



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 03:09 pm BST

PDB ID : 9S3V / pdb_00009s3v
EMDB ID : EMD-54553
Title : Primed-state RyR1 with activating ligand mixture (Calcium/ACP/Caffeine)
in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-25
Resolution : 3.20 Å(reported)
Based on initial model : 7tzc

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

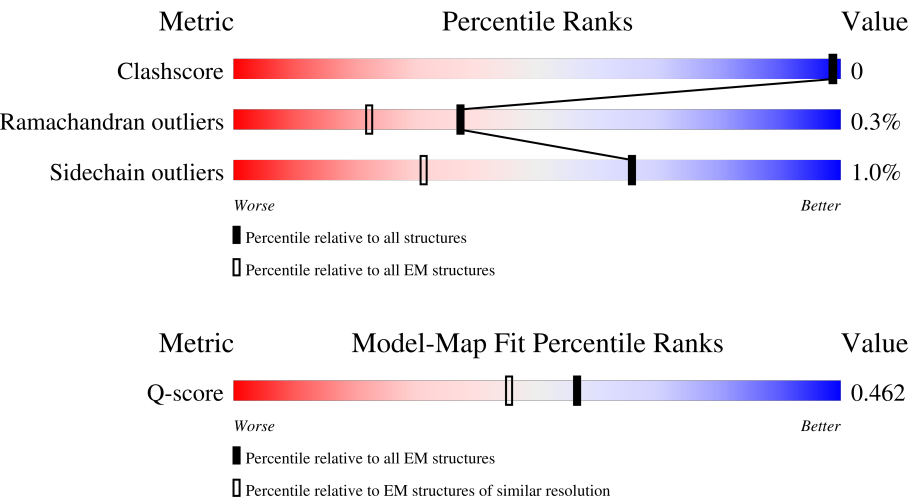
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	A	5037	14% 85% 13%
1	B	5037	14% 85% 13%
1	C	5037	14% 85% 13%
1	D	5037	13% 85% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	6% 97% ..
2	F	108	6% 97% ..
2	G	108	6% 97% ..
2	H	108	6% 97% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 287288 atoms, of which 143004 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	A	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

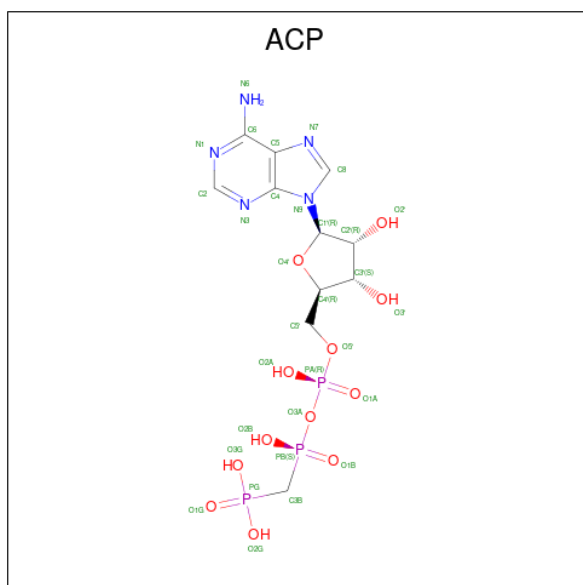
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

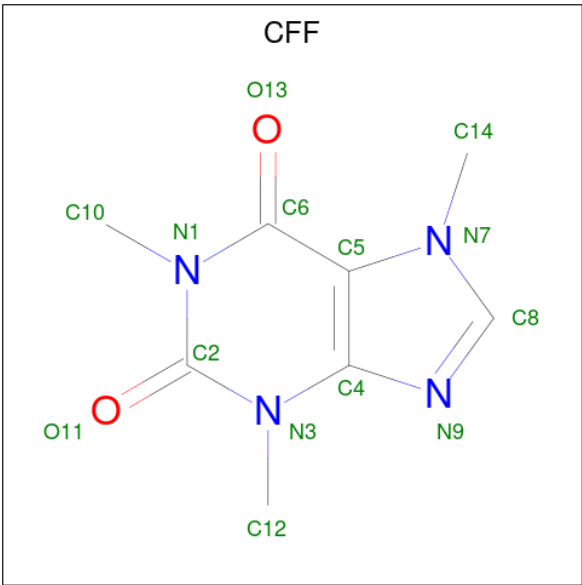
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

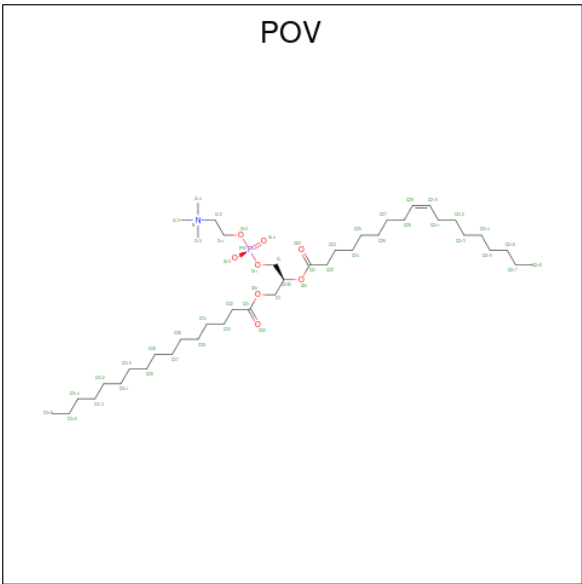
- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	D	1	Total	C	H	N	O	0
			24	8	10	4	2	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).

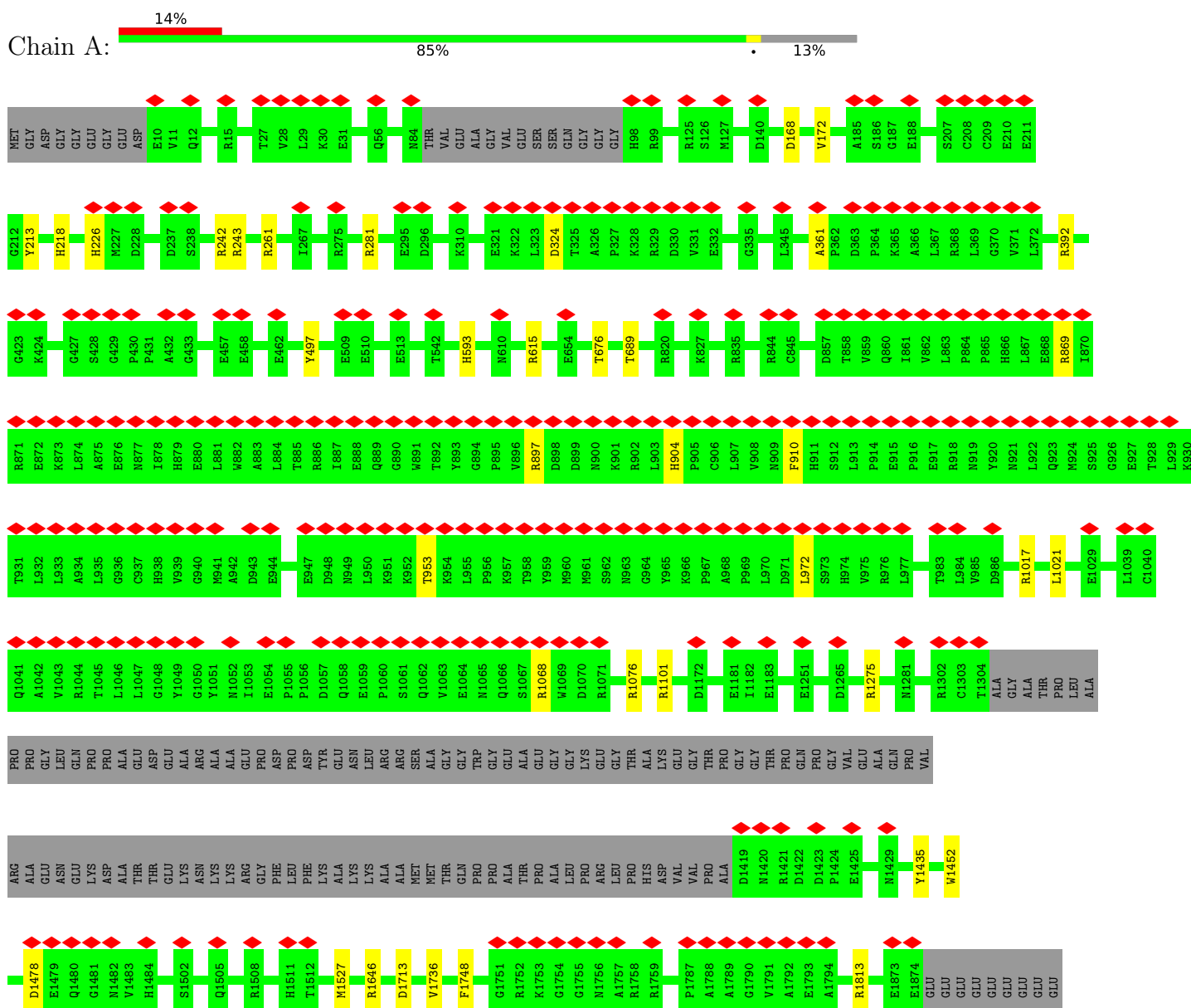


Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	D	1	Total 134	C 42	H 82	N 1	O 8	P 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.

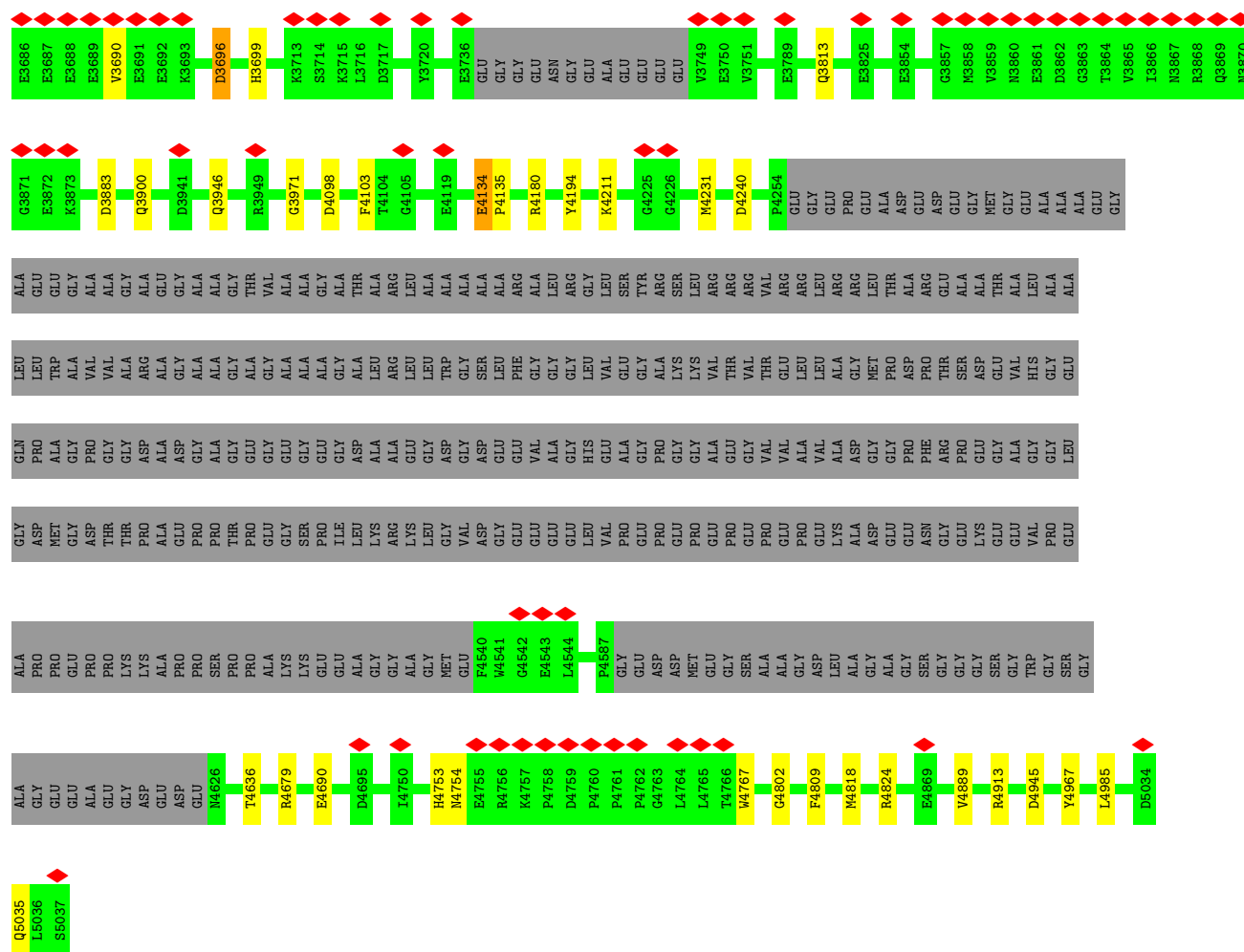
• Molecule 1: Ryanodine receptor 1



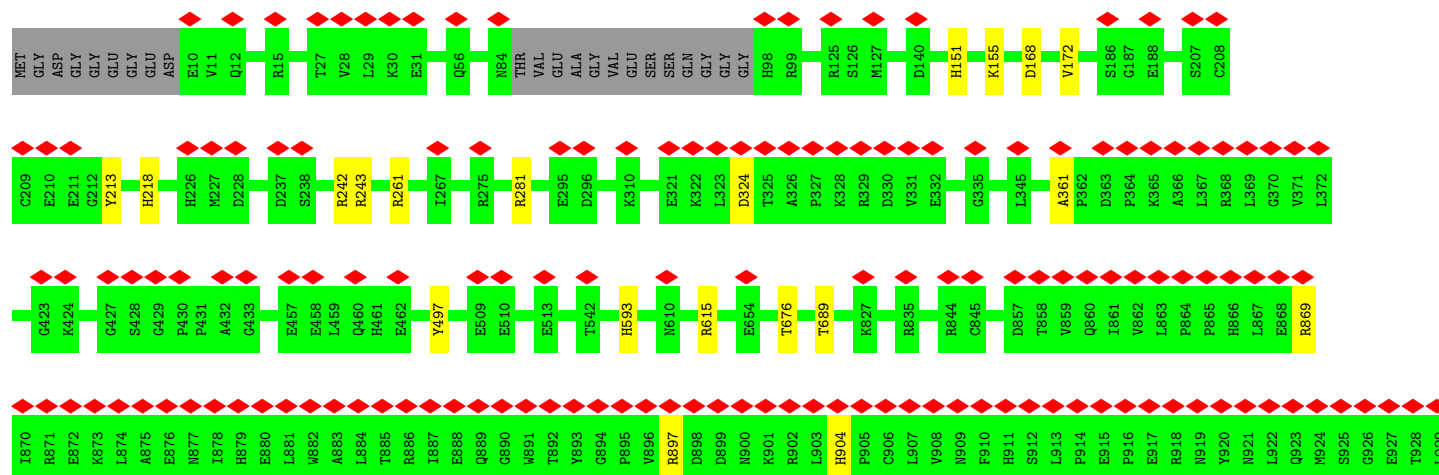
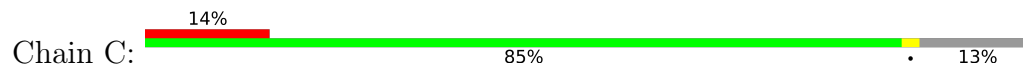




