



wwPDB EM Validation Summary Report ⓘ

Dec 28, 2024 – 11:21 AM EST

PDB ID : 6Z1F
EMDB ID : EMD-11028
Title : CryoEM structure of Rubisco Activase with its substrate Rubisco from Nostoc sp. (strain PCC7120)
Authors : Wang, H.; Bracher, A.; Flecken, M.; Popilka, L.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on : 2020-05-13
Resolution : 2.86 Å(reported)

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

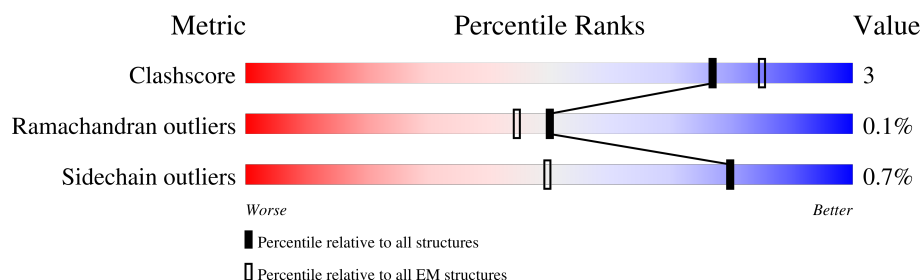
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	290	<div> <div>47%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	2	290	<div> <div>60%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	3	290	<div> <div>82%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	4	290	<div> <div>80%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	5	290	<div> <div>43%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	6	290	<div> <div>35%</div> <div>89%</div> <div>7%</div> <div>5%</div> </div>
2	A	476	<div> <div>92%</div> <div>5%</div> <div>.</div> </div>
2	B	476	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	476	
2	D	476	
2	E	476	
2	F	476	
2	G	476	
2	H	476	
3	I	109	
3	J	109	
3	K	109	
3	L	109	
3	M	109	
3	N	109	
3	O	109	
3	P	109	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49815 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 Ribulose biphosphate carboxylase/oxygenase activase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	280	Total	C	N	O	S	0	0
			2184	1392	380	405	7		
1	2	281	Total	C	N	O	S	0	0
			2215	1411	388	409	7		
1	3	284	Total	C	N	O	S	0	0
			2241	1423	391	420	7		
1	4	281	Total	C	N	O	S	0	0
			2222	1414	389	412	7		
1	5	280	Total	C	N	O	S	0	0
			2206	1405	386	408	7		
1	6	276	Total	C	N	O	S	0	0
			2174	1385	381	401	7		

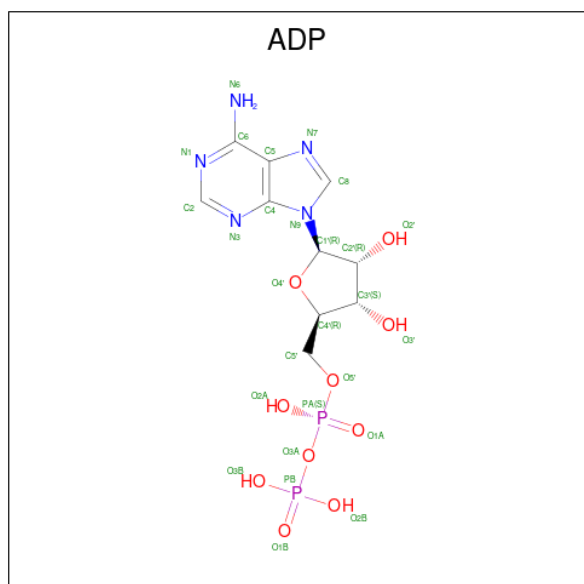
- Molecule 2 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	466	Total	C	N	O	S	0	0
			3665	2329	640	682	14		
2	B	459	Total	C	N	O	S	0	0
			3601	2295	634	659	13		
2	C	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	D	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	E	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	F	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	G	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	H	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		

- Molecule 3 is a protein called Ribulose biphosphate carboxylase small chain.

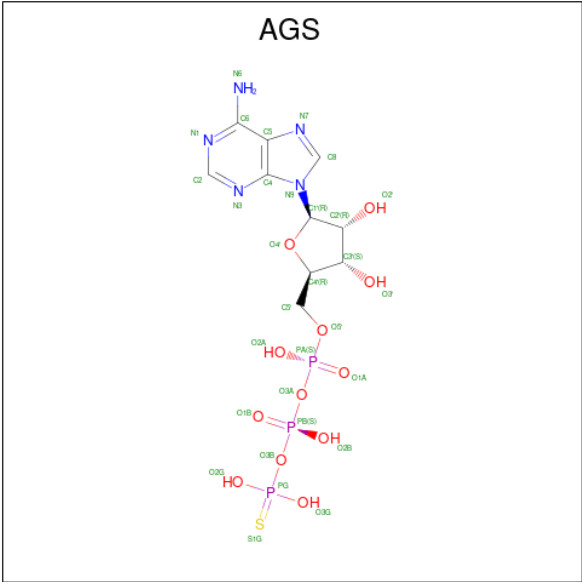
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	J	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	K	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	L	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	M	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	N	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	O	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	P	108	Total	C	N	O	S	0	0
			884	574	145	162	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
5	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	3	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

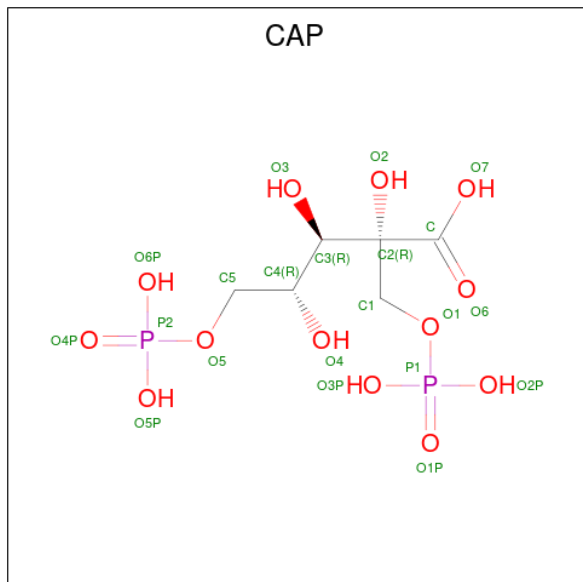
Mol	Chain	Residues	Atoms		AltConf
6	2	1	Total	Mg	0
			1	1	
6	3	1	Total	Mg	0
			1	1	
6	4	1	Total	Mg	0
			1	1	
6	5	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	G	1	Total	Mg	0
			1	1	
6	H	1	Total	Mg	0
			1	1	

- Molecule 7 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			21	6	13	2	
7	C	1	Total	C	O	P	0
			21	6	13	2	
7	D	1	Total	C	O	P	0
			21	6	13	2	
7	E	1	Total	C	O	P	0
			21	6	13	2	
7	F	1	Total	C	O	P	0
			21	6	13	2	
7	G	1	Total	C	O	P	0
			21	6	13	2	

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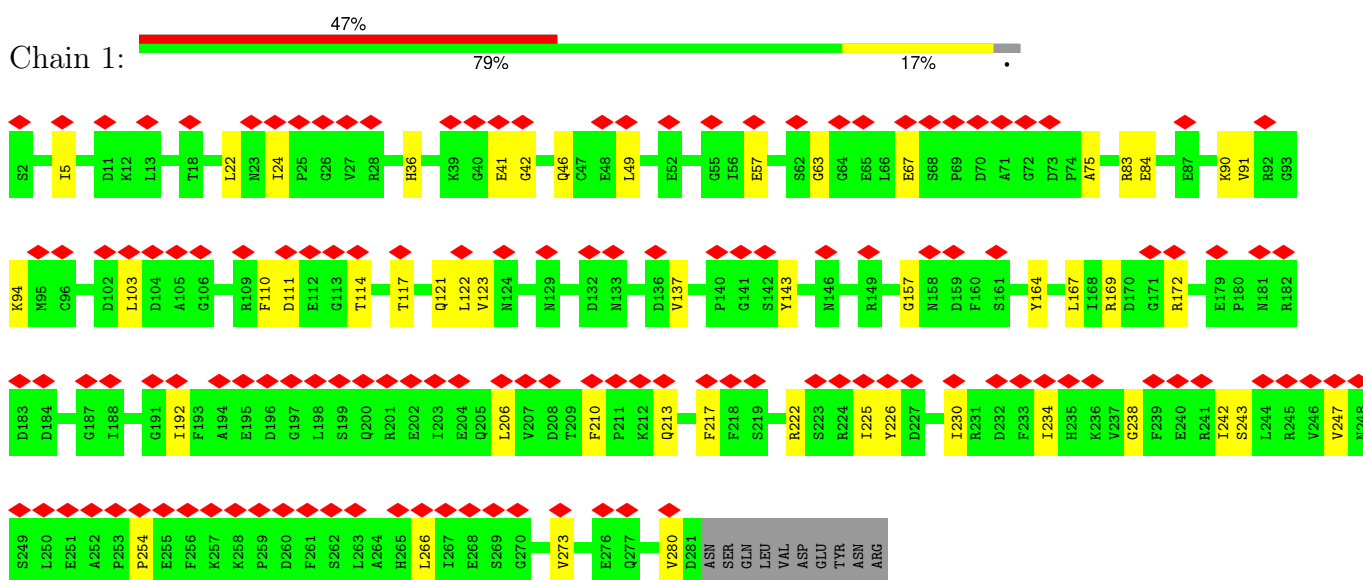
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
7	H	1	21	6	13	2	0

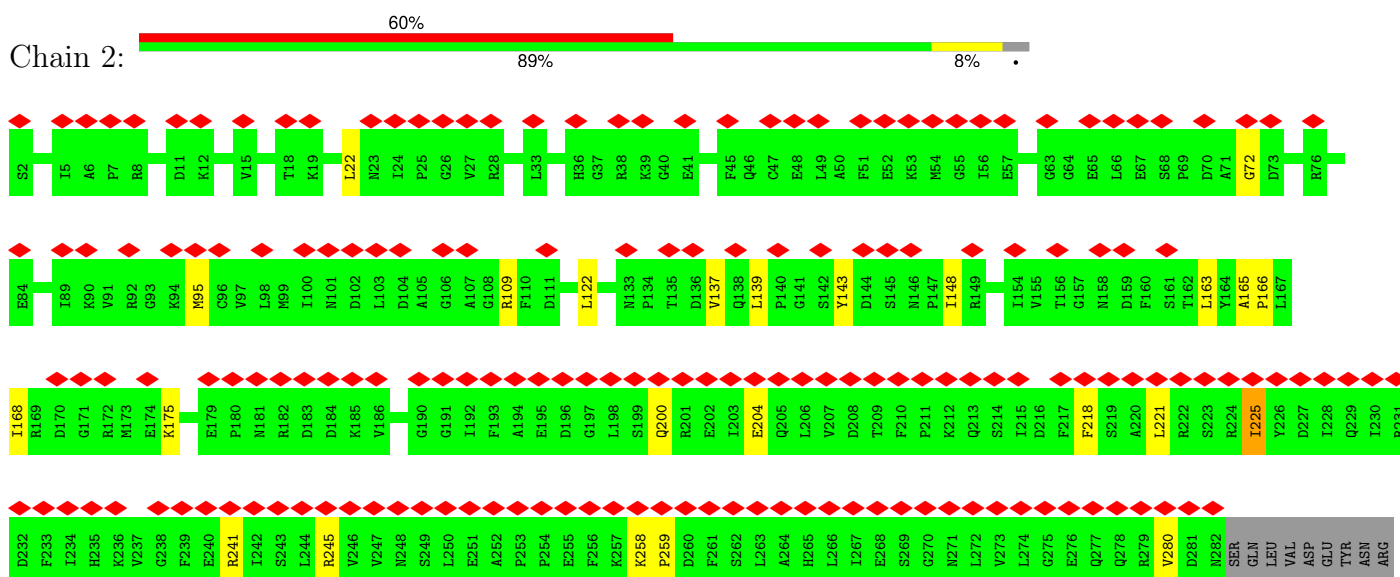
3 Residue-property plots

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: Ribulose biphosphate carboxylase/oxygenase activase

