52,52	0.37	0
8	A1C3Z	C	5307	-	33,34,34	0.19	0	40,50,50	0.33	0
7	PCW	D	5305	-	53,53,53	0.49	0	59,61,61	0.46	0
7	PCW	C	5306	-	53,53,53	0.49	0	59,61,61	0.48	0
8	A1C3Z	D	5307	-	33,34,34	0.19	0	40,50,50	0.33	0
3	ATP	B	5301	-	32,33,33	0.29	0	48,52,52	0.36	0
6	CFF	B	5304	-	15,15,15	0.53	0	23,23,23	0.79	1 (4%)
7	PCW	B	5306	-	53,53,53	0.49	0	59,61,61	0.48	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
7	PCW	A	5306	-	-	21/57/57/57	-
7	PCW	B	5305	-	-	19/57/57/57	-
3	ATP	D	5301	-	-	3/22/38/38	0/3/3/3
7	PCW	C	5305	-	-	19/57/57/57	-
7	PCW	A	5305	-	-	19/57/57/57	-
6	CFF	A	5304	-	-	-	0/2/2/2
3	ATP	C	5301	-	-	3/22/38/38	0/3/3/3
6	CFF	C	5304	-	-	-	0/2/2/2
8	A1C3Z	B	5307	-	-	8/23/35/35	0/3/3/3
7	PCW	D	5306	-	-	21/57/57/57	-
8	A1C3Z	A	5307	-	-	8/23/35/35	0/3/3/3
6	CFF	D	5304	-	-	-	0/2/2/2
3	ATP	A	5301	-	-	3/22/38/38	0/3/3/3
8	A1C3Z	C	5307	-	-	8/23/35/35	0/3/3/3
7	PCW	D	5305	-	-	19/57/57/57	-
7	PCW	C	5306	-	-	21/57/57/57	-
8	A1C3Z	D	5307	-	-	8/23/35/35	0/3/3/3
3	ATP	B	5301	-	-	3/22/38/38	0/3/3/3
6	CFF	B	5304	-	-	-	0/2/2/2
7	PCW	B	5306	-	-	21/57/57/57	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5304	CFF	C12-N3-C2	2.45	121.60	117.33
6	B	5304	CFF	C12-N3-C2	2.45	121.60	117.33
6	C	5304	CFF	C12-N3-C2	2.45	121.60	117.33
6	D	5304	CFF	C12-N3-C2	2.44	121.58	117.33

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

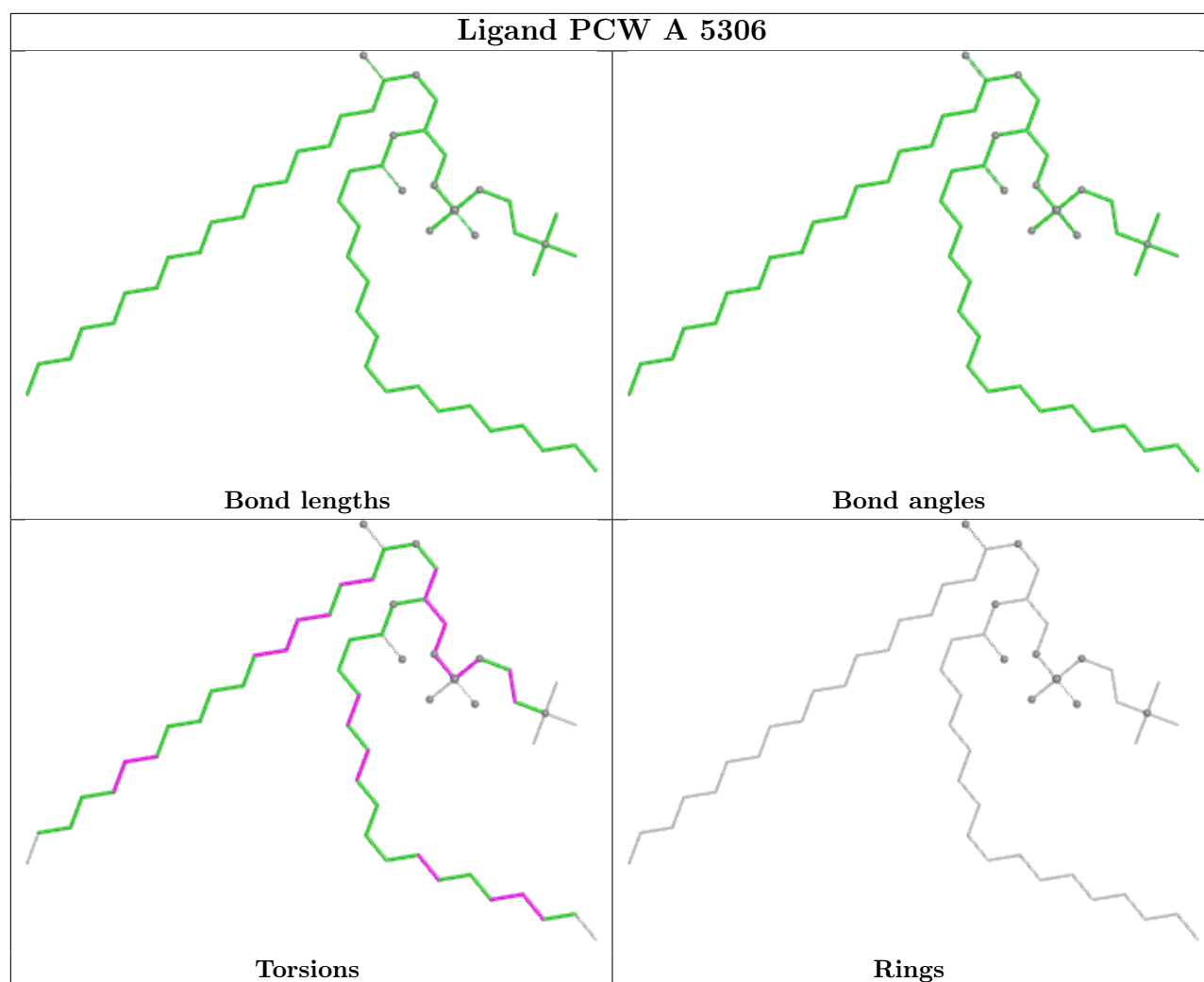
Mol	Chain	Res	Type	Atoms
7	A	5305	PCW	O4P-C4-C5-N
7	A	5305	PCW	C1-O3P-P-O2P
7	A	5305	PCW	C1-O3P-P-O4P
7	A	5305	PCW	C4-O4P-P-O2P
7	A	5306	PCW	C1-O3P-P-O1P

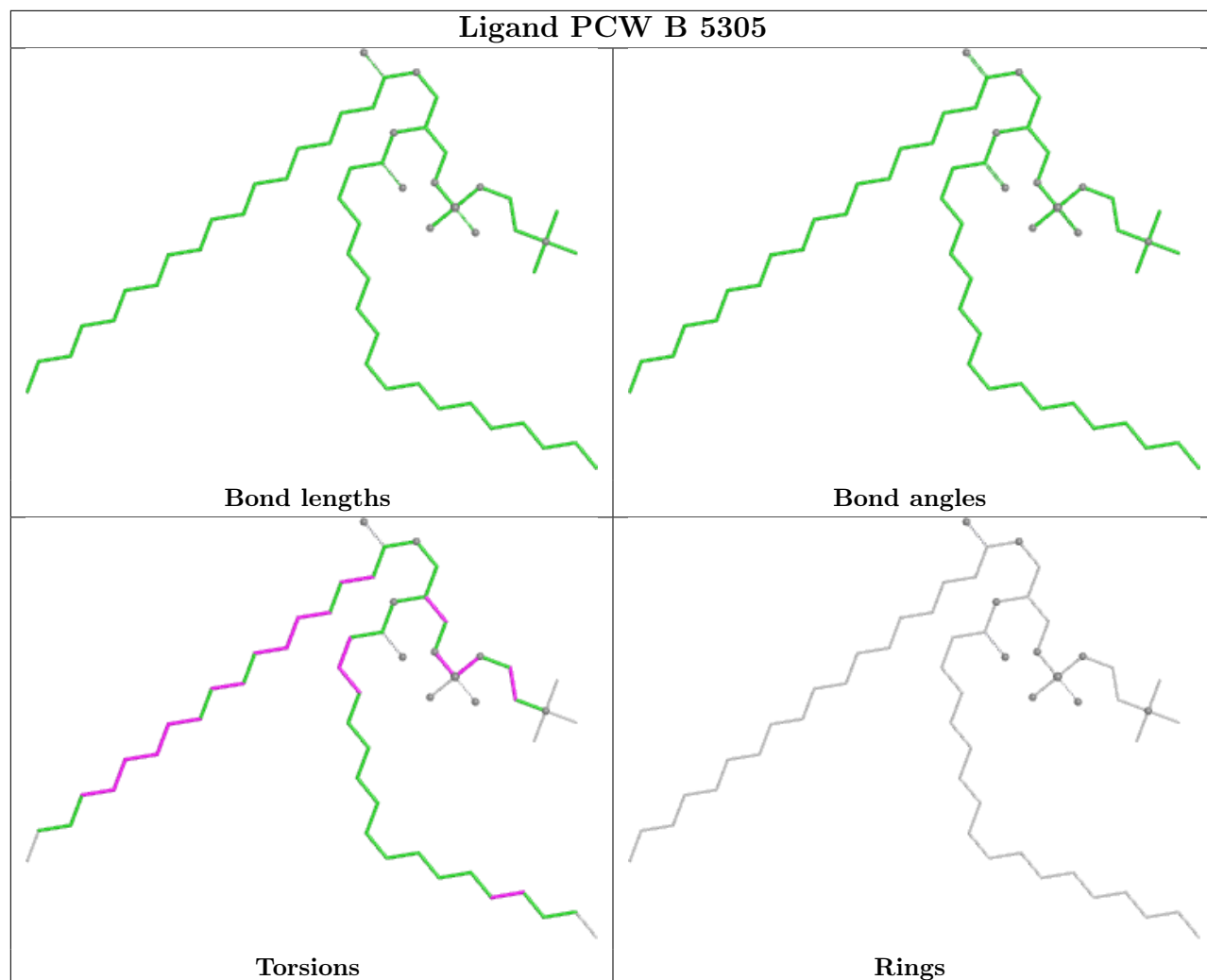
There are no ring outliers.

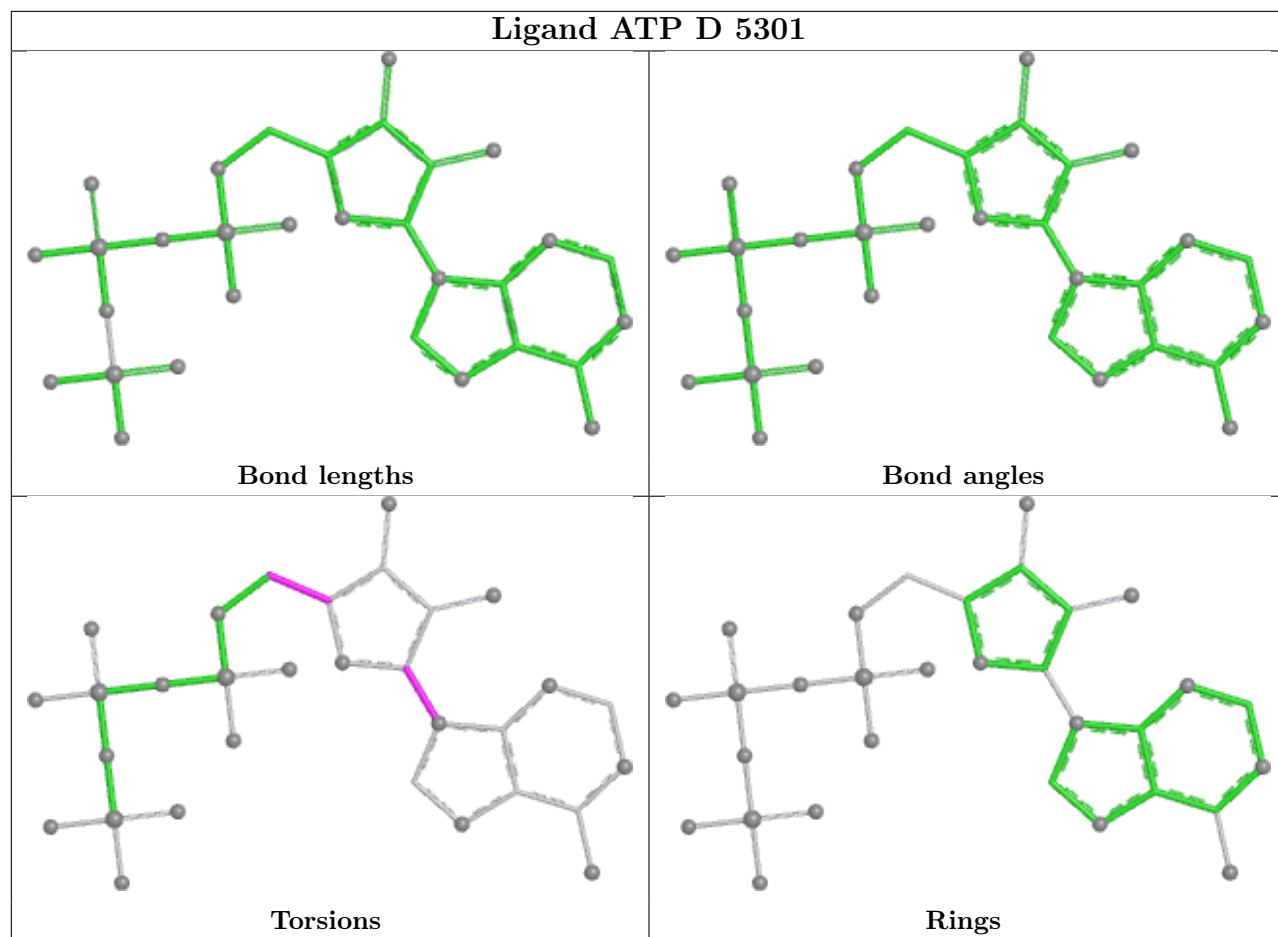
12 monomers are involved in 43 short contacts:

