



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 02:11 AM UTC

PDB ID : 8RRW / pdb_00008rrw
EMDB ID : EMD-19467
Title : Structure of RyR1 in detergent in open state in complex with FKBP and Nb9657.
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-01-23
Resolution : 4.20 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:

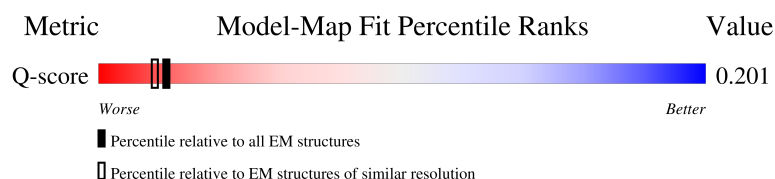
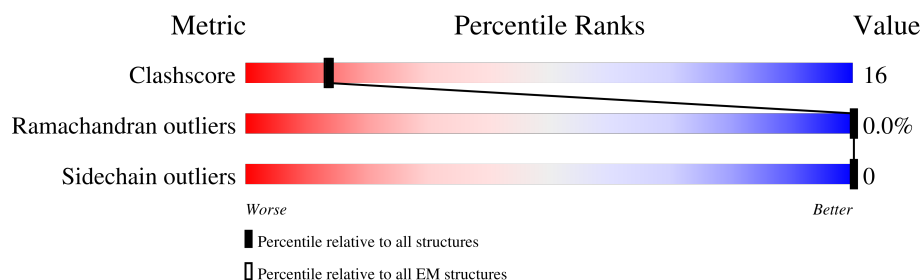
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	5027	
1	E	5027	
1	G	5027	
1	J	5027	

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Mol	Chain	Length	Quality of chain
2	A	107	
2	D	107	
2	H	107	
2	I	107	
3	C	137	
3	F	137	
3	K	137	
3	M	137	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143744 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	E	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	G	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		
1	J	4319	Total	C	N	O	S	1	0
			34104	21737	5881	6261	225		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	I	107	Total	C	N	O	S	0	0
			818	516	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

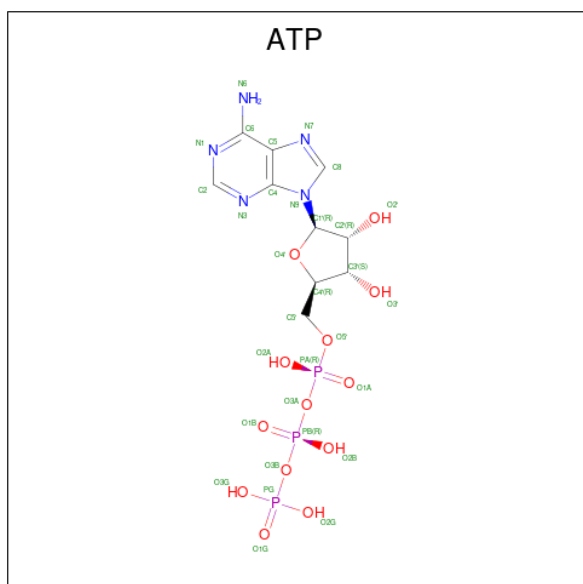
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	F	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	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).



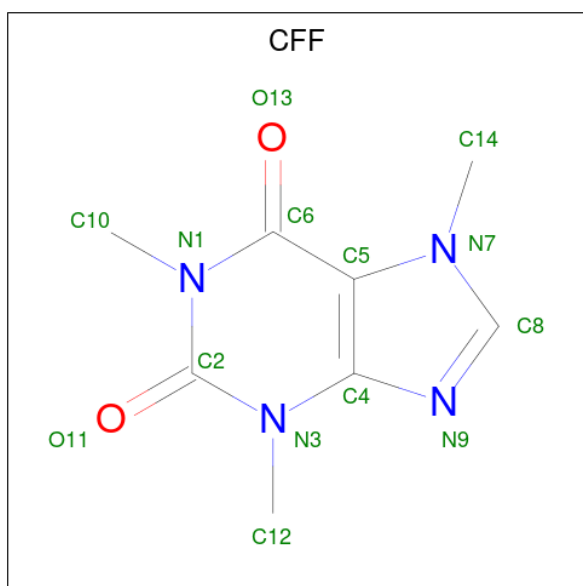
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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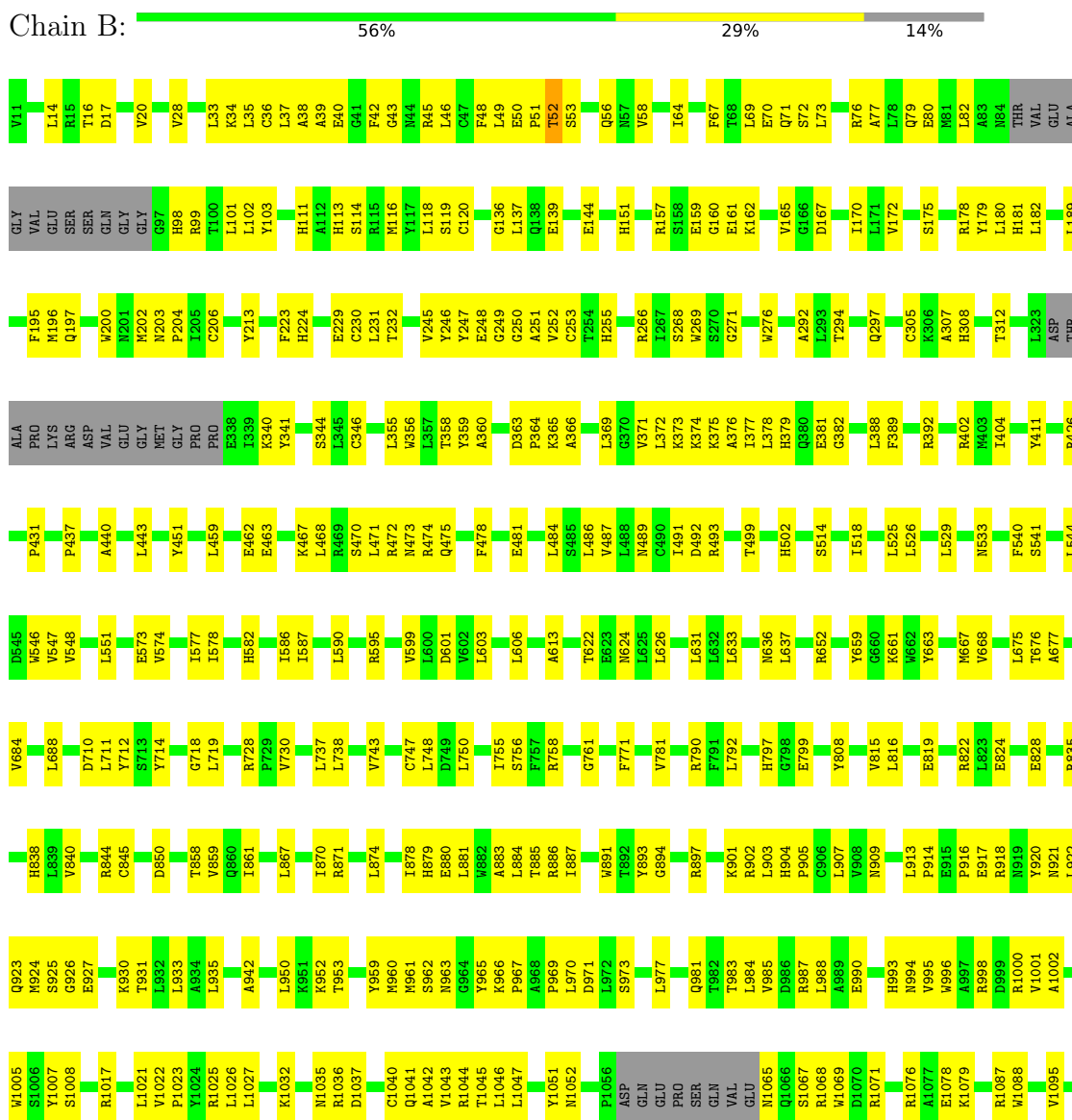
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Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

3 Residue-property plots

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: Ryanodine receptor 1







- Molecule 1: Ryanodine receptor 1

Response	Percentage
Current government is the best	57%
Opposition is the best	29%
Neither is the best	14%









GLU	L4544	A4738	L4843	K4984	L4885	L4843	GLU	L4626	GLU	GLU
GLU	E4545	E4739	F4859	L4985	F4859	F4859	GLU	M4627	GLU	GLU
GLU	V4546	L4745	N4864	M4989	R15	R15	GLU	V4628	GLU	GLU
LEU	V4549	L4748	K4865	L4992	T16	T16	VAL	L4632	LEU	VAL
PRO	K4550	E4749	M4871	M4993	D17	D17	PRO	A4642	PRO	PRO
GLU	M4558	H4753	F4872	L4996	V20	V20	GLU	L4646	GLU	GLU
PRO	L4562	P4761	D4873	K4997	V28	V28	PRO	L4650	PRO	PRO
GLU	L4567	T4766	C4876	K4998	L33	L33	GLU	T4651	GLU	GLU
GLU	F4568	W4767	M4879	D4999	L35	L35	GLU	L4652	GLU	GLU
PRO	L4569	I4771	C4882	E5002	C36	C36	PRO	A4653	PRO	PRO
PRO	L4580	D4772	R4892	H5003	A38	A38	PRO	F4654	PRO	PRO
GLU	K4581	V4773	B4892	E5007	A39	A39	GLU	L4656	GLU	GLU
LYS	D4584	K4774	Q4896	Y5009	E40	E40	LYS	C4657	LYS	LYS
ALA	S4585	K4779	E4900	K5012	G41	G41	ALA	I4658	ALA	ALA
ASP	P4586	F4780	M5013	Y5014	F42	F42	ASP	G4660	ASP	ASP
GLU	P4587	G4781	Y5015	Q5016	G43	G43	GLU	Y4661	GLU	GLU
ASN	GLY	V4782	D4902	E5017	N44	N44	ASN	L4664	ASN	ASN
GLY	GLU	I4783	E4903	R5017	R45	R45	GLY	K4665	GLY	GLY
GLU	ASP	D4786	P4904	C5018	L46	L46	GLU	V4666	GLU	GLU
LYS	ASP	N4787	Y4909	W5019	F48	F48	LYS	P4667	LYS	LYS
GLU	GLY	S4788	R4913	S5037	E50	E50	GLU	L4668	GLU	GLU
VAL	SER	L4792	T4918		P51	P51	VAL	R4673	VAL	VAL
PRO	ALA	M4796	F4922		T52	T52	PRO	E4674	PRO	PRO
ALA	GLY	L4800	L4927		S53	S53	ALA	K4675	ALA	ALA
PRO	ASP	L4801	A4930		Q56	Q56	PRO	E4676	PRO	PRO
GLU	ALA	G4802	A4936		N57	N57	GLU	R4679	GLU	GLU
PRO	GLY	H4803	T4937		V58	V58	PRO	K4680	PRO	PRO
LYS	SER	F4808	L4937		I64	I64	LYS	Q4691	LYS	LYS
ALA	GLY	L4813	G4941		F67	F67	ALA	K4698	ALA	ALA
PRO	GLY	L4815	E4942		T68	T68	PRO	Q4699	PRO	PRO
SER	GLY	I4816	L4943		L69	L69	SER	G4700	SER	SER
PRO	SER	A4817	R4944		G71	G71	PRO	N4701	PRO	PRO
ALA	TRP	L4704	D4945		S72	S72	ALA	D4702	ALA	ALA
LYS	SER	P4712	Q4947		L73	L73	LYS	L4704	LYS	LYS
GLU	GLY	L4823	V4950		R76	R76	GLU	K4718	GLU	GLU
GLU	ALA	T4825	K4951		A77	A77	GLU	GLY	GLU	GLU
ALA	GLY	L4826	E4952		L78	L78	ALA	ALA	ALA	ALA
GLU	GLY	L4827	T4956		Q79	Q79	GLU	GLY	GLY	GLY
GLY	GLY	V4830	T4960		E80	E80	GLY	L4725	GLY	GLY
ALA	GLY	K4835	C4961		L81	L81	ALA	D4726	ALA	ALA
GLY	ASP	M4839	H4983		L82	L82	GLY	H4728	GLY	GLY
GLU	ASP				A83	A83	GLU	E4735	GLU	GLU
ASP	ASP				THR	THR	ASP	R4736	ASP	ASP
					VAL	VAL		L4737		
					ALA	ALA				