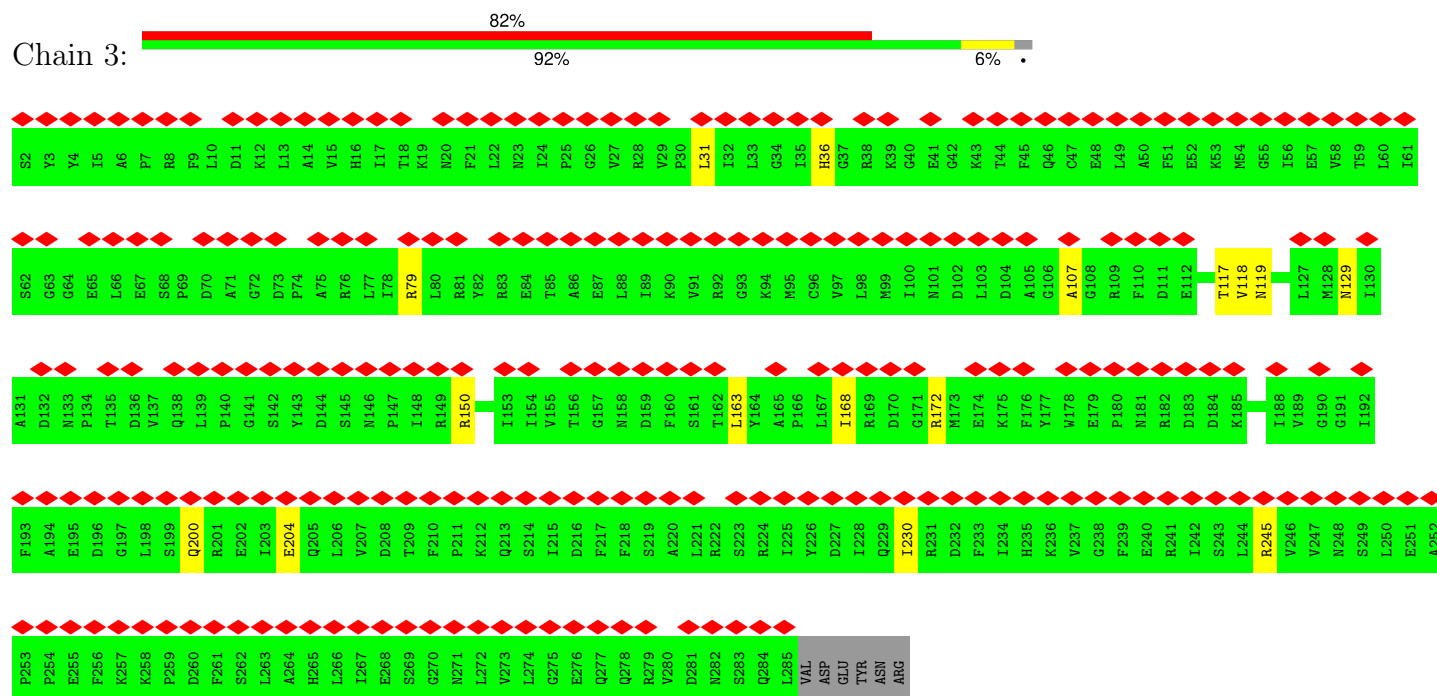


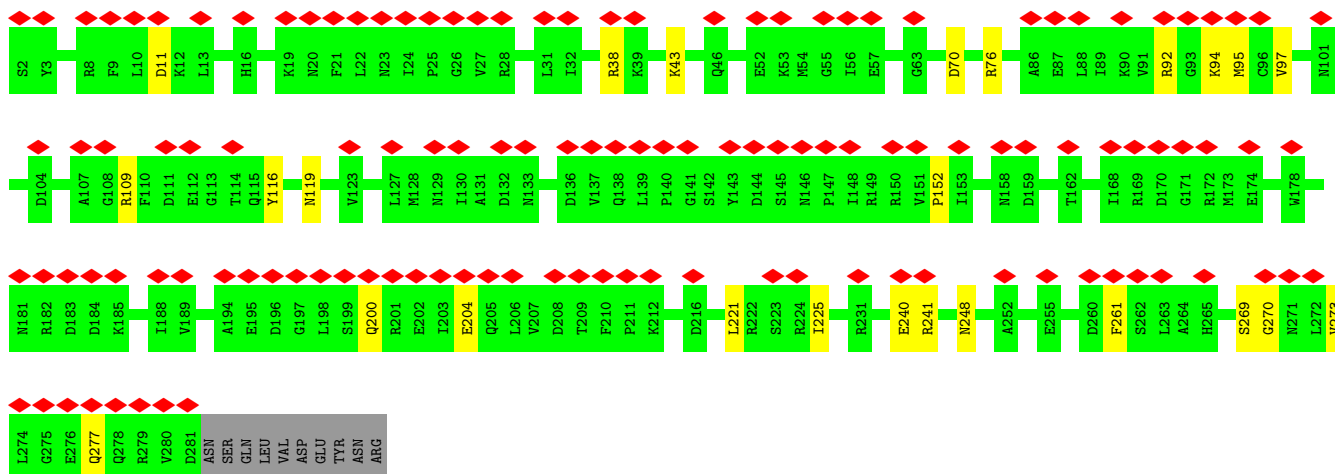
- Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase



• Molecule 1: Ribulose biphosphate carboxylase/oxygenase activase

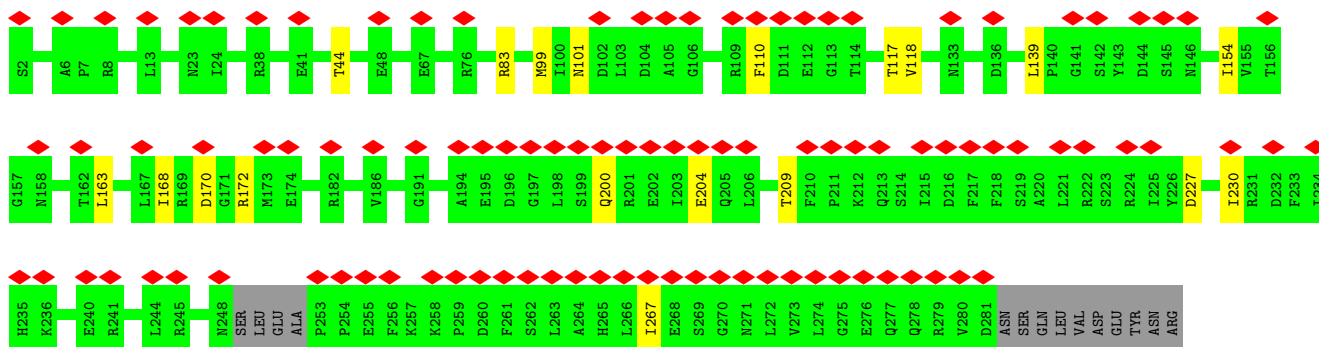
Chain 3:





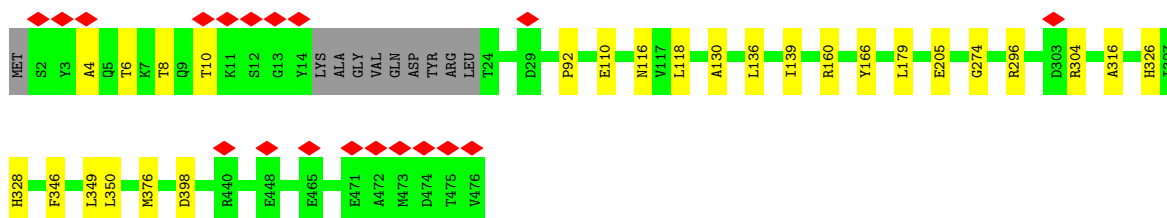
- Molecule 1: Ribulose biphosphate carboxylase/oxygenase activase

Chain 6: 35% 89% 7% 5%



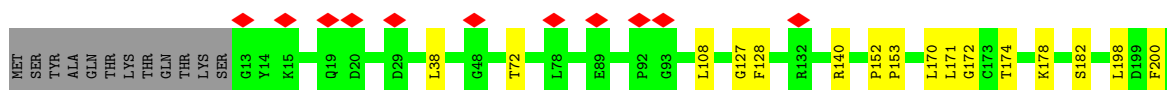
- Molecule 2: Ribulose biphosphate carboxylase large chain

Chain A: 92% 5%



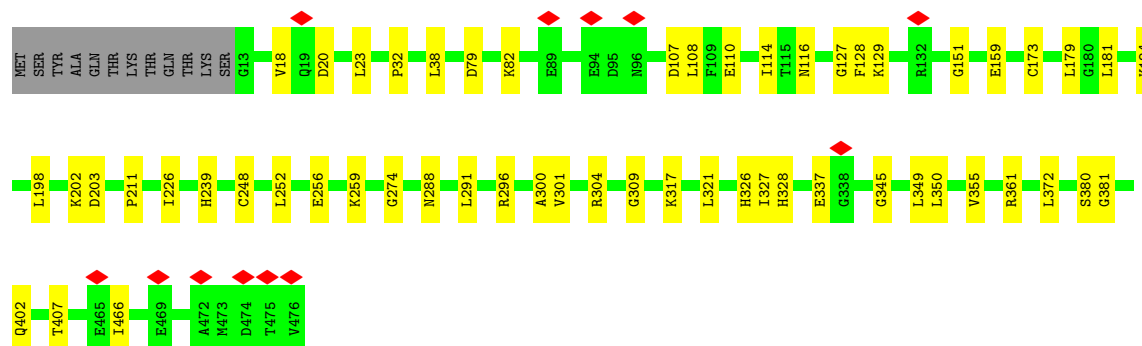
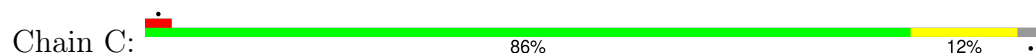
- Molecule 2: Ribulose biphosphate carboxylase large chain

Chain B: 90% 6%

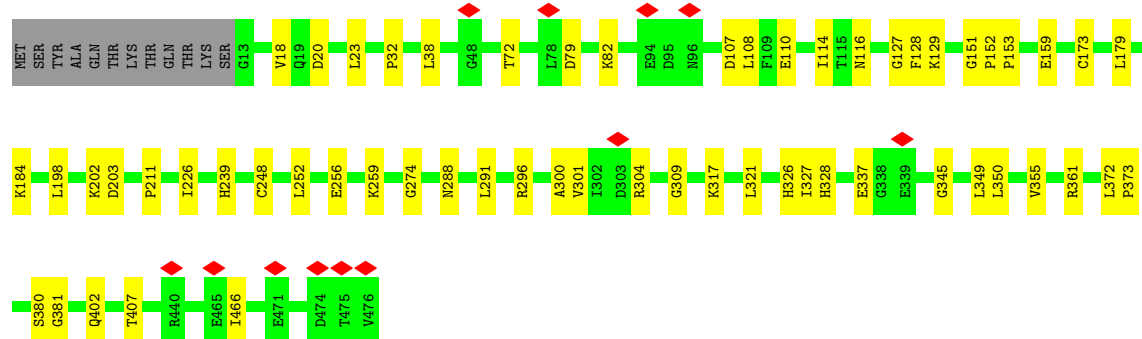
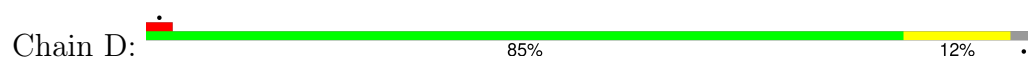




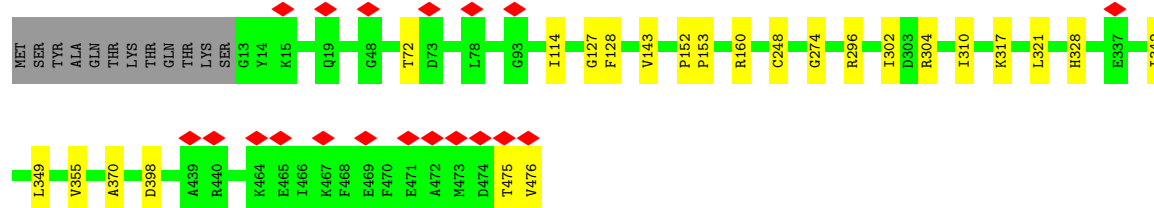
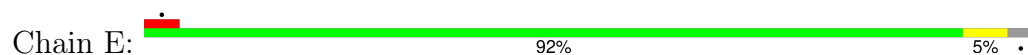
- Molecule 2: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose bisphosphate carboxylase large chain