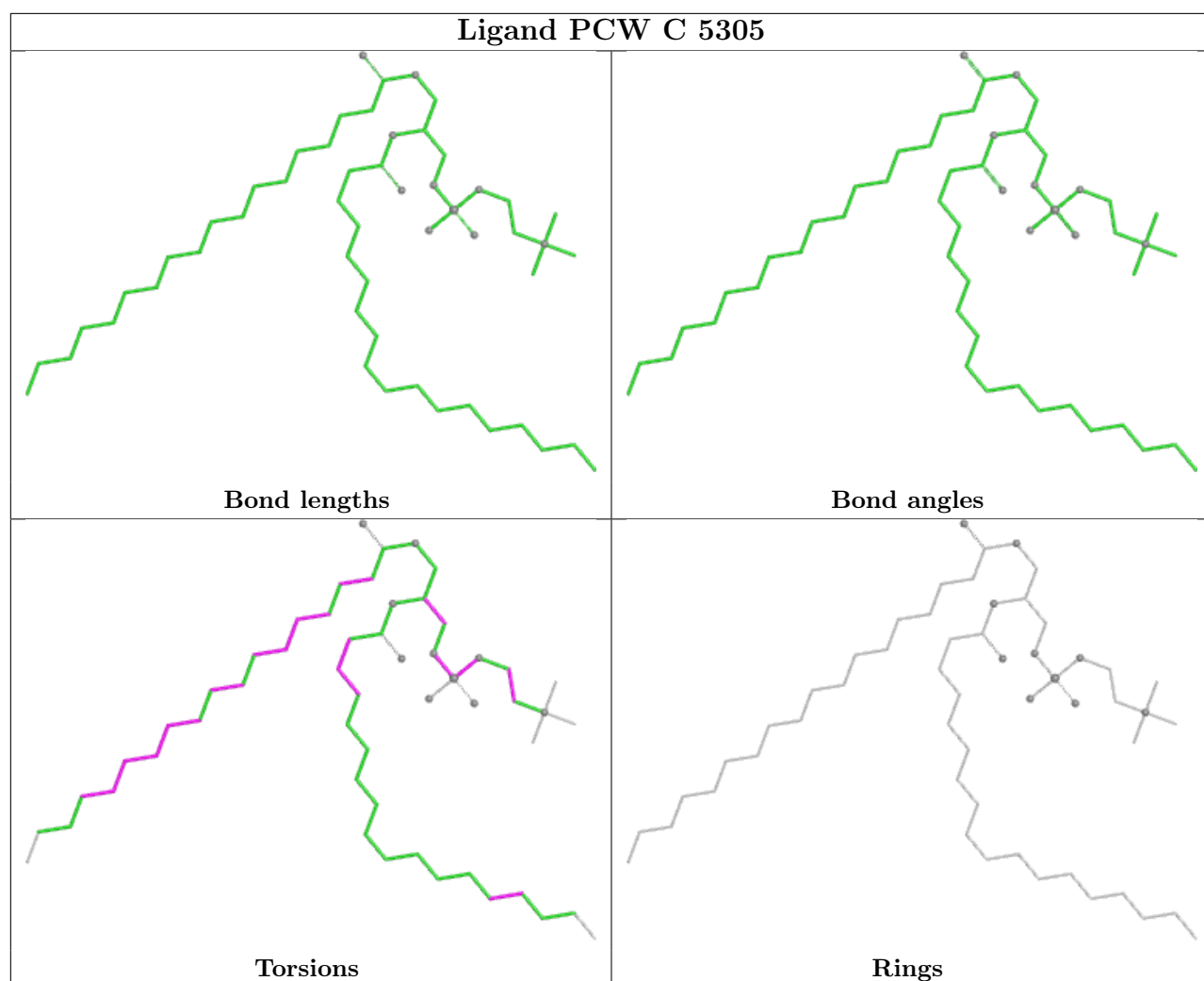
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	5306	PCW	4	0
7	B	5305	PCW	6	0
7	C	5305	PCW	6	0
7	A	5305	PCW	6	0
8	B	5307	A1C3Z	5	0
7	D	5306	PCW	4	0
8	A	5307	A1C3Z	5	0
8	C	5307	A1C3Z	5	0
7	D	5305	PCW	6	0
7	C	5306	PCW	4	0
8	D	5307	A1C3Z	5	0
7	B	5306	PCW	3	0

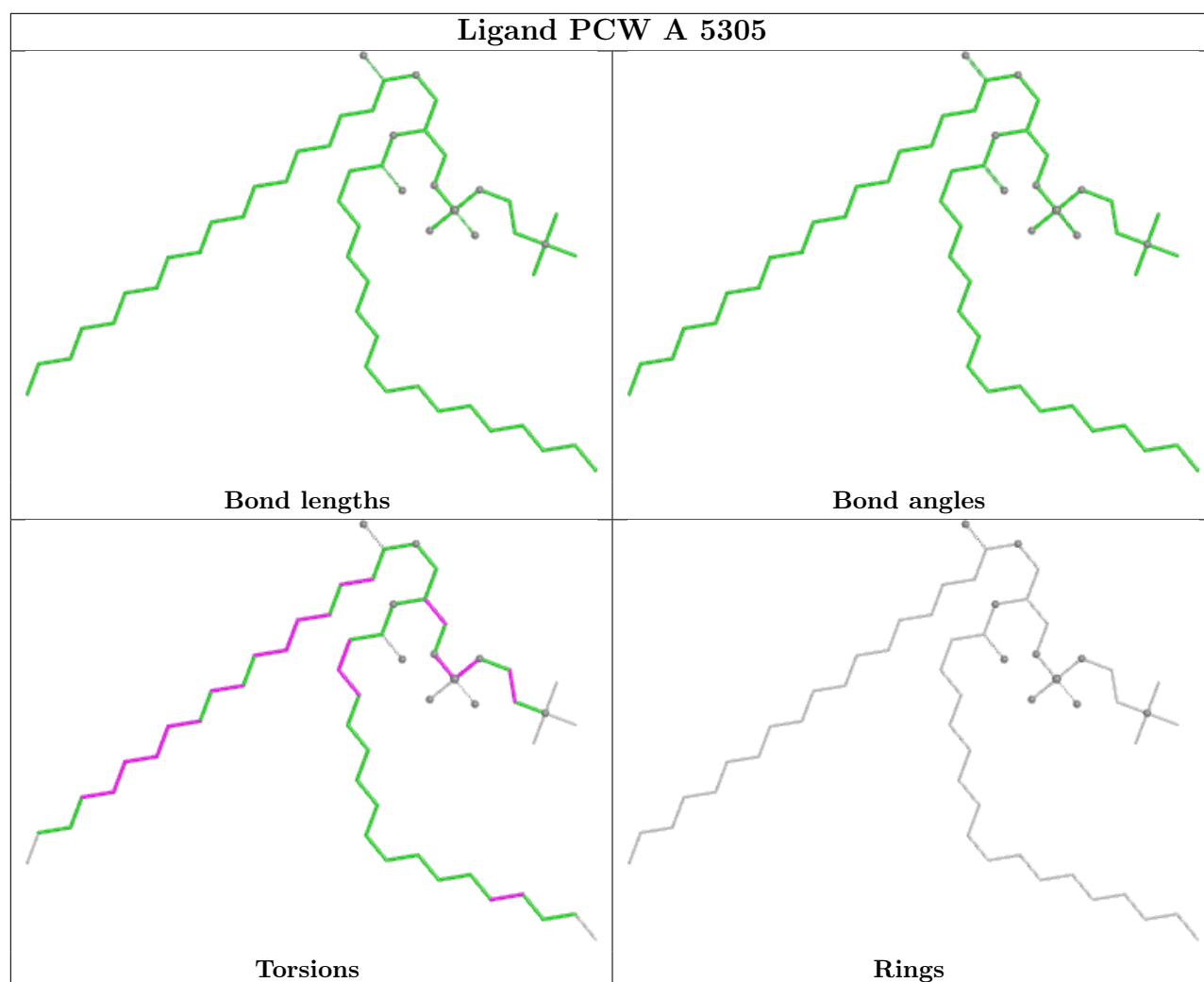
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