• Molecule 1: Ryanodine receptor 1

Chain G:  57% 29% 14%

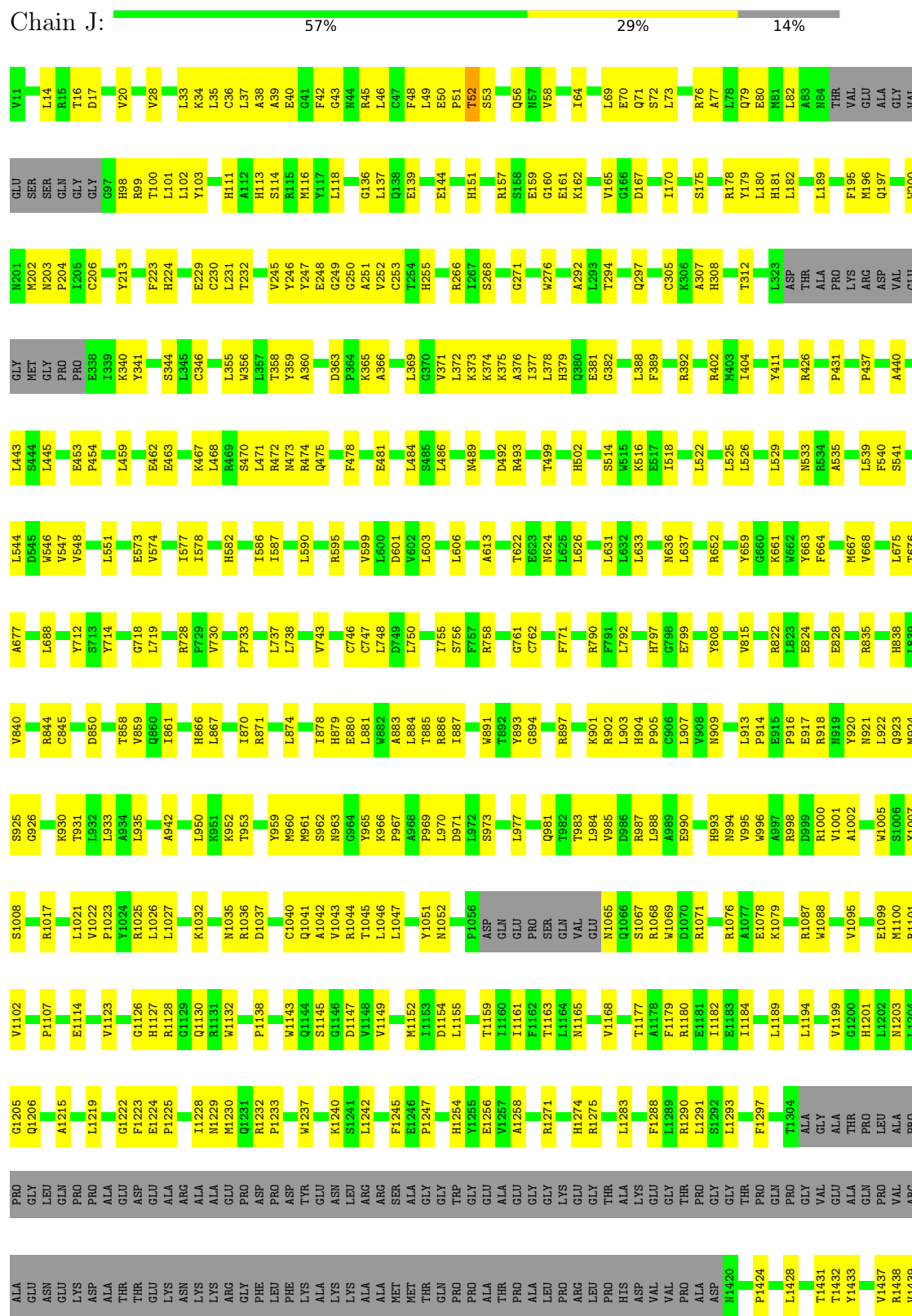
V11	W200	THR	P437	F540	M667	R835
L14	W201	ALA	T438	S541	V668	H838
R15	N202	PRO	E439	L544	L675	L839
T16	N203	LYS	A440	T676	L675	V940
D17	P204	ARG	A440	D545	A677	
V20	L205	ASP	L443	V547	L688	B844
V28	C206	VAL	S444	V548	L688	C845
G97	G97	GLU	L445	L551	D710	D850
H98	H98	GLY	L459	L551	L710	L850
R99	R99	MET	L459	L551	L711	L850
T100	T100	GLY	L459	L551	L712	T858
L101	L101	PRO	E462	E555	S713	V859
L102	L102	PRO	E463	E573	Y714	Q860
Y103	Y103	E538	E463	V574	Y714	I861
H111	H111	Y341	K467	I577	G718	L867
H113	H113	C346	L468	I578	L719	L867
S114	S114	S470	S470	I578	L720	L870
R115	R115	L471	L471	H582	F728	R871
M116	M116	L472	L472	V730	V730	L874
Y117	Y117	N473	N473	I586	L737	L878
L118	L118	R474	R474	I587	L738	L878
G136	G136	Y359	Y359	L590	L738	L879
L137	L137	A360	A360	L590	V743	E880
Q138	Q138	D363	D363	R595	C746	L881
E139	E139	F364	F364	V599	C747	W882
E144	E144	K365	K365	L600	L748	A883
H151	H151	T358	T358	D601	L748	L884
R157	R157	Y359	Y359	Y602	D749	T885
S158	S158	A360	A360	L603	L750	R886
E159	E159	L369	L369	L606	L755	L887
G160	G160	G370	G370	L606	S756	W891
E161	E161	V371	V371	L606	F757	T892
K162	K162	L372	L372	A613	R758	Y893
V165	V165	K373	K373	T622	G761	G894
G168	G168	K374	K374	E623	F771	
D167	D167	K375	K375	N624	L791	K901
I170	I170	A376	A376	L626	R790	L902
S175	S175	L378	L378	N514	L792	L903
R178	R178	H379	H379	N515	L792	H904
Y179	Y179	E381	E381	K516	H797	P905
L180	L180	G382	G382	E517	G798	C906
H181	H181	L388	L388	L518	E799	L907
L182	L182	F389	F389	L522	Y608	V908
L82	L82	R392	R392	L525	Y608	N909
A83	A83	R402	R402	L526	V615	L913
THR	THR	M403	M403	L529	L529	P914
VAL	VAL	L404	L404	G660	R822	E915
ALA	ALA	Y411	Y411	L661	L823	P916
		R426	R426	W662	E924	E917
		A535	A535	F664	E928	R918
		L539	L539			N919
						Y920
						N921





E5007	M4879	P4761	L4652	L4569	GLU	ALA	VAL	ARG	E4253	N4124	L4013	T3812	A3775	K3679	Y3604
S5008	C4882	T4766	V4653	L4654	PRO	GLY	THR	ARG	GLU	F4125	F4014	D3921	M3778	Q3683	H3605
Y5009		W4767	F4655	Y4580	PRO	VAL	THR	VAL	GLY	E4127	E4015	D3921	V3779	E3686	L3606
K5012	R4892	I4771	C4657	K4581	PRO	VAL	LEU	ARG	GLU	F4128	L4016	L3923	I3783		E3607
N5013	G4896	D4772	I4658	D4584	GLU	VAL	LEU	LEU	PRO	R4131	D4018	L3924	M3793	P3695	T3612
Y5014		W4773	I4659	S4585	GLY	VAL	LEU	ARG	ALA	F4132	E4016	L3924	V3794		Y3612
Q5015	E4900	K4774	G4660	P4586	ALA	ASP	ALA	ARG	ASP	I4139	Q4020	R3925	S3795	H3699	L3606
R5017	I4901		Y4661	P4587	ASP	GLY	GLY	LEU	GLU	L4160	M4023	S3929	K3799	Q3700	SER
C5018	D4902	F4782			GLY	GLY	PRO	THR	ASP	I4160	M4023	S3929	S3795	L3701	L3606
N5019	P4904	I4783	L4668	GLY	GLY	GLY	THR	GLU	GLY	F4163	M4044	Y3937	L3800	V3702	L3606
S5037	Y4909	D4786	K4672	GLU	GLY	GLY	ALA	ALA	GLY	A4167	M4047	Y3937	T3804	H3704	VAL
	R4913	L4792	R4673	ALA	VAL	GLY	VAL	ALA	ALA	E4168	M4054	K3940	L3805	T3708	HIS
	F4922	L4796	E4674	GLY	PRO	GLY	GLY	ALA	GLY	E4172	M4054	K3940	E3811	L3710	LEU
	I4927		K4675	GLY	GLY	LEU	GLY	ALA	GLY	E4182	I4058	Y3934	Q3814	Y3720	SER
	A4930	L4800	E4676	ASP	ALA	GLY	GLN	LEU	ALA	I4183	I4059	W3935	K3815	M3723	L3606
	I4936	L4800	PRO	LEU	PRO	ASP	PRO	LEU	GLY	R4188	K4060	G3947	M3816	A3724	ARG
G4941	Q4946	L4801	ALA	GLY	PRO	GLY	GLY	ALA	GLY	F4062	F4061	K3948	L3820	ARG	ARG
E4942	Q4947	L4802	ALA	ALA	PRO	ASP	PRO	VAL	ALA	E4191	D4063	R3949	F3828	I3728	ALA
L4943	Q4948	H4803	GLY	GLY	PRO	THR	GLY	VAL	ALA	R4192	M4064	M3955	F3832	M3729	VAL
R4944	Q4949		THR	THR	PRO	THR	GLY	VAL	GLY	I4193	M4064	F3962	L3832	A3730	VAL
D4945	Q4950	L4816	LYS	GLY	ALA	ALA	ALA	ALA	ALA	N4201	K4067	N3963	L3835	K3731	ALA
Q4946	V4950	A4817	PRO	PRO	PRO	GLY	ASP	GLY	GLY	M4207	V4072	S3964	C3839	S3732	CYS
V4950	K4951	T4822	SER	SER	SER	PRO	GLY	ALA	ALA	P4208	F4077	T3966	C3839	C3733	PHE
E4952	C4952	L4823	TRP	TRP	PRO	THR	GLY	ALA	GLY	Q4209	Q4078	E3967	L3842	H3734	ARG
T4956		L4824	ALA	ALA	PRO	GLY	GLY	ALA	VAL	K4211	V4210	I3969	A3846		MET
I4960		T4825	LYS	LYS	LYS	GLY	GLY	ALA	ALA	R4215	Y4080	Q3970	F3847	GLU	L3641
C4961		I4826	GLY	GLY	GLY	SER	GLY	ALA	ALA	F4219	R4085	T3874	K3873	ALA	R3648
R4983		L4827	LEU	LEU	GLU	PRO	GLY	ALA	GLY	Q3978	T4088	Q3978	Y3874	GLU	K3652
N4984		V4830	ALA	ALA	ALA	LYS	ASP	ALA	ALA	V4222	D4092	S3979	D3877	GLU	K3658
L4985		K4835	GLY	GLY	GLY	ARG	GLY	LEU	ARG	E4227	F4093	A3980	F3880		A3659
M4989		H4839	LEU	LEU	GLY	LYS	GLY	LEU	LEU	K4230	Q4094	H3982	F3880	E3755	K3660
L4992		L4843	ASP	ASP	VAL	GLY	GLY	TRP	ALA	F4234	K4095	S3983	L3884	K3756	K3661
M4993		F4859	GLY	GLY	GLY	ASP	GLY	LEU	ALA	D4240	A4096	R3984	F3886	E3757	L3662
I4996		K4864	GLY	GLY	GLY	GLY	GLY	ALA	ALA	T4241	Q4100	L3985	F3887	M3758	T3664
N4997		K4865	GLY	GLY	GLY	GLY	GLY	LEU	ALA	F4242	F4103	W3986	L3888	Q3761	H3667
K4998		L4745	LEU	LEU	LEU	GLY	VAL	GLY	ARG	F4243	T4104	F3996	Q3889		S3668
D4999		E4871	VAL	VAL	VAL	GLY	GLY	ALA	ALA	F4244	Q4105	H3998	L3891	Y3765	F3669
		P4872	PRO	PRO	PRO	GLY	HIS	LEU	GLY	M4245	I4108	M3999	C3892	D3671	E3670
E5002		D4873	GLY	GLY	GLY	VAL	VAL	LEU	GLY	M4246	Q4109	M4000	N3896	S3768	R3672
H5003		C4876	PRO	PRO	PRO	GLY	GLY	GLY	ALA	I4247	Q4121	M4001	N3896	R3769	K3673
			GLY	GLY	GLY	ALA	GLY	ALA	GLY	I4251	M4122	K4002	L3903	H3771	L3674
			LYS	LYS	SER	LYS	LYS	SER	ARG	S4252	N4123	L4003	L3903	T3772	D3675
			LYS	LYS	LEU	LEU	LYS	LYS	LEU			Q4009	Q3906	G3774	

● Molecule 1: Ryanodine receptor 1

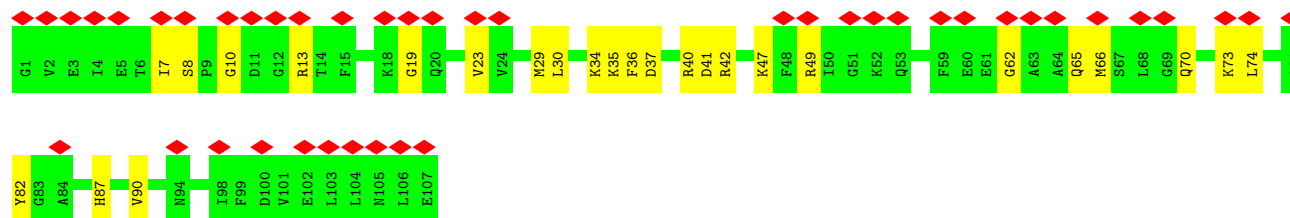
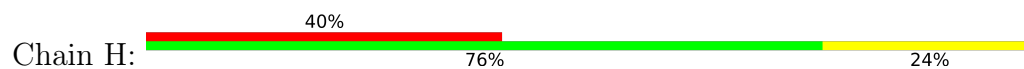