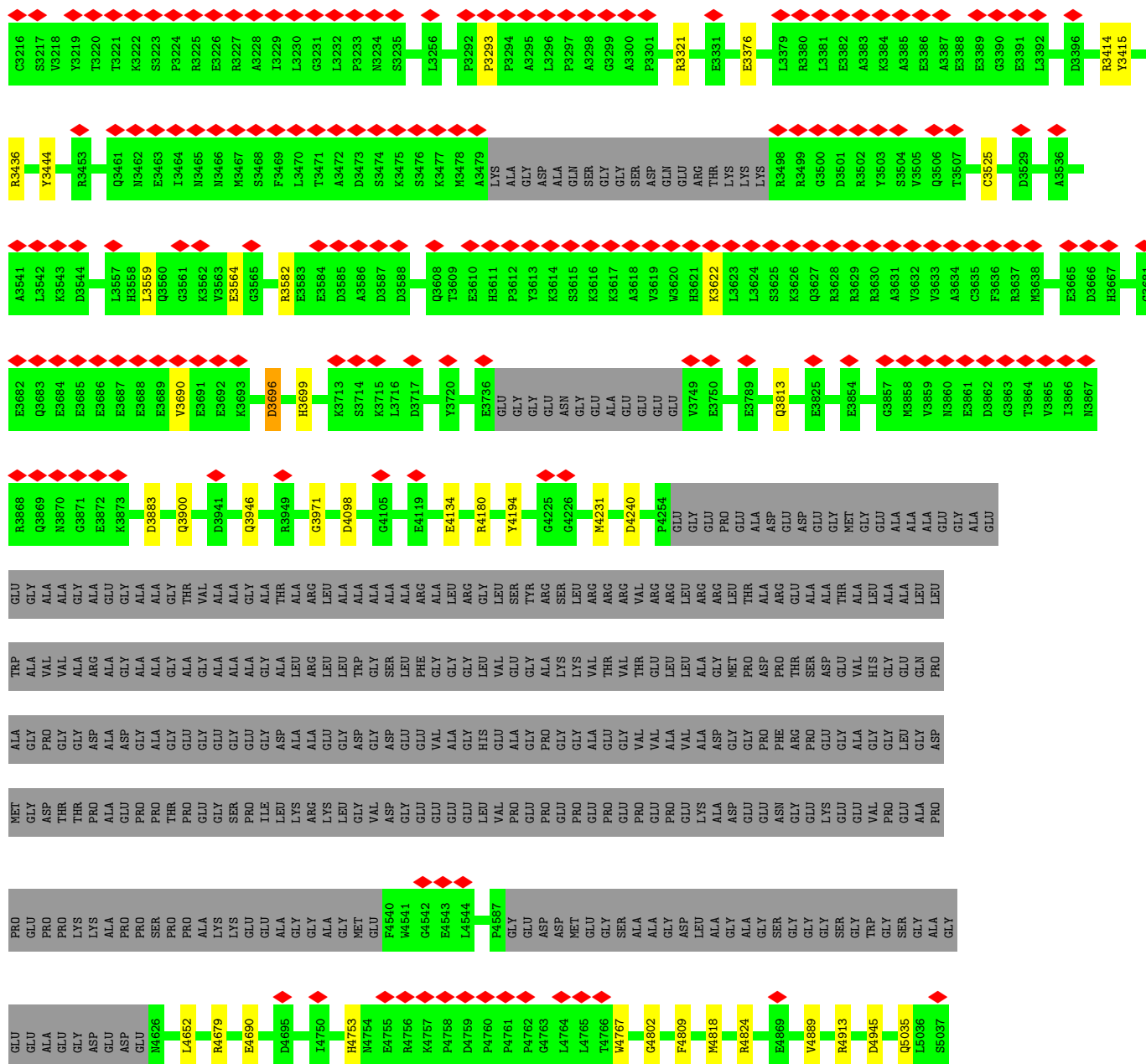




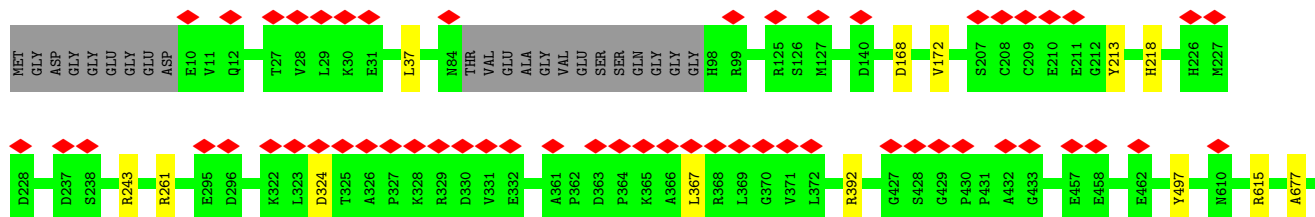
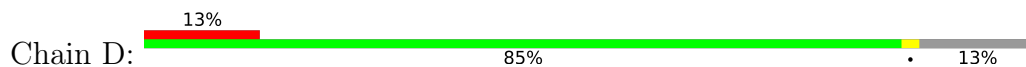
• Molecule 1: Ryanodine receptor 1



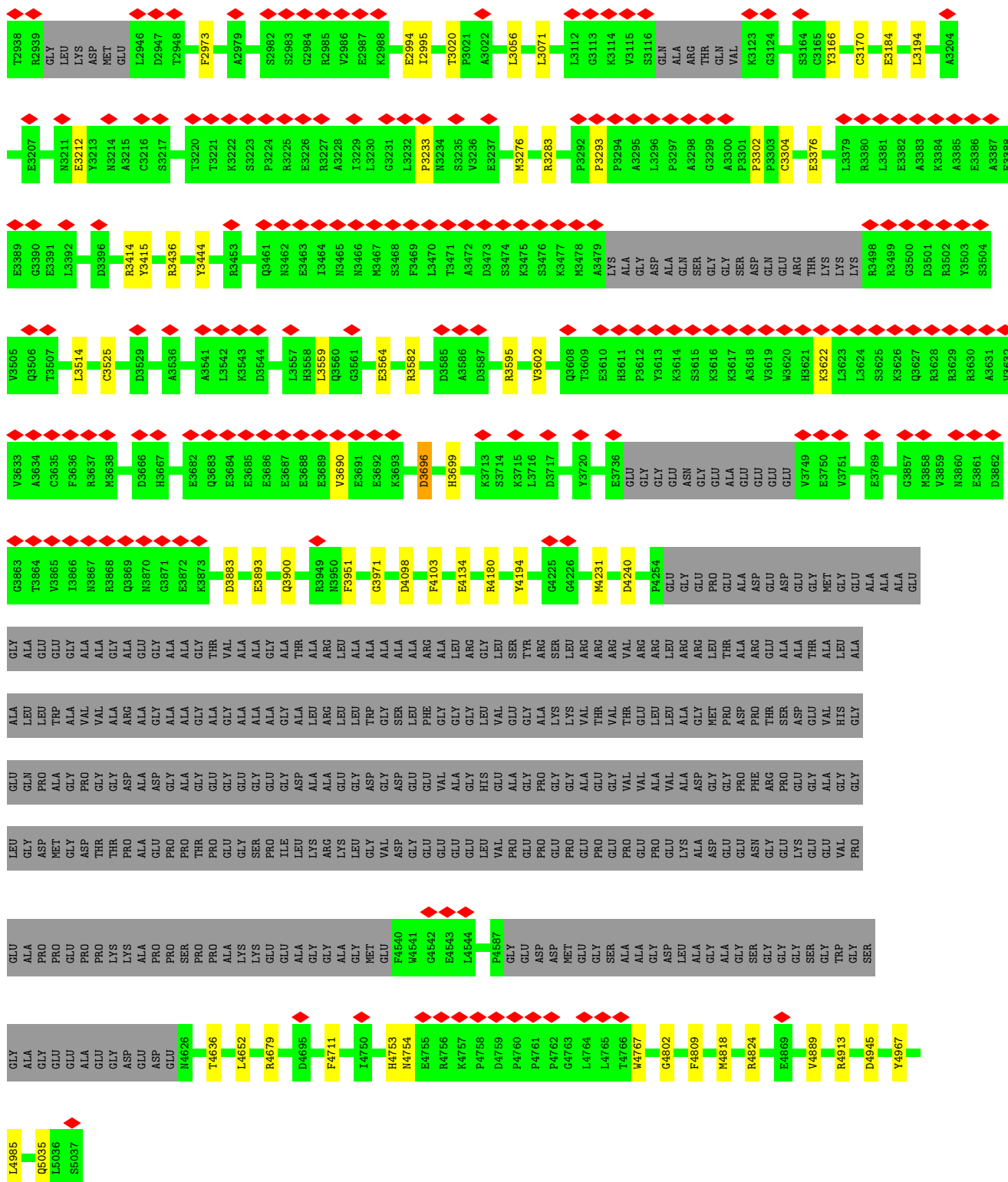




● Molecule 1: Ryanodine receptor 1







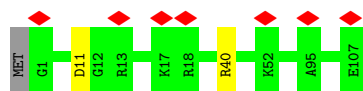
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





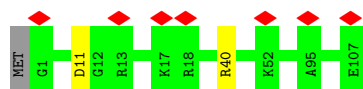
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 6% 97% ..



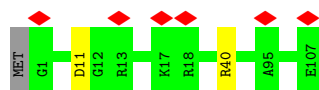
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 6% 97% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 6% 97% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	69502	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 ($e^-/\text{\AA}^2$)	67.44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	16.338	Depositor
Minimum map value	0.000	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.293	Depositor
Recommended contour level	1	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, CA, CFF, ACP, 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	0.76	0/35885	1.29	54/48603 (0.1%)
1	B	0.76	0/35885	1.29	55/48603 (0.1%)
1	C	0.76	0/35885	1.29	54/48603 (0.1%)
1	D	0.76	0/35885	1.30	46/48603 (0.1%)
2	E	0.78	0/851	1.36	2/1146 (0.2%)
2	F	0.79	0/851	1.37	2/1146 (0.2%)
2	G	0.78	0/851	1.37	2/1146 (0.2%)
2	H	0.78	0/851	1.37	2/1146 (0.2%)
All	All	0.76	0/146944	1.30	217/198996 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	14
1	C	0	12
1	D	0	11
All	All	0	51

There are no bond length outliers.

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2797	PHE	CA-CB-CG	8.93	122.73	113.80
1	B	2797	PHE	CA-CB-CG	8.93	122.73	113.80
1	C	2797	PHE	CA-CB-CG	8.80	122.60	113.80
1	D	2797	PHE	CA-CB-CG	8.14	121.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	615	ARG	N-CA-C	7.76	119.82	111.36
1	D	3293	PRO	N-CA-C	7.18	119.46	110.70
1	B	3293	PRO	N-CA-C	7.10	119.36	110.70
1	A	3293	PRO	N-CA-C	7.09	119.35	110.70
1	C	3293	PRO	N-CA-C	7.06	119.31	110.70
1	C	615	ARG	N-CA-C	6.97	120.26	111.69
1	B	615	ARG	N-CA-C	6.96	120.25	111.69
1	A	615	ARG	N-CA-C	6.92	120.20	111.69
1	D	3436	ARG	NE-CZ-NH2	6.64	125.17	119.20
1	B	2355	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	B	3696	ASP	CA-CB-CG	6.46	119.06	112.60
1	C	2355	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	C	3436	ARG	NE-CZ-NH2	6.36	124.93	119.20
1	B	3436	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	A	3436	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	B	4098	ASP	CA-CB-CG	6.22	118.83	112.60
1	D	4098	ASP	CA-CB-CG	6.20	118.80	112.60
1	C	3696	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	4098	ASP	CA-CB-CG	6.16	118.76	112.60
1	D	261	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	A	4753	HIS	CA-CB-CG	6.08	119.88	113.80
1	B	1275	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	D	324	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	1813	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	C	1748	PHE	CA-C-N	6.03	124.06	119.66
1	C	1748	PHE	C-N-CA	6.03	124.06	119.66
2	F	11	ASP	CA-CB-CG	6.03	118.62	112.60
2	E	11	ASP	CA-CB-CG	6.02	118.62	112.60
2	G	11	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	1813	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	C	1275	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	1813	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	1275	ARG	NE-CZ-NH2	5.99	124.59	119.20
2	H	11	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	4098	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	261	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	C	1813	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	D	4753	HIS	CA-CB-CG	5.91	119.71	113.80
1	C	4753	HIS	CA-CB-CG	5.89	119.69	113.80
1	C	261	ARG	NE-CZ-NH2	5.87	124.49	119.20
1	D	1275	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	B	261	ARG	NE-CZ-NH2	5.83	124.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1748	PHE	CA-C-N	5.83	123.92	119.66
1	B	1748	PHE	C-N-CA	5.83	123.92	119.66
1	A	1748	PHE	CA-C-N	5.79	123.89	119.66
1	A	1748	PHE	C-N-CA	5.79	123.89	119.66
1	B	4753	HIS	CA-CB-CG	5.75	119.55	113.80
1	B	3883	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	3883	ASP	CA-CB-CG	5.73	118.33	112.60
1	D	2593	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	3883	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	3883	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	1736	VAL	N-CA-C	5.64	114.16	107.73
1	C	3813	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	4103	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	1736	VAL	N-CA-C	5.61	114.12	107.73
1	D	3696	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	3900	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	C	1736	VAL	N-CA-C	5.59	114.10	107.73
2	H	40	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	B	3813	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	C	151	HIS	CA-C-N	5.58	125.55	120.03
1	C	151	HIS	C-N-CA	5.58	125.55	120.03
1	D	2795	LYS	N-CA-C	5.58	118.08	111.33
1	C	3900	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	C	3321	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	3900	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	D	3414	ARG	NE-CZ-NH2	5.56	124.21	119.20
1	A	3414	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	2593	ARG	NE-CZ-NH2	5.55	124.20	119.20
2	G	40	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	A	3696	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	2575	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	B	869	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	D	2738	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	C	2593	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	2738	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	324	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	1736	VAL	N-CA-C	5.49	113.99	107.73
1	D	4945	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	869	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	3321	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	D	4103	PHE	CA-CB-CG	5.47	119.27	113.80
2	E	40	ARG	NE-CZ-NH2	5.47	124.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	2738	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	A	2973	PHE	CA-CB-CG	5.45	119.25	113.80
1	C	869	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	4945	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	1101	ARG	NE-CZ-NH2	5.43	124.09	119.20
2	F	40	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	2593	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	D	2244	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	1101	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	4945	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	2136	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	2738	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	3321	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	3414	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	C	4945	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	2575	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	B	1101	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	D	1101	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	C	2136	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	2136	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	C	3414	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	2575	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	D	2973	PHE	CA-CB-CG	5.37	119.17	113.80
1	D	1017	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	2973	PHE	CA-CB-CG	5.36	119.16	113.80
1	D	3900	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	C	2575	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	243	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	324	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	243	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	243	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	2973	PHE	CA-CB-CG	5.31	119.11	113.80
1	D	2126	ARG	NE-CZ-NH2	5.31	123.97	119.20
1	A	2385	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	3582	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	C	4240	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	1076	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	3813	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	D	4240	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	4240	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	1017	ARG	NE-CZ-NH2	5.25	123.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2584	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	B	3582	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	1076	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	D	3595	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	1017	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	3582	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	D	2584	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	2355	ARG	CD-NE-CZ	5.23	131.73	124.40
1	B	2600	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	3946	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	4240	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	1017	ARG	NE-CZ-NH2	5.22	123.89	119.20
1	B	2385	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	1076	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	2355	ARG	CD-NE-CZ	5.20	131.68	124.40
1	C	2600	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	4690	GLU	N-CA-C	5.20	118.08	111.69
1	D	2167	ILE	CB-CA-C	5.19	119.81	111.29
1	B	3271	GLU	N-CA-C	5.19	118.08	111.69
1	C	4824	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	3271	GLU	N-CA-C	5.18	118.06	111.69
1	C	3946	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	4824	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	1478	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	2588	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	B	1076	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	C	3582	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	2629	ASP	CA-C-N	5.16	123.49	120.24
1	B	2629	ASP	C-N-CA	5.16	123.49	120.24
1	D	243	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	B	2588	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	C	3093	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	C	1478	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	242	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	C	593	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	C	1646	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	4824	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	2629	ASP	CA-C-N	5.12	123.47	120.24
1	D	2629	ASP	C-N-CA	5.12	123.47	120.24
1	C	1068	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	2600	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	4824	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1646	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	3946	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	D	1478	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	2806	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	3699	HIS	CB-CG-CD2	-5.11	124.55	131.20
1	B	2806	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	2584	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	904	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	904	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	3699	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	A	1068	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	904	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	2806	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	392	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	2588	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	C	2629	ASP	CA-C-N	5.08	123.44	120.24
1	C	2629	ASP	C-N-CA	5.08	123.44	120.24
1	A	593	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	B	593	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	D	3893	GLU	N-CA-CB	-5.08	103.39	110.29
1	C	2516	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	2584	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	4690	GLU	N-CA-C	5.07	117.93	111.69
1	D	3699	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	1646	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	1068	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	3595	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	D	904	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	B	1478	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	2588	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	2629	ASP	CA-C-N	5.03	123.41	120.24
1	A	2629	ASP	C-N-CA	5.03	123.41	120.24
1	B	242	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	2716	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	3699	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	242	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	4103	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	4690	GLU	N-CA-C	5.03	117.87	111.69
1	A	1646	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	4548	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	D	2041	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	2167	ILE	CB-CA-C	5.01	119.51	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	392	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	D	3233	PRO	CA-C-N	5.01	127.24	120.38
1	D	3233	PRO	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2199	ARG	Sidechain
1	A	2355	ARG	Sidechain
1	A	2452	ARG	Sidechain
1	A	2553	TYR	Sidechain
1	A	2593	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	3415	TYR	Sidechain
1	A	3444	TYR	Sidechain
1	A	4180	ARG	Sidechain
1	A	4194	TYR	Sidechain
1	A	4913	ARG	Sidechain
1	A	4967	TYR	Sidechain
1	A	497	TYR	Sidechain
1	A	897	ARG	Sidechain
1	B	2199	ARG	Sidechain
1	B	2452	ARG	Sidechain
1	B	2553	TYR	Sidechain
1	B	2593	ARG	Sidechain
1	B	2761	TYR	Sidechain
1	B	281	ARG	Sidechain
1	B	3415	TYR	Sidechain
1	B	3444	TYR	Sidechain
1	B	4180	ARG	Sidechain
1	B	4194	TYR	Sidechain
1	B	4913	ARG	Sidechain
1	B	4967	TYR	Sidechain
1	B	497	TYR	Sidechain
1	B	897	ARG	Sidechain
1	C	2199	ARG	Sidechain
1	C	2452	ARG	Sidechain
1	C	2553	TYR	Sidechain
1	C	2593	ARG	Sidechain
1	C	281	ARG	Sidechain
1	C	3415	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	3444	TYR	Sidechain
1	C	4180	ARG	Sidechain
1	C	4194	TYR	Sidechain
1	C	4913	ARG	Sidechain
1	C	497	TYR	Sidechain
1	C	897	ARG	Sidechain
1	D	2199	ARG	Sidechain
1	D	2452	ARG	Sidechain
1	D	3166	TYR	Sidechain
1	D	3283	ARG	Sidechain
1	D	3415	TYR	Sidechain
1	D	3444	TYR	Sidechain
1	D	4180	ARG	Sidechain
1	D	4194	TYR	Sidechain
1	D	4913	ARG	Sidechain
1	D	4967	TYR	Sidechain
1	D	497	TYR	Sidechain

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	35088	34734	34715	7	0
1	B	35088	34734	34715	8	0
1	C	35088	34734	34715	6	0
1	D	35088	34734	34715	10	0
2	E	832	829	831	0	0
2	F	832	829	831	0	0
2	G	832	829	831	0	0
2	H	832	829	831	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	14	14	1	0
5	B	31	14	14	1	0
5	C	31	14	14	0	0
5	D	31	14	14	1	0
6	A	14	10	10	0	0
6	B	14	10	10	0	0
6	C	14	10	10	0	0
6	D	14	10	10	0	0
7	A	104	164	164	0	0
7	B	104	164	164	0	0
7	C	104	164	164	0	0
7	D	104	164	164	0	0
All	All	144284	143004	142936	31	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 0.