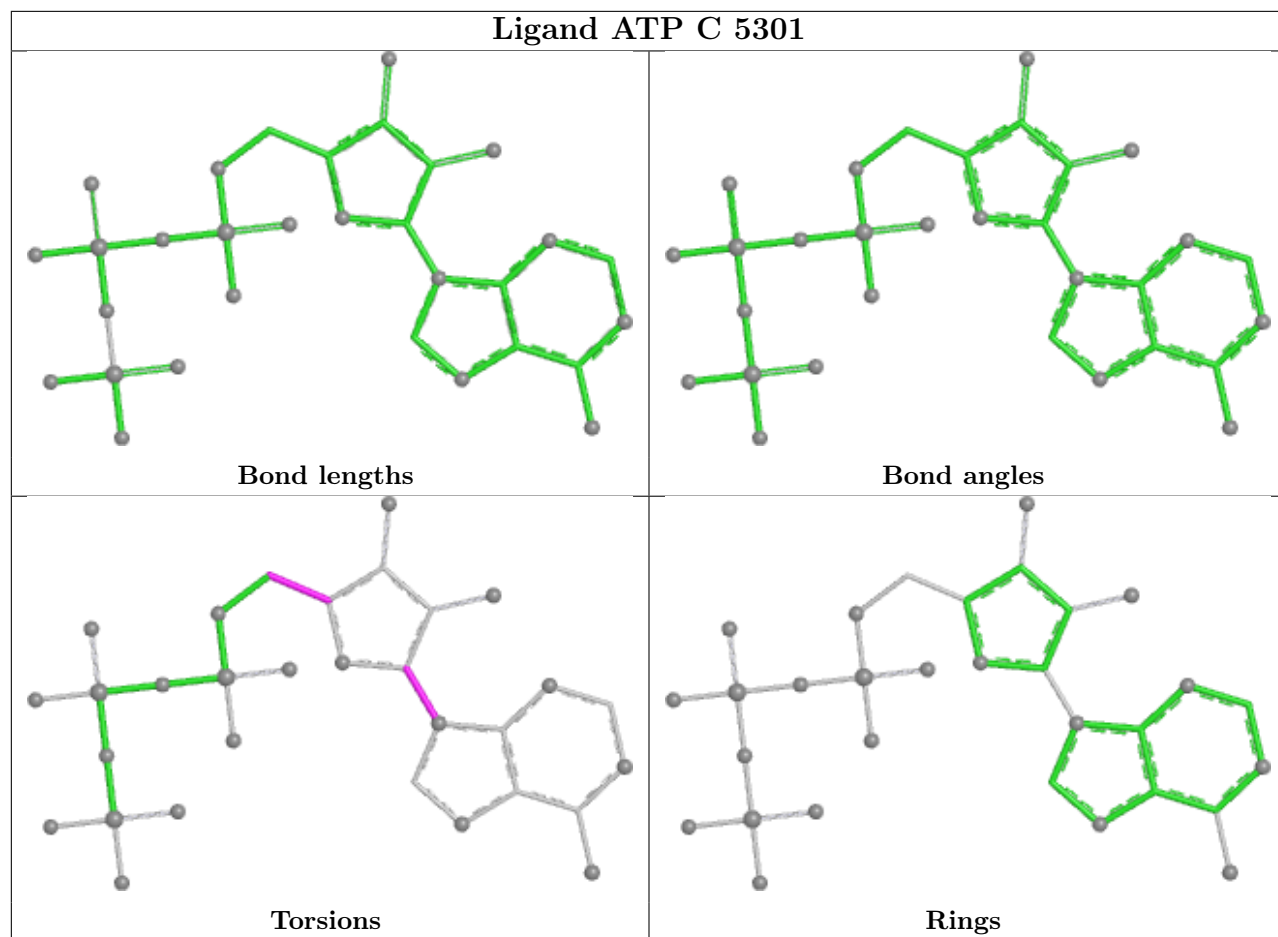




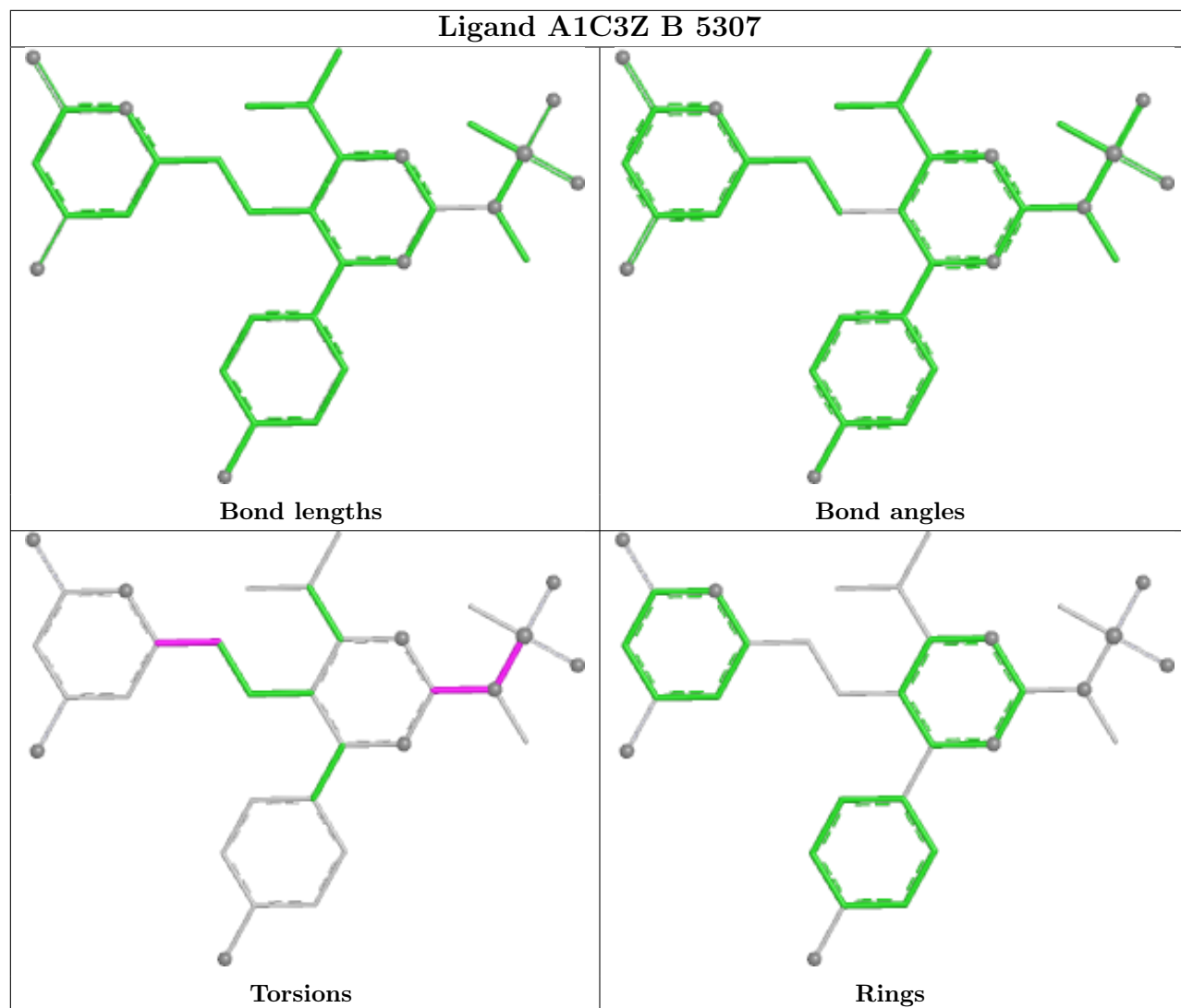


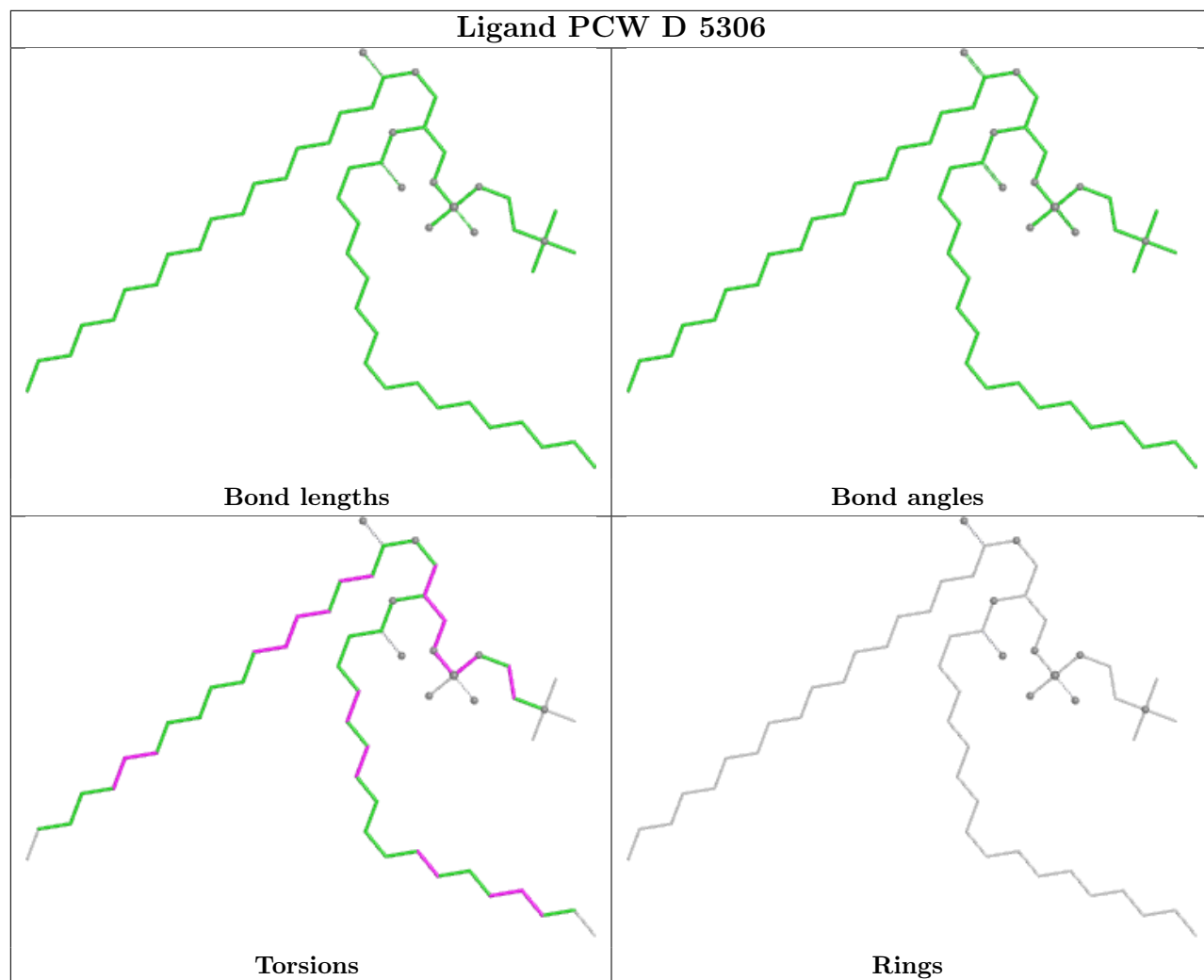




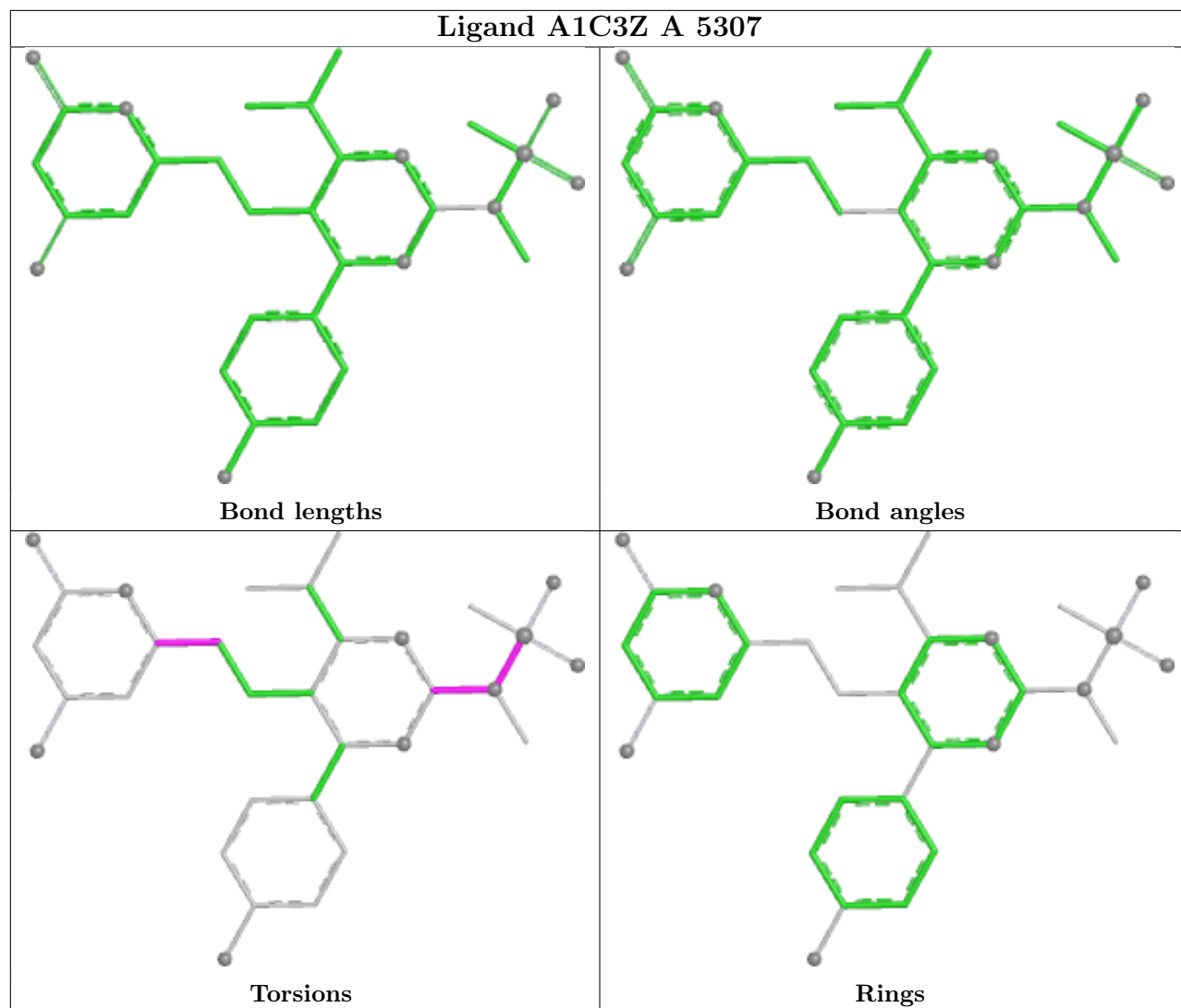


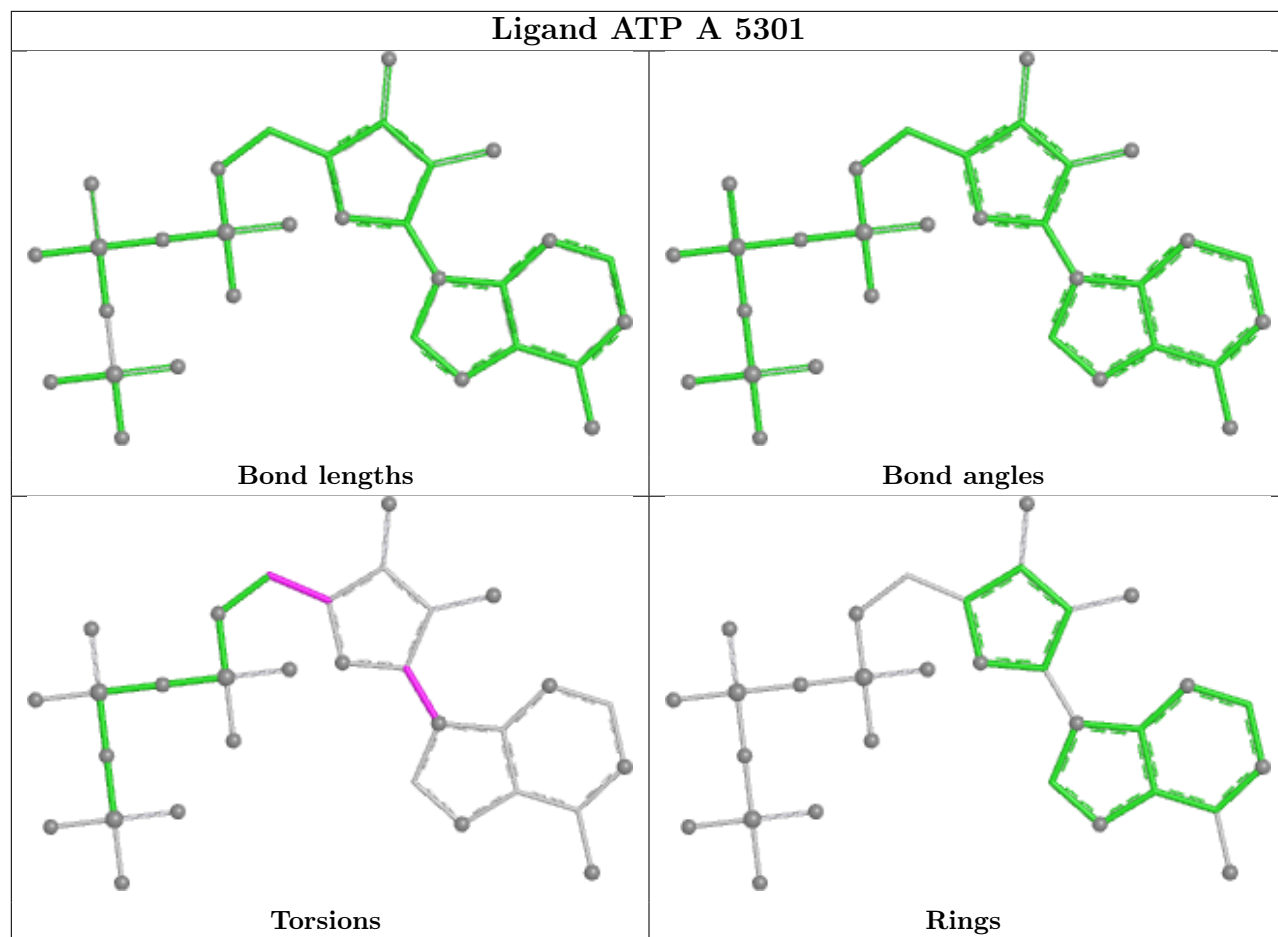
Ligand A1C3Z B 5307

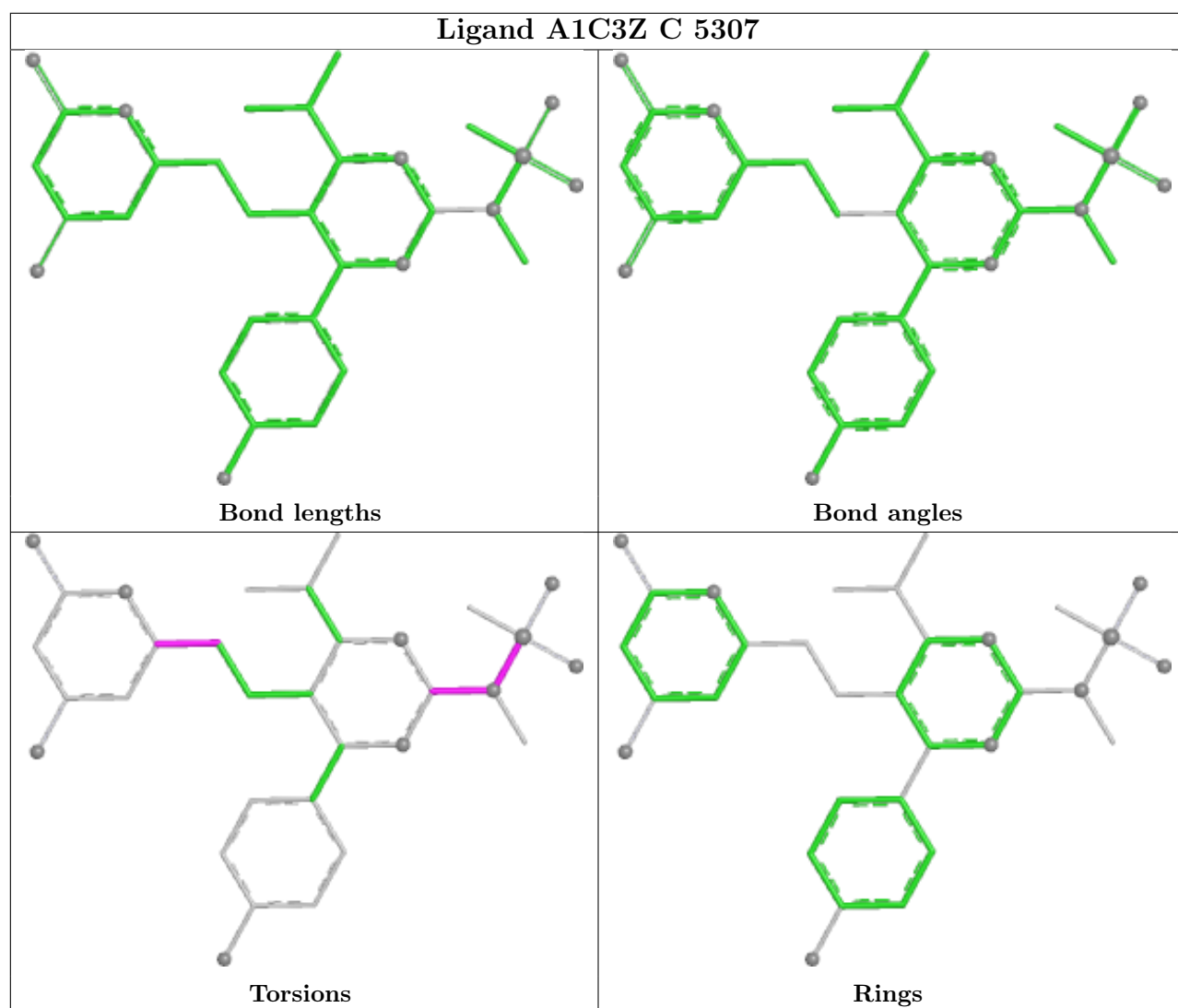