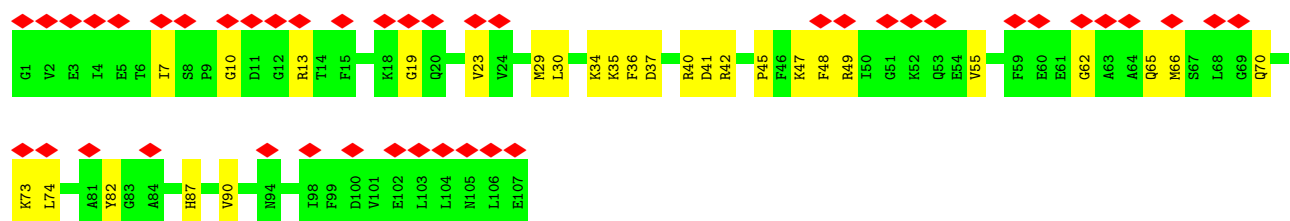
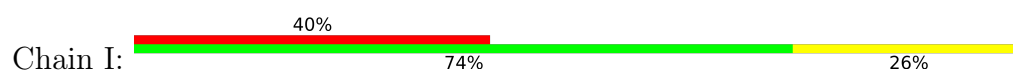
V4025	K3940	L3800	T3708	TRP	K3517	E3440	P3233	I3147	L3071	V2908	TLE
M4026	I3943	I3804	A3709	HIS	Q3521	I3441	R3234	H3150	A3072	L2911	SER
L4027	I3944	L3805	L3710	LEU	K3524	F3442	V3235	R3151	R3073	T2912	GLN
L4030	E3945	L3905	L3710	LEU	K3524	A3342	V3236	F3152	S3074	A2913	THR
I4040	Q3946	E3811	Y3720	SER	K3524	L3345	E3237	V3156	R3078	K2914	ALA
M4044	G3947	Q3814	K3723	GLN	P3527	V3346	E3238	I3157	T3079	E2915	THR
M4044	K3948	K3815	A3724	ARG	T3528	F3451	V3245	L3158	V3080	K2916	TTR
M4047	R3949	M3816	Y3725	ARG	K3530	K3452	L3246	D3159	M3081	A2917	ASP
M4054	M3955	A3726	A3726	ARG	D3531	R3453	D3247	P3162	P3085	R2920	PRO
M4063	F3962	D3727	L3532	ALA	L3532	R3248	R3248	Q3163	E3086	E2921	ARG
M4064	N3963	L3728	L3533	VAL	K3534	K3457	K3250	V3163	I3087	GLY	GLY
M4064	N3963	K3729	K3534	VAL	K3534	F3458	M3250	S3164	V3088	Y2855	
M4067	F3962	K3730	L3535	VAL	L3535	V3459	G3165	G3165	L3003	E2856	
V4072	N3963	A3731	L3535	ALA	L3535	F3460	V3166	P3167	E2925	P2857	
F4077	L3965	S3732	CYS	CYS	A3536	K3461	R3167	Y3009	L2926	P2858	
Q4078	T3966	S3732	PHE	PHE	K3537	Q3461	T3168	L3015	L2927	Q2858	
D4079	T3967	C3733	ARG	ARG	T3538	R3464	I3172	Y3016	F2928	P2859	
V4081	L3835	H3734	MET	MET	Y3540	I3464	P3262	L3018	F3095	R2860	
R4085	C3839	E3740	T3639	T3639	A3541	M3467	M3266	L3021	F3096	D2861	
I4088	L3842	GLY	L3641	L3641	L3542	K3475	P3267	L3025	E3097	L2862	
D4092	T3974	GLU	R3648	R3648	E3547	SER	H3268	L3031	R3098	Q2864	
Q4093	G3975	ALA	E3548	ALA	F3548	LYS	V3269	L3034	A3099	V2865	
Q4094	N3976	GLU	V3549	MET	V3549	MET	I3270	L3035	S3100	T2866	
A4096	Q3977	GLU	R3652	R3652	R3550	ALA	I3271	L3037	E3101	L2867	
Q4100	Q3978	E3747	K3658	K3658	L3551	LYS	E3272	A3031	D3102	S2868	
F4103	S3978	E3747	A3659	A3659	K3384	ALA	I3186	L3032	L3032	Q2872	
T4104	L3980	S3752	A3660	A3660	A3385	ALA	L3186	L3033	F3035	A2873	
G4105	A3981	S3752	V3661	V3661	E3386	GLY	R3187	L3036	K3036	L2878	
D4092	R3877	E3752	I3662	I3662	E3391	ASP	P3275	L3042	L3037	E2880	
Q4093	S3982	E3755	L3663	L3663	V3394	GLN	Y3280	L3046	L3042	N2881	
Q4095	H3982	K3756	L3663	L3663	V3394	GLN	L3281	F3043	F3043	Y2882	
A4096	R3985	E3757	T3664	T3664	R3395	SER	R3282	K2953	K2953	H2883	
Q4100	L3985	K3758	H3667	H3667	K3571	GLY	R3283	L3046	L3046	N2884	
F4103	Q3986	E3761	S3668	S3668	F3573	GLY	V3284	F2957	F2957	T2885	
T4104	F3986	Q3765	L3669	L3669	K3573	ASP	R3287	G2958	G2958	Q2887	
G4105	A3987	Y3765	E3670	E3670	V3400	GLU	E3290	Q2961	Q2961	R2888	
I4108	H3988	S3768	D3671	D3671	L3401	GLU	C3304	R3051	R3051	K2889	
Q4109	N3989	R3769	M3673	M3673	R3414	LYS	A3204	H3052	H3052	Q2892	
E4121	M3999	L3770	I3674	I3674	Y3415	LYS	V3307	R3053	R3053	L2894	
I4123	Q3900	H3771	D3675	D3675	V3416	ARG	T3309	V3054	V3054	E2895	
N4124	K4002	L3772	D3676	D3676	Q3597	ARG	L3312	F3057	F3057	A2896	
F4125	L4003	R3773	K3679	K3679	Y3604	GLY	L3315	D3060	D3060	K2897	
E4126	Q4009	A3775	Q3683	Q3683	L3606	ASP	L3316	A3061	A3061	Q2898	
E4127	L4013	K3778	E3686	E3686	L3606	ASP	L3316	V3065	V3065	Q2899	
F4128	K4014	Y3779	K3686	K3686	E3607	TRP	K3222	L3070	L3070	H2902	
	L4016	Q3782	P3695	P3695	P3612	TRP	S3223	A2975	A2975	P2903	
	D4018	L3783	K3699	K3699	Y3511	LYS	R3321	F3062	F3062	L2904	
	L4019	S3784	SER	SER	A3512	ALA	R3324	V3065	V3065	V2906	
	Q4020	A3785	L3701	L3701	L3513	LYS	R3325	L3068	L3068	P2907	
	K4021	C3786	V3702	V3702	K3514	LYS	R3327	H3069	H3069		
	D4022	K3787	ALA	ALA	K3516	VAL	A3322				
	Y4024	K3793	H3704	H3704	K3516		L3232				



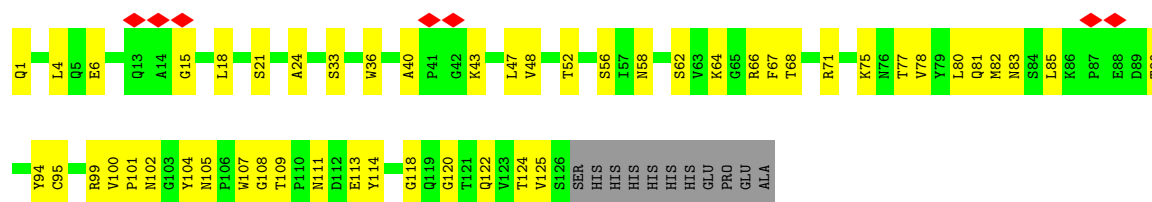
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



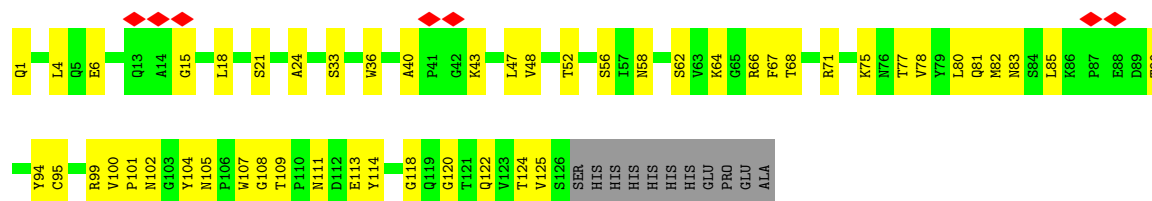
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



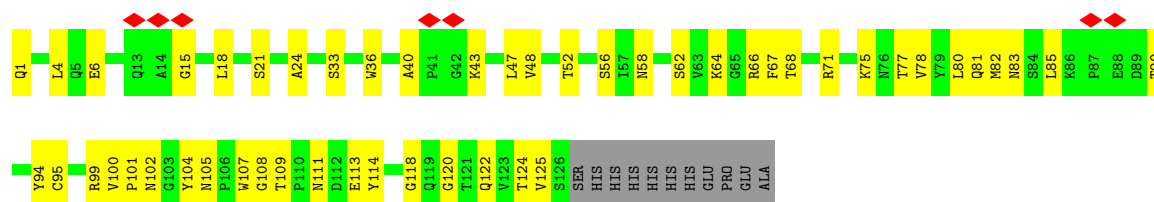
• Molecule 3: Nanobody 9657



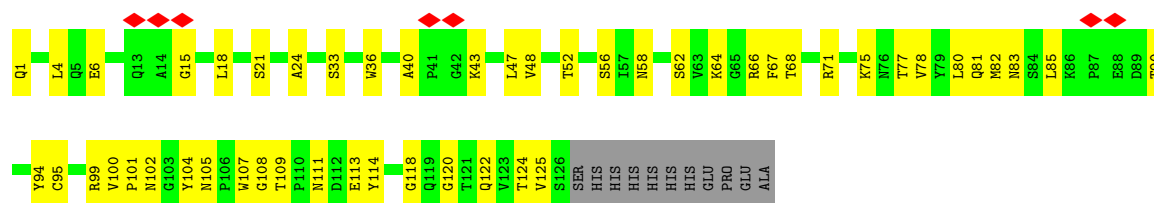
• Molecule 3: Nanobody 9657



Chain K:



Chain M:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29246	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	4.150	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.061	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.28	Depositor
Map size ($\text{\AA}$)	500.64, 500.64, 500.64	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, CFF, CA, 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	B	0.13	0/34879	0.34	2/47278 (0.0%)
1	E	0.13	0/34879	0.34	2/47278 (0.0%)
1	G	0.13	0/34879	0.34	2/47278 (0.0%)
1	J	0.13	0/34879	0.34	1/47278 (0.0%)
2	A	0.11	0/834	0.34	0/1123
2	D	0.11	0/834	0.34	0/1123
2	H	0.11	0/834	0.34	0/1123
2	I	0.11	0/834	0.34	0/1123
3	C	0.17	0/987	0.44	0/1340
3	F	0.17	0/987	0.44	0/1340
3	K	0.17	0/987	0.44	0/1340
3	M	0.17	0/987	0.44	0/1340
All	All	0.13	0/146800	0.34	7/198964 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1503	PRO	N-CA-CB	6.12	110.06	103.33
1	E	1503	PRO	N-CA-CB	6.12	110.06	103.33
1	G	1503	PRO	N-CA-CB	6.12	110.06	103.33
1	J	1503	PRO	N-CA-CB	6.12	110.06	103.33
1	G	2635	GLU	CB-CA-C	-5.37	109.92	117.23

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	B	34104	0	33492	1093	0
1	E	34104	0	33492	1083	0
1	G	34104	0	33492	1087	0
1	J	34104	0	33492	1080	0
2	A	818	0	824	20	0
2	D	818	0	824	22	0
2	H	818	0	824	22	0
2	I	818	0	824	21	0
3	C	967	0	916	45	0
3	F	967	0	916	47	0
3	K	967	0	916	46	0
3	M	967	0	916	47	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	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
5	J	31	0	12	1	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	G	14	0	10	4	0
6	J	14	0	10	1	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	143744	0	141016	4498	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 16.