All (31) 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:C:4231:MET:HA	1:C:4231:MET:HE2	1.87	0.56
1:B:4231:MET:HA	1:B:4231:MET:HE2	1.87	0.56
1:A:4231:MET:HA	1:A:4231:MET:HE2	1.87	0.55
1:D:4231:MET:HE2	1:D:4231:MET:HA	1.87	0.55
1:D:3194:LEU:HD21	1:D:3276:MET:HE2	1.92	0.52
1:C:1931:LEU:HD22	1:C:1931:LEU:H	1.80	0.46
1:C:1452:TRP:CD1	1:C:1527:MET:CE	3.00	0.45
1:D:1452:TRP:CD1	1:D:1527:MET:CE	3.00	0.44
1:A:1452:TRP:CD1	1:A:1527:MET:CE	3.00	0.44
1:A:1931:LEU:H	1:A:1931:LEU:HD22	1.83	0.44
1:B:1931:LEU:H	1:B:1931:LEU:HD22	1.83	0.44
1:D:1931:LEU:H	1:D:1931:LEU:HD22	1.83	0.43
1:B:1452:TRP:CD1	1:B:1527:MET:CE	3.01	0.43
1:A:4802:GLY:HA3	1:A:4809:PHE:CE2	2.54	0.43
1:B:4679:ARG:HH21	1:B:4679:ARG:HG2	1.84	0.43
1:A:4679:ARG:HG2	1:A:4679:ARG:HH21	1.84	0.42
1:C:4818:MET:C	1:C:4818:MET:SD	3.03	0.42
1:B:4985:LEU:H	5:B:5103:ACP:HN61	1.68	0.42
1:D:4818:MET:SD	1:D:4818:MET:C	3.03	0.42
1:C:4679:ARG:HH21	1:C:4679:ARG:HG2	1.84	0.42
1:D:4679:ARG:HG2	1:D:4679:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4802:GLY:HA3	1:B:4809:PHE:CE2	2.55	0.42
1:D:4802:GLY:HA3	1:D:4809:PHE:CE2	2.54	0.42
1:A:4985:LEU:H	5:A:5103:ACP:HN61	1.68	0.42
1:C:4802:GLY:HA3	1:C:4809:PHE:CE2	2.55	0.42
1:A:4818:MET:C	1:A:4818:MET:SD	3.02	0.41
1:B:4818:MET:C	1:B:4818:MET:SD	3.02	0.41
1:B:4134:GLU:H	1:B:4135:PRO:HD2	1.85	0.41
1:D:4711:PHE:CD1	1:D:4711:PHE:C	2.99	0.41
1:D:4985:LEU:H	5:D:5103:ACP:HN61	1.67	0.41
1:D:3514:LEU:HD21	1:D:3602:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	4195 (96%)	167 (4%)	14 (0%)	36	68
1	B	4376/5037 (87%)	4187 (96%)	178 (4%)	11 (0%)	36	68
1	C	4376/5037 (87%)	4193 (96%)	173 (4%)	10 (0%)	43	73
1	D	4376/5037 (87%)	4190 (96%)	173 (4%)	13 (0%)	36	68
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17924/20580 (87%)	17173 (96%)	703 (4%)	48 (0%)	37	68

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	A	2663	ASN
1	B	213	TYR
1	C	213	TYR
1	D	213	TYR
1	A	972	LEU
1	A	3622	LYS
1	A	4134	GLU
1	B	972	LEU
1	B	2663	ASN
1	B	3622	LYS
1	B	4134	GLU
1	C	972	LEU
1	C	2663	ASN
1	C	3622	LYS
1	C	4134	GLU
1	D	677	ALA
1	D	972	LEU
1	D	2663	ASN
1	D	3622	LYS
1	D	4134	GLU
1	A	2092	GLN
1	A	2750	LYS
1	B	2092	GLN
1	B	2750	LYS
1	C	2092	GLN
1	C	2750	LYS
1	D	2092	GLN
1	D	3690	VAL
1	A	226	HIS
1	A	2572	THR
1	A	3735	LEU
1	C	361	ALA
1	D	2413	GLU
1	D	2750	LYS
1	D	3304	CYS
1	A	361	ALA
1	B	361	ALA
1	C	3690	VAL
1	D	3302	PRO
1	B	3690	VAL
1	A	3233	PRO
1	B	3971	GLY

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Mol	Chain	Res	Type
1	C	3971	GLY
1	A	3690	VAL
1	A	3971	GLY
1	B	3233	PRO
1	D	3971	GLY

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	3827/4276 (90%)	3791 (99%)	36 (1%)	70	81
1	B	3827/4276 (90%)	3788 (99%)	39 (1%)	68	80
1	C	3827/4276 (90%)	3789 (99%)	38 (1%)	68	80
1	D	3827/4276 (90%)	3784 (99%)	43 (1%)	65	79
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15664/17464 (90%)	15508 (99%)	156 (1%)	65	80

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	A	172	VAL
1	A	218	HIS
1	A	676	THR
1	A	689	THR
1	A	910	PHE
1	A	953	THR
1	A	1021	LEU
1	A	1435	TYR
1	A	1713	ASP

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Mol	Chain	Res	Type
1	A	1931	LEU
1	A	1963	GLU
1	A	2088	GLU
1	A	2157	GLU
1	A	2168	VAL
1	A	2224	ARG
1	A	2386	ILE
1	A	2509	VAL
1	A	2545	GLU
1	A	2635	GLU
1	A	2644	LEU
1	A	2694	GLU
1	A	2880	GLU
1	A	2994	GLU
1	A	3020	THR
1	A	3056	LEU
1	A	3170	CYS
1	A	3376	GLU
1	A	3525	CYS
1	A	3564	GLU
1	A	3696	ASP
1	A	4636	THR
1	A	4652	LEU
1	A	4767	TRP
1	A	4889	VAL
1	A	5035	GLN
1	B	168	ASP
1	B	172	VAL
1	B	218	HIS
1	B	676	THR
1	B	689	THR
1	B	832	GLU
1	B	910	PHE
1	B	950	LEU
1	B	953	THR
1	B	1021	LEU
1	B	1435	TYR
1	B	1713	ASP
1	B	1931	LEU
1	B	1963	GLU
1	B	2088	GLU
1	B	2157	GLU

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Mol	Chain	Res	Type
1	B	2168	VAL
1	B	2224	ARG
1	B	2386	ILE
1	B	2509	VAL
1	B	2545	GLU
1	B	2635	GLU
1	B	2644	LEU
1	B	2880	GLU
1	B	2994	GLU
1	B	3020	THR
1	B	3056	LEU
1	B	3170	CYS
1	B	3376	GLU
1	B	3525	CYS
1	B	3559	LEU
1	B	3564	GLU
1	B	3696	ASP
1	B	4211	LYS
1	B	4636	THR
1	B	4754	ASN
1	B	4767	TRP
1	B	4889	VAL
1	B	5035	GLN
1	C	155	LYS
1	C	168	ASP
1	C	172	VAL
1	C	218	HIS
1	C	676	THR
1	C	689	THR
1	C	953	THR
1	C	1021	LEU
1	C	1435	TYR
1	C	1713	ASP
1	C	1931	LEU
1	C	1963	GLU
1	C	1995	THR
1	C	2088	GLU
1	C	2157	GLU
1	C	2168	VAL
1	C	2386	ILE
1	C	2414	ASN
1	C	2509	VAL

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Mol	Chain	Res	Type
1	C	2545	GLU
1	C	2635	GLU
1	C	2644	LEU
1	C	2694	GLU
1	C	2880	GLU
1	C	2994	GLU
1	C	2995	ILE
1	C	3020	THR
1	C	3056	LEU
1	C	3170	CYS
1	C	3376	GLU
1	C	3525	CYS
1	C	3559	LEU
1	C	3564	GLU
1	C	3696	ASP
1	C	4652	LEU
1	C	4767	TRP
1	C	4889	VAL
1	C	5035	GLN
1	D	37	LEU
1	D	168	ASP
1	D	172	VAL
1	D	218	HIS
1	D	367	LEU
1	D	689	THR
1	D	961	MET
1	D	1435	TYR
1	D	1603	VAL
1	D	1721	GLU
1	D	1733	GLU
1	D	1931	LEU
1	D	2088	GLU
1	D	2157	GLU
1	D	2168	VAL
1	D	2169	GLN
1	D	2509	VAL
1	D	2545	GLU
1	D	2635	GLU
1	D	2644	LEU
1	D	2694	GLU
1	D	2763	HIS
1	D	2880	GLU

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Mol	Chain	Res	Type
1	D	2994	GLU
1	D	2995	ILE
1	D	3020	THR
1	D	3056	LEU
1	D	3071	LEU
1	D	3170	CYS
1	D	3184	GLU
1	D	3212	GLU
1	D	3376	GLU
1	D	3525	CYS
1	D	3559	LEU
1	D	3564	GLU
1	D	3696	ASP
1	D	3951	PHE
1	D	4636	THR
1	D	4652	LEU
1	D	4754	ASN
1	D	4767	TRP
1	D	4889	VAL
1	D	5035	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	278	GLN
1	A	581	ASN
1	A	617	ASN
1	A	838	HIS
1	A	921	ASN
1	A	1035	ASN
1	A	1158	ASN
1	A	1220	GLN
1	A	1563	GLN
1	A	1629	GLN
1	A	1631	GLN
1	A	1719	HIS
1	A	1756	ASN
1	A	1824	GLN
1	A	1973	GLN
1	A	2005	GLN
1	A	2487	GLN

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Mol	Chain	Res	Type
1	A	2780	ASN
1	A	2993	GLN
1	A	3109	ASN
1	A	3127	GLN
1	A	3450	ASN
1	A	3466	ASN
1	A	3611	HIS
1	A	3867	ASN
1	A	4094	GLN
1	A	4102	GLN
1	A	4574	ASN
1	A	4662	ASN
1	B	57	ASN
1	B	278	GLN
1	B	383	HIS
1	B	581	ASN
1	B	812	HIS
1	B	838	HIS
1	B	921	ASN
1	B	1220	GLN
1	B	1563	GLN
1	B	1629	GLN
1	B	1631	GLN
1	B	1719	HIS
1	B	1756	ASN
1	B	1824	GLN
1	B	1973	GLN
1	B	2005	GLN
1	B	2487	GLN
1	B	2756	ASN
1	B	2780	ASN
1	B	2993	GLN
1	B	3109	ASN
1	B	3450	ASN
1	B	3457	ASN
1	B	3466	ASN
1	B	3611	HIS
1	B	3897	ASN
1	B	4094	GLN
1	B	4162	ASN
1	B	4574	ASN
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	278	GLN
1	C	383	HIS
1	C	581	ASN
1	C	812	HIS
1	C	838	HIS
1	C	921	ASN
1	C	1058	GLN
1	C	1158	ASN
1	C	1563	GLN
1	C	1629	GLN
1	C	1631	GLN
1	C	1719	HIS
1	C	1824	GLN
1	C	1973	GLN
1	C	2005	GLN
1	C	2487	GLN
1	C	2744	ASN
1	C	2756	ASN
1	C	2763	HIS
1	C	2780	ASN
1	C	2993	GLN
1	C	3109	ASN
1	C	3127	GLN
1	C	3466	ASN
1	C	3611	HIS
1	C	3867	ASN
1	C	3889	GLN
1	C	3897	ASN
1	C	3960	GLN
1	C	4094	GLN
1	C	4574	ASN
1	D	32	GLN
1	D	57	ASN
1	D	278	GLN
1	D	379	HIS
1	D	581	ASN
1	D	624	ASN
1	D	812	HIS
1	D	838	HIS
1	D	921	ASN
1	D	1133	HIS
1	D	1220	GLN

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Mol	Chain	Res	Type
1	D	1563	GLN
1	D	1629	GLN
1	D	1631	GLN
1	D	1719	HIS
1	D	1756	ASN
1	D	1824	GLN
1	D	1953	HIS
1	D	2284	ASN
1	D	2744	ASN
1	D	2780	ASN
1	D	2961	GLN
1	D	2962	GLN
1	D	2993	GLN
1	D	3109	ASN
1	D	3450	ASN
1	D	3456	GLN
1	D	3457	ASN
1	D	3466	ASN
1	D	3867	ASN
1	D	3897	ASN
1	D	3927	GLN
1	D	4574	ASN
2	E	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	5104	-	15,15,15	0.83	0	23,23,23	0.99	1 (4%)
5	ACP	B	5103	-	30,33,33	1.37	3 (10%)	45,52,52	1.25	6 (13%)
7	POV	B	5106	-	51,51,51	0.70	0	57,59,59	0.48	0
7	POV	C	5105	-	51,51,51	0.66	0	57,59,59	0.64	1 (1%)
5	ACP	C	5103	-	30,33,33	1.39	4 (13%)	45,52,52	1.40	7 (15%)
5	ACP	A	5103	-	30,33,33	1.37	4 (13%)	45,52,52	1.47	8 (17%)
6	CFF	D	5104	-	15,15,15	0.84	0	23,23,23	1.00	2 (8%)
7	POV	B	5105	-	51,51,51	0.65	0	57,59,59	0.63	1 (1%)
7	POV	C	5106	-	51,51,51	0.72	0	57,59,59	0.48	0
7	POV	D	5105	-	51,51,51	0.66	0	57,59,59	0.66	1 (1%)
6	CFF	C	5102	-	15,15,15	0.82	0	23,23,23	1.00	1 (4%)
7	POV	A	5105	-	51,51,51	0.67	0	57,59,59	0.63	1 (1%)
7	POV	A	5106	-	51,51,51	0.71	0	57,59,59	0.48	0
5	ACP	D	5103	-	30,33,33	1.37	3 (10%)	45,52,52	1.36	8 (17%)
6	CFF	A	5104	-	15,15,15	0.83	0	23,23,23	0.97	1 (4%)
7	POV	D	5106	-	51,51,51	0.69	0	57,59,59	0.49	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
6	CFF	B	5104	-	-	-	0/2/2/2
5	ACP	B	5103	-	-	7/19/38/38	0/3/3/3
7	POV	B	5106	-	-	16/55/55/55	-
6	CFF	A	5104	-	-	-	0/2/2/2
5	ACP	C	5103	-	-	1/19/38/38	0/3/3/3
5	ACP	A	5103	-	-	5/19/38/38	0/3/3/3
7	POV	B	5105	-	-	13/55/55/55	-
7	POV	C	5106	-	-	15/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	D	5105	-	-	15/55/55/55	-
6	CFF	D	5104	-	-	-	0/2/2/2
7	POV	A	5105	-	-	13/55/55/55	-
7	POV	A	5106	-	-	14/55/55/55	-
6	CFF	C	5102	-	-	-	0/2/2/2
5	ACP	D	5103	-	-	7/19/38/38	0/3/3/3
7	POV	C	5105	-	-	14/55/55/55	-
7	POV	D	5106	-	-	12/55/55/55	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5103	ACP	PB-O2B	-3.21	1.48	1.56
5	A	5103	ACP	PB-O2B	-3.13	1.49	1.56
5	C	5103	ACP	PG-O3G	-3.12	1.47	1.54
5	C	5103	ACP	PG-O2G	-3.10	1.47	1.54
5	C	5103	ACP	PB-O2B	-3.07	1.49	1.56
5	D	5103	ACP	PB-O2B	-3.06	1.49	1.56
5	A	5103	ACP	PG-O3G	-3.05	1.47	1.54
5	B	5103	ACP	PG-O2G	-3.03	1.48	1.54
5	A	5103	ACP	PG-O2G	-2.85	1.48	1.54
5	D	5103	ACP	PG-O2G	-2.82	1.48	1.54
5	D	5103	ACP	PG-O3G	-2.82	1.48	1.54
5	B	5103	ACP	PG-O3G	-2.71	1.48	1.54
5	C	5103	ACP	C5-C4	-2.11	1.35	1.39
5	A	5103	ACP	C5-C4	-2.09	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5103	ACP	O3G-PG-C3B	4.18	116.54	106.40
5	C	5103	ACP	O2G-PG-C3B	3.45	114.76	106.40
5	C	5103	ACP	C4-C5-N7	3.12	114.42	110.62
5	D	5103	ACP	O1B-PB-C3B	3.12	117.32	109.07
5	A	5103	ACP	C4-C5-N7	3.10	114.39	110.62
5	D	5103	ACP	C5-C4-N3	-2.98	122.86	126.75
5	C	5103	ACP	PB-O3A-PA	-2.96	123.18	132.56
5	B	5103	ACP	C5-C4-N3	-2.92	122.94	126.75
7	D	5105	POV	C2-O21-C21	2.89	124.92	117.79
5	D	5103	ACP	C4-C5-N7	2.88	114.13	110.62
5	B	5103	ACP	C4-C5-N7	2.85	114.09	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5103	ACP	C5-C4-N3	-2.77	123.14	126.75
7	C	5105	POV	C2-O21-C21	2.68	124.39	117.79
7	B	5105	POV	C2-O21-C21	2.63	124.28	117.79
5	D	5103	ACP	O1G-PG-C3B	2.61	116.87	111.24
5	B	5103	ACP	PB-O3A-PA	-2.61	124.29	132.56
7	A	5105	POV	C2-O21-C21	2.61	124.21	117.79
5	A	5103	ACP	PB-O3A-PA	-2.59	124.36	132.56
5	D	5103	ACP	C5-C6-N1	2.53	122.83	117.39
5	C	5103	ACP	C5-C4-N3	-2.53	123.45	126.75
5	C	5103	ACP	C5-C6-N1	2.53	122.82	117.39
5	B	5103	ACP	C5-C6-N1	2.50	122.76	117.39
5	A	5103	ACP	C5-C6-N1	2.48	122.72	117.39
6	D	5104	CFF	C12-N3-C2	2.39	121.50	117.31
6	B	5104	CFF	C12-N3-C2	2.32	121.38	117.31
5	C	5103	ACP	O3G-PG-O1G	-2.28	106.36	112.39
5	C	5103	ACP	C2-N1-C6	-2.27	114.88	118.77
5	A	5103	ACP	O1G-PG-C3B	-2.26	106.37	111.24
6	A	5104	CFF	C12-N3-C2	2.25	121.25	117.31
6	C	5102	CFF	C12-N3-C2	2.23	121.22	117.31
5	B	5103	ACP	C2-N1-C6	-2.23	114.94	118.77
5	D	5103	ACP	N6-C6-N1	-2.22	113.49	118.35
5	D	5103	ACP	C2-N1-C6	-2.19	115.00	118.77
5	B	5103	ACP	N6-C6-N1	-2.13	113.69	118.35
5	D	5103	ACP	PB-O3A-PA	-2.11	125.87	132.56
6	D	5104	CFF	C12-N3-C4	-2.07	117.52	120.69
5	A	5103	ACP	N6-C6-N1	-2.04	113.87	118.35
5	A	5103	ACP	C2-N1-C6	-2.01	115.31	118.77