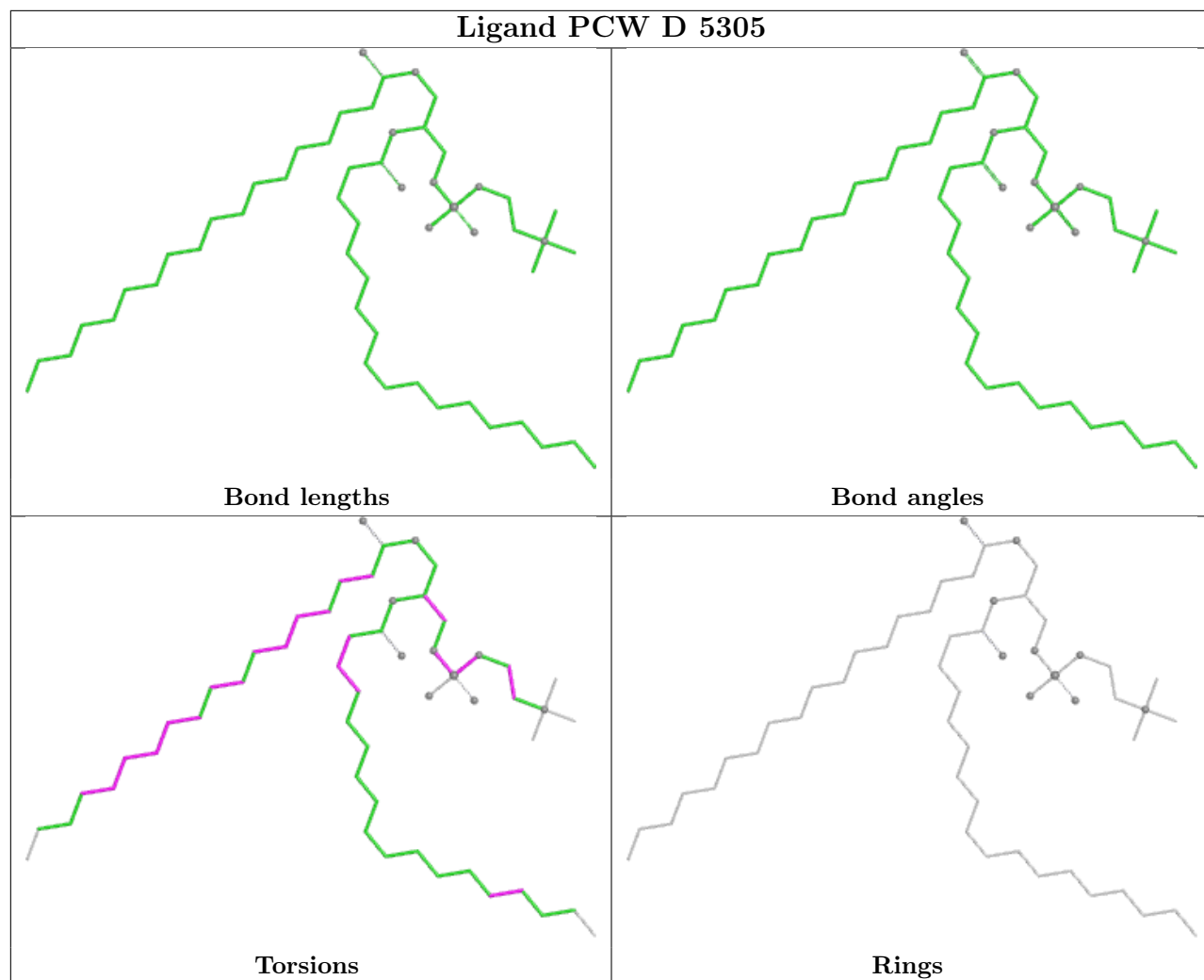


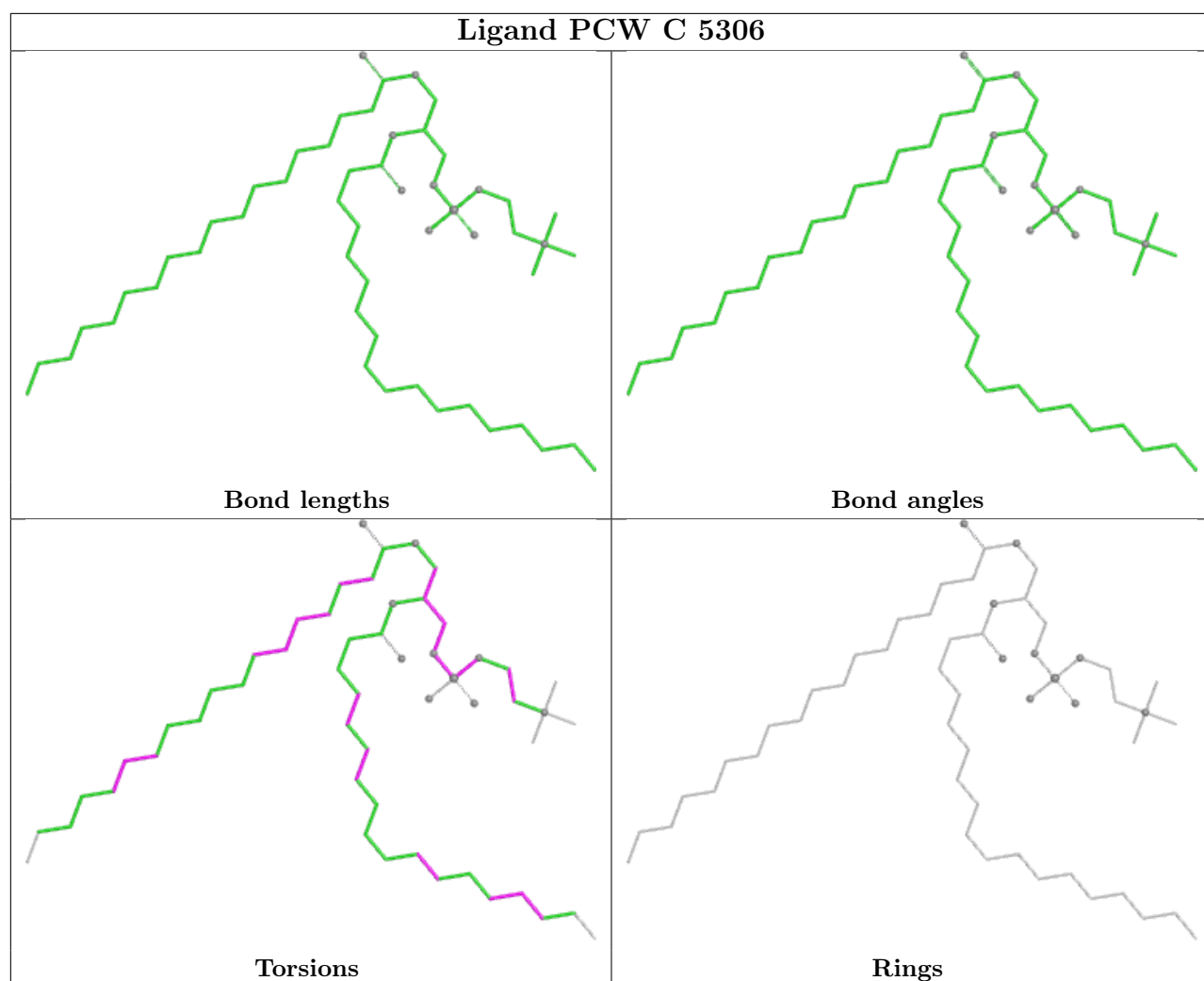
Ligand A1C3Z A 5307



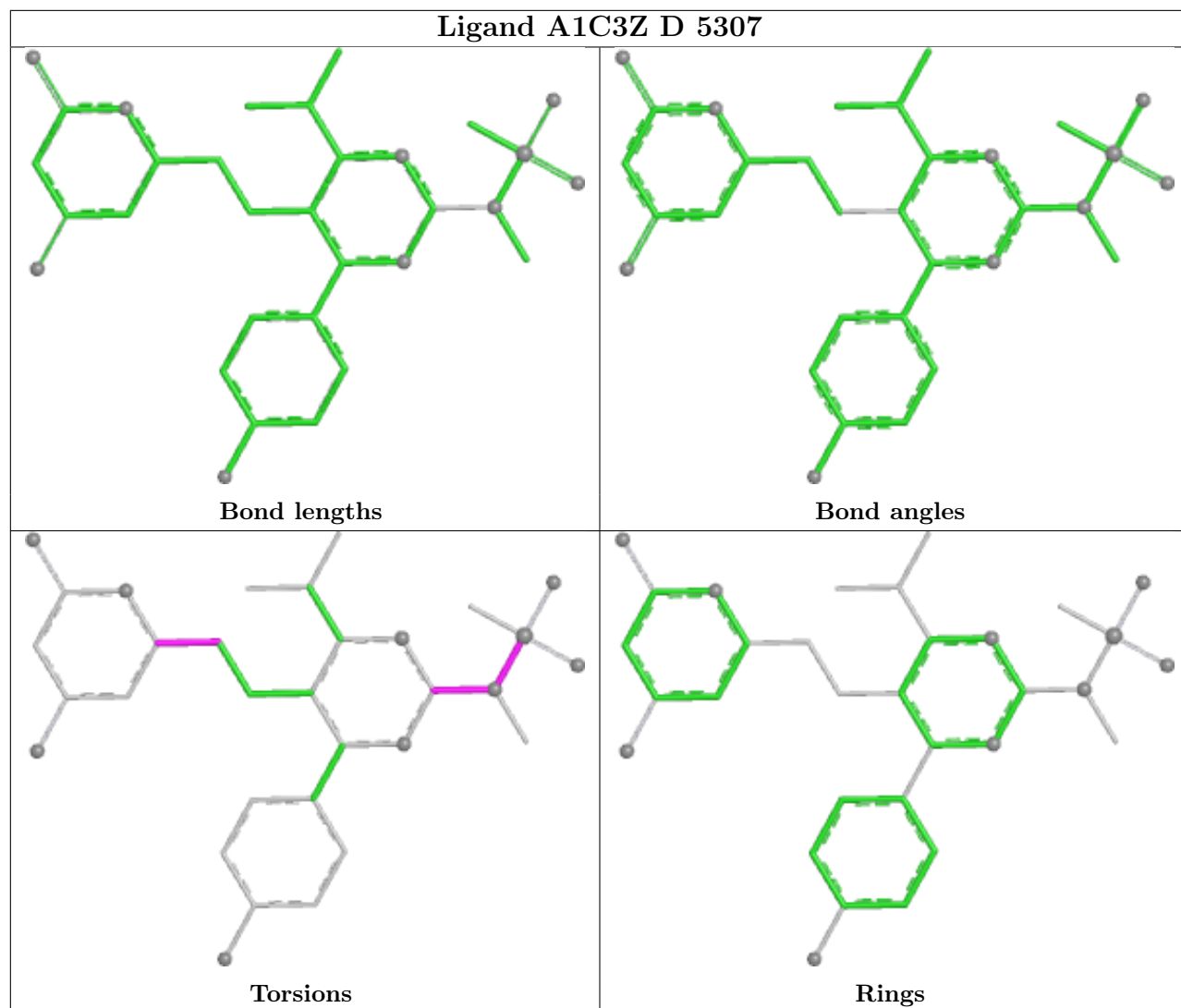


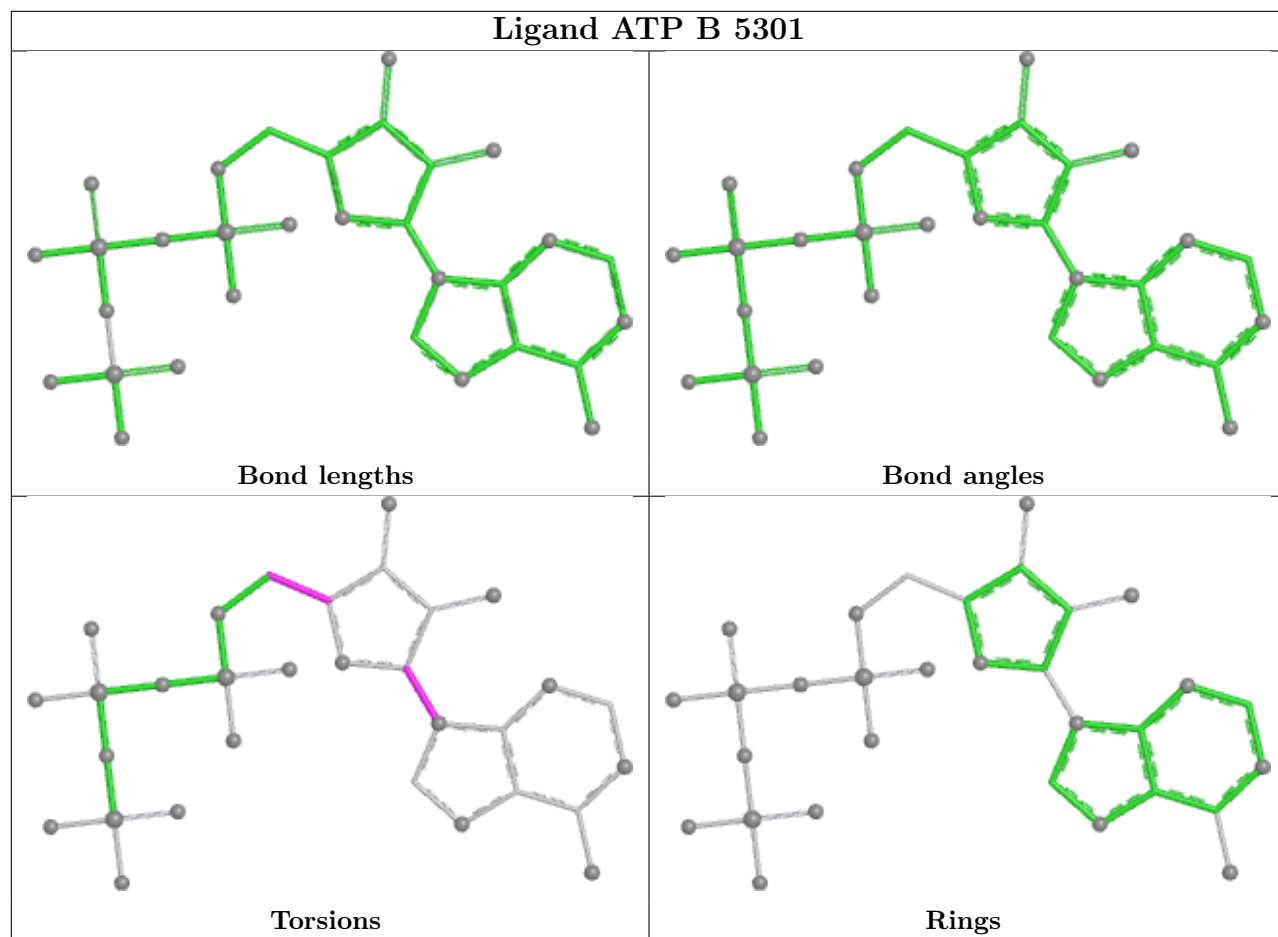


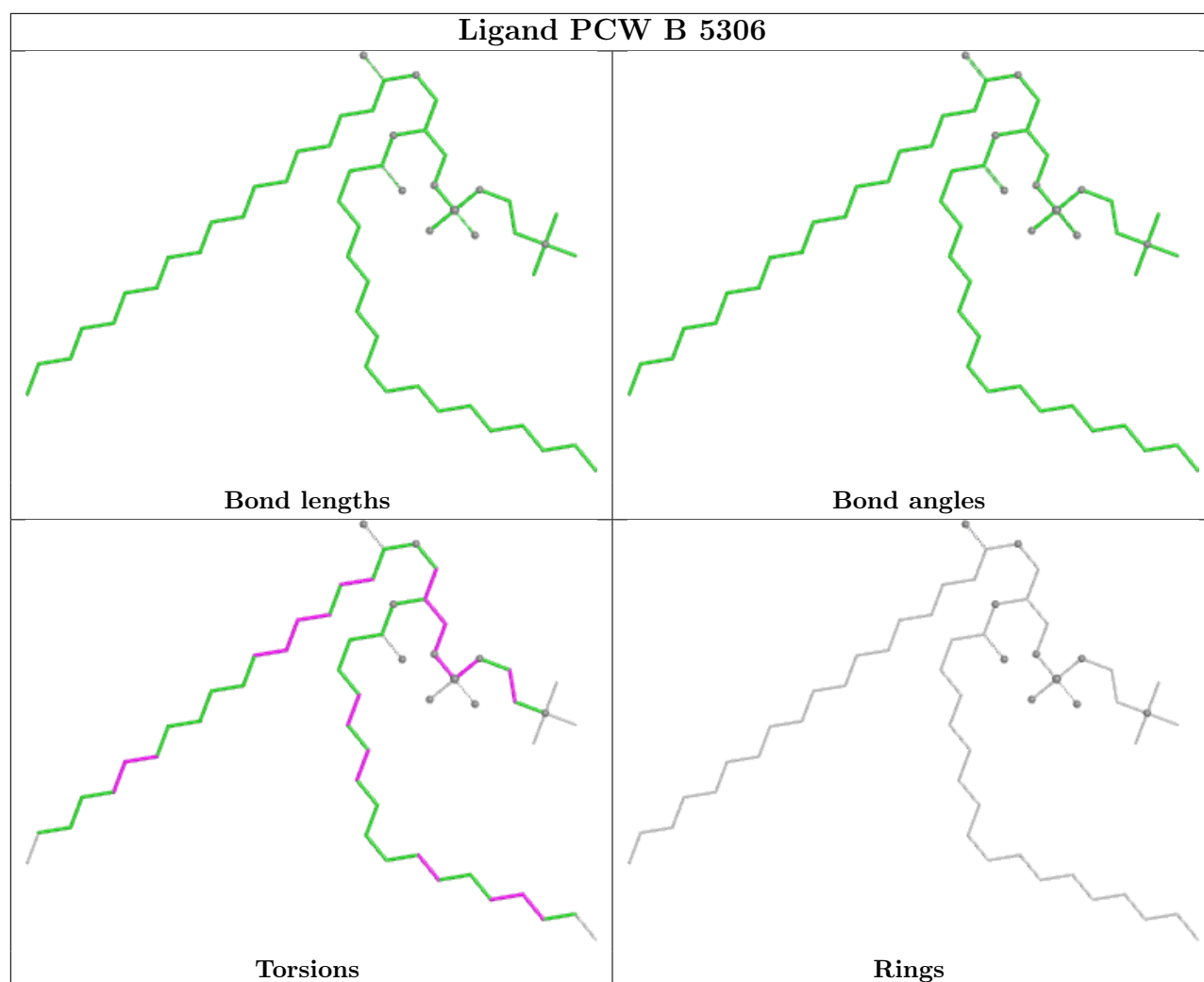




Ligand A1C3Z D 5307







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.

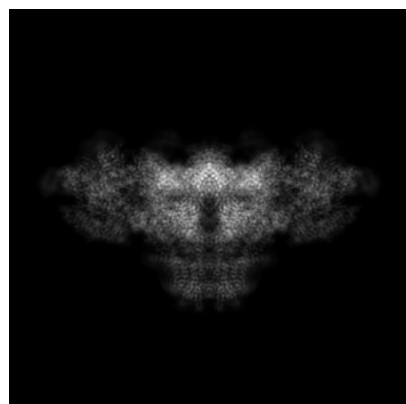
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74486. These allow visual inspection of the internal detail of the map and identification of artifacts.