The worst 5 of 4498 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:E:2911:LEU:HD13	1:E:2915:GLU:HG3	1.53	0.90
1:G:3197:LEU:O	1:G:3201:MET:HB2	1.71	0.90
1:J:3197:LEU:O	1:J:3201:MET:HB2	1.71	0.90
1:J:2911:LEU:HD13	1:J:2915:GLU:HG3	1.53	0.90
1:G:2911:LEU:HD13	1:G:2915:GLU:HG3	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
1	E	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
1	G	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
1	J	4280/5027 (85%)	4178 (98%)	100 (2%)	2 (0%)	100	100
2	A	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	D	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	I	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	C	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	F	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	K	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
3	M	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
All	All	18036/21084 (86%)	17584 (98%)	444 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2867	LEU

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Mol	Chain	Res	Type
1	E	2867	LEU
1	G	2867	LEU
1	J	2867	LEU
1	B	52	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	3659/4270 (86%)	3659 (100%)	0	100	100
1	E	3659/4270 (86%)	3659 (100%)	0	100	100
1	G	3659/4270 (86%)	3659 (100%)	0	100	100
1	J	3659/4270 (86%)	3659 (100%)	0	100	100
2	A	88/88 (100%)	88 (100%)	0	100	100
2	D	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
2	I	88/88 (100%)	88 (100%)	0	100	100
3	C	104/114 (91%)	104 (100%)	0	100	100
3	F	104/114 (91%)	104 (100%)	0	100	100
3	K	104/114 (91%)	104 (100%)	0	100	100
3	M	104/114 (91%)	104 (100%)	0	100	100
All	All	15404/17888 (86%)	15404 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	1691	GLN
2	I	87	HIS
1	J	2308	GLN
1	J	3882	GLN

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Mol	Chain	Res	Type
3	C	122	GLN

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	$\# Z > 2$
6	CFF	B	5103	-	15,15,15	0.50	0	23,23,23	0.71	1 (4%)
5	ATP	B	5102	-	32,33,33	0.27	0	48,52,52	0.31	0
6	CFF	J	5103	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
6	CFF	G	5103	-	15,15,15	1.67	4 (26%)	23,23,23	1.76	5 (21%)
5	ATP	J	5102	-	32,33,33	0.27	0	48,52,52	0.31	0
5	ATP	G	5102	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	E	5102	-	32,33,33	0.26	0	48,52,52	0.31	0
6	CFF	E	5103	-	15,15,15	0.50	0	23,23,23	0.72	1 (4%)

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
6	CFF	B	5103	-	-	-	0/2/2/2
5	ATP	B	5102	-	-	5/22/38/38	0/3/3/3
6	CFF	J	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
5	ATP	J	5102	-	-	5/22/38/38	0/3/3/3
5	ATP	G	5102	-	-	5/22/38/38	0/3/3/3
5	ATP	E	5102	-	-	5/22/38/38	0/3/3/3
6	CFF	E	5103	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5103	CFF	C5-N7	-2.91	1.33	1.38
6	G	5103	CFF	C4-N3	-2.80	1.33	1.38
6	G	5103	CFF	C5-C4	2.69	1.45	1.37
6	G	5103	CFF	C5-C6	2.08	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5103	CFF	N3-C2-N1	4.23	122.42	117.14
6	G	5103	CFF	C6-N1-C2	-2.91	120.92	125.66
6	G	5103	CFF	N3-C4-N9	2.84	130.74	126.27
6	G	5103	CFF	C5-C4-N9	-2.45	107.24	112.10
6	J	5103	CFF	C12-N3-C2	2.29	121.31	117.33

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

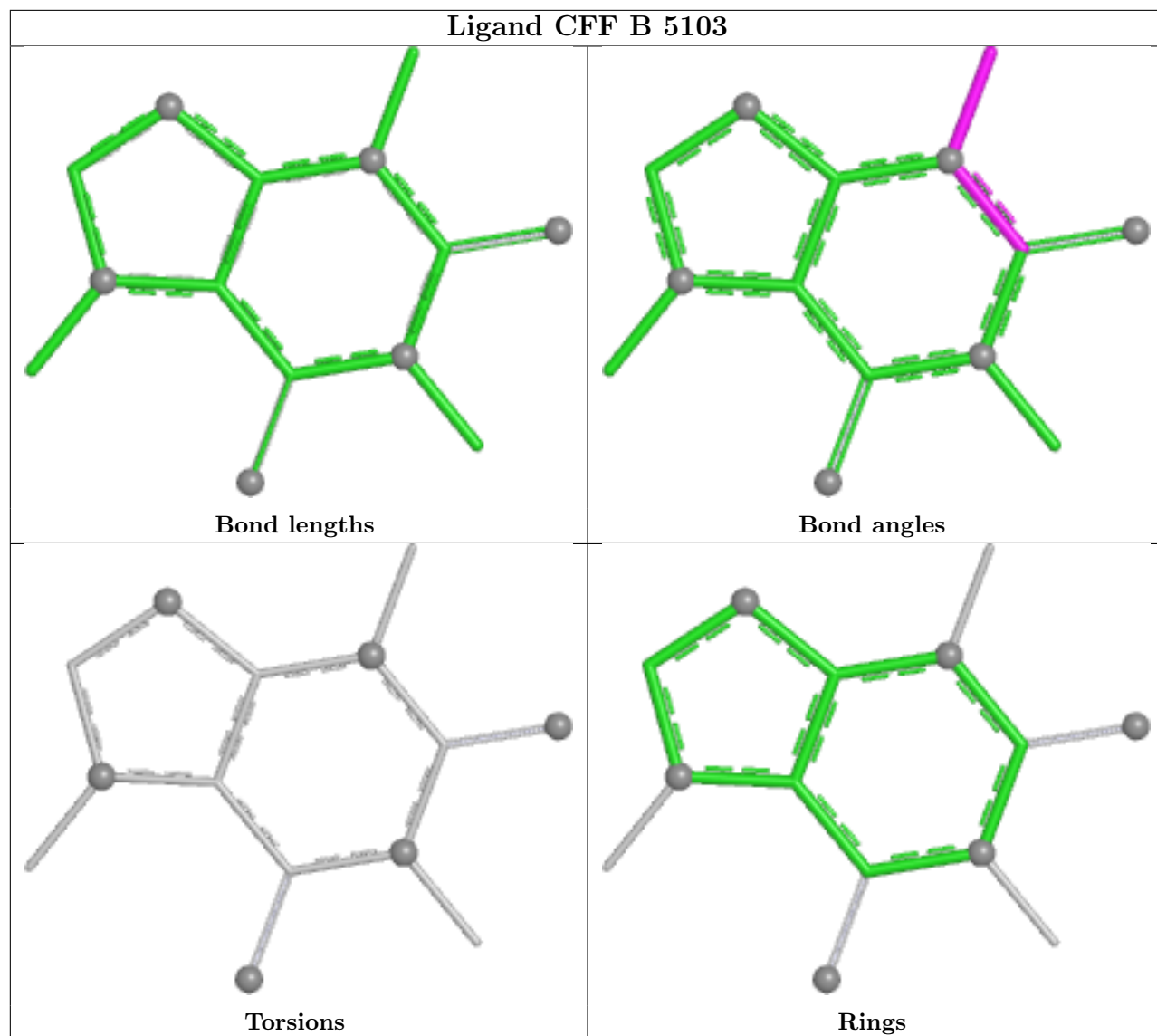
Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	PB-O3B-PG-O2G
5	B	5102	ATP	PB-O3B-PG-O3G
5	B	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	C5'-O5'-PA-O2A
5	B	5102	ATP	C5'-O5'-PA-O3A

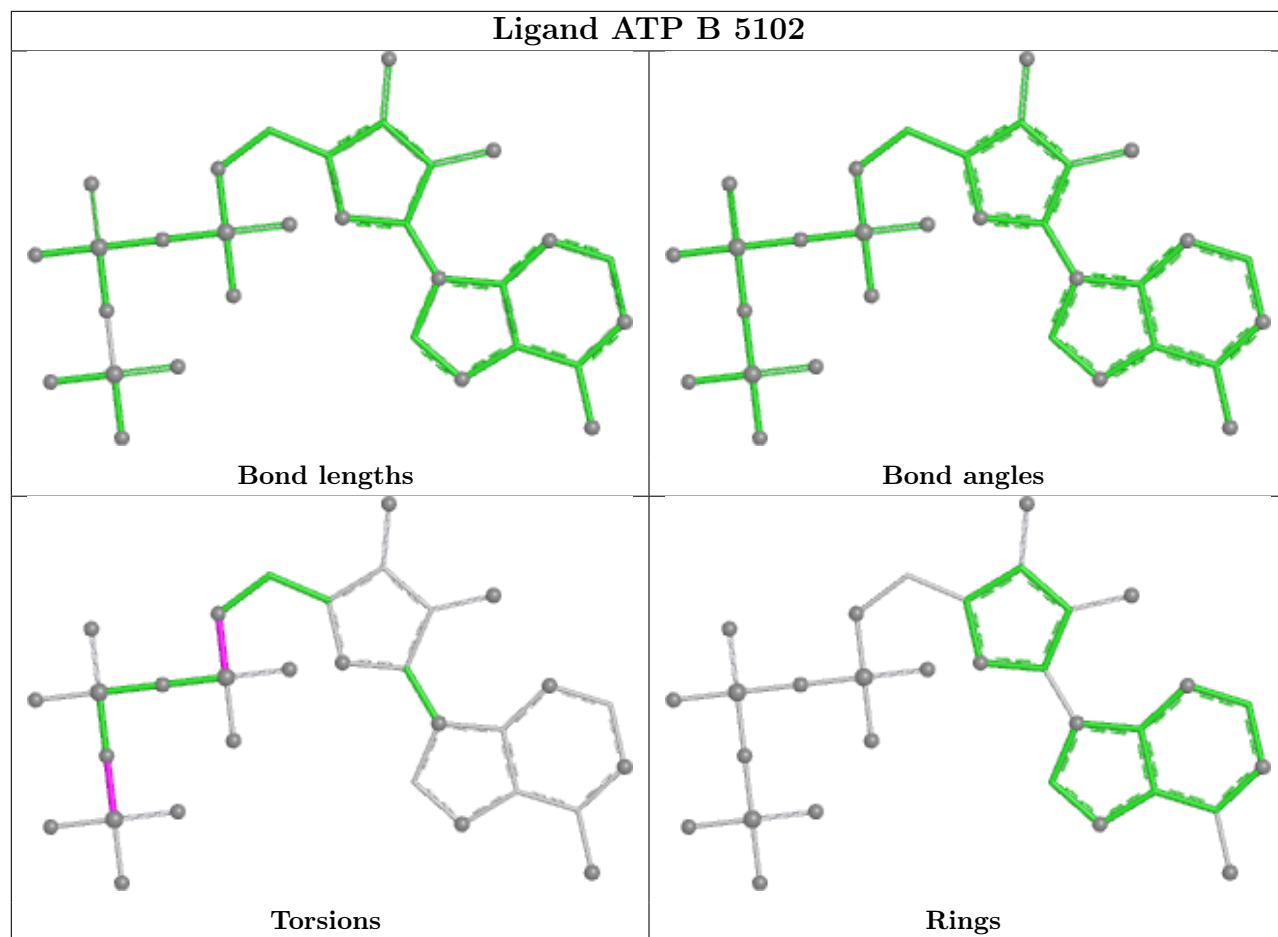
There are no ring outliers.

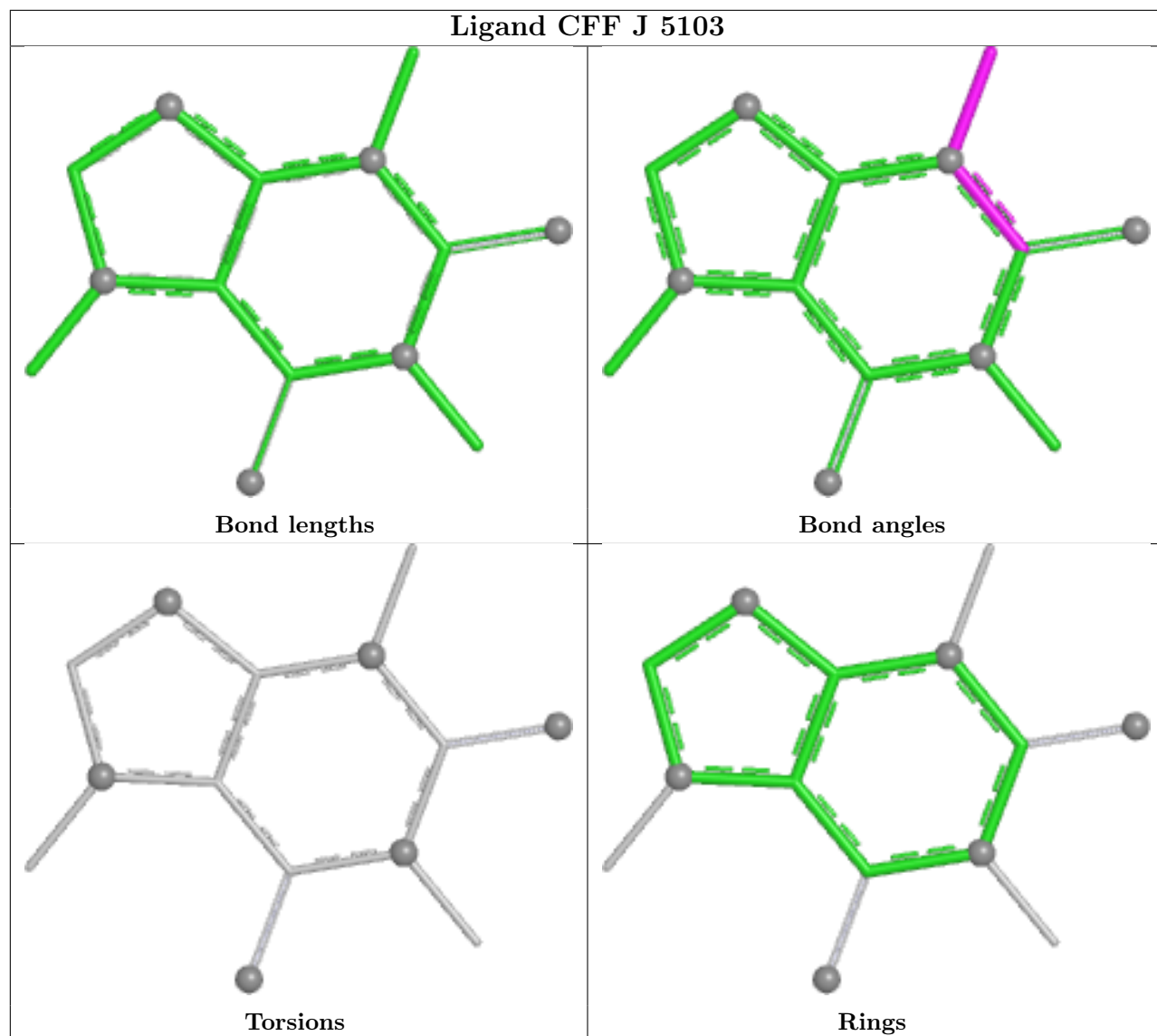
8 monomers are involved in 11 short contacts:

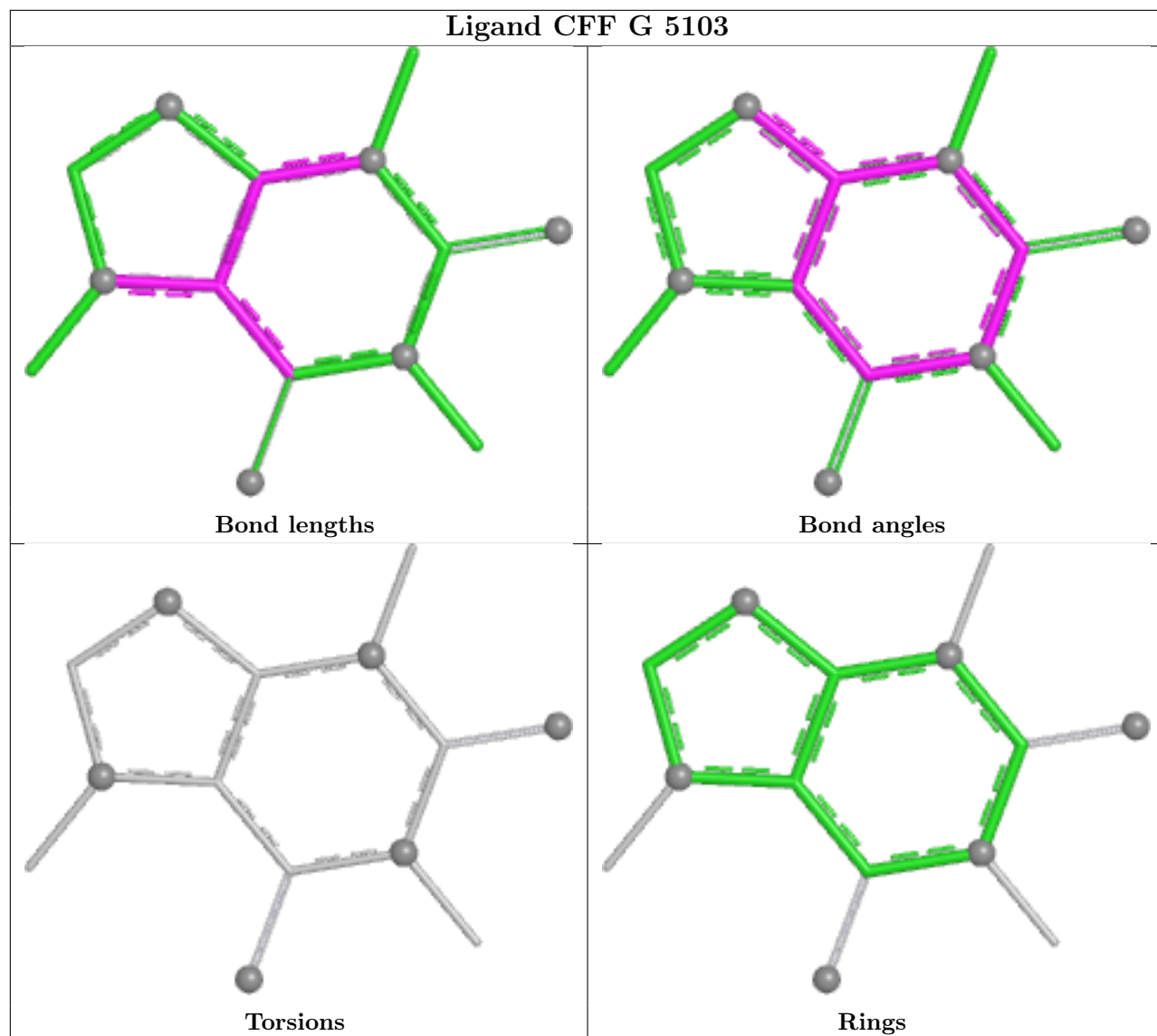
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5103	CFF	1	0
5	B	5102	ATP	1	0
6	J	5103	CFF	1	0
6	G	5103	CFF	4	0
5	J	5102	ATP	1	0
5	G	5102	ATP	1	0
5	E	5102	ATP	1	0
6	E	5103	CFF	1	0

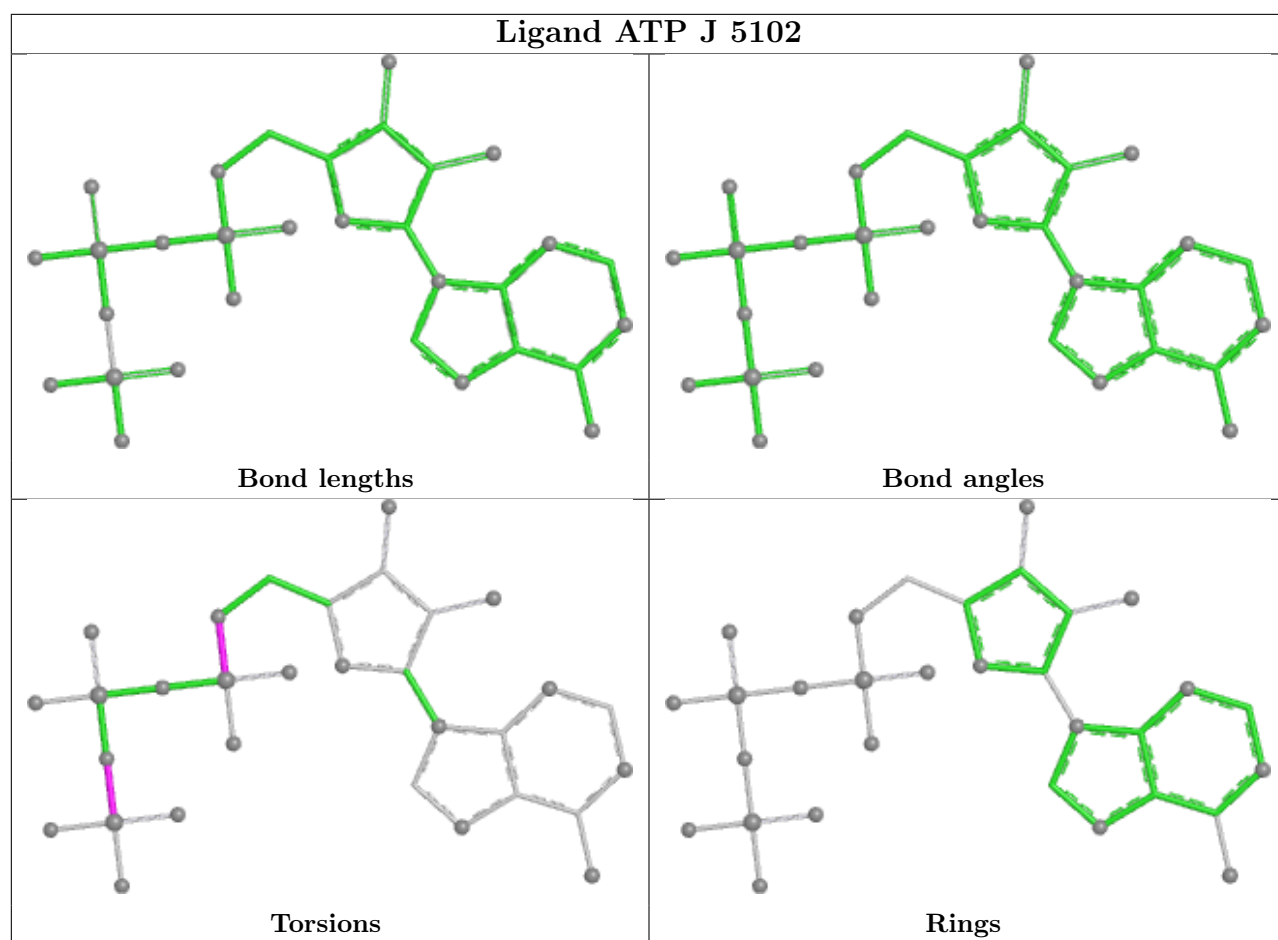
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