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5103	ACP	PB-C3B-PG-O1G
5	A	5103	ACP	C4'-C5'-O5'-PA
5	B	5103	ACP	C5'-O5'-PA-O1A
5	B	5103	ACP	O4'-C4'-C5'-O5'
5	D	5103	ACP	PG-C3B-PB-O1B
5	D	5103	ACP	PG-C3B-PB-O2B
5	D	5103	ACP	PG-C3B-PB-O3A
5	D	5103	ACP	O4'-C4'-C5'-O5'
5	D	5103	ACP	C3'-C4'-C5'-O5'
7	A	5105	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
7	A	5105	POV	C22-C21-O21-C2
7	A	5105	POV	O22-C21-O21-C2
7	A	5106	POV	C11-O12-P-O14
7	B	5105	POV	O12-C11-C12-N
7	B	5105	POV	C22-C21-O21-C2
7	B	5105	POV	O22-C21-O21-C2
7	B	5106	POV	C11-O12-P-O14
7	C	5105	POV	O12-C11-C12-N
7	C	5105	POV	C22-C21-O21-C2
7	C	5105	POV	O22-C21-O21-C2
7	C	5106	POV	C11-O12-P-O14
7	D	5105	POV	O12-C11-C12-N
7	D	5105	POV	C22-C21-O21-C2
7	D	5105	POV	O22-C21-O21-C2
7	D	5106	POV	C11-O12-P-O14
5	B	5103	ACP	C3'-C4'-C5'-O5'
7	A	5106	POV	C311-C312-C313-C314
7	B	5106	POV	C311-C312-C313-C314
7	C	5106	POV	C311-C312-C313-C314
7	A	5106	POV	O21-C2-C3-O31
7	C	5106	POV	C33-C34-C35-C36
7	D	5106	POV	C33-C34-C35-C36
7	B	5106	POV	C11-O12-P-O11
5	D	5103	ACP	C4'-C5'-O5'-PA
7	B	5106	POV	C33-C34-C35-C36
7	B	5106	POV	C312-C313-C314-C315
7	B	5105	POV	C1-C2-C3-O31
7	A	5106	POV	C33-C34-C35-C36
7	C	5106	POV	C31-C32-C33-C34
7	C	5106	POV	C312-C313-C314-C315
7	D	5106	POV	C31-C32-C33-C34
7	A	5106	POV	C27-C28-C29-C210
7	C	5106	POV	C27-C28-C29-C210
7	B	5106	POV	O21-C2-C3-O31
7	C	5106	POV	O21-C2-C3-O31
7	D	5106	POV	O21-C2-C3-O31
7	A	5106	POV	C312-C313-C314-C315
7	B	5106	POV	C27-C28-C29-C210
7	D	5106	POV	C27-C28-C29-C210
7	B	5106	POV	C31-C32-C33-C34
7	C	5105	POV	C1-C2-C3-O31
7	D	5105	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
5	A	5103	ACP	PB-O3A-PA-O1A
7	A	5105	POV	O21-C2-C3-O31
7	B	5105	POV	O21-C2-C3-O31
7	C	5105	POV	O21-C2-C3-O31
7	D	5105	POV	O21-C2-C3-O31
5	B	5103	ACP	C4'-C5'-O5'-PA
5	C	5103	ACP	C4'-C5'-O5'-PA
7	A	5106	POV	C29-C210-C211-C212
7	B	5106	POV	C29-C210-C211-C212
7	C	5105	POV	C31-C32-C33-C34
7	A	5105	POV	C1-C2-C3-O31
7	C	5106	POV	C29-C210-C211-C212
7	D	5106	POV	C29-C210-C211-C212
5	B	5103	ACP	C5'-O5'-PA-O3A
7	A	5106	POV	C11-O12-P-O11
7	C	5106	POV	C11-O12-P-O11
7	A	5105	POV	C2-C1-O11-P
7	B	5105	POV	C2-C1-O11-P
7	C	5105	POV	C2-C1-O11-P
7	D	5105	POV	C2-C1-O11-P
5	B	5103	ACP	C5'-O5'-PA-O2A
7	A	5106	POV	C11-O12-P-O13
7	B	5106	POV	C11-O12-P-O13
7	C	5106	POV	C11-O12-P-O13
7	D	5106	POV	C11-O12-P-O13
7	A	5106	POV	C31-C32-C33-C34
7	A	5106	POV	C12-C11-O12-P
7	B	5106	POV	C12-C11-O12-P
7	C	5106	POV	C12-C11-O12-P
7	D	5106	POV	C12-C11-O12-P
5	A	5103	ACP	PB-C3B-PG-O2G
7	A	5106	POV	C1-C2-C3-O31
7	D	5106	POV	C1-C2-C3-O31
7	D	5106	POV	C39-C310-C311-C312
7	A	5105	POV	C11-O12-P-O11
7	B	5105	POV	C11-O12-P-O11
7	C	5105	POV	C11-O12-P-O11
7	D	5105	POV	C11-O12-P-O11
7	D	5106	POV	C11-O12-P-O11
7	B	5106	POV	C1-C2-C3-O31
7	C	5106	POV	C1-C2-C3-O31
7	A	5106	POV	C37-C38-C39-C310

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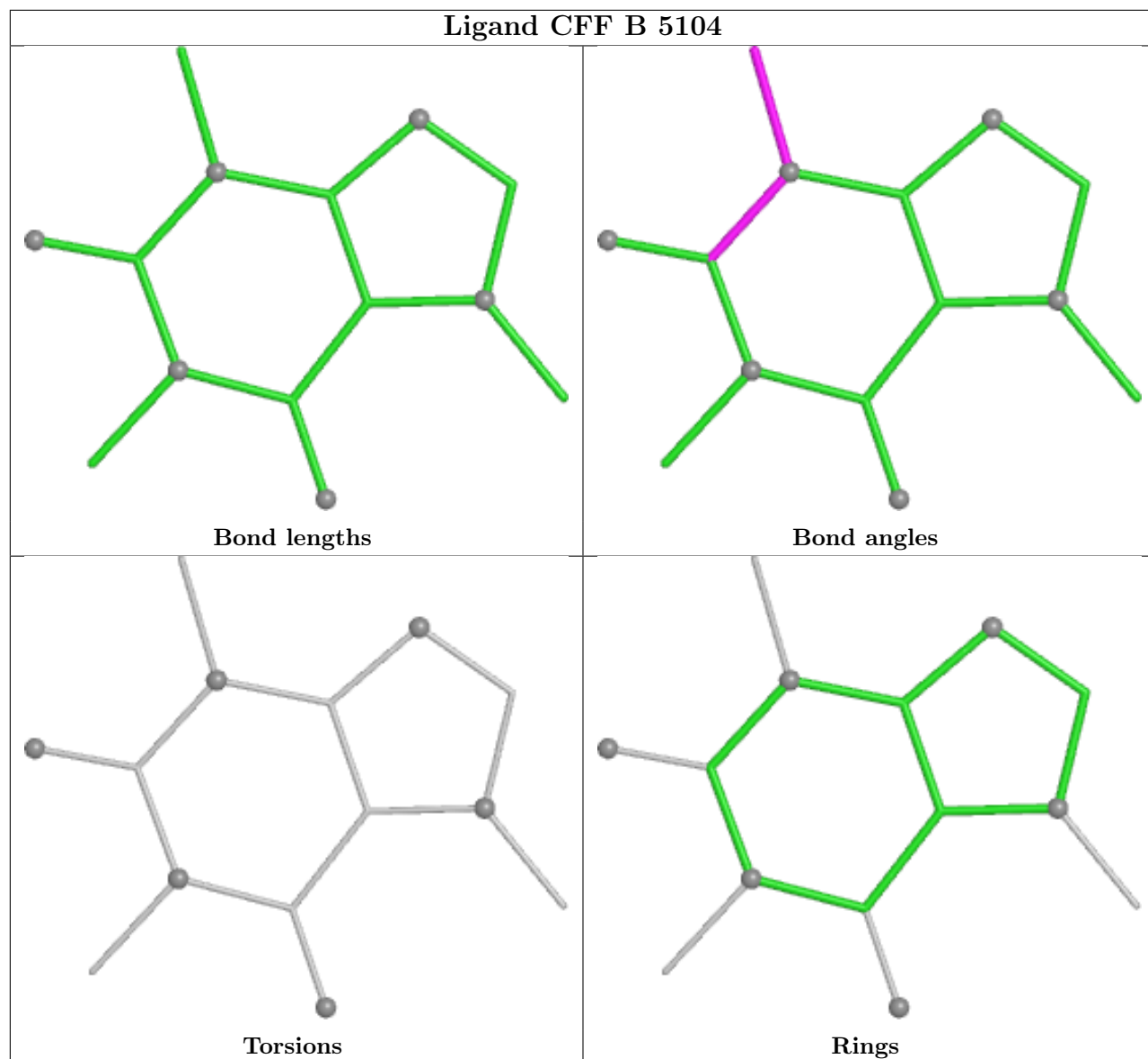
Mol	Chain	Res	Type	Atoms
7	D	5105	POV	C24-C25-C26-C27
7	D	5105	POV	C25-C26-C27-C28
5	B	5103	ACP	PB-O3A-PA-O2A
7	C	5106	POV	C37-C38-C39-C310
7	B	5106	POV	C37-C38-C39-C310
7	A	5105	POV	C31-C32-C33-C34
7	D	5105	POV	C31-C32-C33-C34
7	B	5106	POV	O11-C1-C2-C3
7	C	5106	POV	O11-C1-C2-C3
7	D	5105	POV	C34-C35-C36-C37
7	C	5105	POV	C25-C26-C27-C28
7	A	5105	POV	C34-C35-C36-C37
7	B	5106	POV	C26-C27-C28-C29
7	B	5106	POV	O11-C1-C2-O21
7	C	5106	POV	O11-C1-C2-O21
7	C	5105	POV	C34-C35-C36-C37
7	D	5105	POV	C37-C38-C39-C310
7	C	5105	POV	C24-C25-C26-C27
7	A	5106	POV	O11-C1-C2-C3
7	D	5106	POV	O11-C1-C2-C3
7	C	5105	POV	O31-C31-C32-C33
7	B	5105	POV	C24-C25-C26-C27
7	D	5105	POV	O31-C31-C32-C33
5	A	5103	ACP	C5'-O5'-PA-O3A
5	D	5103	ACP	C5'-O5'-PA-O3A
7	B	5105	POV	C34-C35-C36-C37
7	A	5105	POV	C24-C25-C26-C27
7	B	5105	POV	C25-C26-C27-C28
7	A	5105	POV	O31-C31-C32-C33
7	A	5105	POV	C12-C11-O12-P
7	B	5105	POV	C12-C11-O12-P
7	C	5105	POV	C12-C11-O12-P
7	D	5105	POV	C12-C11-O12-P
7	B	5105	POV	C37-C38-C39-C310
7	C	5105	POV	O32-C31-C32-C33
7	D	5105	POV	O32-C31-C32-C33
7	A	5105	POV	C37-C38-C39-C310
7	B	5105	POV	O31-C31-C32-C33