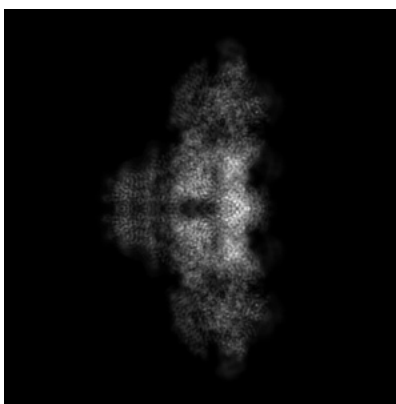
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

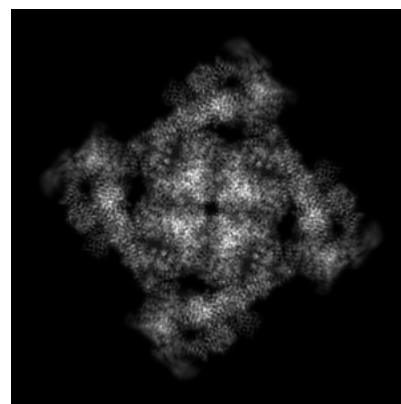
6.1.1 Primary map



X

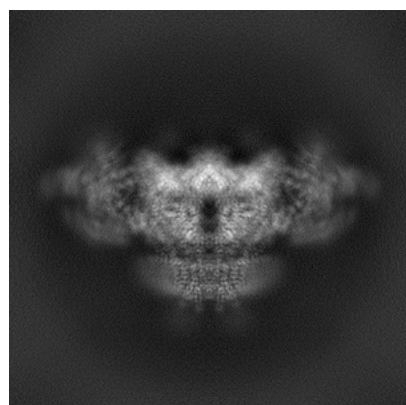


Y

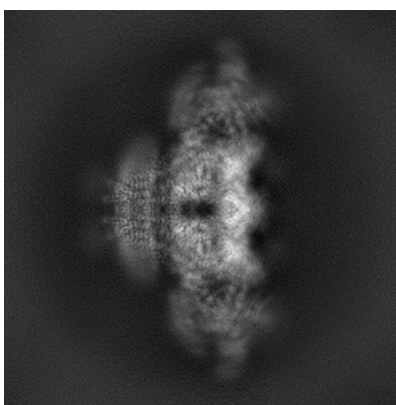


Z

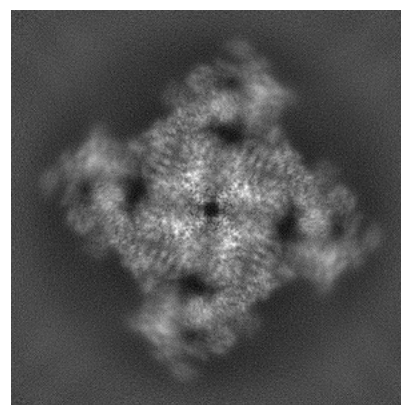
6.1.2 Raw map



X



Y

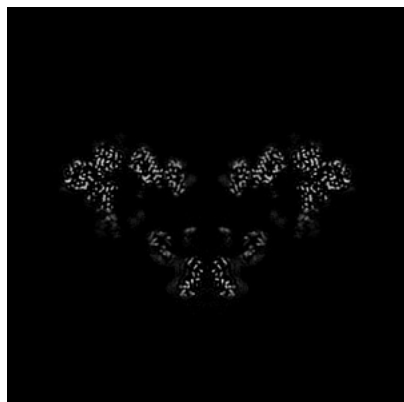


Z

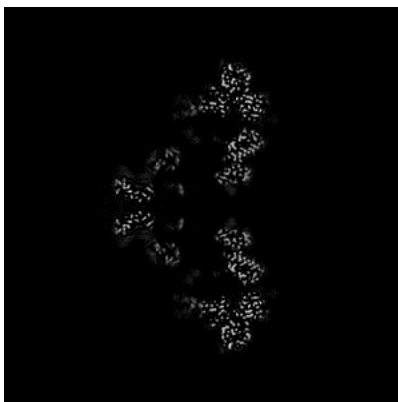
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

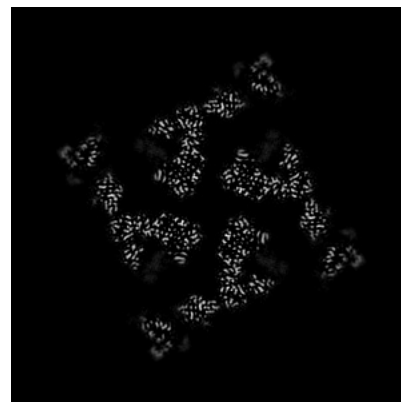
6.2.1 Primary map



X Index: 256

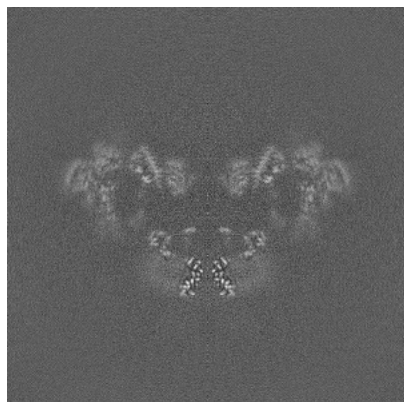


Y Index: 256

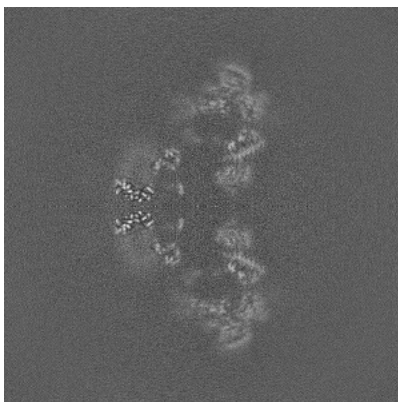


Z Index: 256

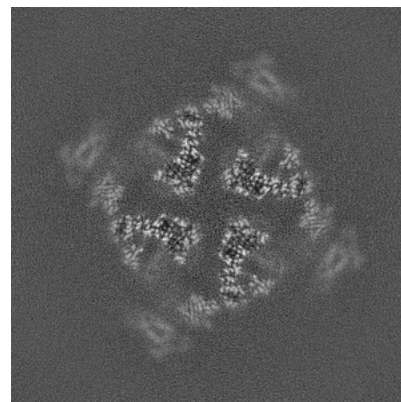
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

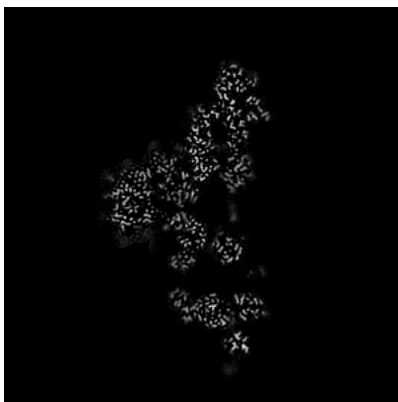
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

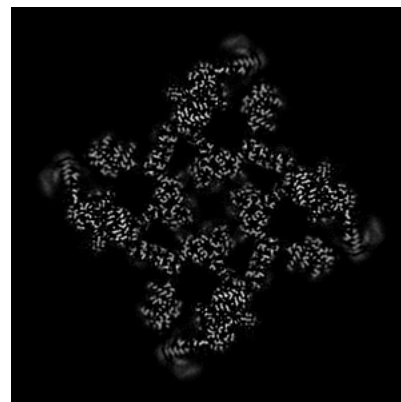
6.3.1 Primary map



X Index: 238

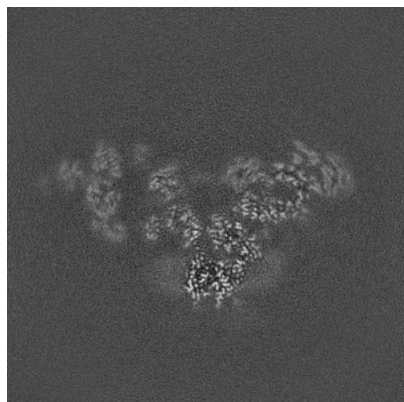


Y Index: 274

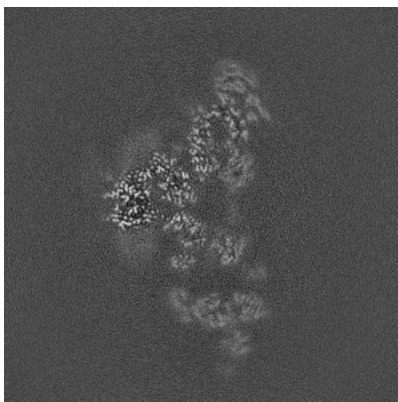


Z Index: 287

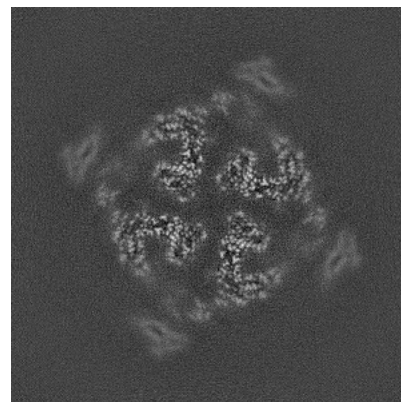
6.3.2 Raw map



X Index: 239



Y Index: 273

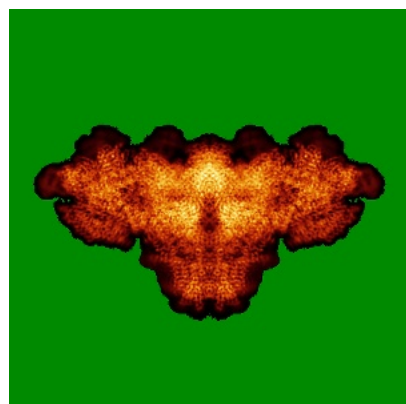


Z Index: 249

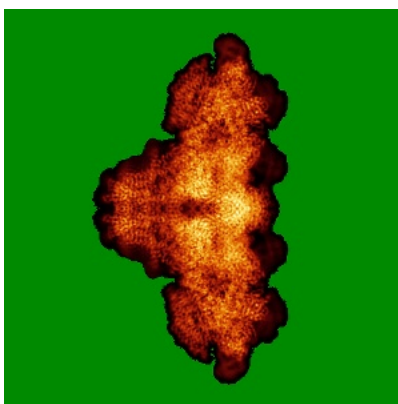
The images above show the largest variance slices of the map in three orthogonal directions.

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

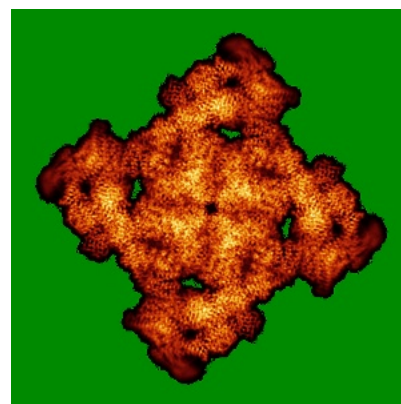
6.4.1 Primary map



X

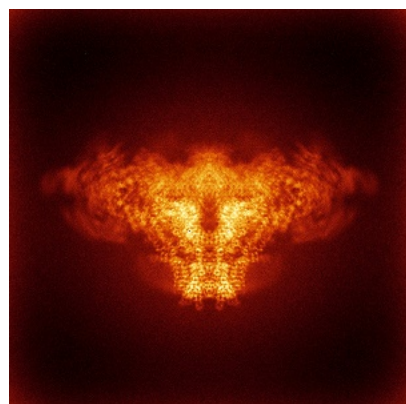


Y

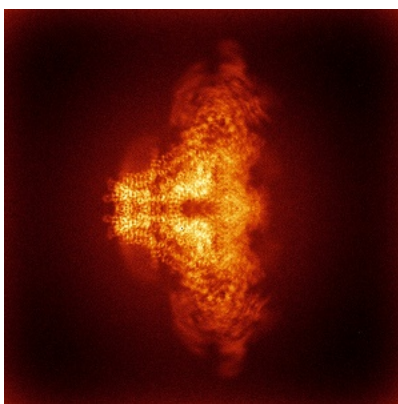


Z

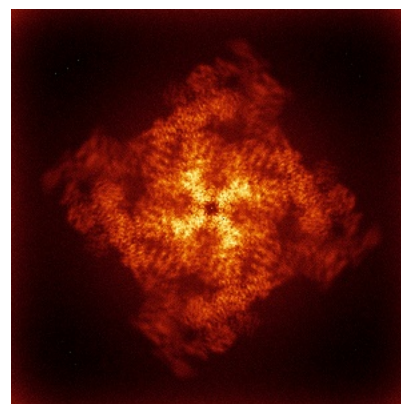
6.4.2 Raw map



X



Y

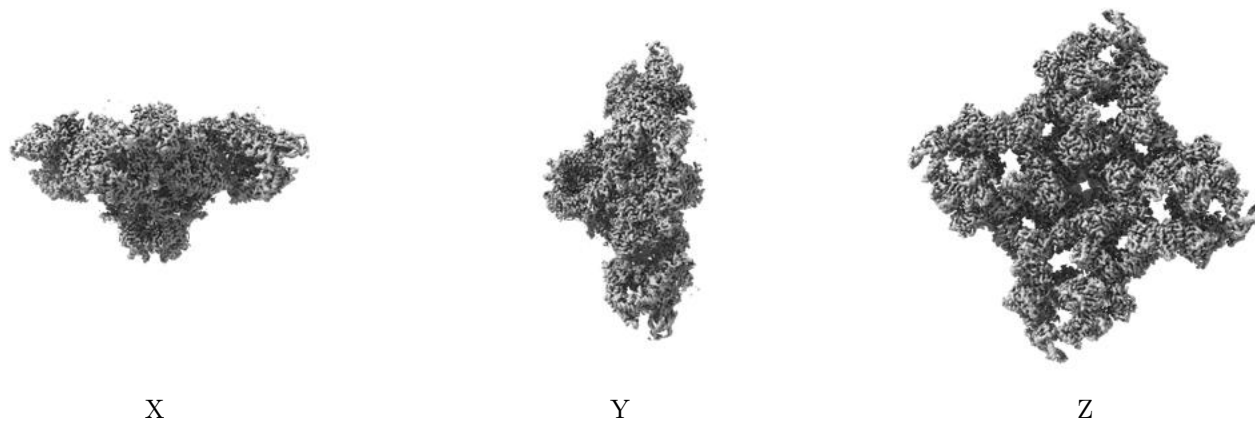


Z

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.