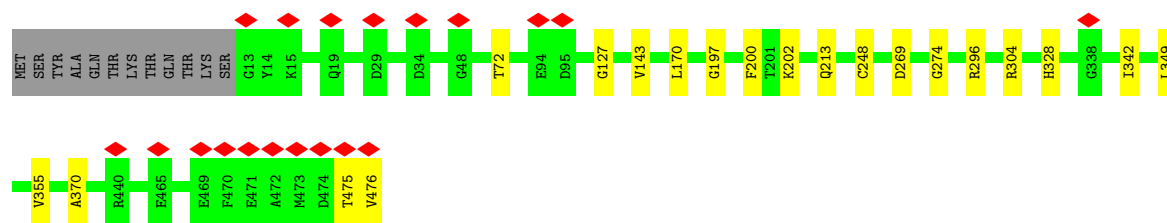


- Molecule 2: Ribulose bisphosphate carboxylase large chain

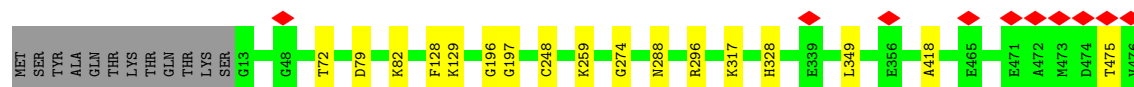


- Molecule 2: Ribulose bisphosphate carboxylase large chain

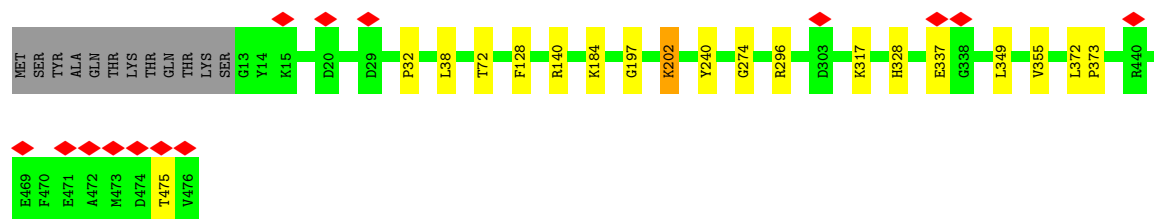




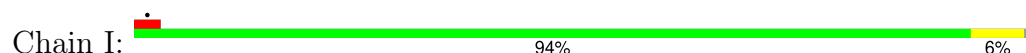
- Molecule 2: Ribulose biphosphate carboxylase large chain



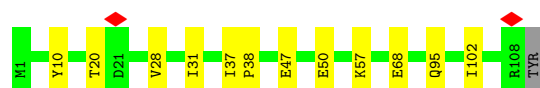
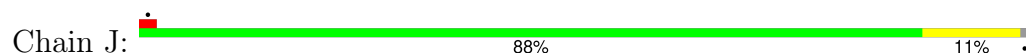
- Molecule 2: Ribulose biphosphate carboxylase large chain



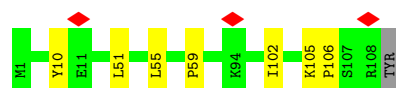
- Molecule 3: Ribulose biphosphate carboxylase small chain



- Molecule 3: Ribulose biphosphate carboxylase small chain



- Molecule 3: Ribulose biphosphate carboxylase small chain



- Molecule 3: Ribulose biphosphate carboxylase small chain



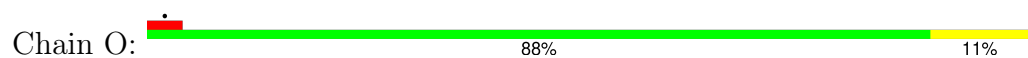
- Molecule 3: Ribulose biphosphate carboxylase small chain



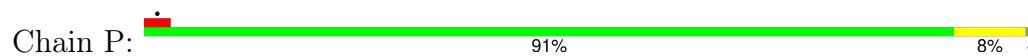
- Molecule 3: Ribulose biphosphate carboxylase small chain



- Molecule 3: Ribulose biphosphate carboxylase small chain



- Molecule 3: Ribulose biphosphate carboxylase small chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	306.432, 306.432, 306.432	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85120004, 0.85120004, 0.85120004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, CAP, KCX, MG, ADP

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	1	0.26	0/2227	0.57	0/3018
1	2	0.26	0/2258	0.57	0/3054
1	3	0.27	0/2284	0.58	0/3090
1	4	0.26	0/2265	0.58	0/3063
1	5	0.26	0/2249	0.57	0/3043
1	6	0.26	0/2216	0.58	0/2997
2	A	0.40	0/3740	0.58	0/5074
2	B	0.41	0/3677	0.57	0/4992
2	C	0.40	0/3725	0.59	0/5055
2	D	0.40	0/3725	0.59	0/5055
2	E	0.41	0/3725	0.57	0/5055
2	F	0.40	0/3725	0.57	0/5055
2	G	0.41	0/3725	0.57	0/5055
2	H	0.41	0/3725	0.57	0/5055
3	I	0.42	0/908	0.56	0/1237
3	J	0.42	0/908	0.56	0/1237
3	K	0.41	0/908	0.58	0/1237
3	L	0.41	0/908	0.58	0/1237
3	M	0.42	0/908	0.56	0/1237
3	N	0.42	0/908	0.55	0/1237
3	O	0.41	0/908	0.56	0/1237
3	P	0.42	0/908	0.56	0/1237
All	All	0.37	0/50530	0.57	0/68557

There are no bond length outliers.

There are no bond angle outliers.

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	1	2184	0	2169	53	0
1	2	2215	0	2225	33	0
1	3	2241	0	2237	11	0
1	4	2222	0	2233	16	0
1	5	2206	0	2212	19	0
1	6	2174	0	2172	17	0
2	A	3665	0	3586	21	0
2	B	3601	0	3527	25	0
2	C	3649	0	3573	36	0
2	D	3649	0	3573	38	0
2	E	3649	0	3573	12	0
2	F	3649	0	3573	8	0
2	G	3649	0	3573	7	0
2	H	3649	0	3573	10	0
3	I	884	0	878	2	0
3	J	884	0	878	12	0
3	K	884	0	878	4	0
3	L	884	0	878	5	0
3	M	884	0	878	3	0
3	N	884	0	878	3	0
3	O	884	0	878	5	0
3	P	884	0	878	5	0
4	1	27	0	12	1	0
5	2	31	0	12	6	0
5	3	31	0	12	1	0
5	4	31	0	12	1	0
5	5	31	0	12	2	0
5	6	31	0	12	2	0
6	2	1	0	0	0	0
6	3	1	0	0	0	0
6	4	1	0	0	0	0
6	5	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	21	0	9	0	0
7	C	21	0	9	0	0
7	D	21	0	9	0	0
7	E	21	0	9	0	0
7	F	21	0	9	0	0
7	G	21	0	9	0	0
7	H	21	0	9	0	0
All	All	49815	0	48958	277	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 3.

The worst 5 of 277 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)
5:2:301:AGS:PG	5:2:301:AGS:S1G	1.53	1.53
1:1:84:GLU:CD	2:B:464:LYS:HG3	1.64	1.17
1:1:247:VAL:HG21	1:2:95:MET:HG2	1.11	1.11
1:2:143:TYR:HB3	3:P:1:MET:HB2	1.36	1.03
1:1:247:VAL:CG2	1:2:95:MET:HG2	1.88	1.01

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	1	278/290 (96%)	269 (97%)	9 (3%)	0	100	100
1	2	279/290 (96%)	257 (92%)	21 (8%)	1 (0%)	30	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	282/290 (97%)	263 (93%)	19 (7%)	0	100	100
1	4	279/290 (96%)	269 (96%)	10 (4%)	0	100	100
1	5	278/290 (96%)	261 (94%)	17 (6%)	0	100	100
1	6	272/290 (94%)	264 (97%)	7 (3%)	1 (0%)	30	49
2	A	461/476 (97%)	437 (95%)	24 (5%)	0	100	100
2	B	456/476 (96%)	439 (96%)	17 (4%)	0	100	100
2	C	461/476 (97%)	449 (97%)	11 (2%)	1 (0%)	44	63
2	D	461/476 (97%)	449 (97%)	11 (2%)	1 (0%)	44	63
2	E	461/476 (97%)	447 (97%)	14 (3%)	0	100	100
2	F	461/476 (97%)	448 (97%)	12 (3%)	1 (0%)	44	63
2	G	461/476 (97%)	446 (97%)	14 (3%)	1 (0%)	44	63
2	H	461/476 (97%)	448 (97%)	12 (3%)	1 (0%)	44	63
3	I	106/109 (97%)	102 (96%)	4 (4%)	0	100	100
3	J	106/109 (97%)	102 (96%)	4 (4%)	0	100	100
3	K	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
3	L	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
3	M	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
3	N	106/109 (97%)	102 (96%)	4 (4%)	0	100	100
3	O	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
3	P	106/109 (97%)	102 (96%)	4 (4%)	0	100	100
All	All	6199/6420 (97%)	5962 (96%)	230 (4%)	7 (0%)	50	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	381	GLY
2	D	381	GLY
1	6	110	PHE
1	2	225	ILE
2	H	197	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	1	233/252 (92%)	233 (100%)	0	100	100
1	2	239/252 (95%)	239 (100%)	0	100	100
1	3	243/252 (96%)	242 (100%)	1 (0%)	89	95
1	4	241/252 (96%)	239 (99%)	2 (1%)	79	90
1	5	238/252 (94%)	238 (100%)	0	100	100
1	6	234/252 (93%)	234 (100%)	0	100	100
2	A	377/385 (98%)	374 (99%)	3 (1%)	79	90
2	B	366/385 (95%)	363 (99%)	3 (1%)	79	90
2	C	373/385 (97%)	371 (100%)	2 (0%)	86	94
2	D	373/385 (97%)	371 (100%)	2 (0%)	86	94
2	E	373/385 (97%)	369 (99%)	4 (1%)	70	85
2	F	373/385 (97%)	368 (99%)	5 (1%)	65	83
2	G	373/385 (97%)	369 (99%)	4 (1%)	70	85
2	H	373/385 (97%)	370 (99%)	3 (1%)	79	90
3	I	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	J	99/102 (97%)	98 (99%)	1 (1%)	73	87
3	K	99/102 (97%)	99 (100%)	0	100	100
3	L	99/102 (97%)	99 (100%)	0	100	100
3	M	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	N	99/102 (97%)	98 (99%)	1 (1%)	73	87
3	O	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	P	99/102 (97%)	98 (99%)	1 (1%)	73	87
All	All	5201/5408 (96%)	5163 (99%)	38 (1%)	80	91

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	475	THR
3	O	20	THR
3	I	20	THR
3	M	20	THR