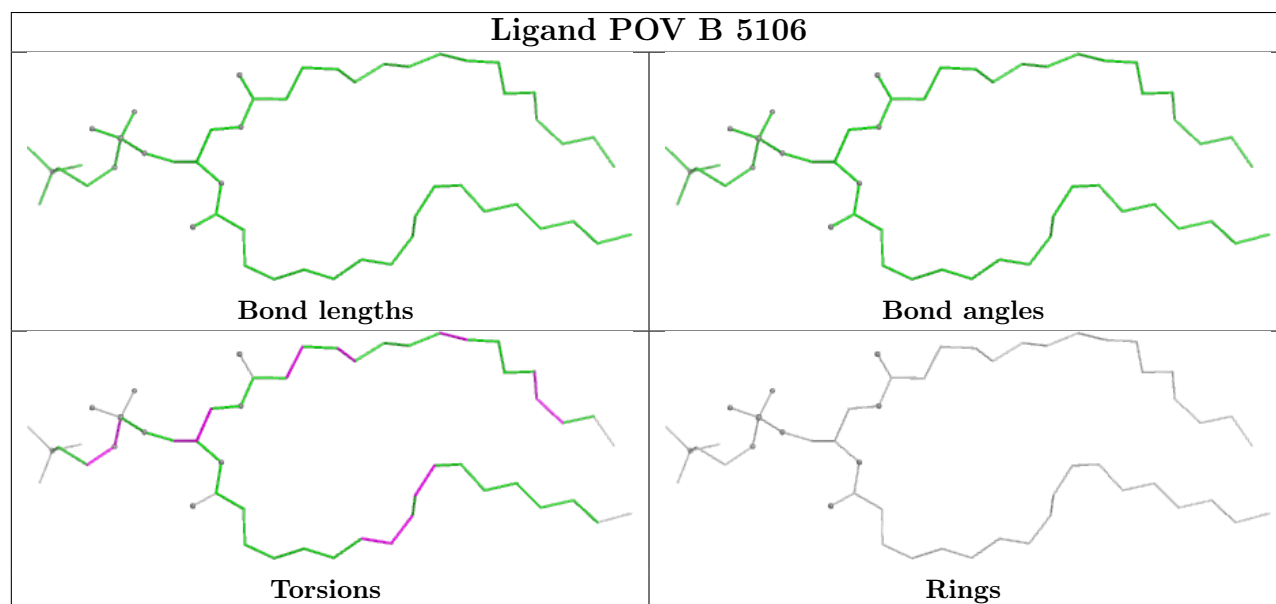
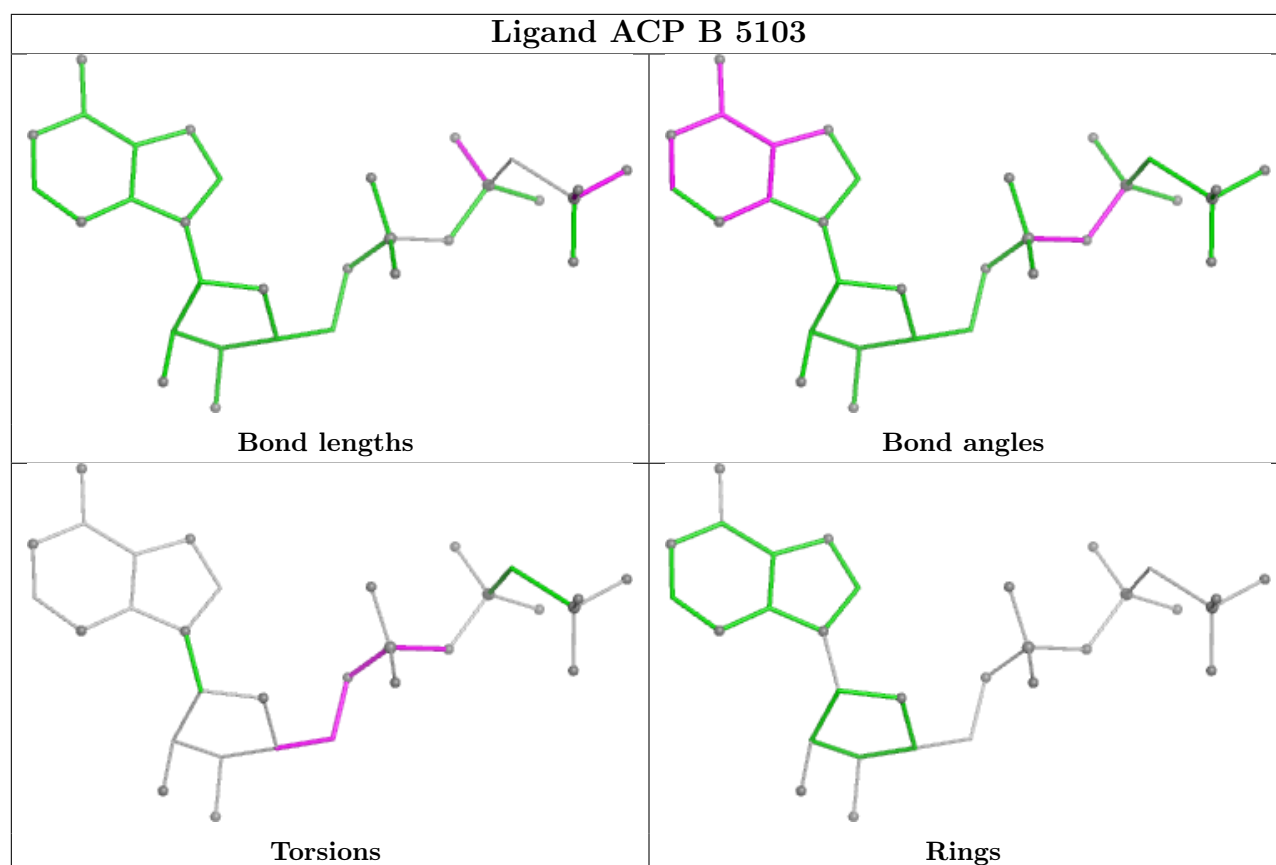
There are no ring outliers.

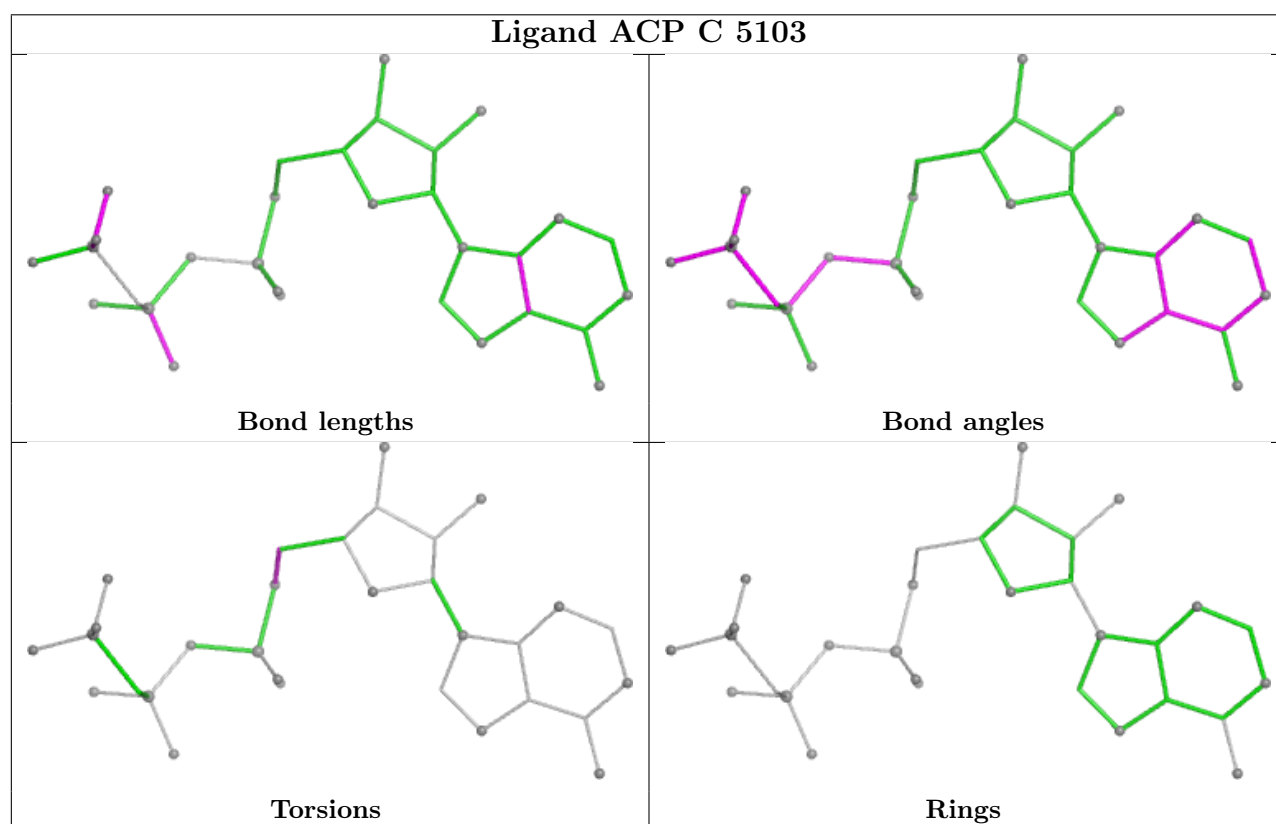
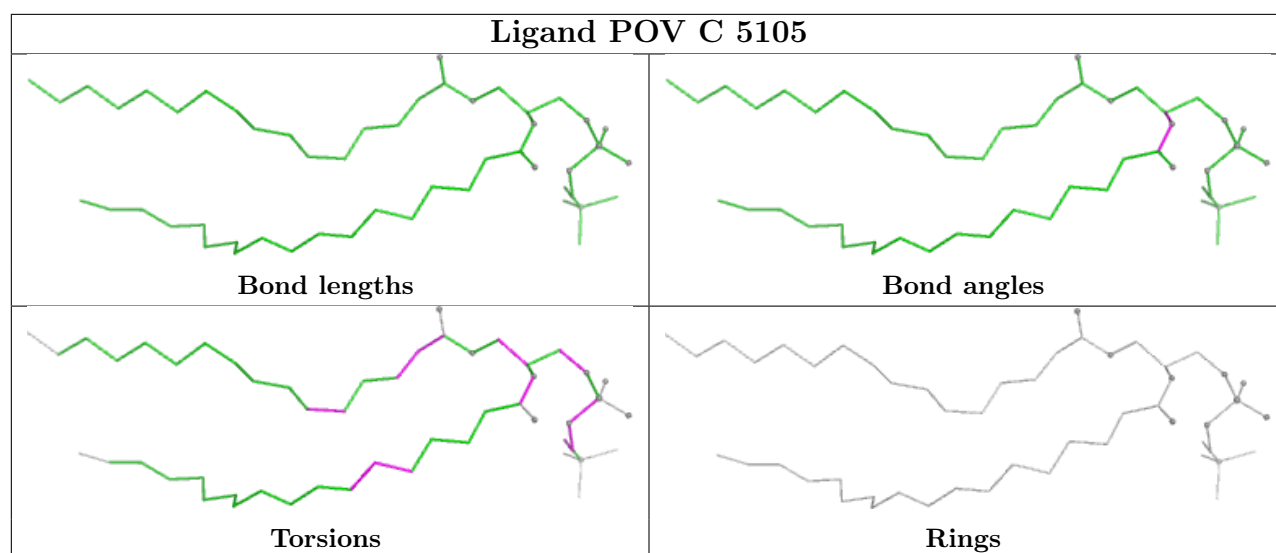
3 monomers are involved in 3 short contacts:

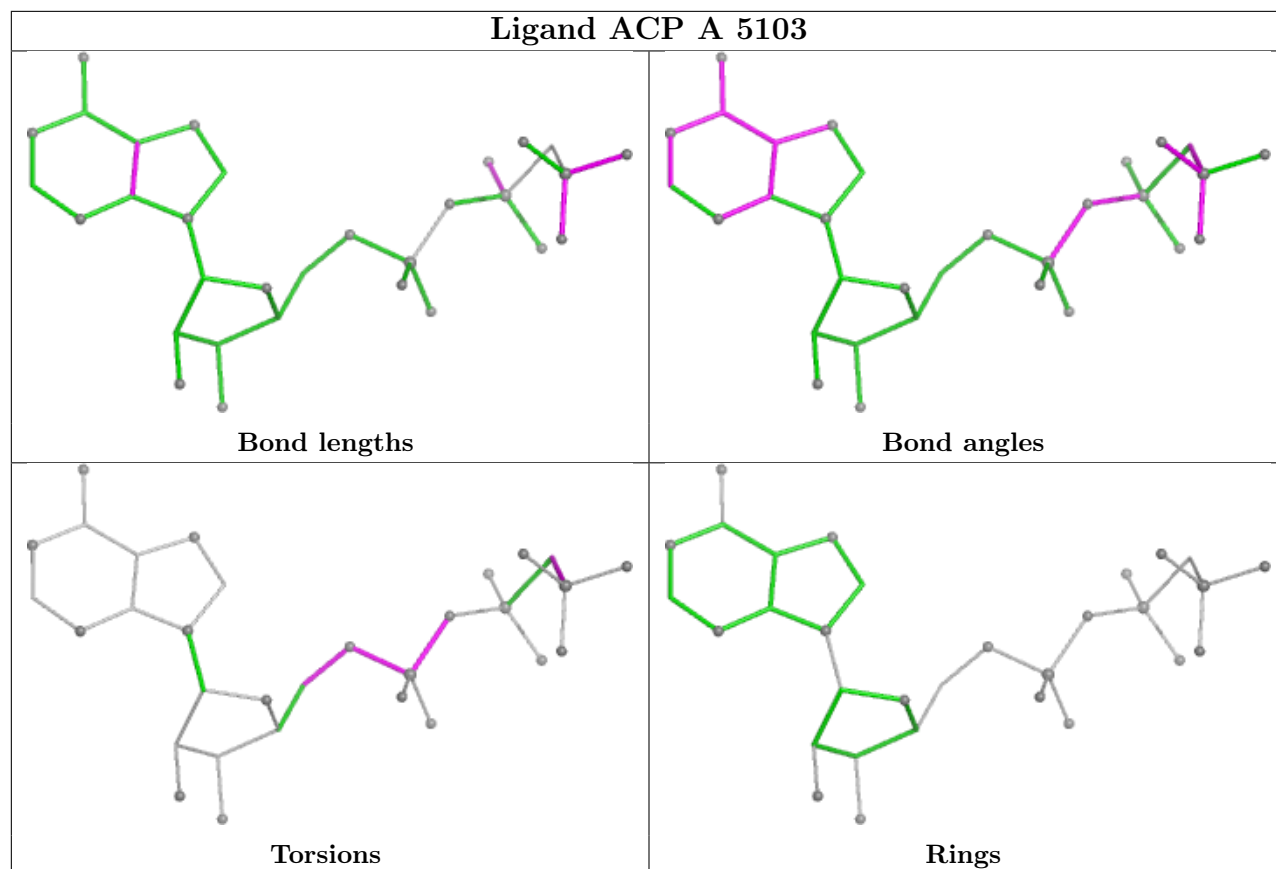
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5103	ACP	1	0
5	A	5103	ACP	1	0
5	D	5103	ACP	1	0

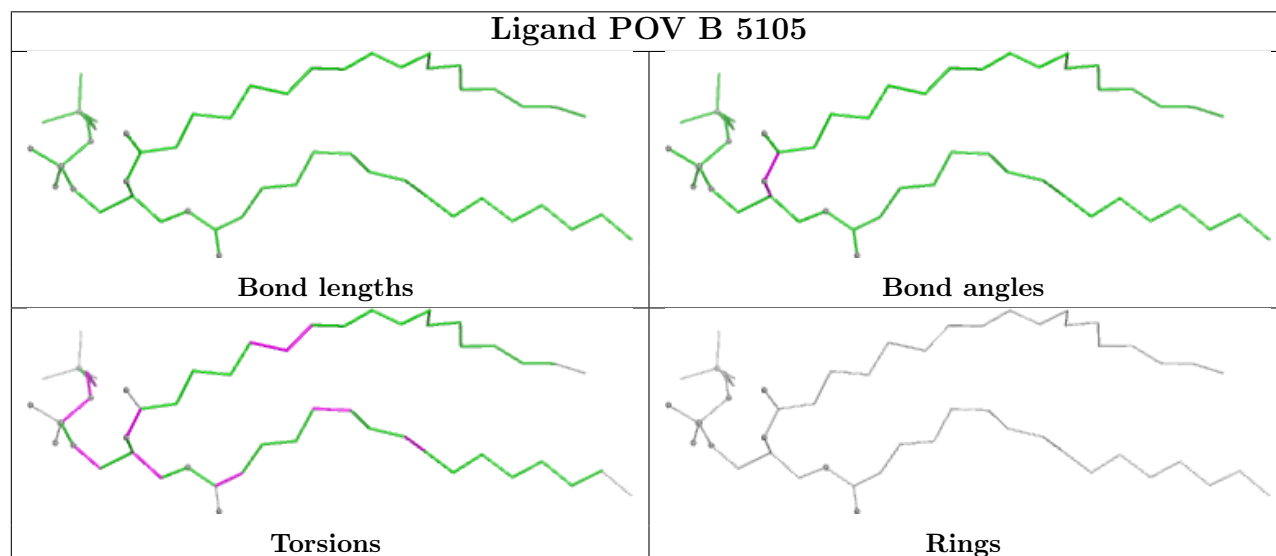
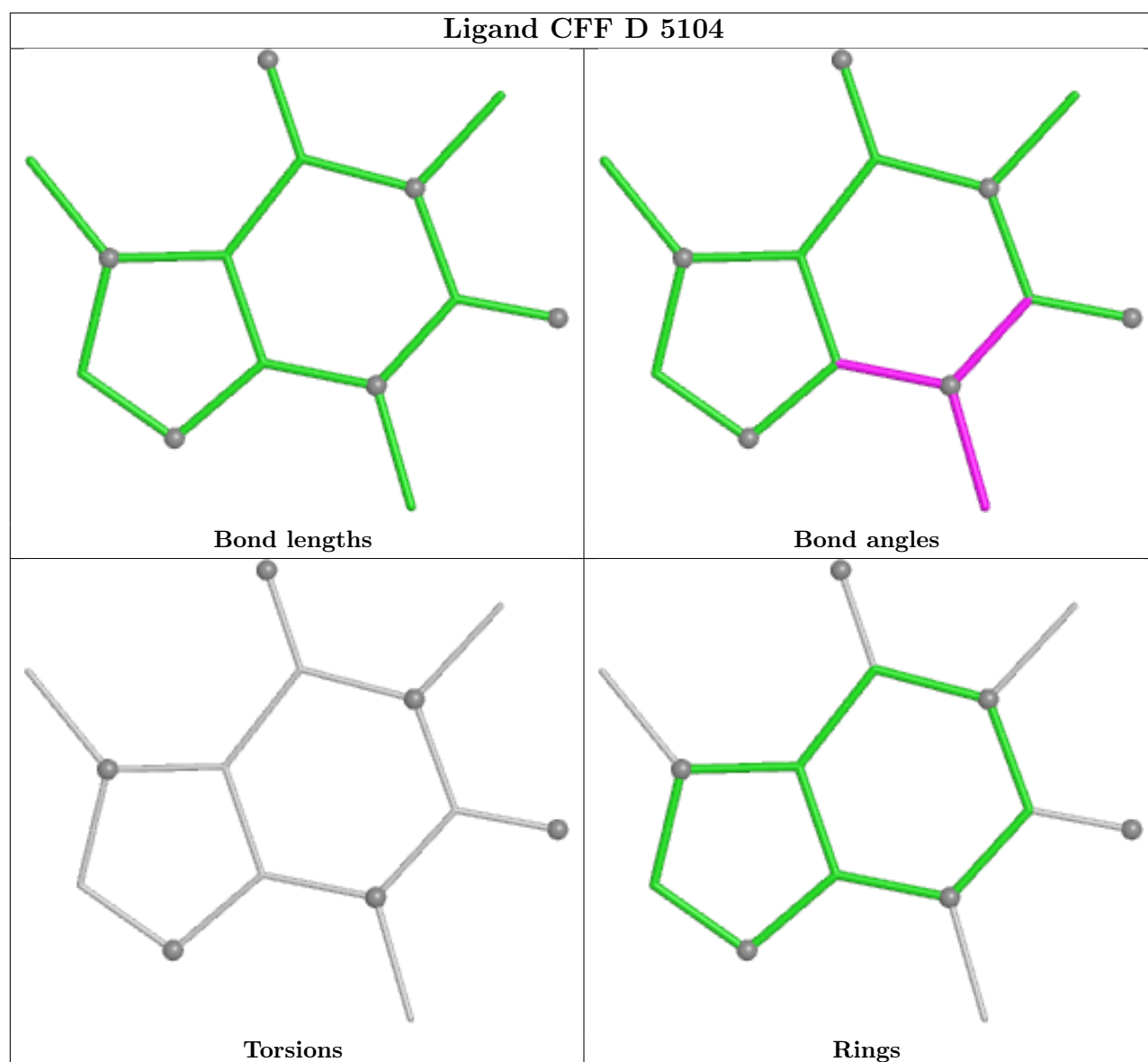
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