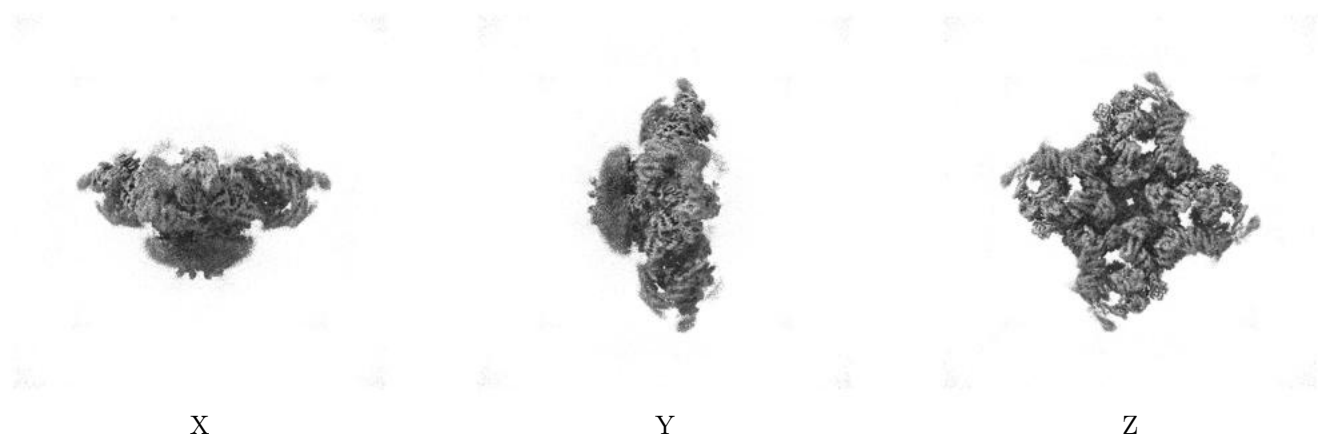
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

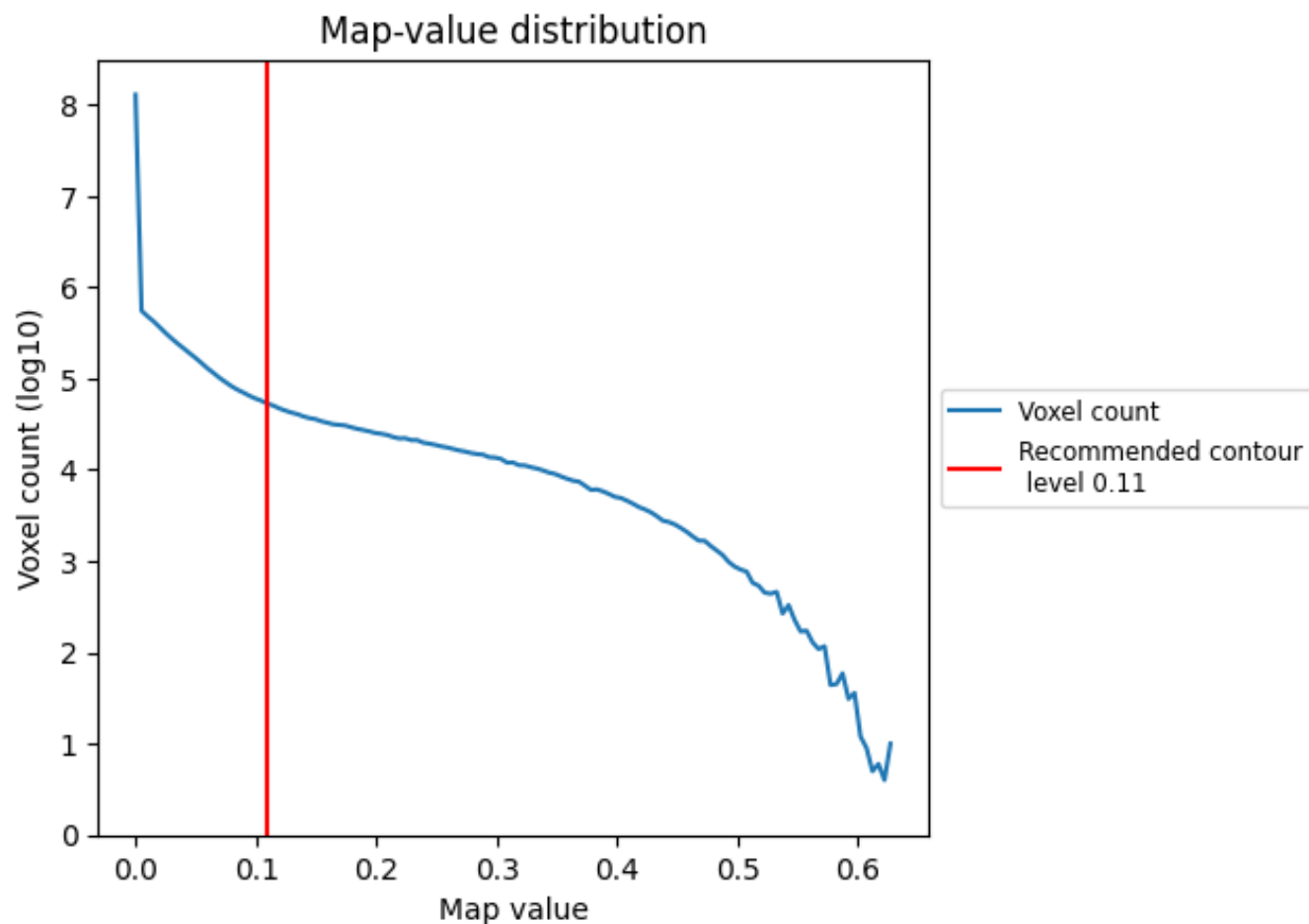
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

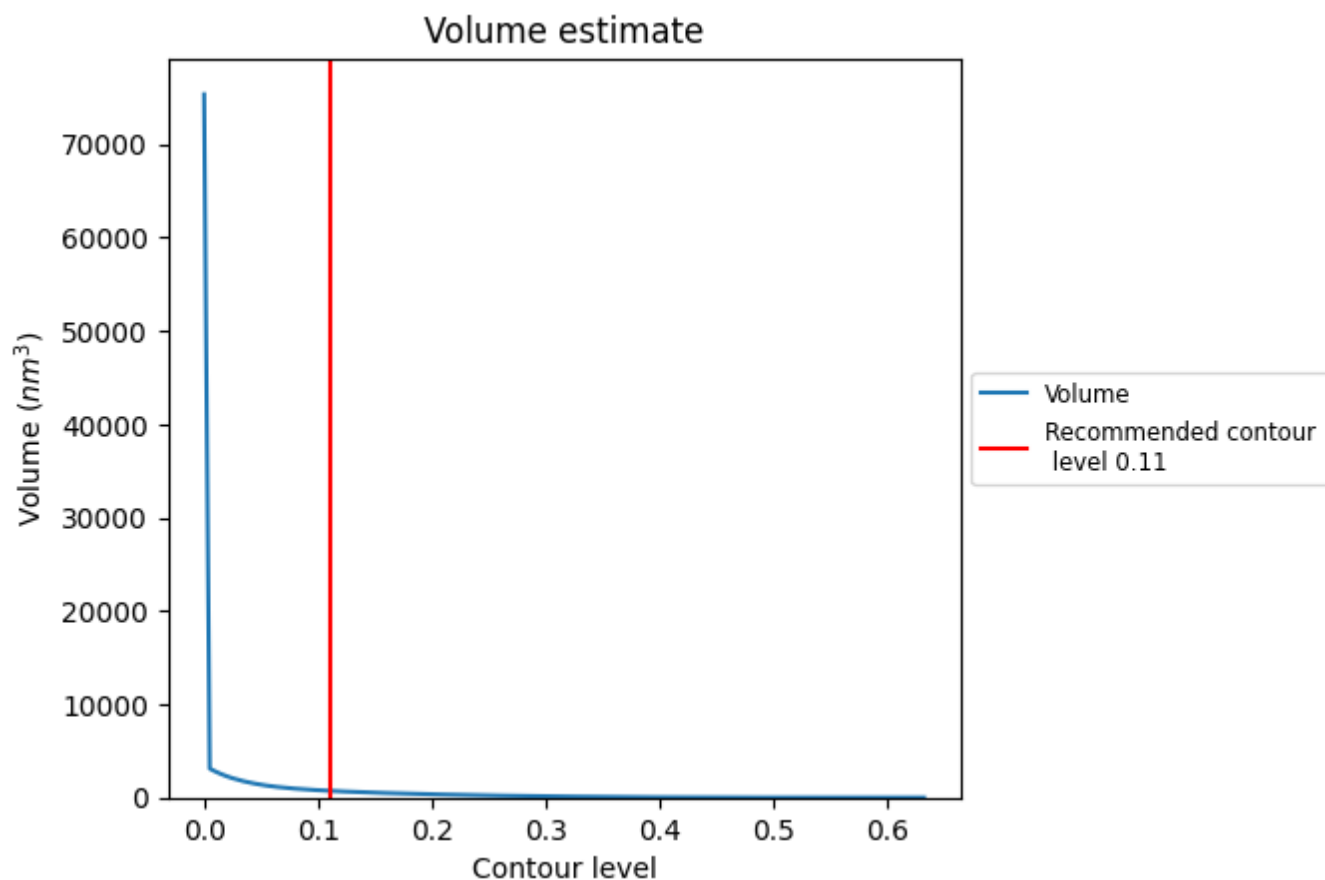
This section contains the results of statistical analysis of the map.

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.

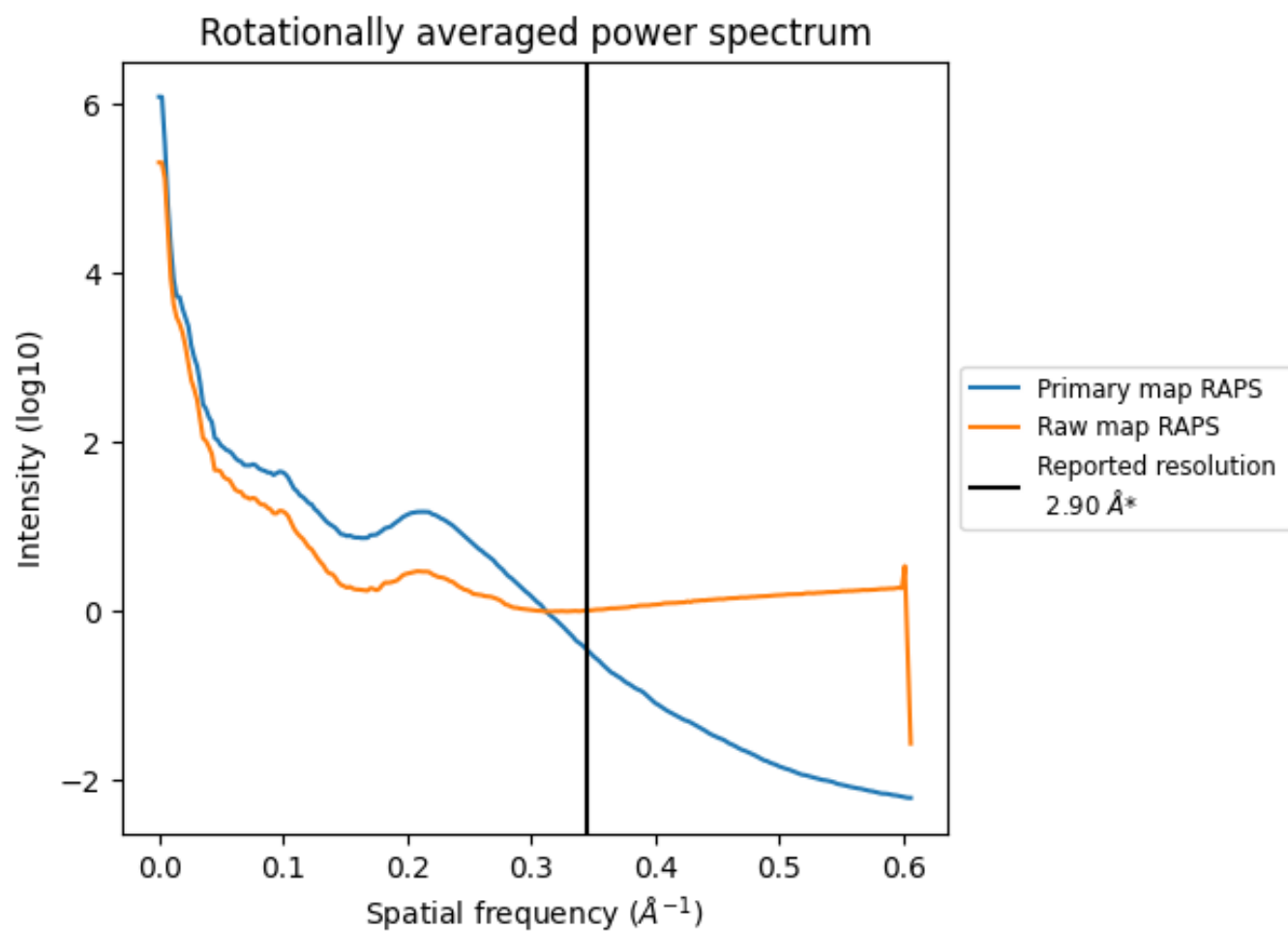
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm³; this corresponds to an approximate mass of 654 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 ⓘ