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Mol	Chain	Res	Type
3	P	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	116	ASN
2	H	116	ASN
2	D	213	GLN
2	H	213	GLN
2	G	116	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KCX	H	202	2,6	10,11,12	2.14	1 (10%)	6,12,14	1.94	1 (16%)
2	KCX	C	202	2,6	10,11,12	0.51	0	6,12,14	1.24	1 (16%)
2	KCX	F	202	2,6	10,11,12	2.16	1 (10%)	6,12,14	1.96	1 (16%)
2	KCX	B	202	2,6	10,11,12	2.13	1 (10%)	6,12,14	1.98	1 (16%)
2	KCX	A	202	2,6	10,11,12	0.50	0	6,12,14	0.86	0
2	KCX	E	202	2,6	10,11,12	0.52	0	6,12,14	0.97	0
2	KCX	D	202	2,6	10,11,12	2.13	1 (10%)	6,12,14	2.17	2 (33%)
2	KCX	G	202	2,6	10,11,12	0.52	0	6,12,14	0.88	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
2	KCX	H	202	2,6	-	3/9/10/12	-
2	KCX	C	202	2,6	-	4/9/10/12	-
2	KCX	F	202	2,6	-	4/9/10/12	-
2	KCX	B	202	2,6	-	3/9/10/12	-
2	KCX	A	202	2,6	-	2/9/10/12	-
2	KCX	E	202	2,6	-	5/9/10/12	-
2	KCX	D	202	2,6	-	4/9/10/12	-
2	KCX	G	202	2,6	-	4/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	202	KCX	OQ1-CX	6.51	1.33	1.21
2	H	202	KCX	OQ1-CX	6.45	1.33	1.21
2	B	202	KCX	OQ1-CX	6.45	1.33	1.21
2	D	202	KCX	OQ1-CX	6.43	1.33	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	KCX	OQ1-CX-NZ	-4.40	118.24	124.92
2	B	202	KCX	OQ1-CX-NZ	-4.24	118.48	124.92
2	F	202	KCX	OQ1-CX-NZ	-4.23	118.50	124.92
2	H	202	KCX	OQ1-CX-NZ	-4.10	118.69	124.92
2	C	202	KCX	CE-NZ-CX	2.31	125.91	121.98

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	KCX	C-CA-CB-CG
2	B	202	KCX	C-CA-CB-CG
2	C	202	KCX	N-CA-CB-CG
2	C	202	KCX	C-CA-CB-CG
2	C	202	KCX	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	202	KCX	1	0
2	B	202	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	AGS	3	301	6	28,33,33	2.06	5 (17%)	31,52,52	1.87	5 (16%)
7	CAP	C	502	6	18,20,20	0.79	0	23,31,31	1.11	1 (4%)
7	CAP	G	502	6	18,20,20	0.79	0	23,31,31	1.12	1 (4%)
7	CAP	A	502	6	18,20,20	0.76	0	23,31,31	1.18	2 (8%)
4	ADP	1	301	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
7	CAP	E	502	6	18,20,20	0.78	0	23,31,31	1.18	2 (8%)
7	CAP	H	502	6	18,20,20	0.73	0	23,31,31	1.31	2 (8%)
5	AGS	6	301	-	28,33,33	2.65	9 (32%)	31,52,52	1.78	4 (12%)
5	AGS	5	301	6	28,33,33	2.80	7 (25%)	31,52,52	1.93	5 (16%)
7	CAP	D	502	6	18,20,20	0.76	0	23,31,31	1.29	2 (8%)
7	CAP	F	502	6	18,20,20	0.77	0	23,31,31	1.29	2 (8%)
5	AGS	2	301	6	28,33,33	3.79	6 (21%)	31,52,52	1.84	5 (16%)
5	AGS	4	301	6	28,33,33	2.42	6 (21%)	31,52,52	1.86	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	3	301	6	-	5/17/38/38	0/3/3/3
7	CAP	C	502	6	-	6/29/29/29	-
7	CAP	G	502	6	-	8/29/29/29	-
7	CAP	A	502	6	-	6/29/29/29	-
4	ADP	1	301	-	-	1/12/32/32	0/3/3/3
7	CAP	E	502	6	-	6/29/29/29	-
7	CAP	H	502	6	-	7/29/29/29	-
5	AGS	6	301	-	-	7/17/38/38	0/3/3/3
5	AGS	5	301	6	-	1/17/38/38	0/3/3/3
7	CAP	D	502	6	-	6/29/29/29	-
7	CAP	F	502	6	-	8/29/29/29	-
5	AGS	2	301	6	-	5/17/38/38	0/3/3/3
5	AGS	4	301	6	-	3/17/38/38	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	301	AGS	PG-S1G	-16.97	1.53	1.90
5	5	301	AGS	PG-S1G	-10.59	1.67	1.90
5	6	301	AGS	PG-S1G	9.27	2.10	1.90
5	4	301	AGS	PG-S1G	8.34	2.08	1.90
5	3	301	AGS	C2-N3	6.25	1.41	1.32

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	301	AGS	N3-C2-N1	-7.68	118.24	128.67
5	4	301	AGS	N3-C2-N1	-7.63	118.32	128.67
5	3	301	AGS	N3-C2-N1	-7.45	118.56	128.67
5	2	301	AGS	N3-C2-N1	-7.24	118.85	128.67
5	6	301	AGS	N3-C2-N1	-7.06	119.08	128.67

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2	301	AGS	C5'-O5'-PA-O1A
5	2	301	AGS	C5'-O5'-PA-O3A
5	3	301	AGS	C5'-O5'-PA-O3A
5	4	301	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
7	A	502	CAP	O6-C-C2-C1

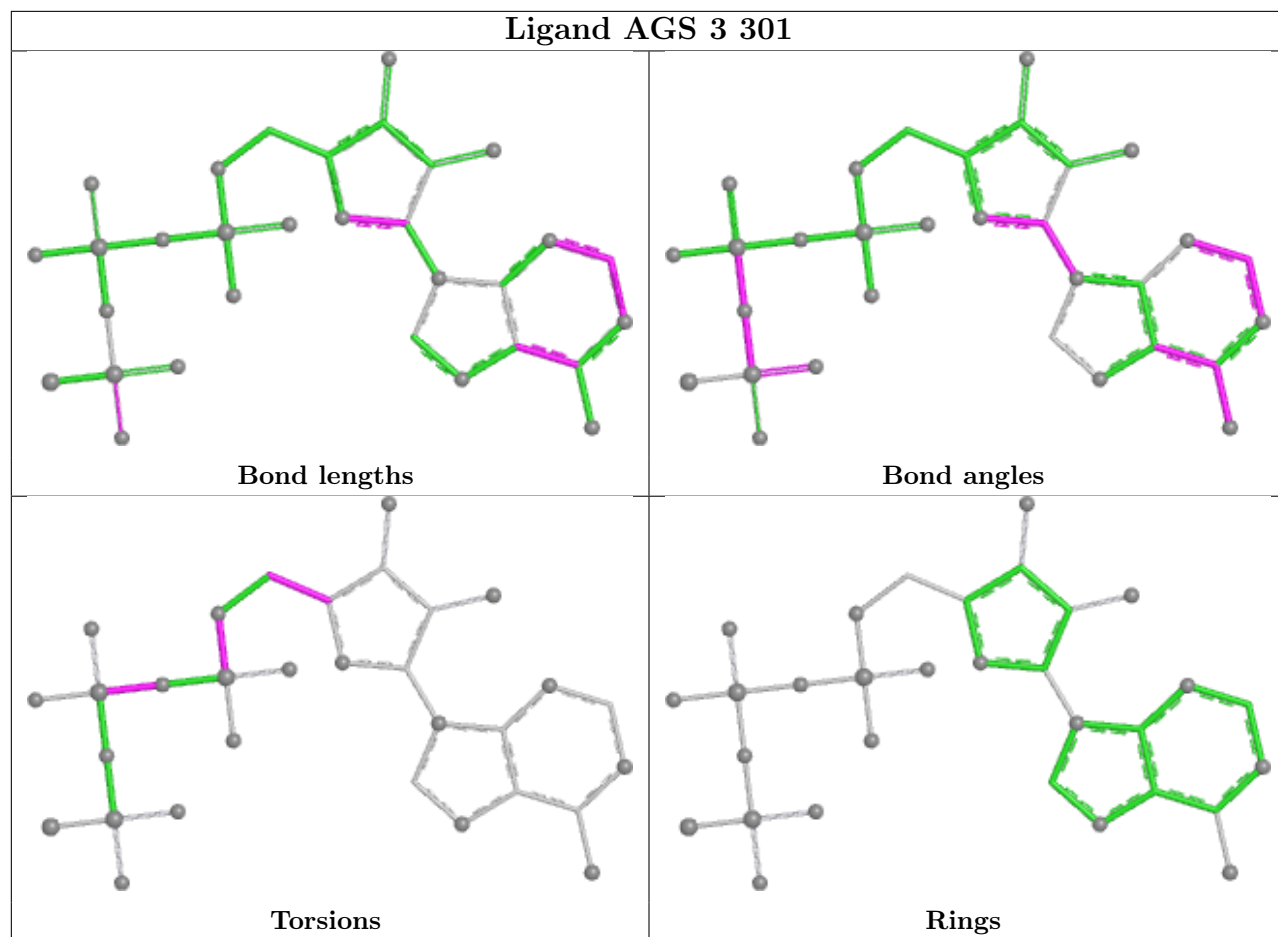
There are no ring outliers.

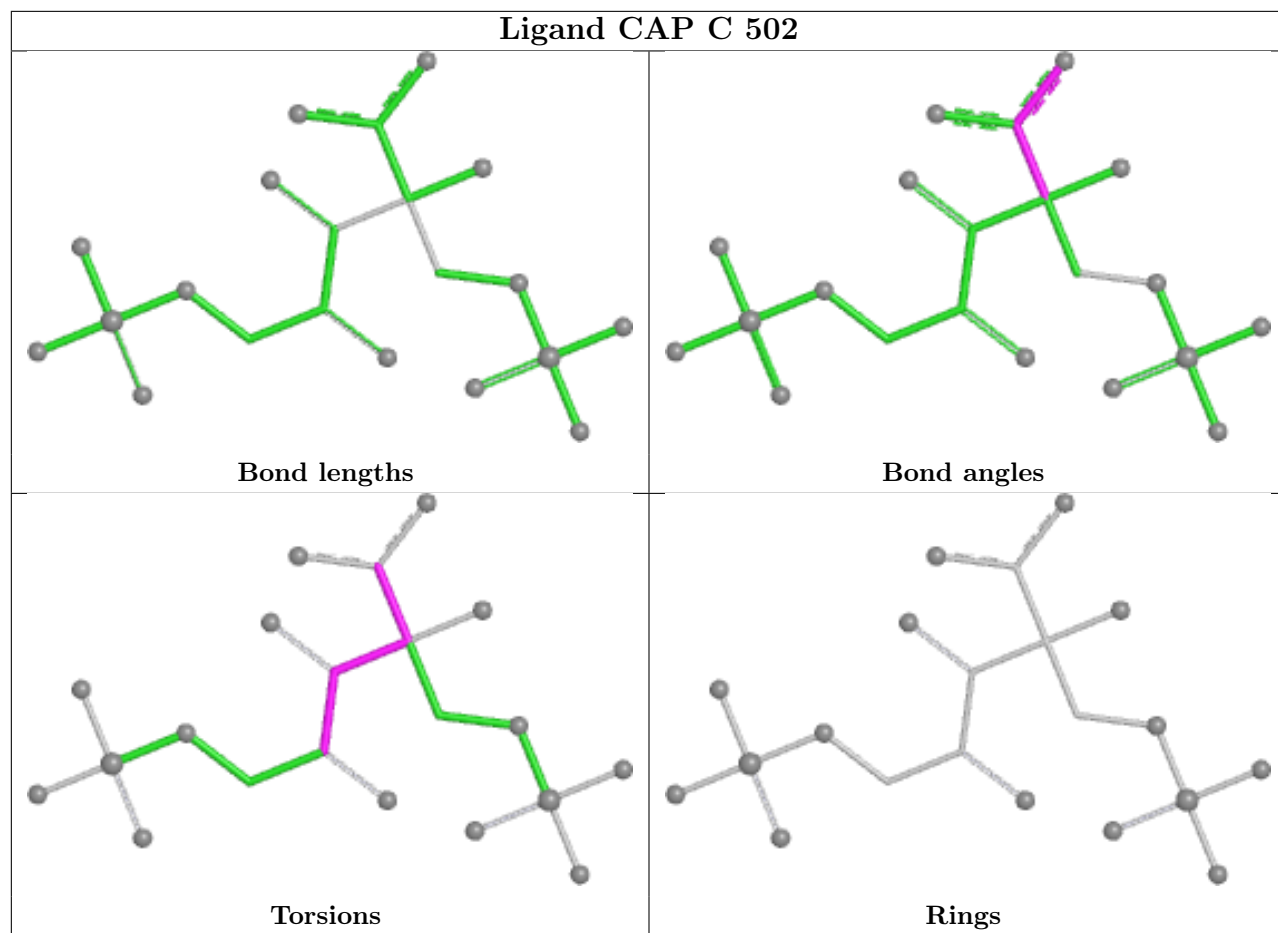
6 monomers are involved in 13 short contacts:

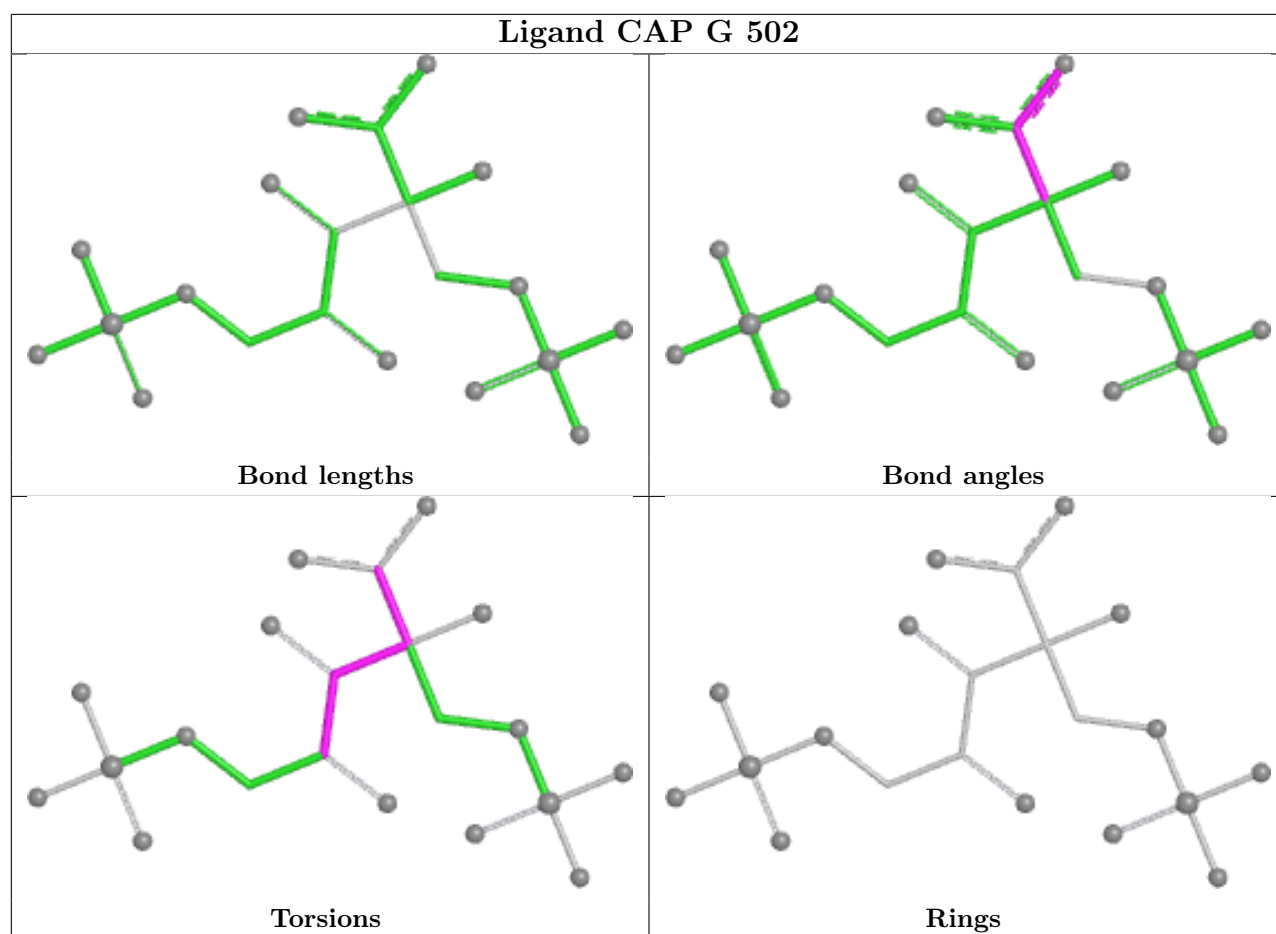
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	301	AGS	1	0
4	1	301	ADP	1	0
5	6	301	AGS	2	0
5	5	301	AGS	2	0
5	2	301	AGS	6	0
5	4	301	AGS	1	0

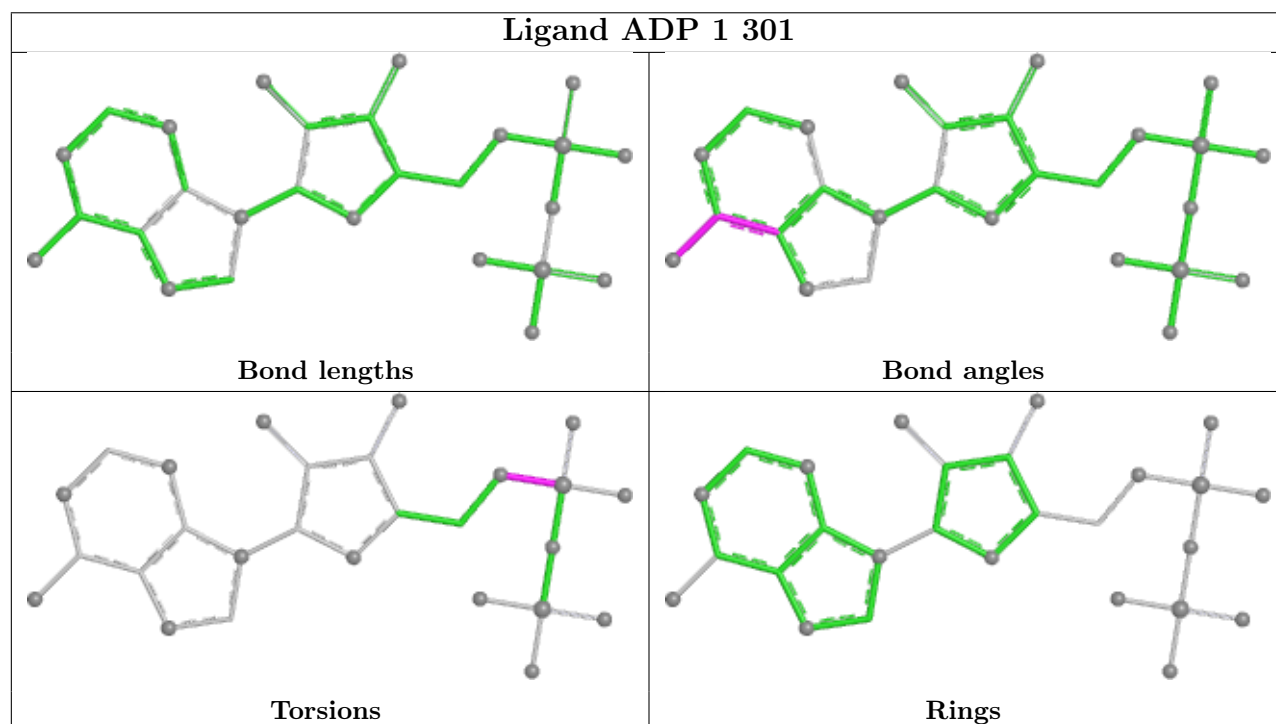
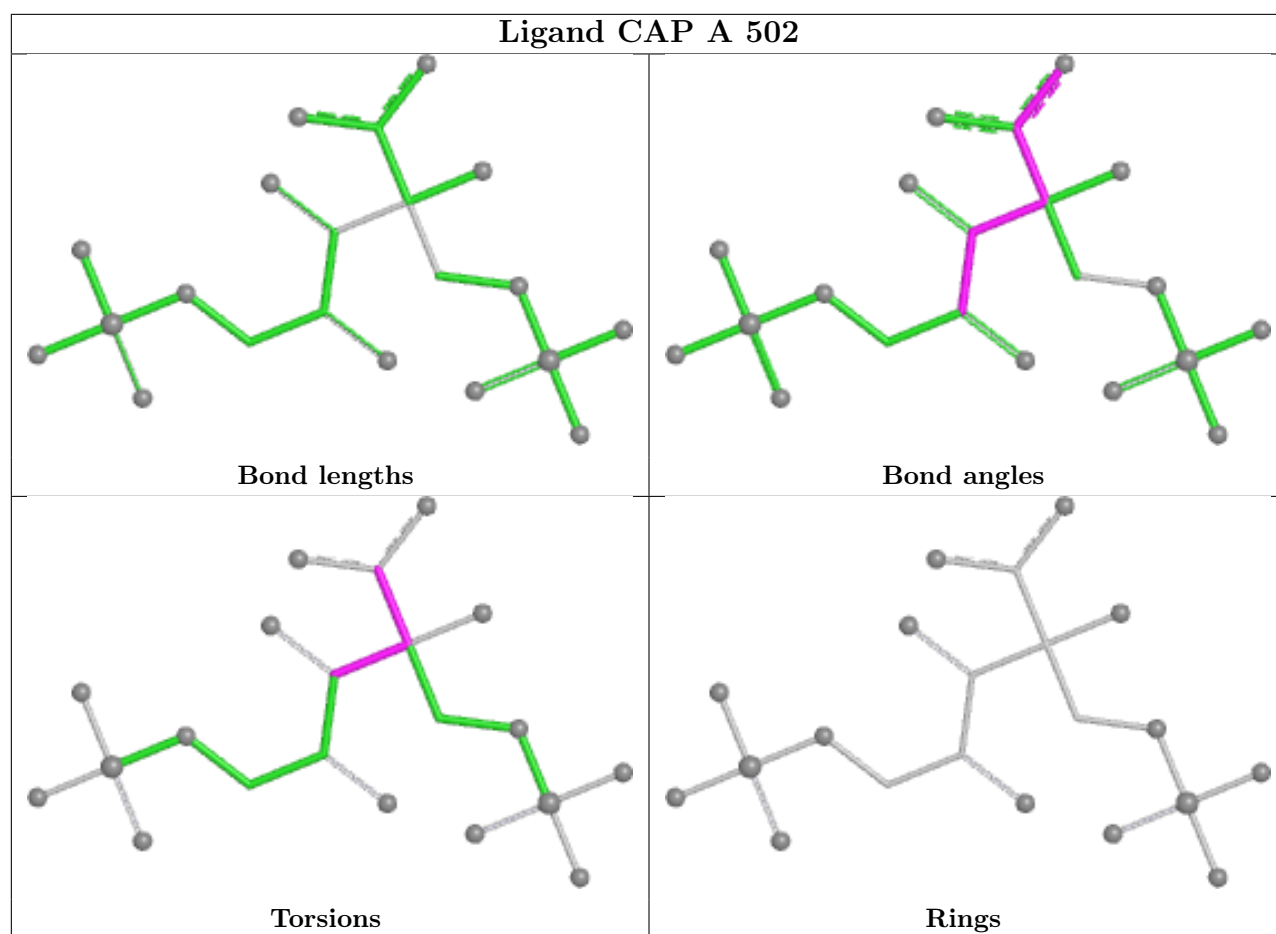
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