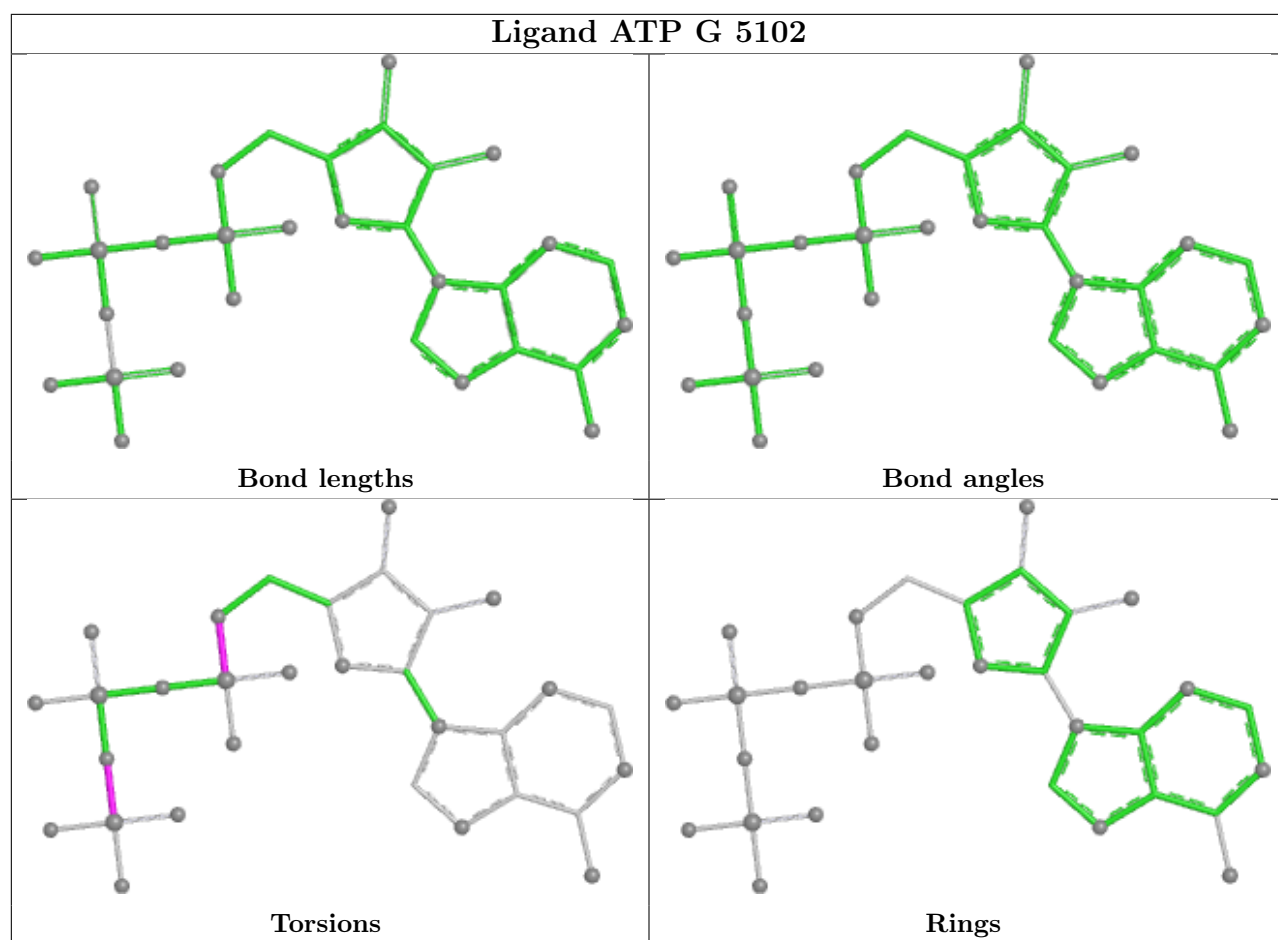


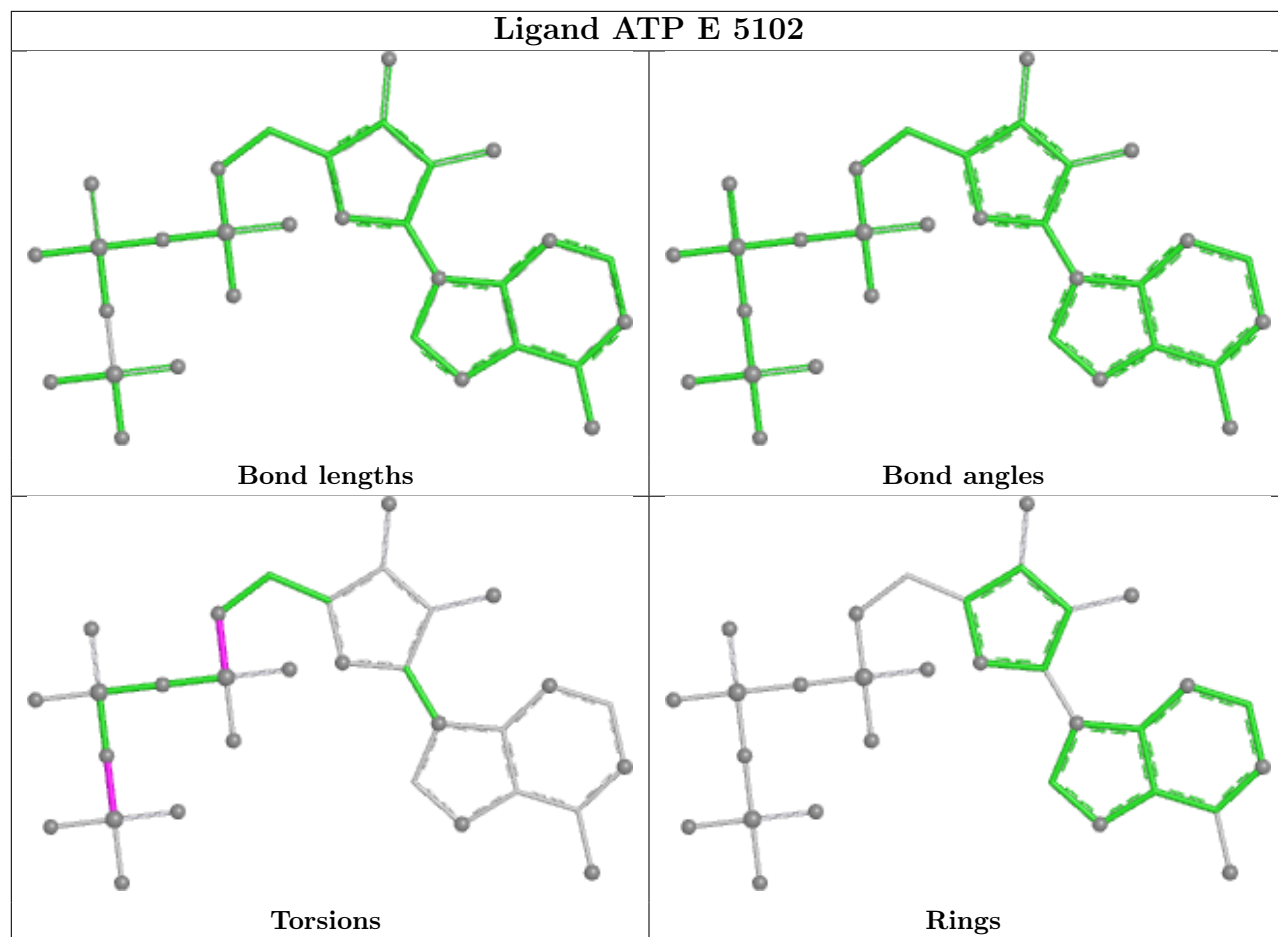


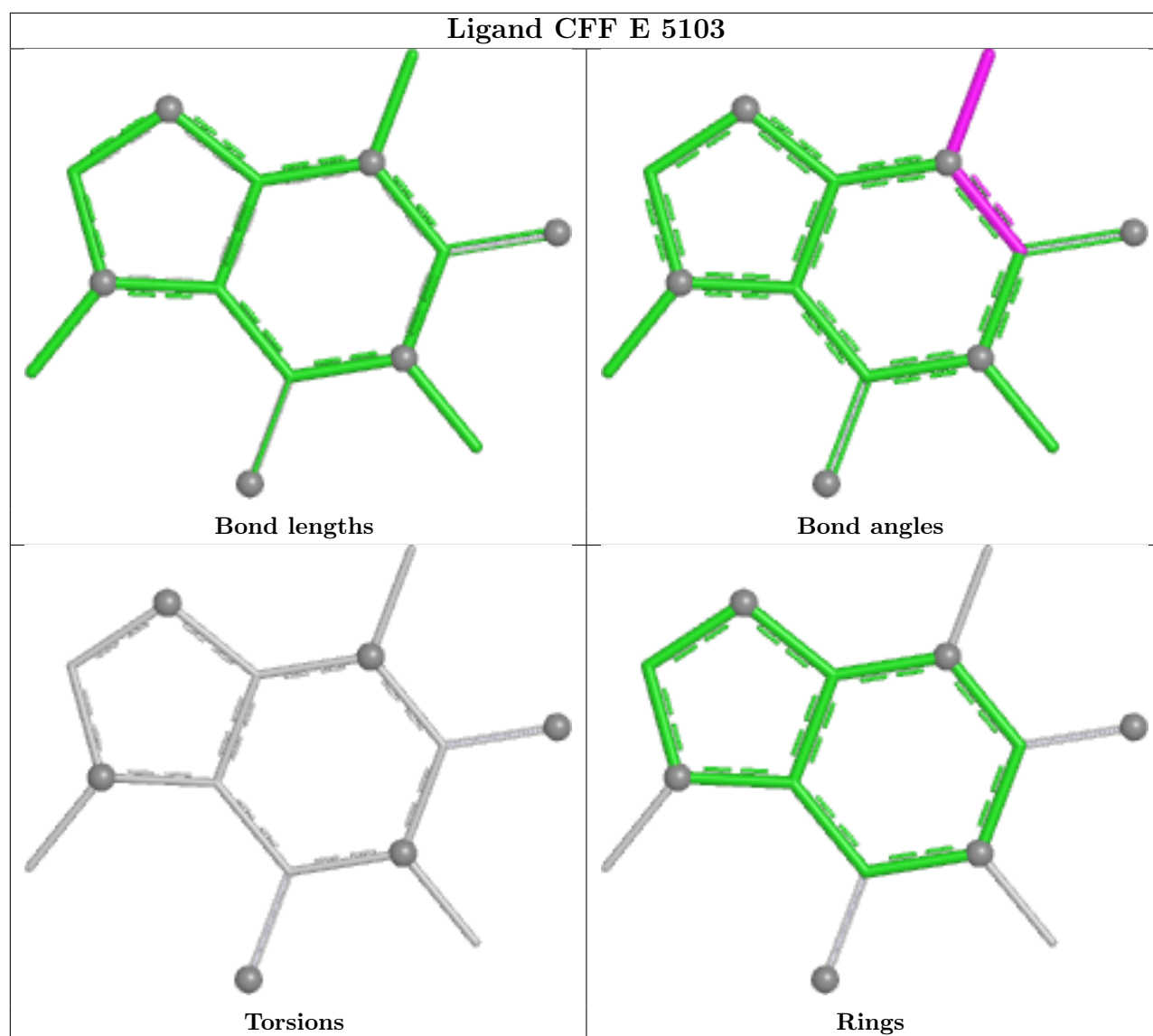












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

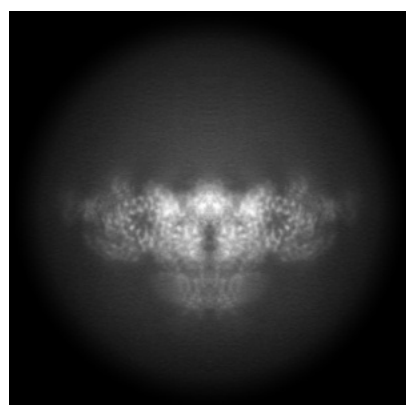
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19467. These allow visual inspection of the internal detail of the map and identification of artifacts.

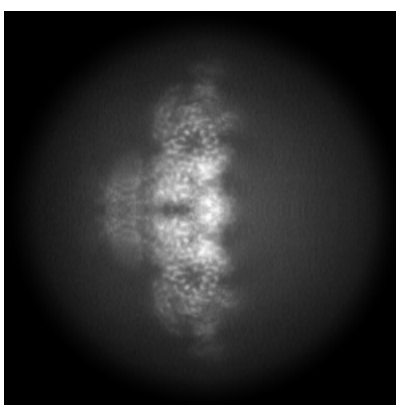
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

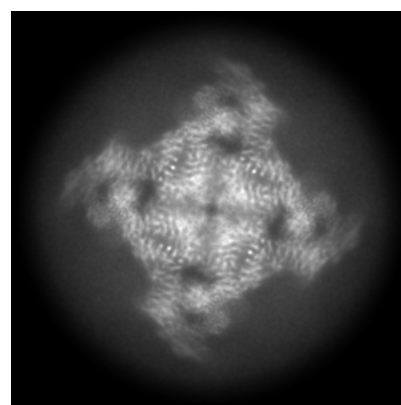
6.1.1 Primary map



X



Y

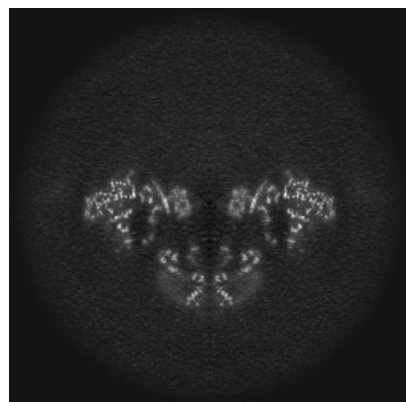


Z

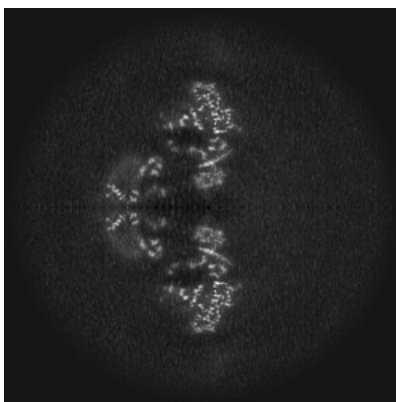
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

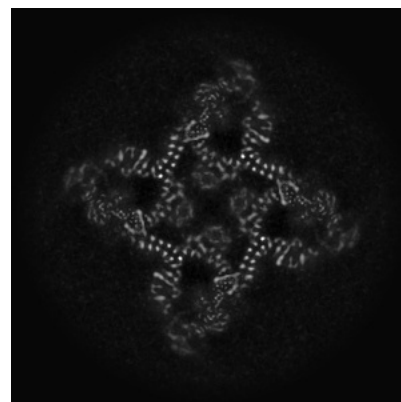
6.2.1 Primary map



X Index: 168



Y Index: 168

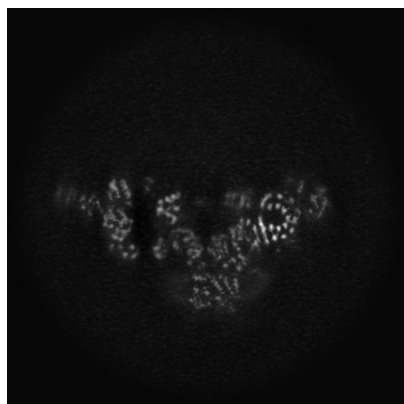


Z Index: 168

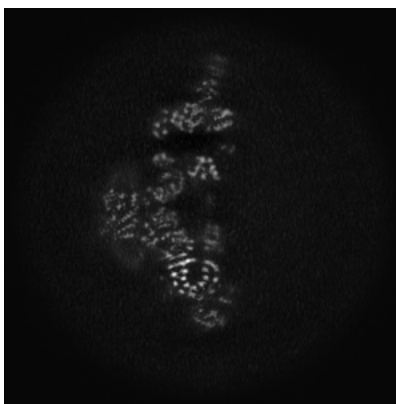
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

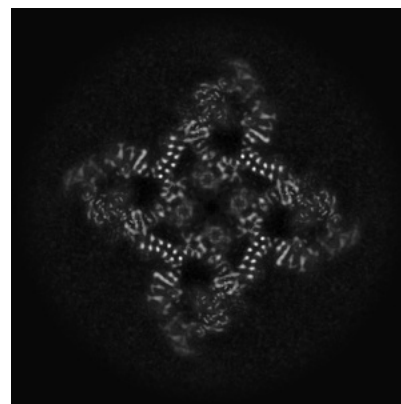
6.3.1 Primary map



X Index: 157



Y Index: 157

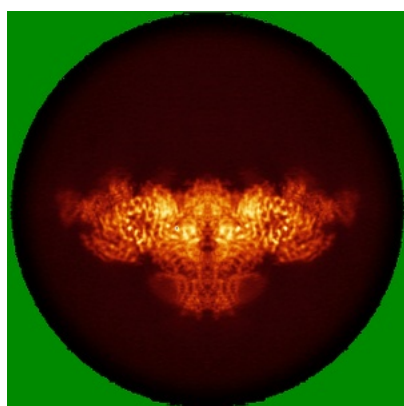


Z Index: 167

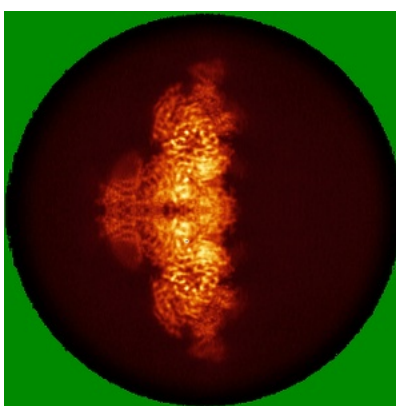
The images above show the largest variance slices of the map in three orthogonal directions.