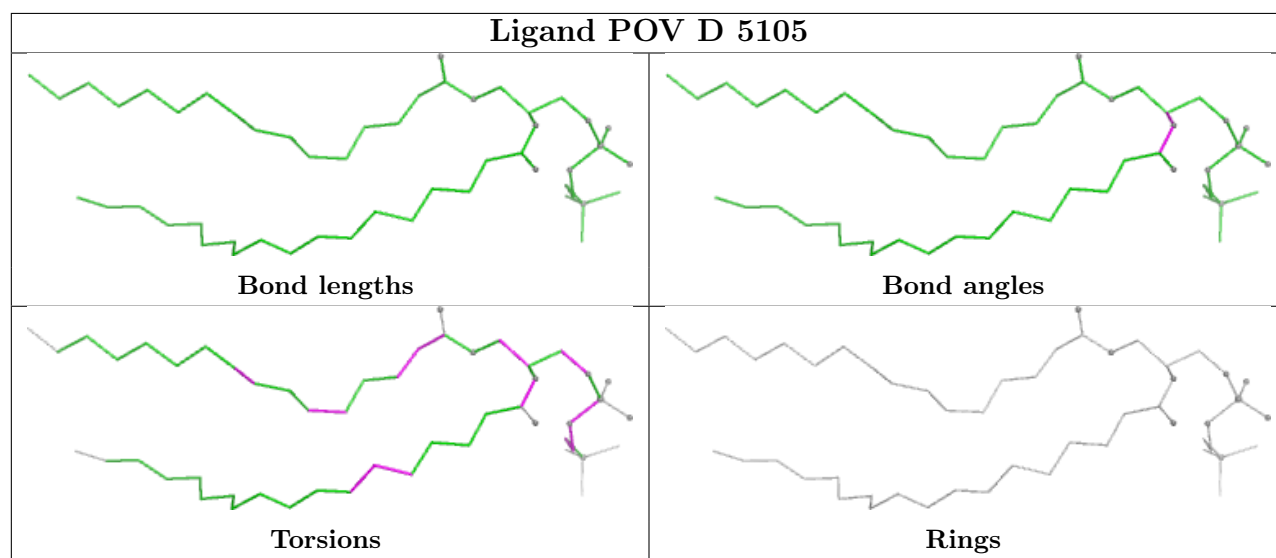
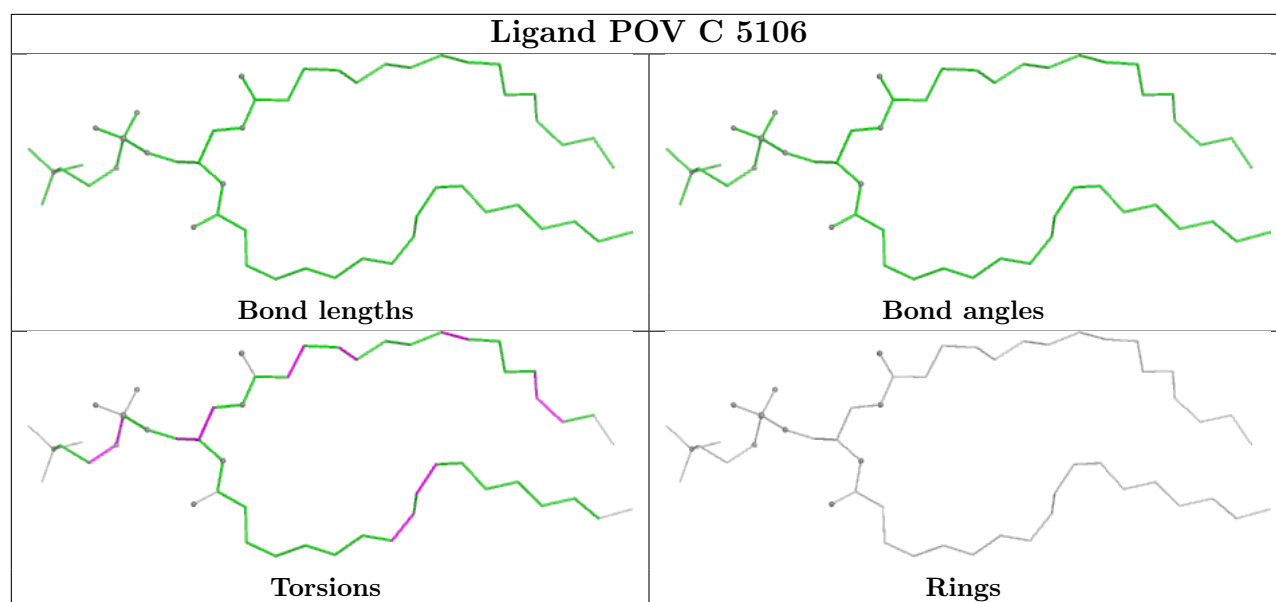


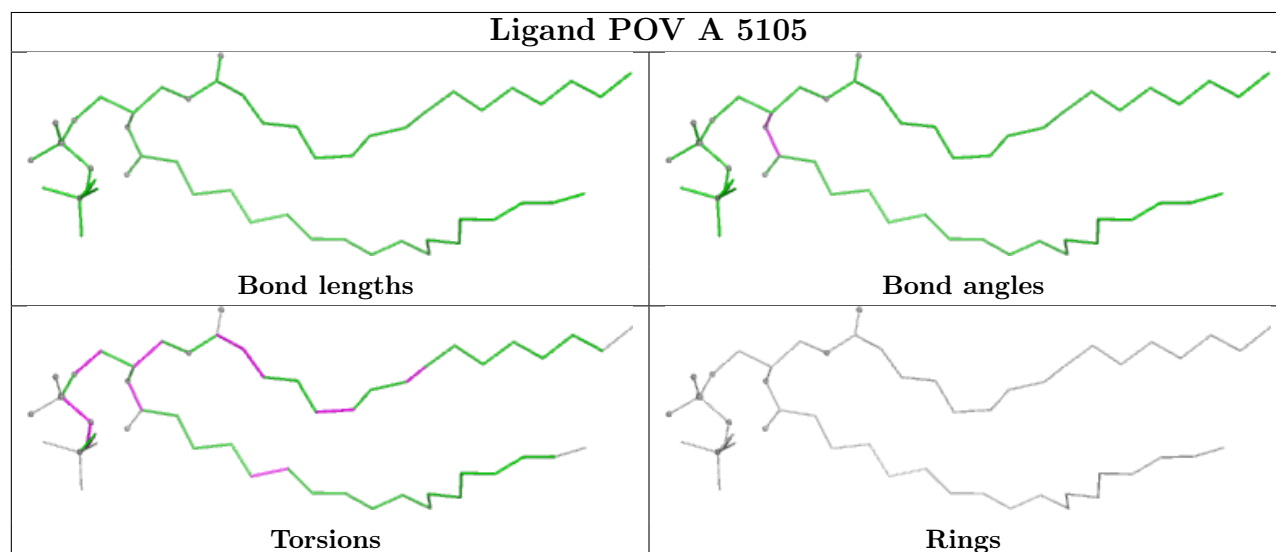
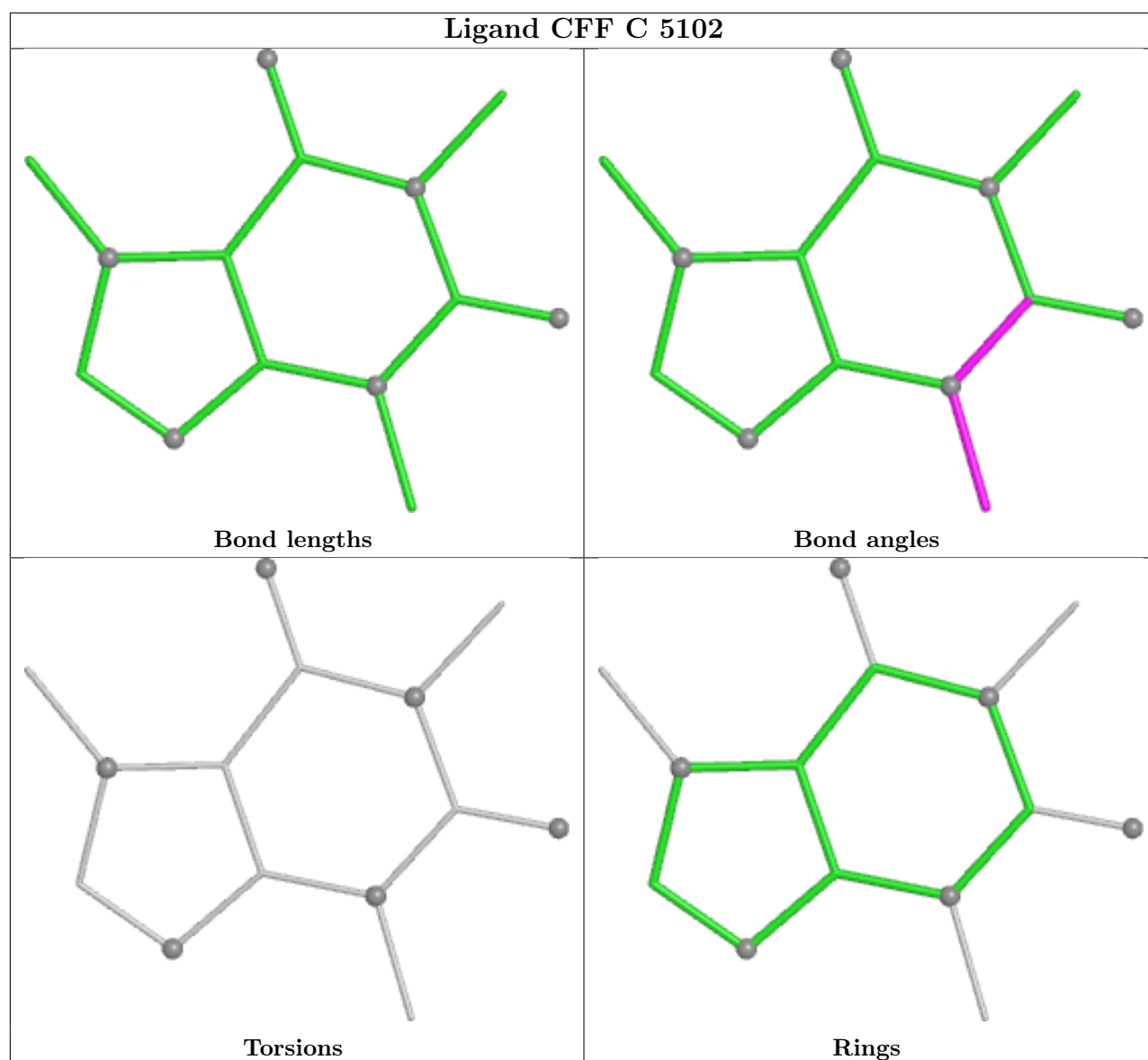


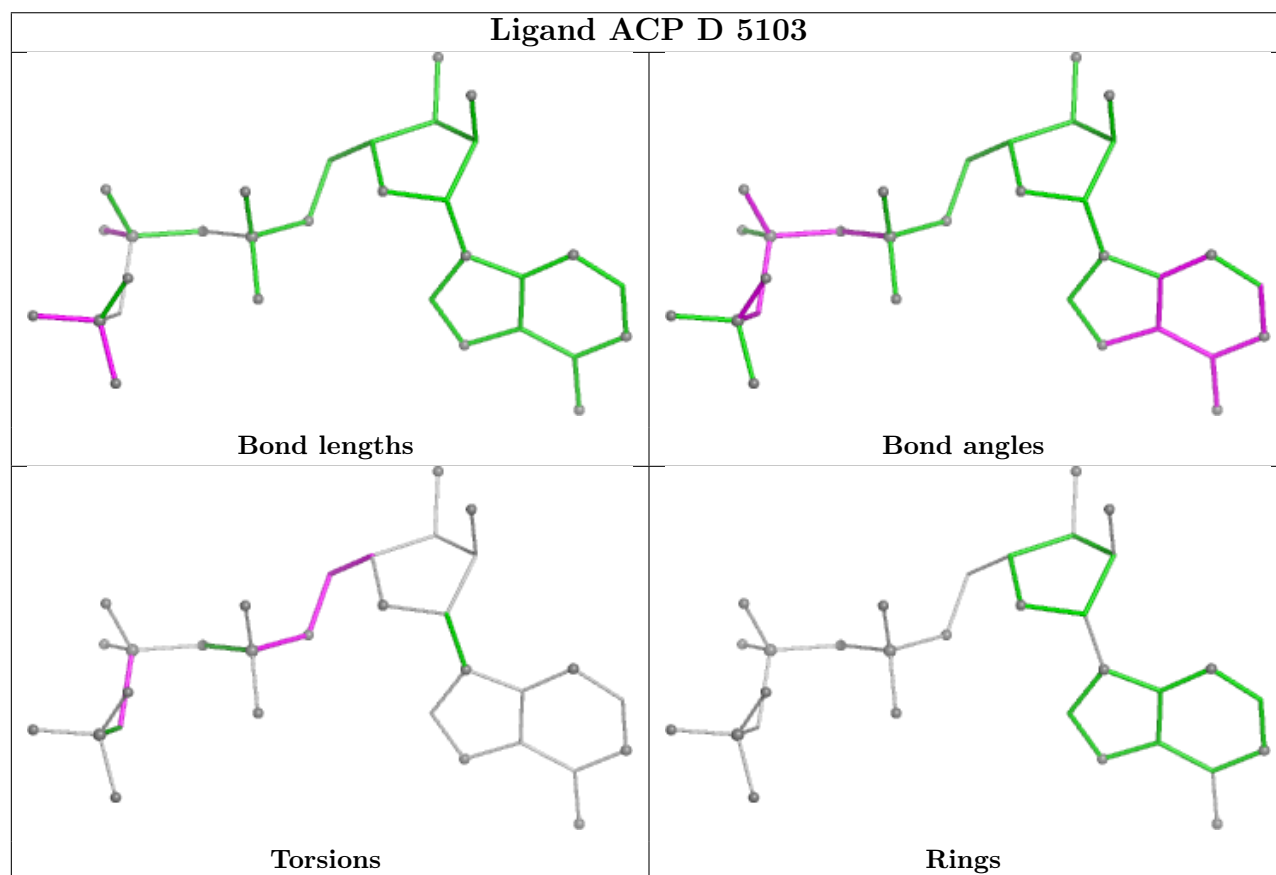
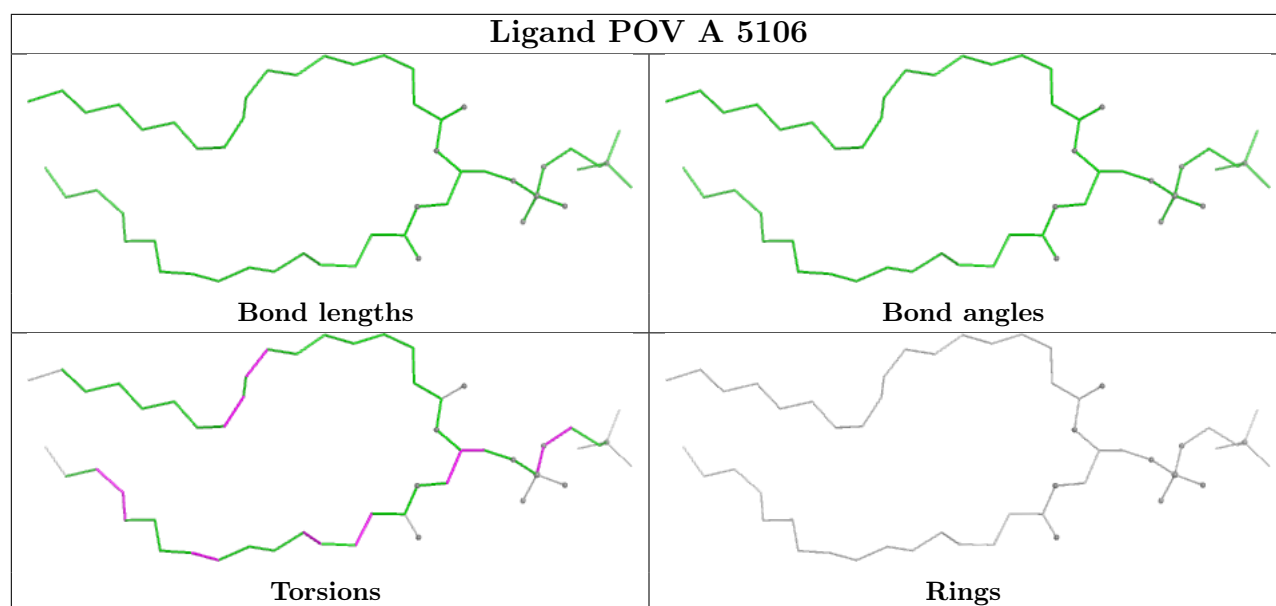