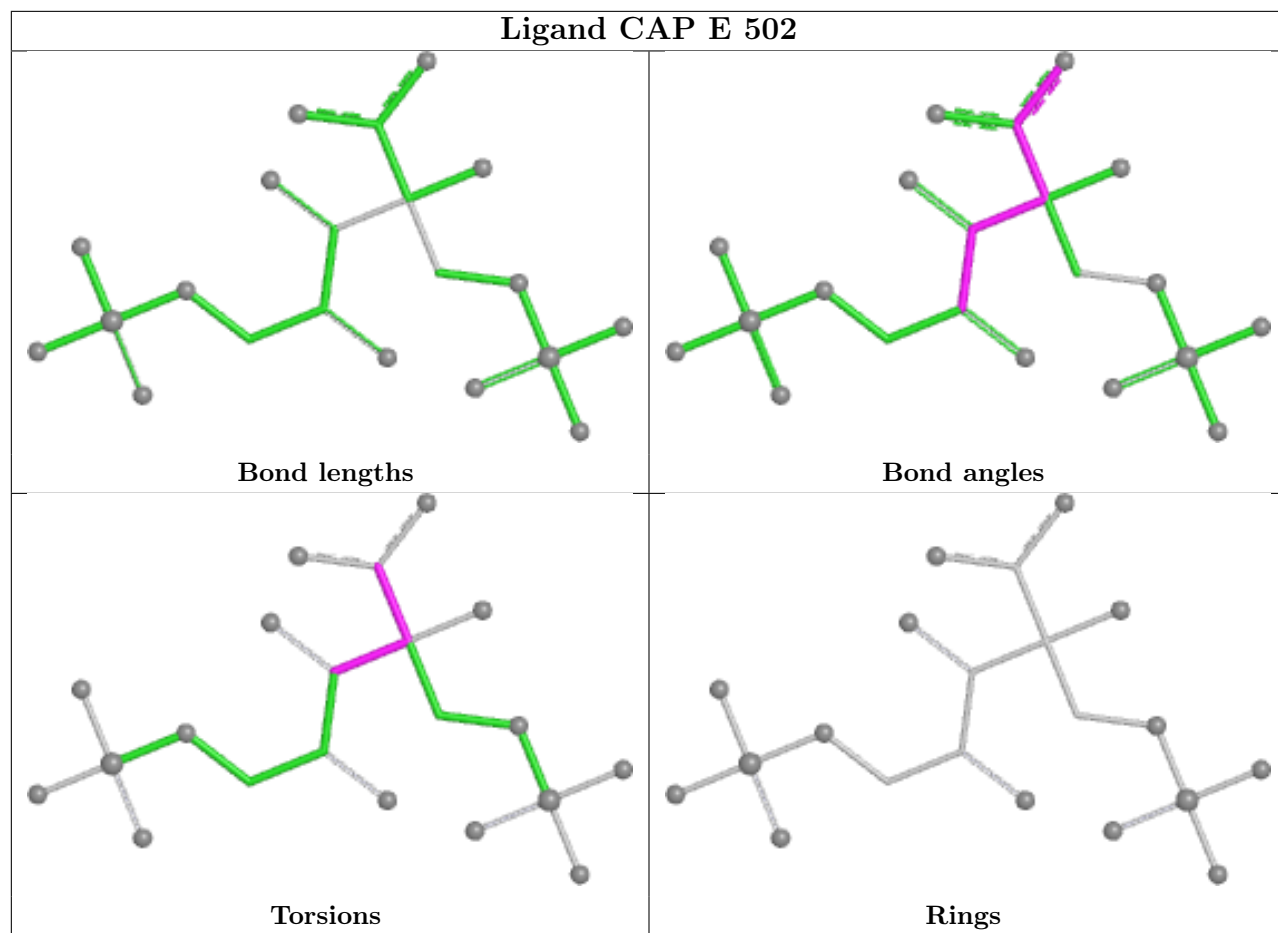
Ligand AGS 3 301

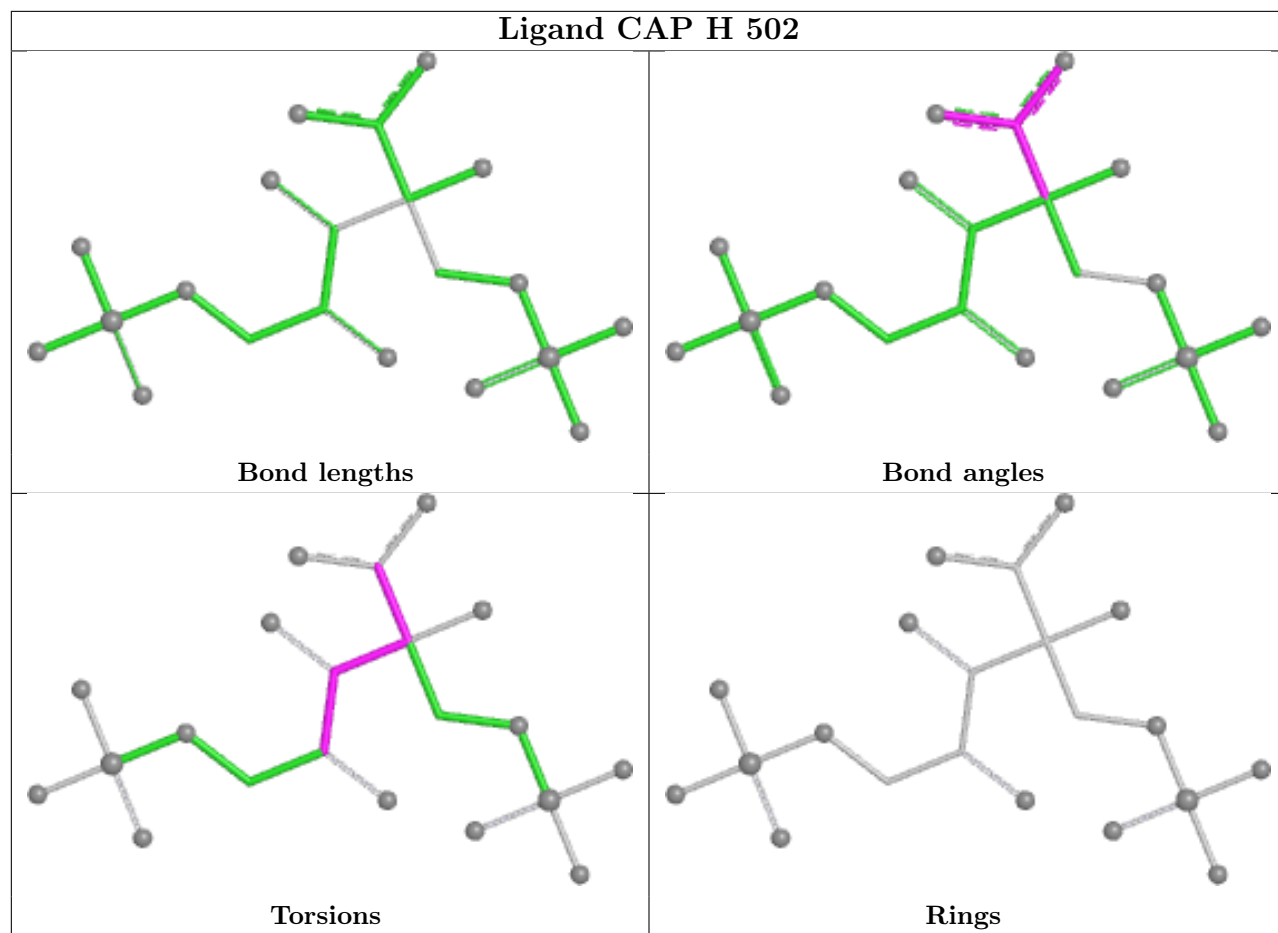




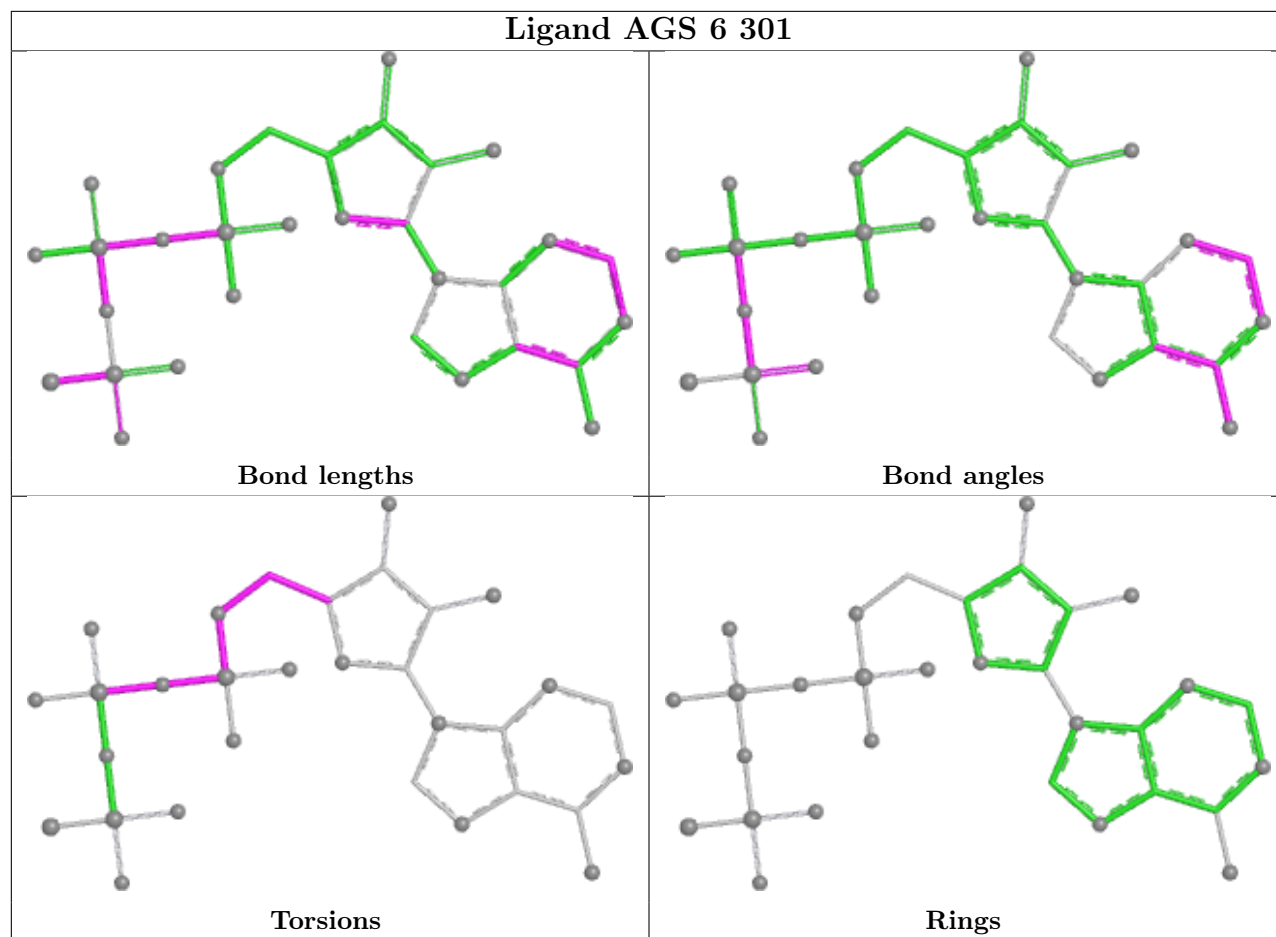




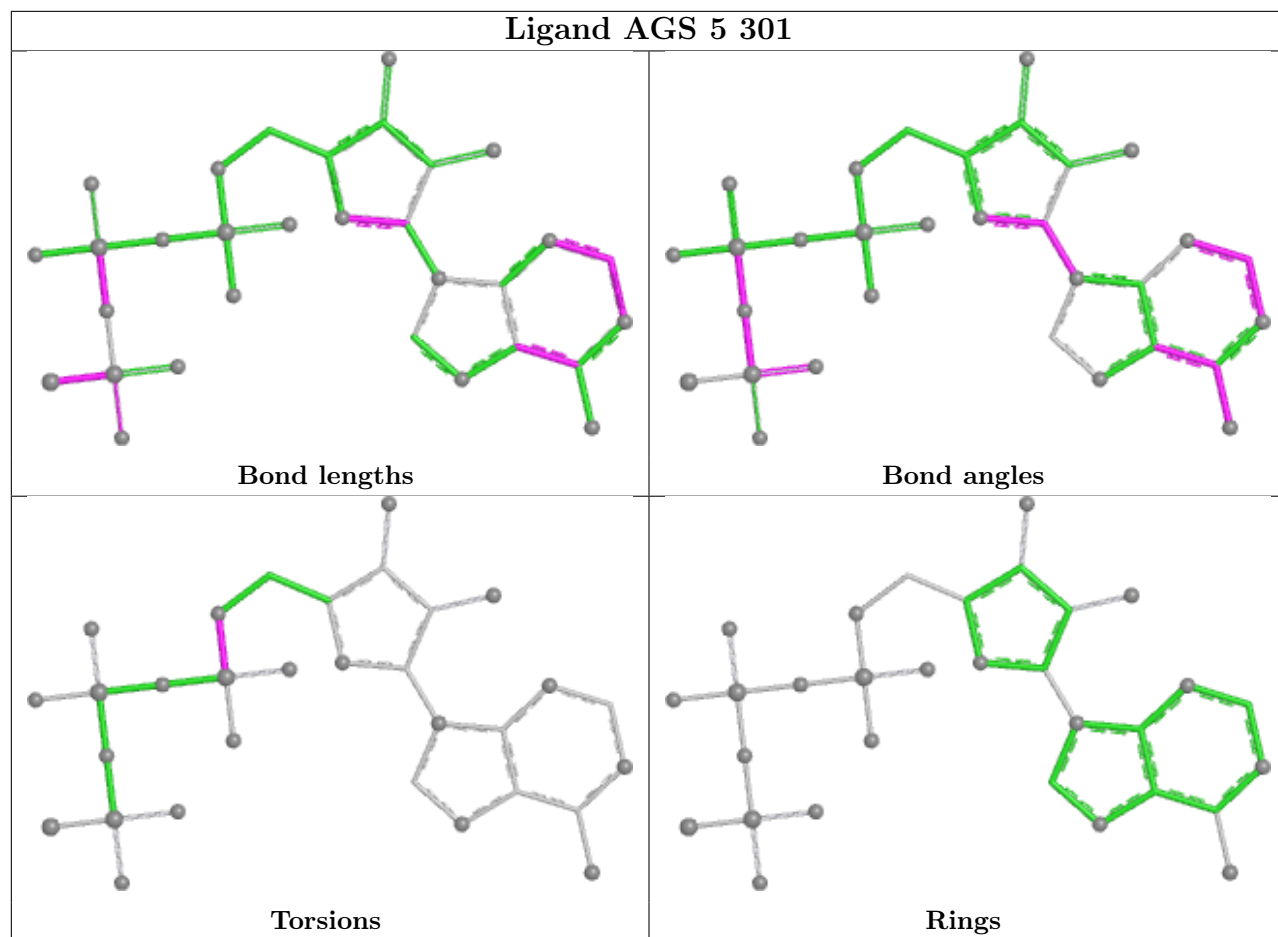


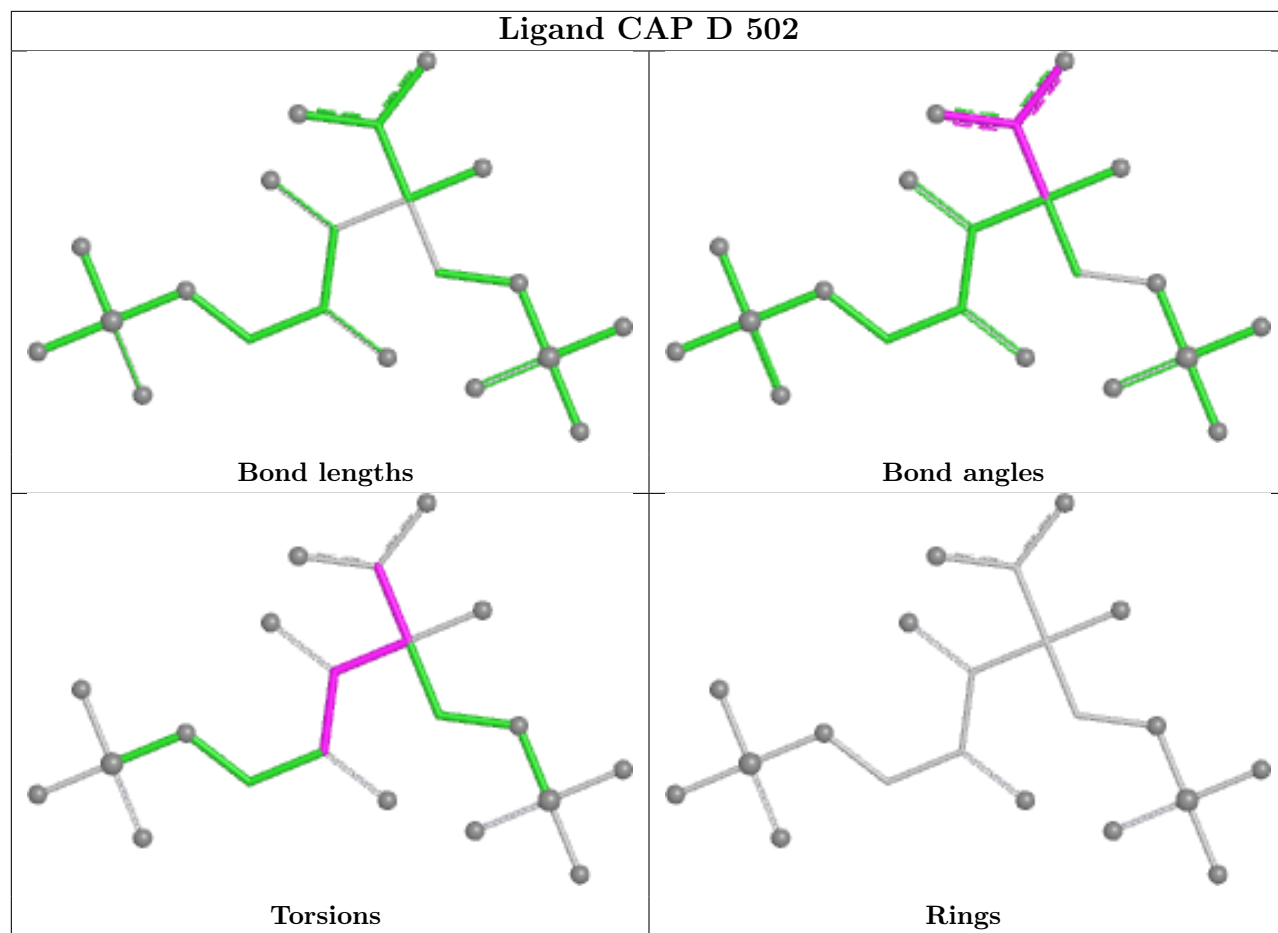


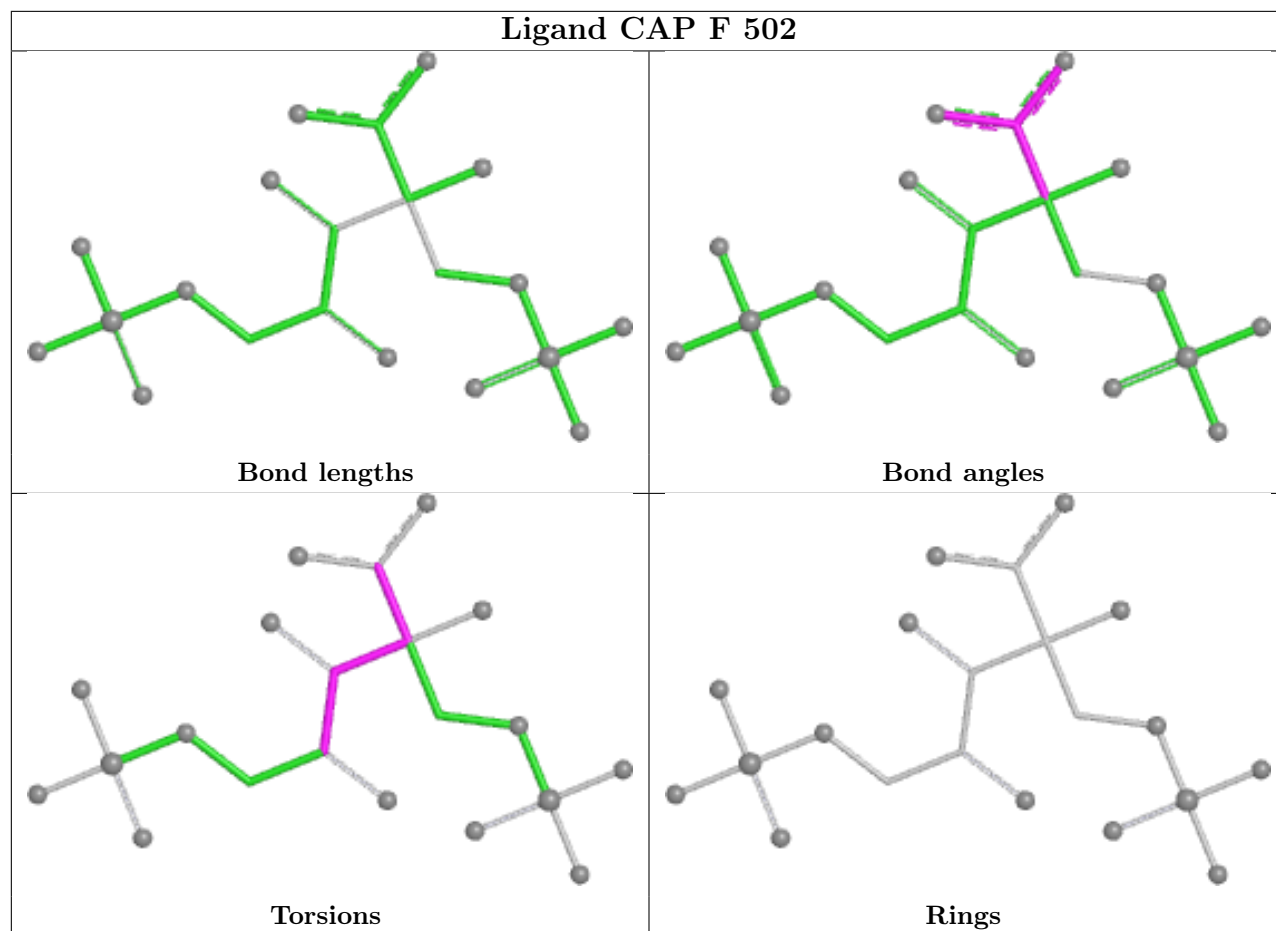
Ligand AGS 6 301



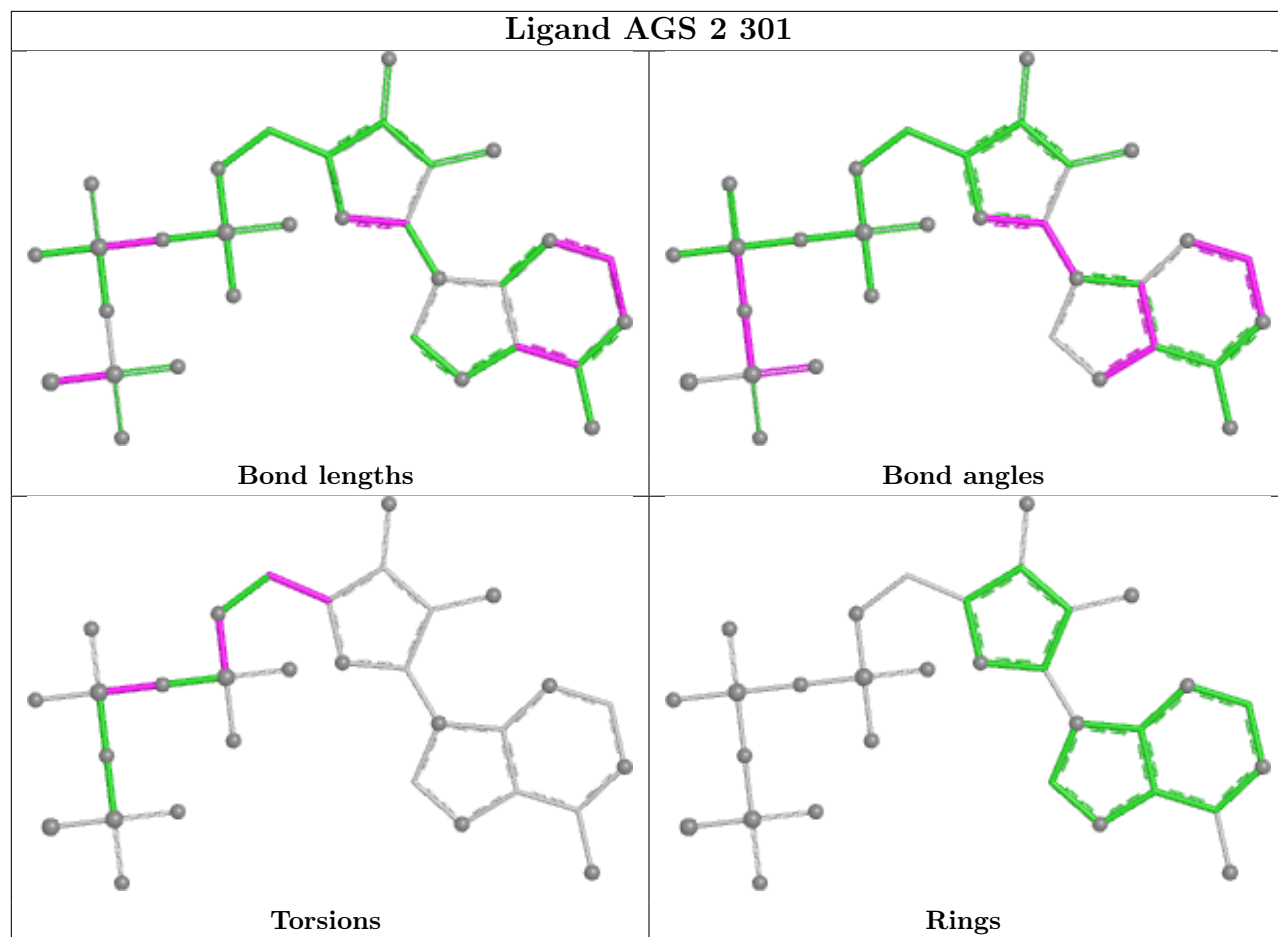
Ligand AGS 5 301

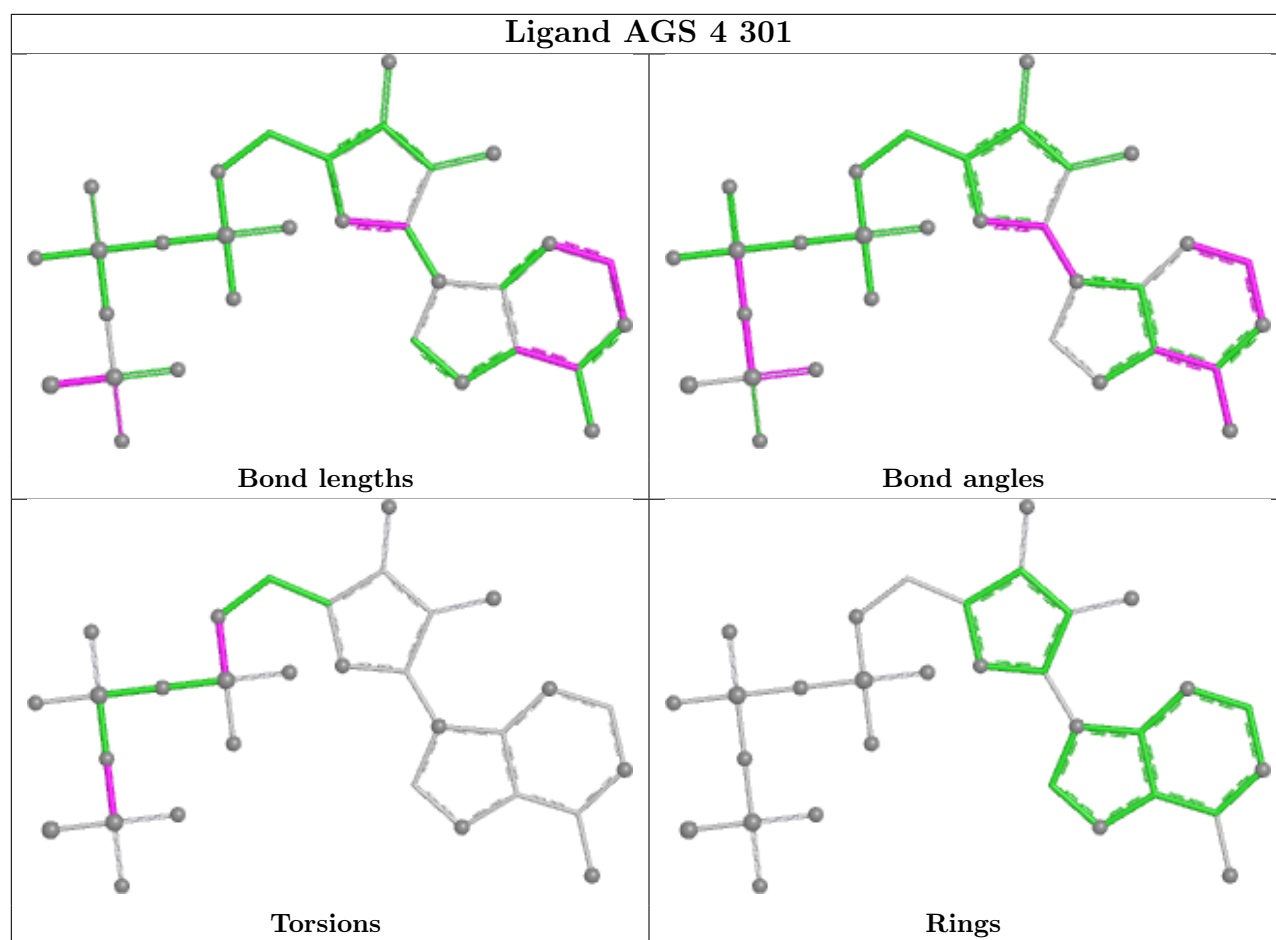






Ligand AGS 2 301





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.

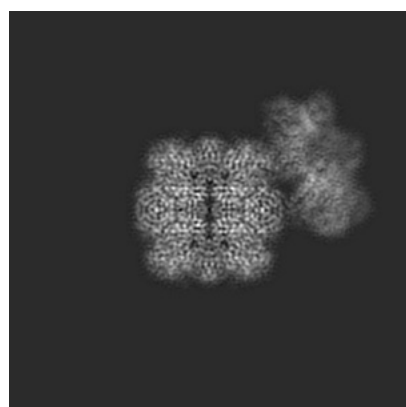