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

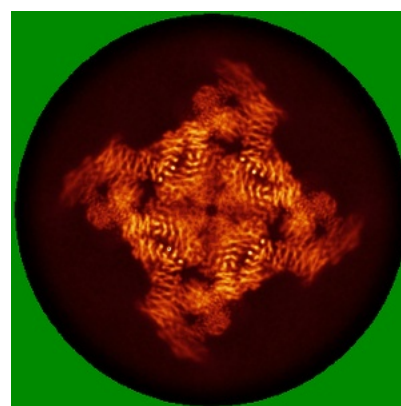
6.4.1 Primary map



X



Y

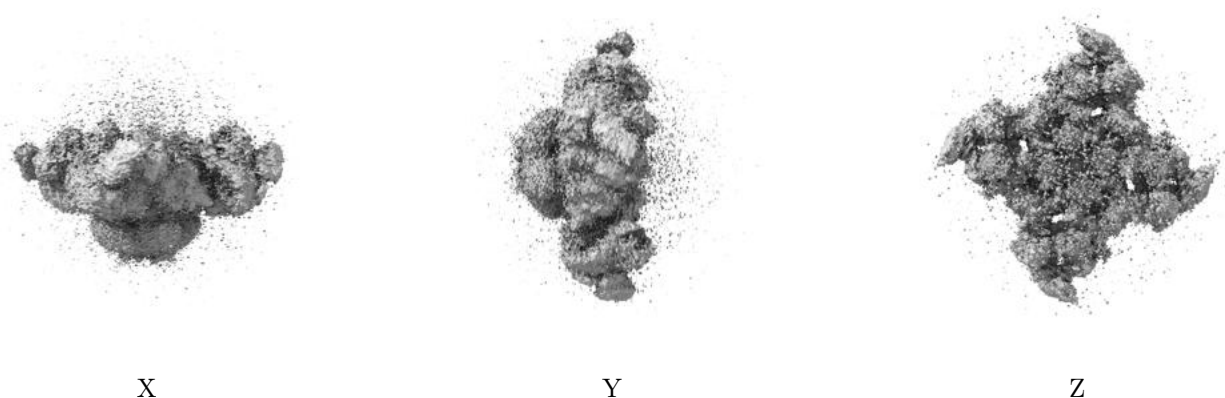


Z

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

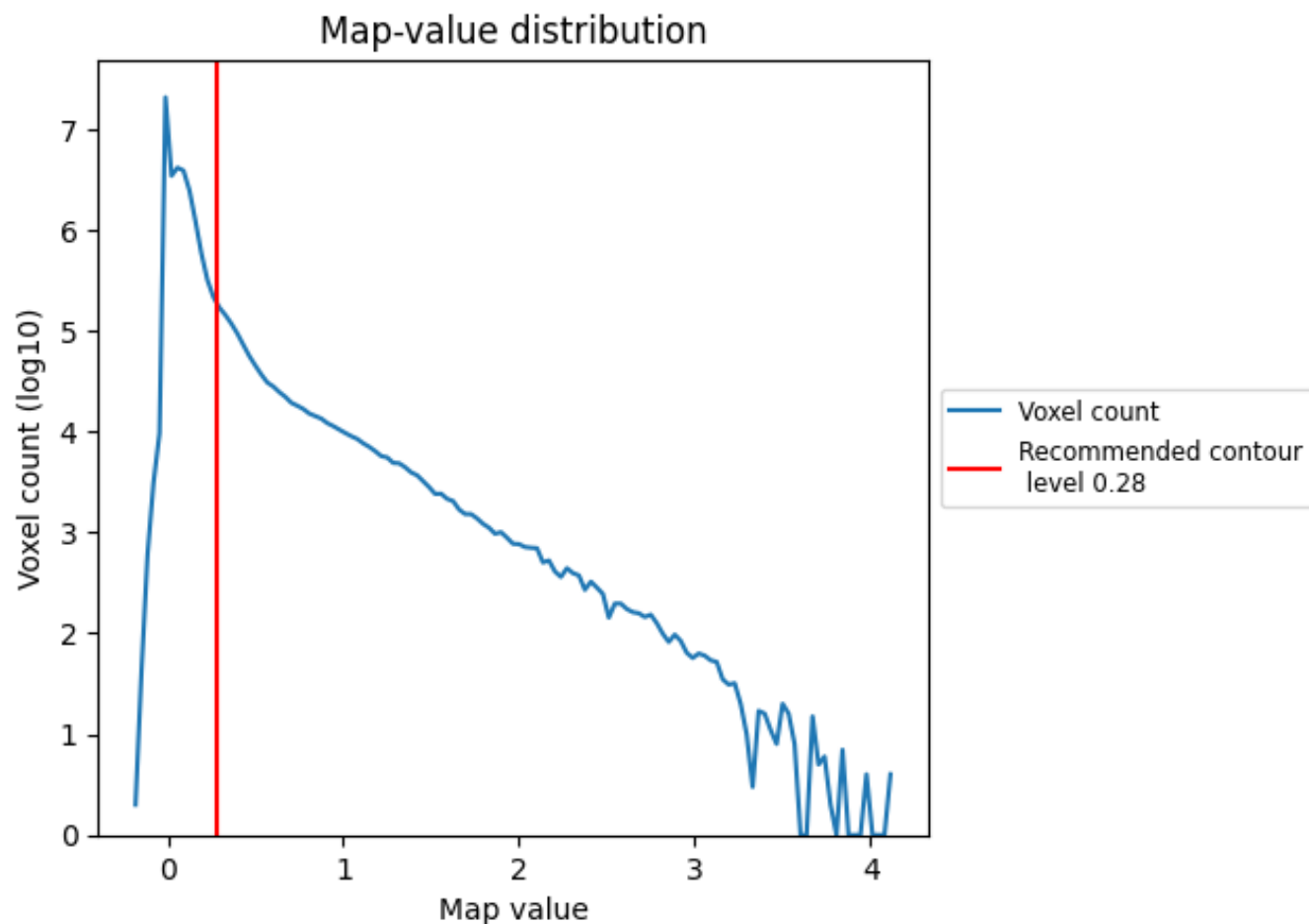
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

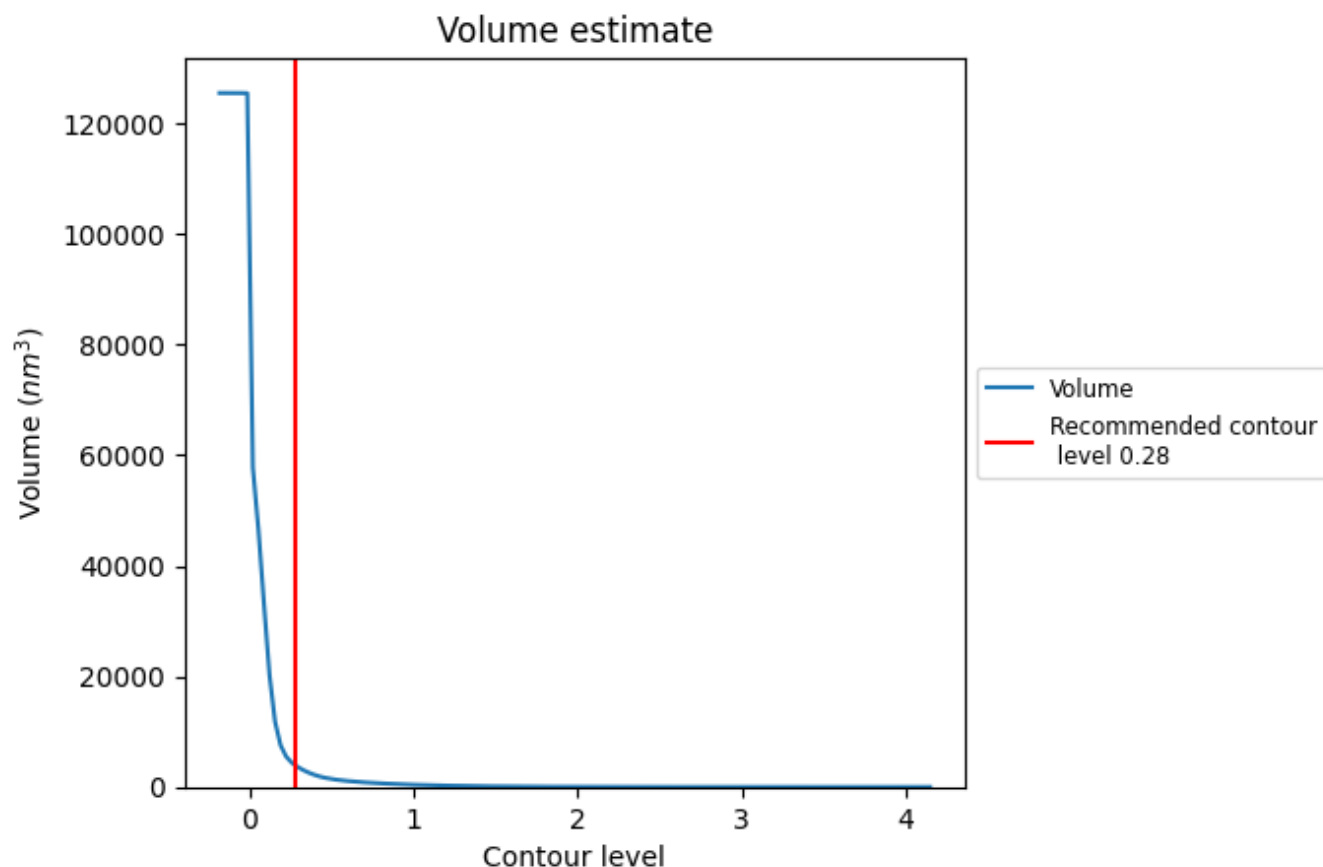
This section contains the results of statistical analysis of the map.

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.

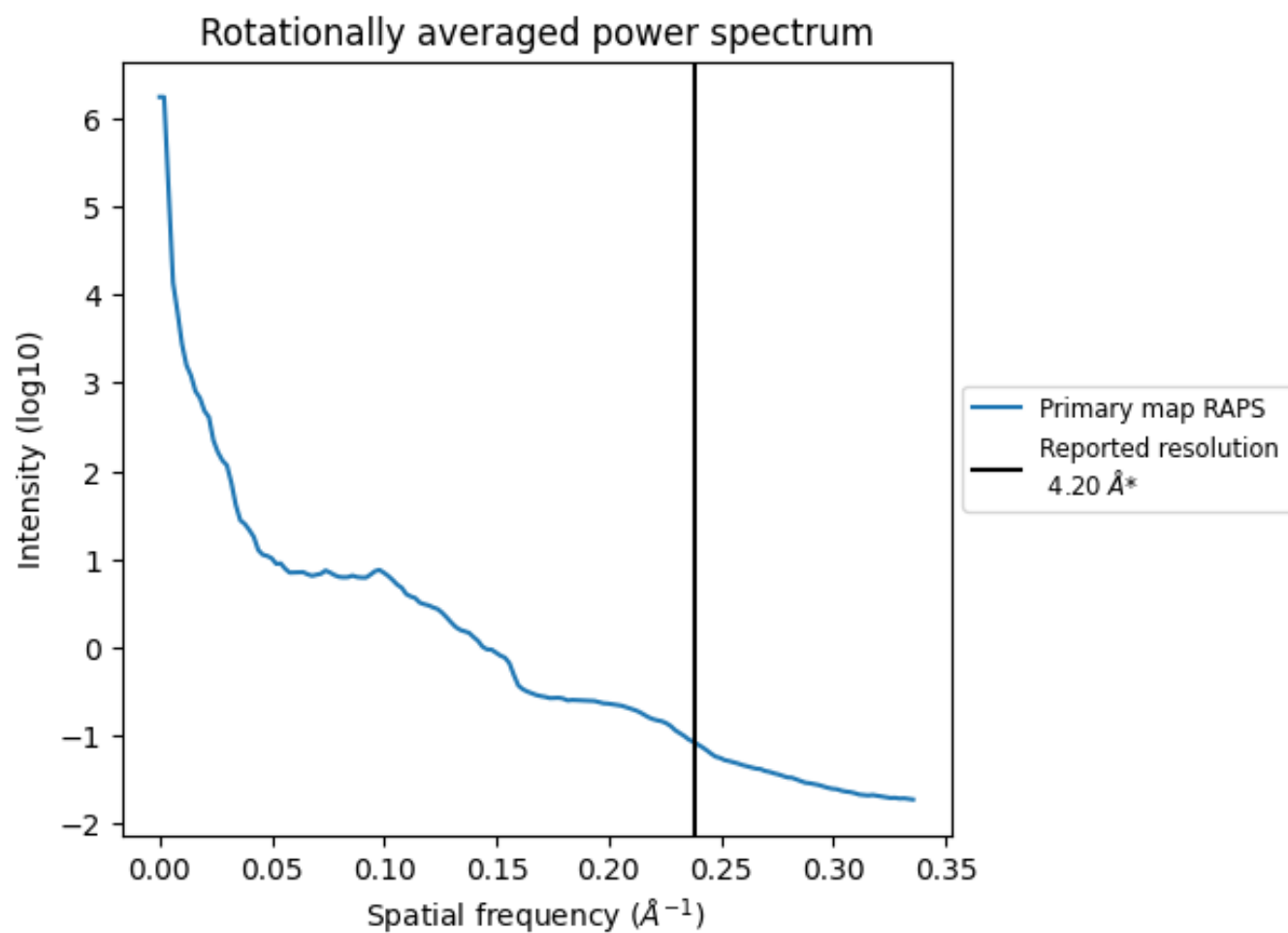
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3900 nm³; this corresponds to an approximate mass of 3523 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 ⓘ