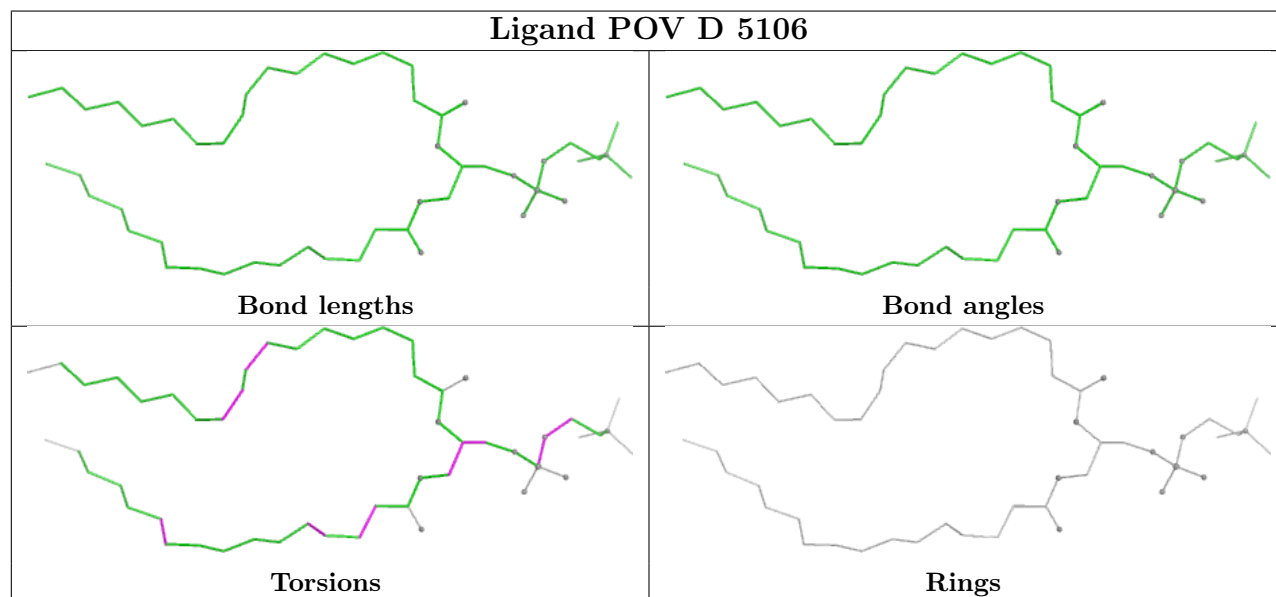
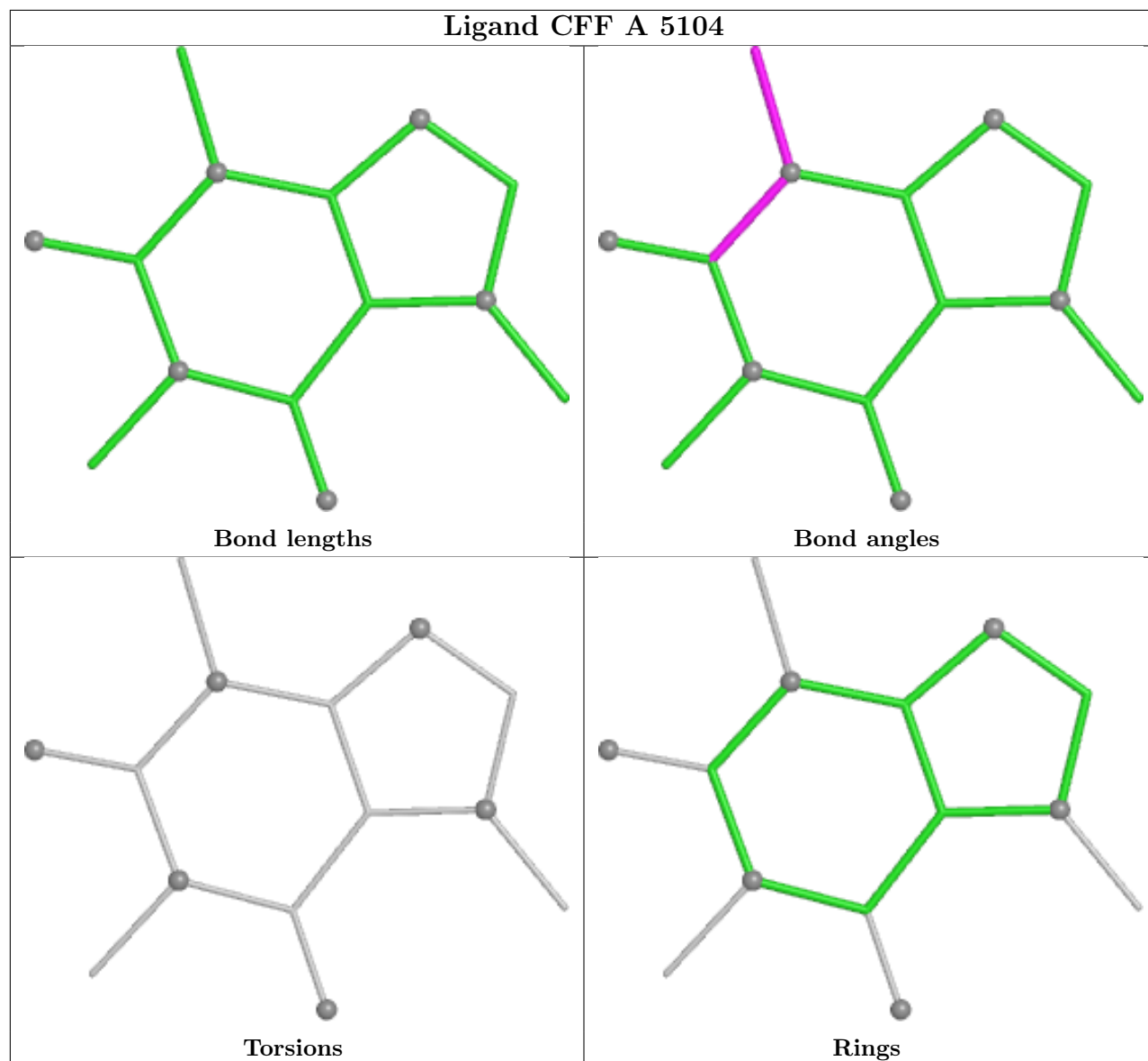












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

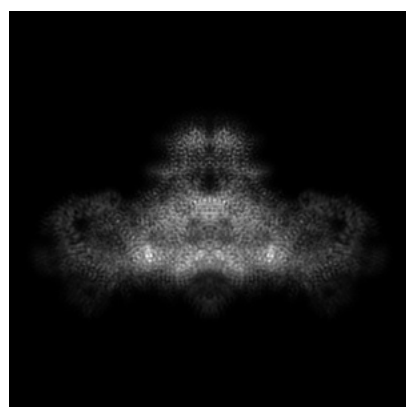
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54553. These allow visual inspection of the internal detail of the map and identification of artifacts.

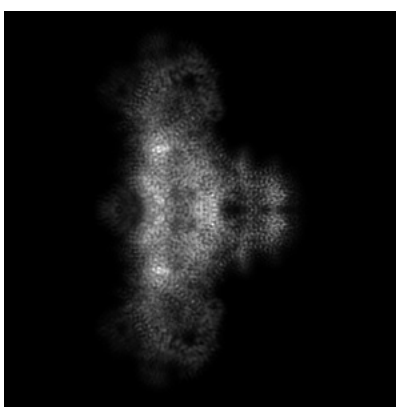
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

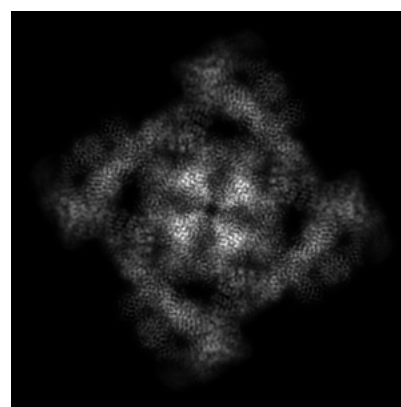
6.1.1 Primary map



X



Y

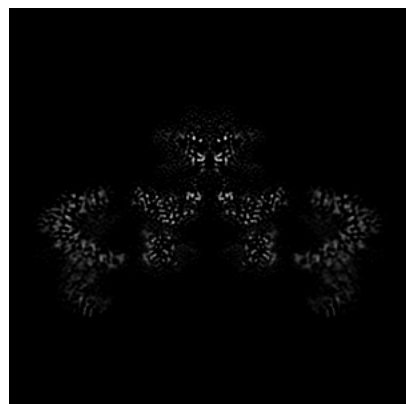


Z

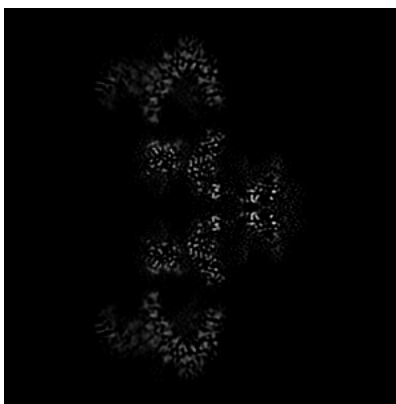
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 167



Y Index: 133

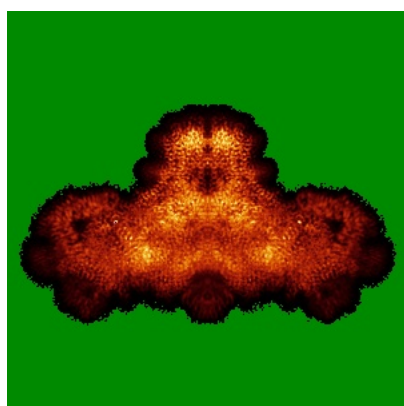


Z Index: 115

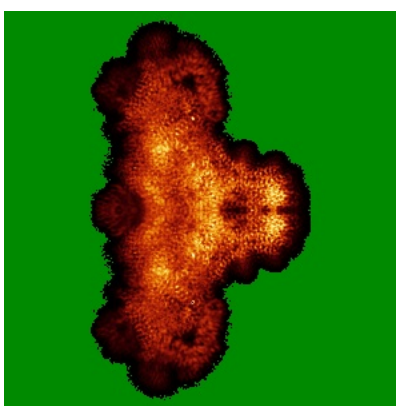
The images above show the largest variance slices of the map in three orthogonal directions.

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

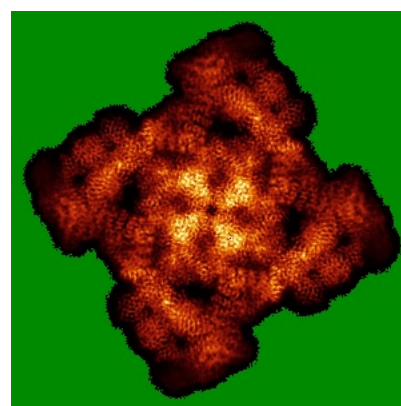
6.4.1 Primary map



X



Y

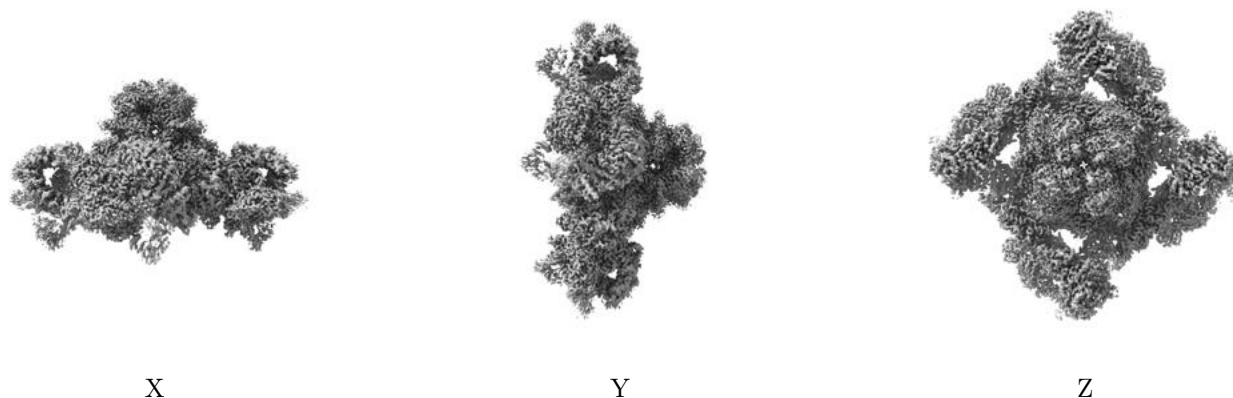


Z

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

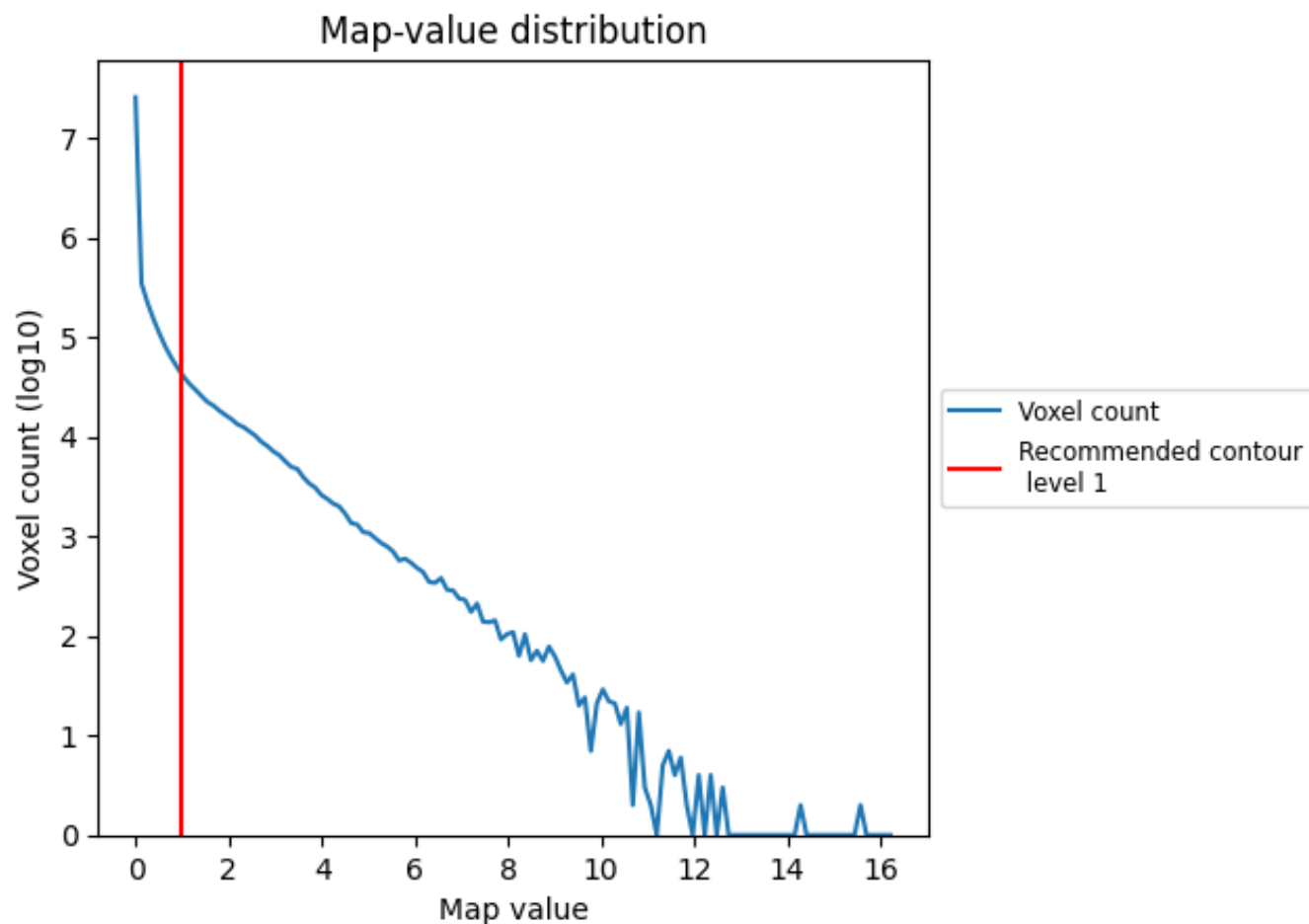
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