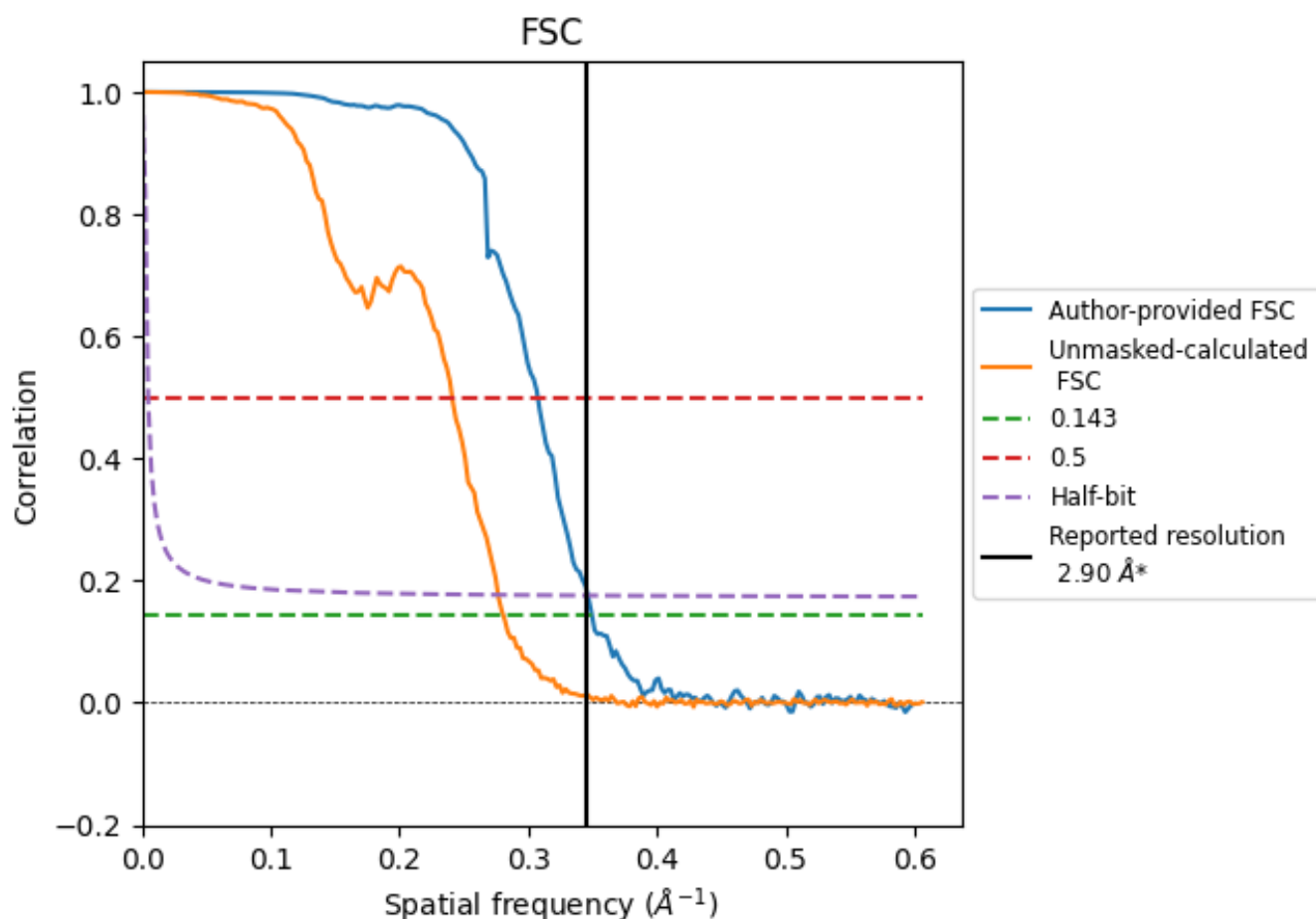


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

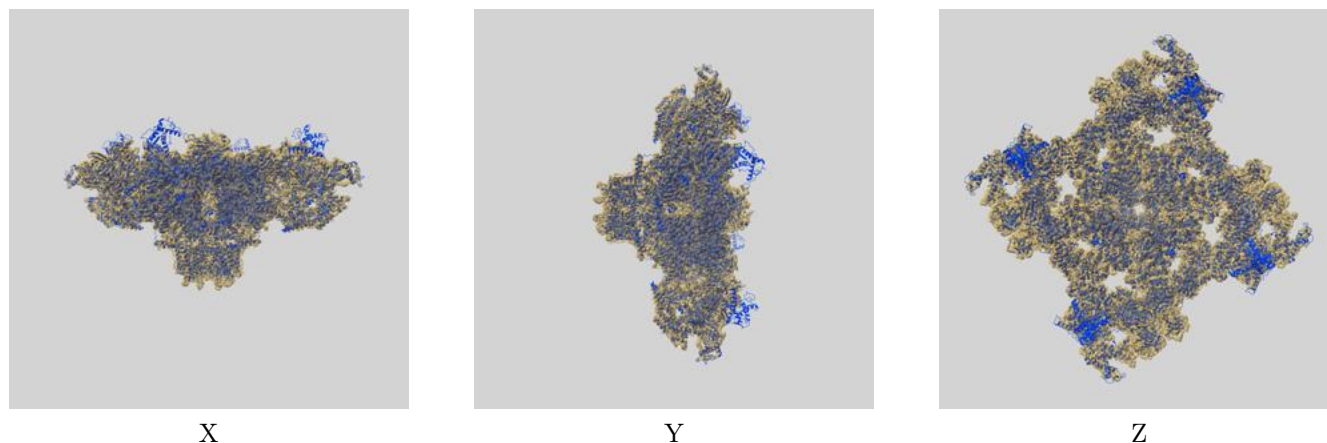
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.25	2.89
Unmasked-calculated*	3.56	4.15	3.62

*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 3.56 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

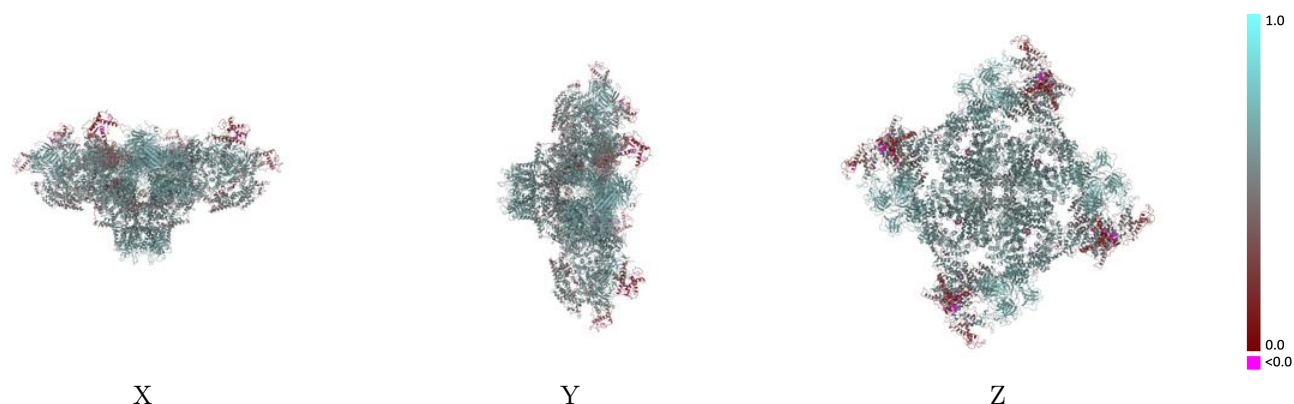
This section contains information regarding the fit between EMDB map EMD-74486 and PDB model 9ZOE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



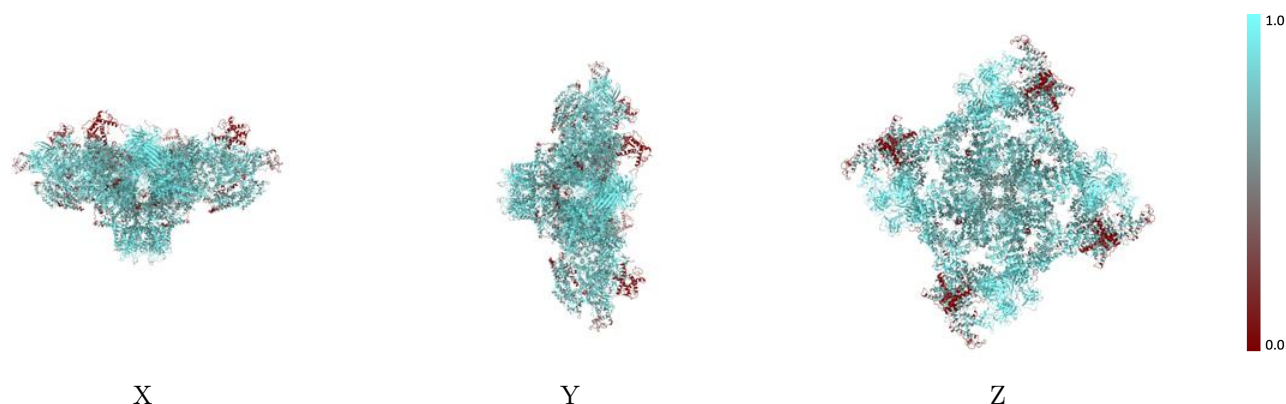
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



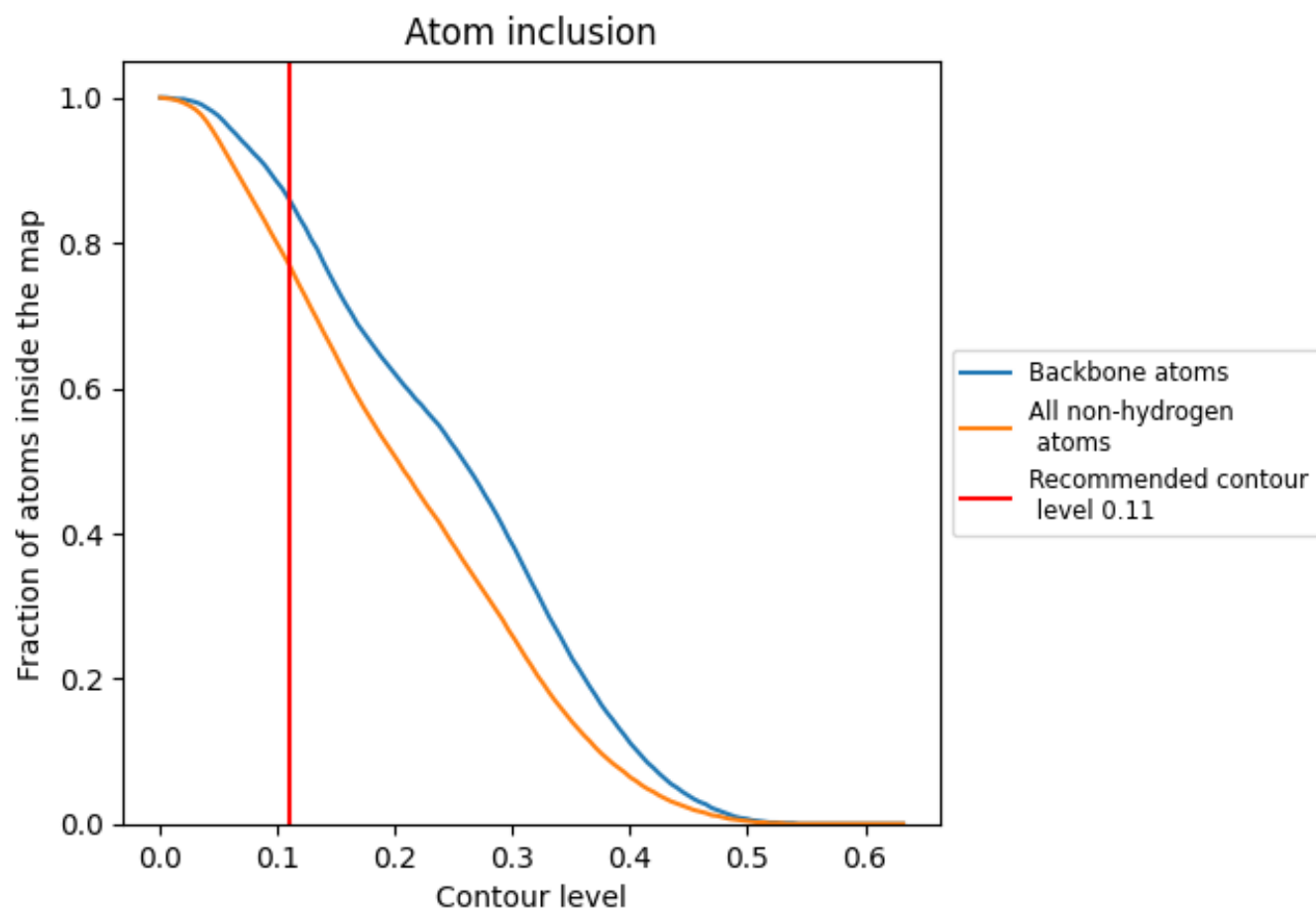
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.5450
A	0.7670	0.5430
B	0.7670	0.5430
C	0.7670	0.5430
D	0.7670	0.5430
E	0.8480	0.6220
F	0.8500	0.6210
G	0.8480	0.6210
H	0.8500	0.6240

1.0

0.0

<0.0