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11028. These allow visual inspection of the internal detail of the map and identification of artifacts.

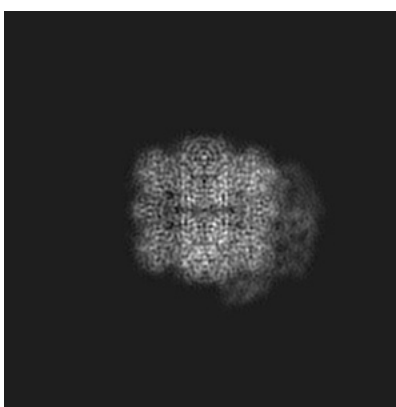
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

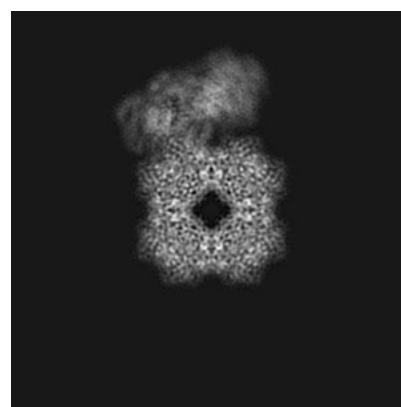
6.1.1 Primary map



X



Y

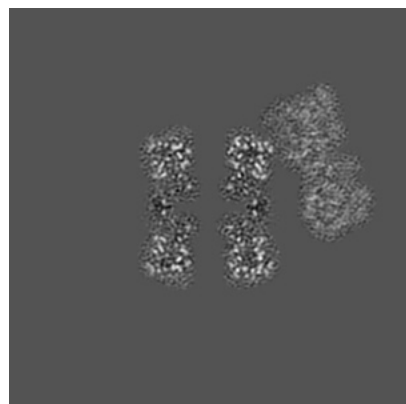


Z

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

6.2 Central slices [i](#)

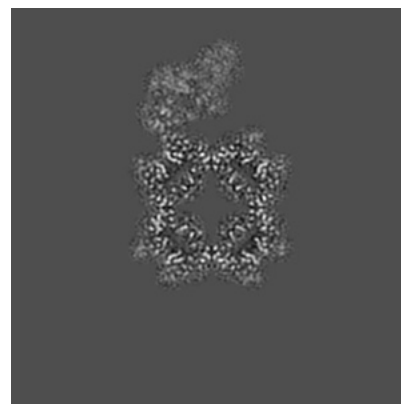
6.2.1 Primary map



X Index: 180



Y Index: 180