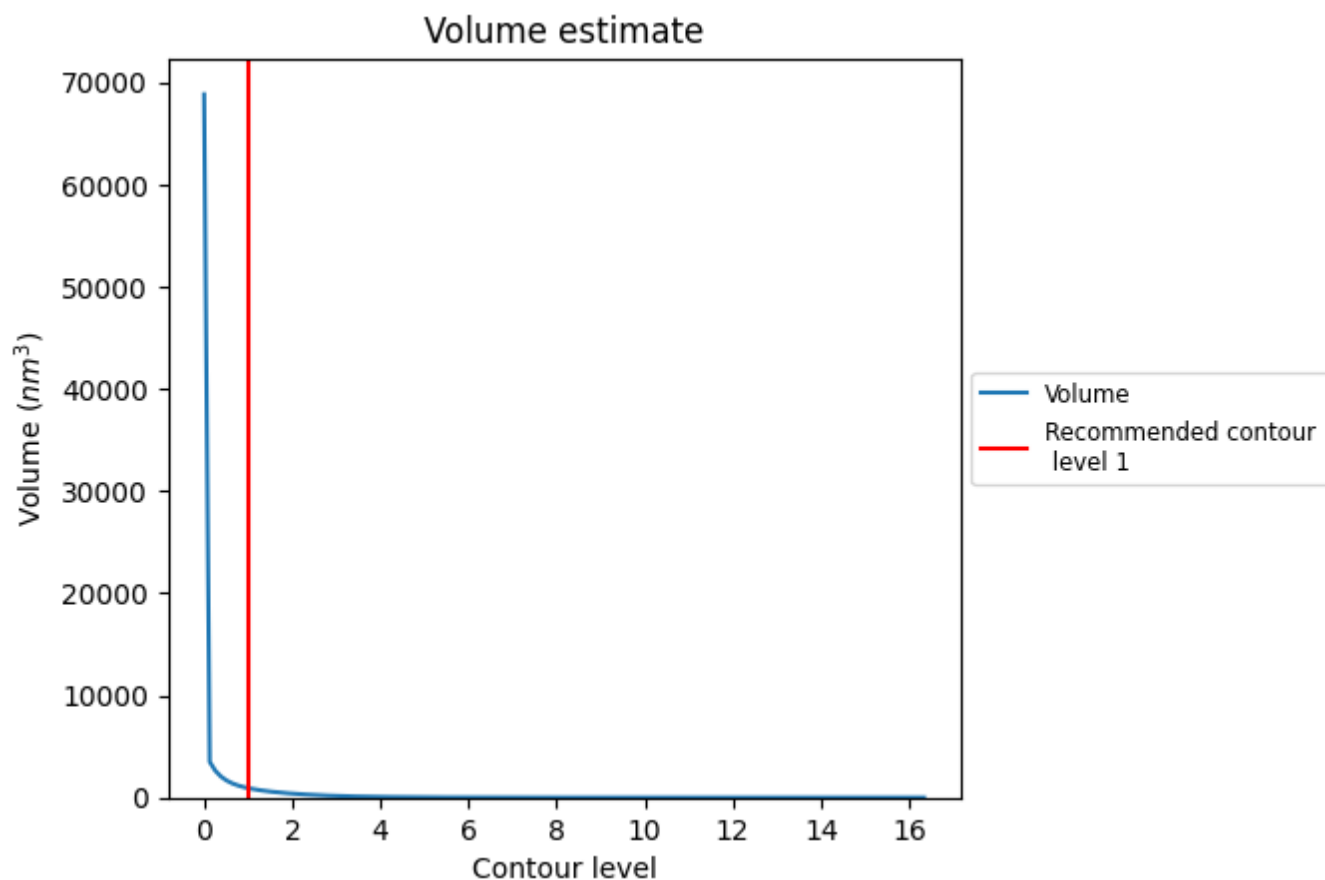
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

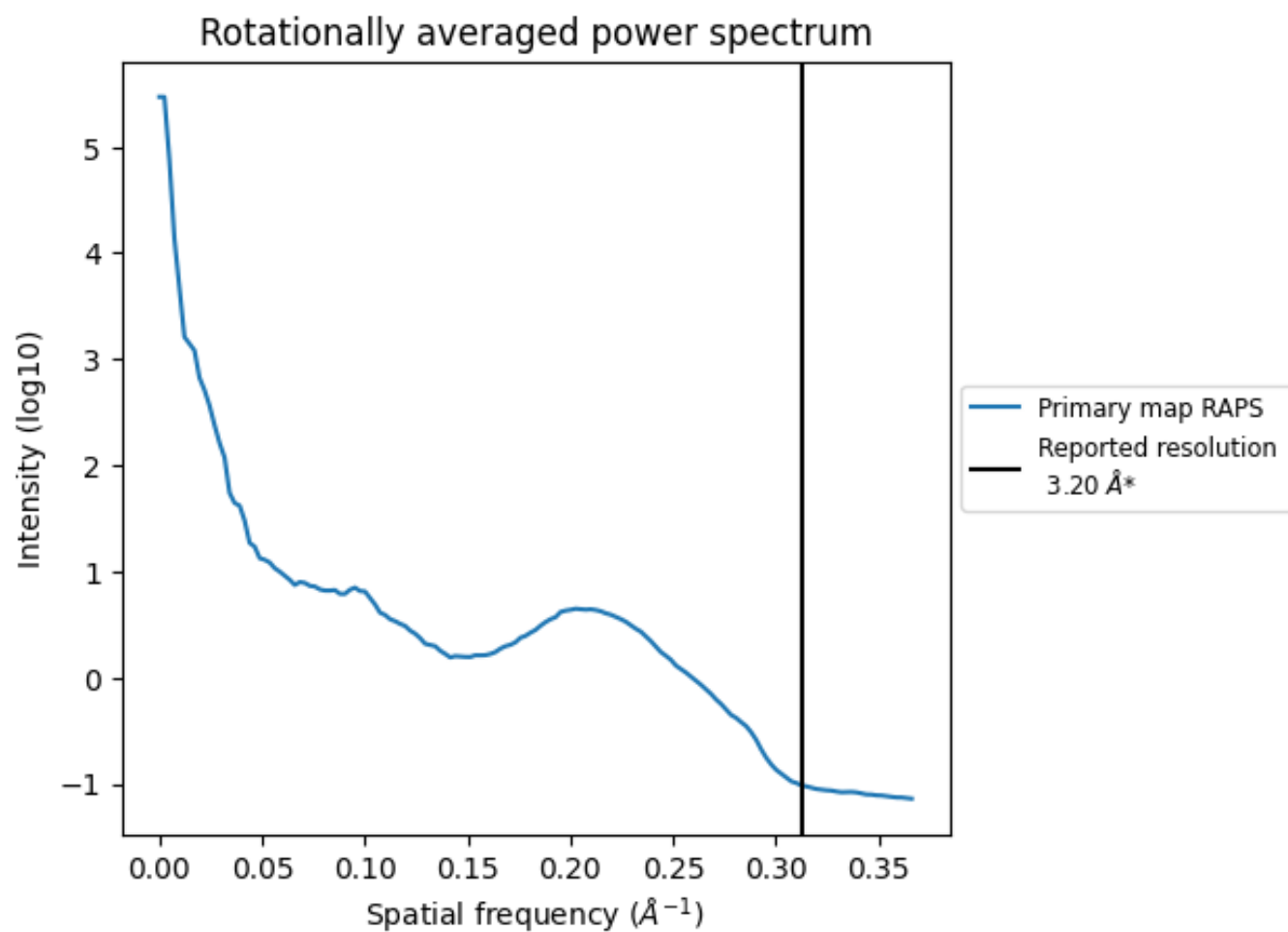
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 925 nm³; this corresponds to an approximate mass of 835 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 0.312 Å⁻¹

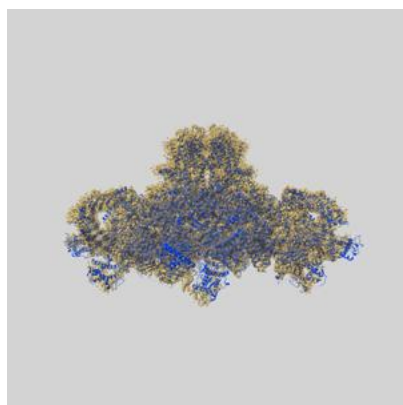
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

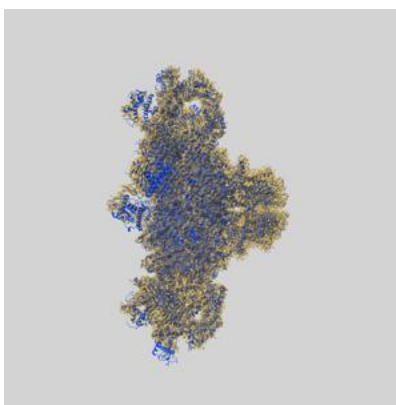
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54553 and PDB model 9S3V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

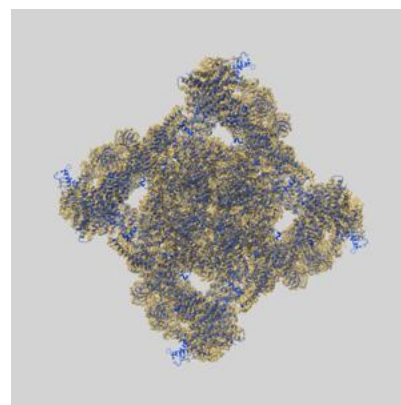
9.1 Map-model overlay [i](#)



X



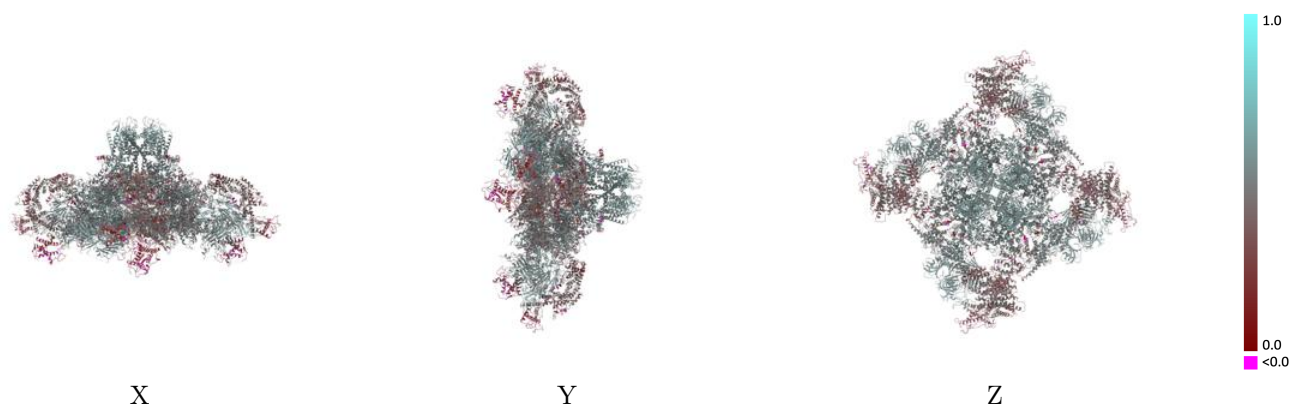
Y



Z

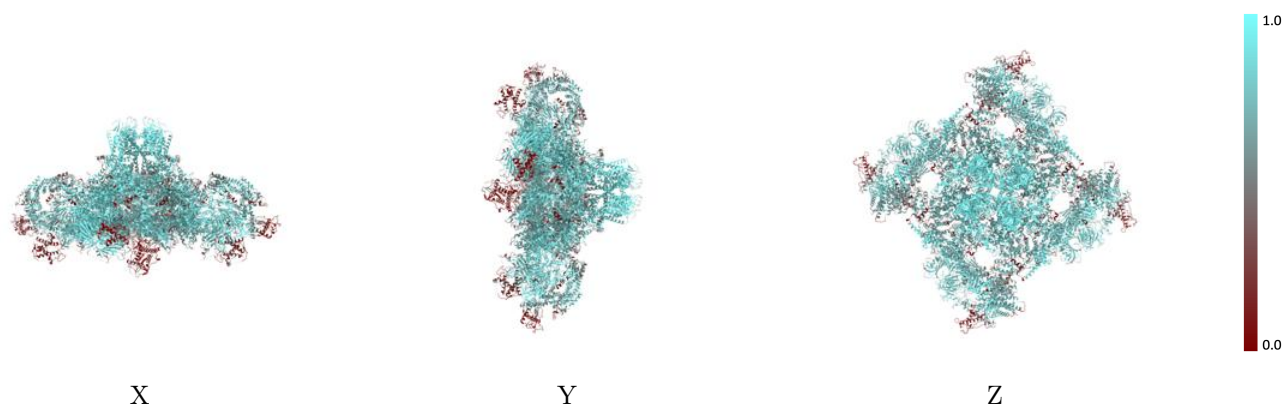
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



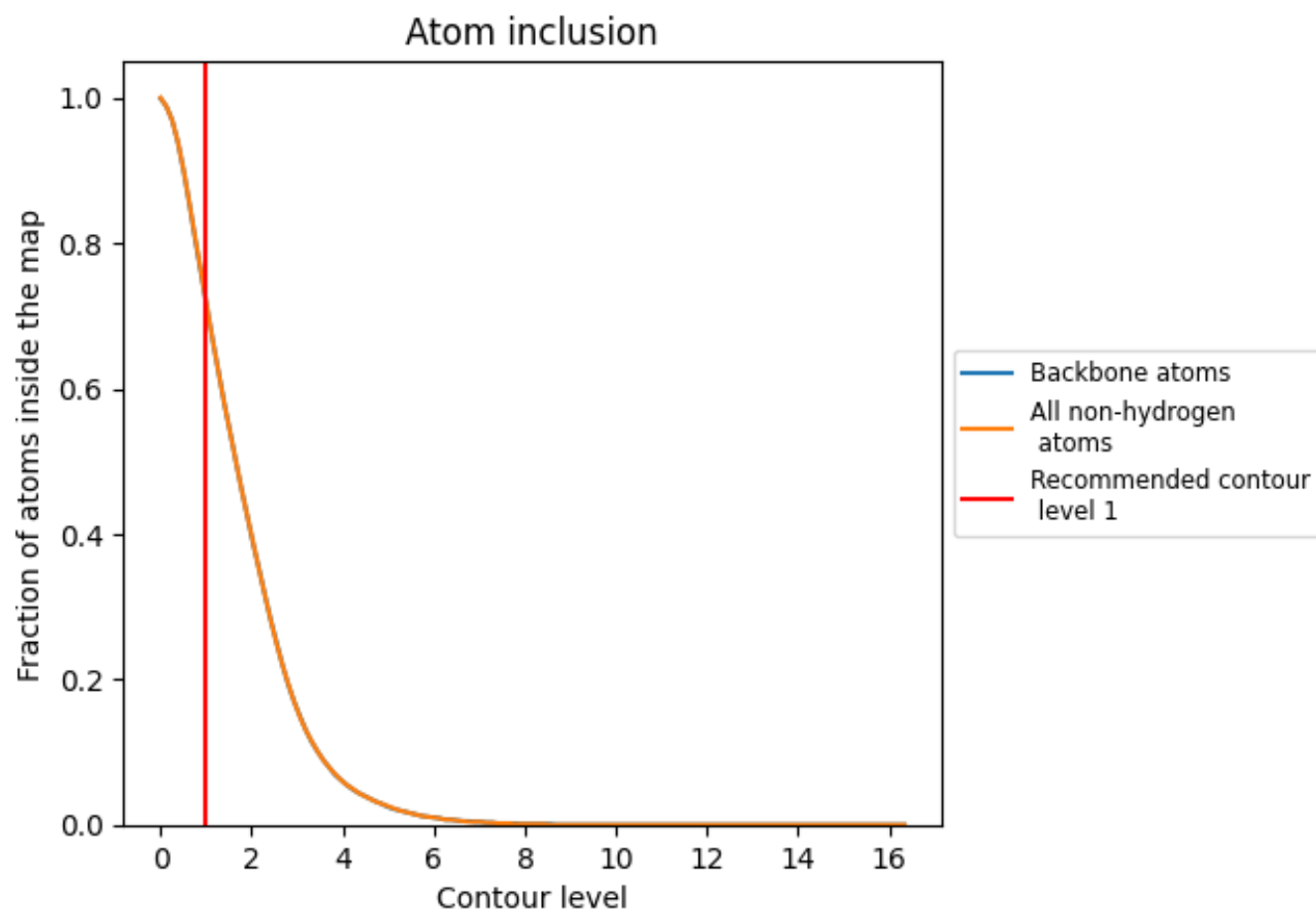
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.4620
A	0.7160	0.4600
B	0.7160	0.4590
C	0.7180	0.4590
D	0.7470	0.4640
E	0.7620	0.5360
F	0.7660	0.5370
G	0.7650	0.5370
H	0.7840	0.5390

1.0

0.0

<0.0