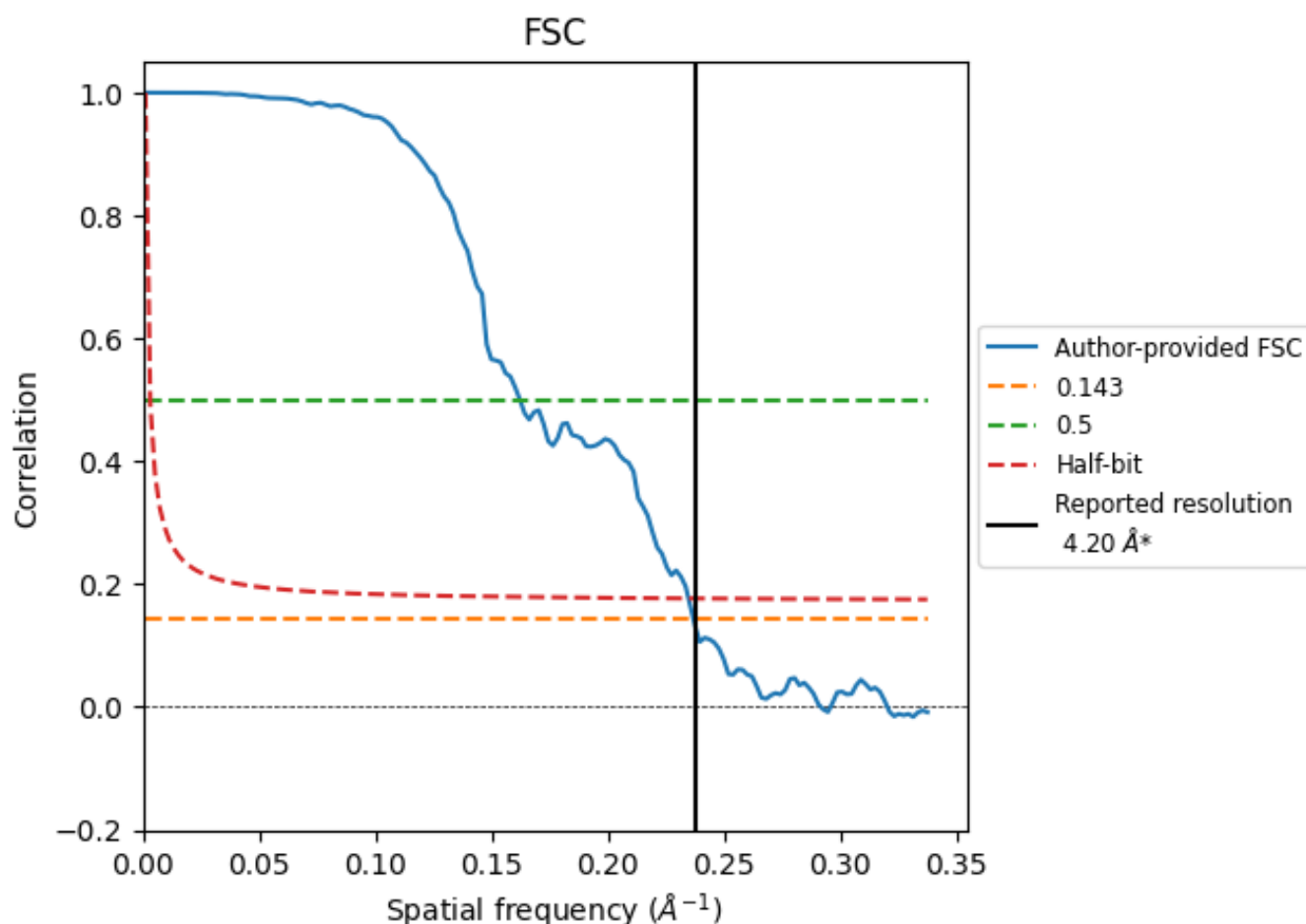


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

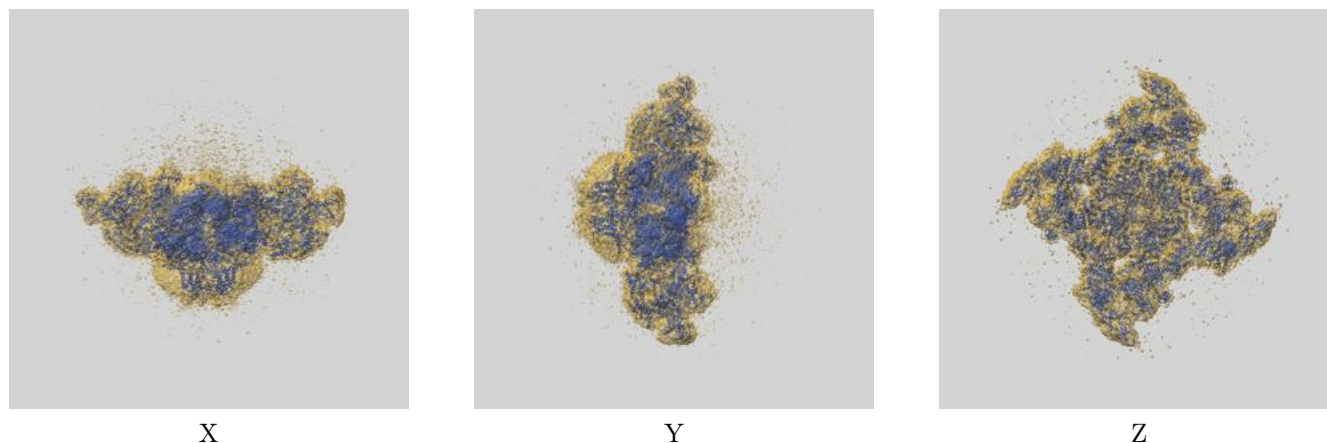
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.17	4.26
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

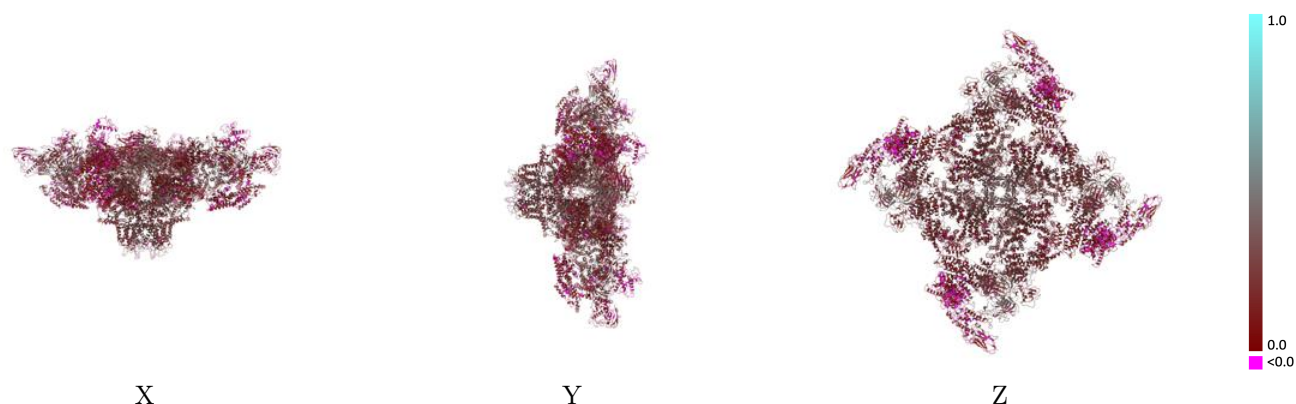
This section contains information regarding the fit between EMDB map EMD-19467 and PDB model 8RRW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



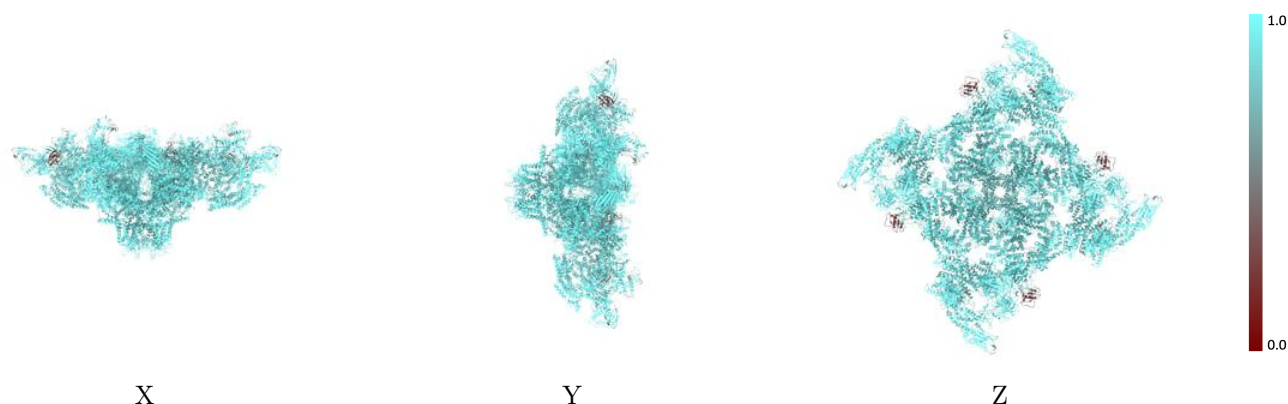
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



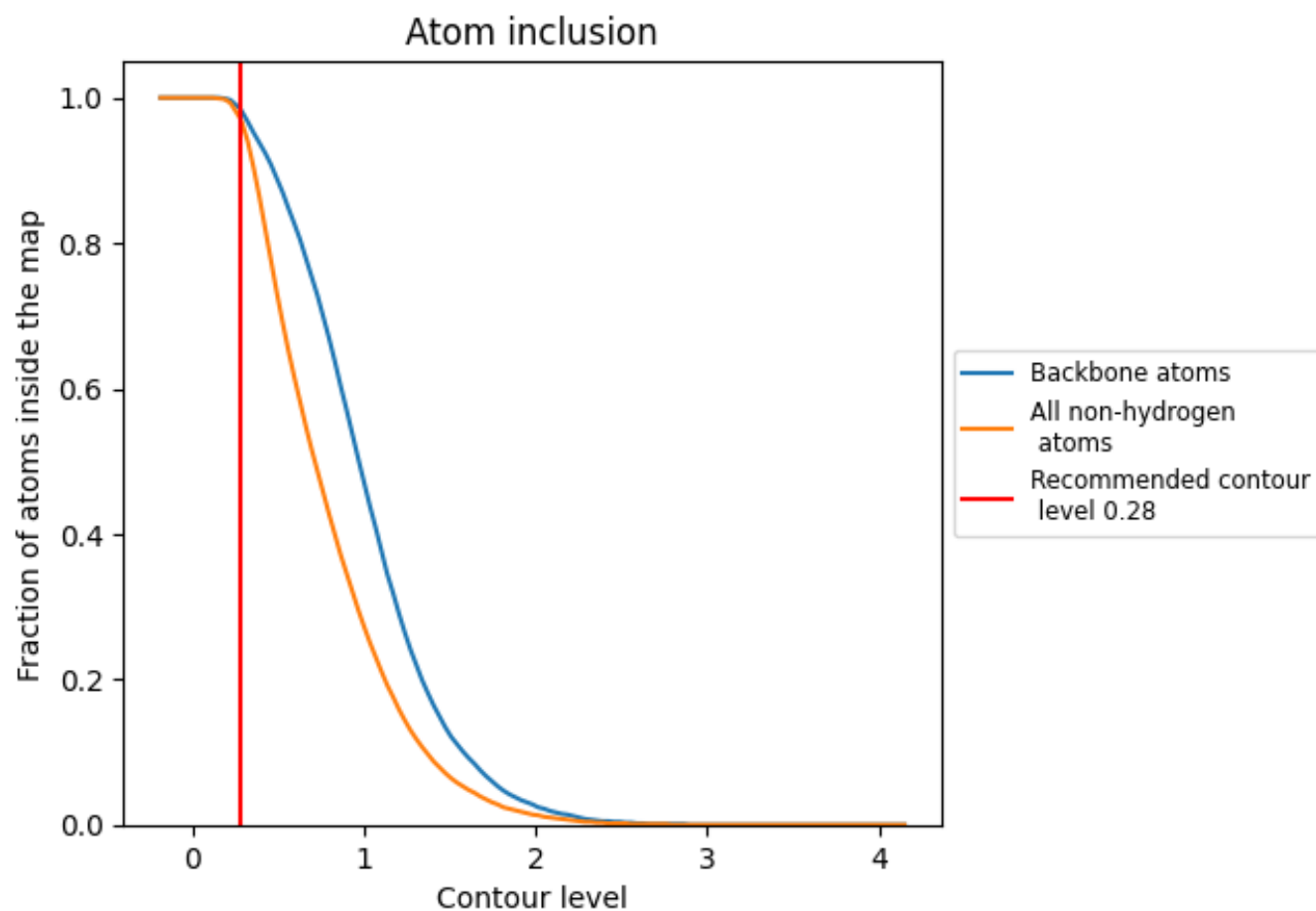
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.2010
A	0.5280	0.2090
B	0.9840	0.2030
C	0.9250	0.1360
D	0.5240	0.2080
E	0.9840	0.2030
F	0.9240	0.1370
G	0.9840	0.2030
H	0.5320	0.2130
I	0.5300	0.2090
J	0.9840	0.2030
K	0.9250	0.1380
M	0.9250	0.1360

1.0

0.0

<0.0