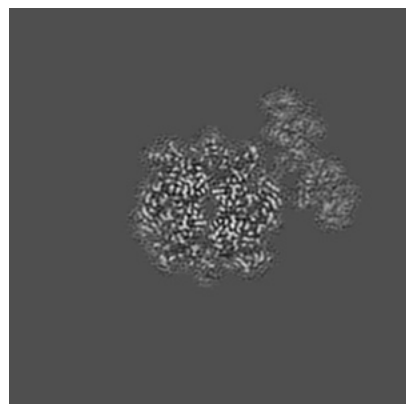


Z Index: 180

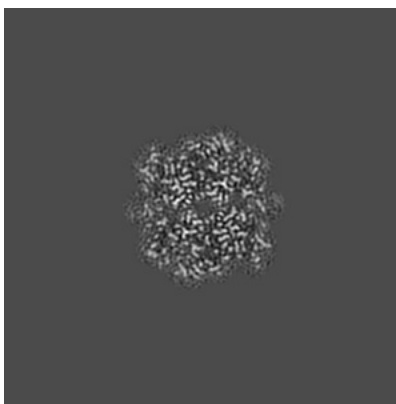
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

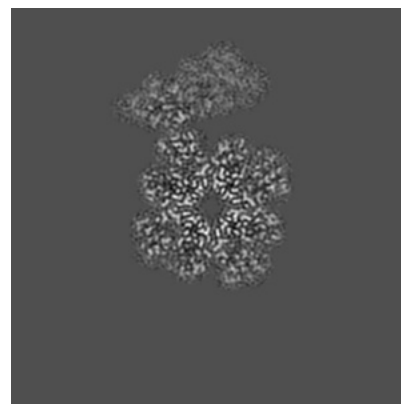
6.3.1 Primary map



X Index: 158



Y Index: 201

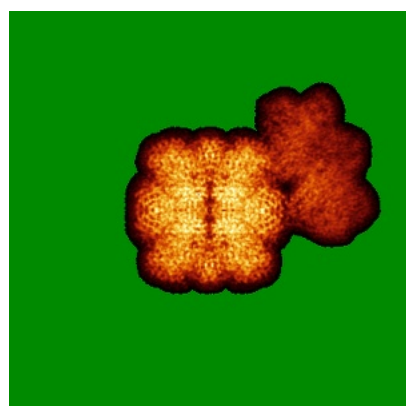


Z Index: 194

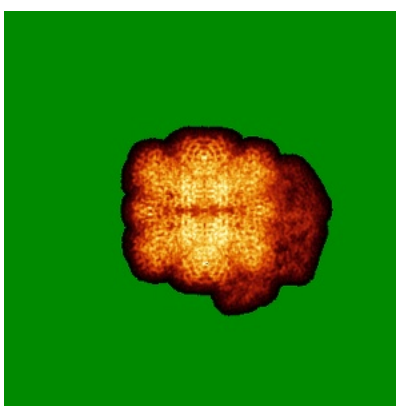
The images above show the largest variance slices of the map in three orthogonal directions.

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

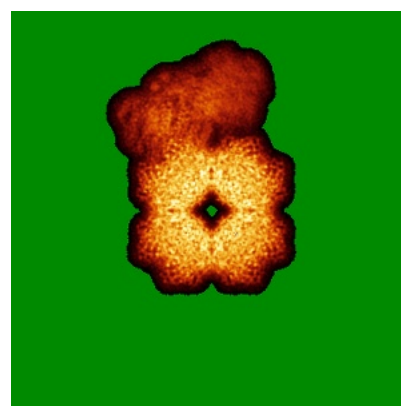
6.4.1 Primary map



X



Y

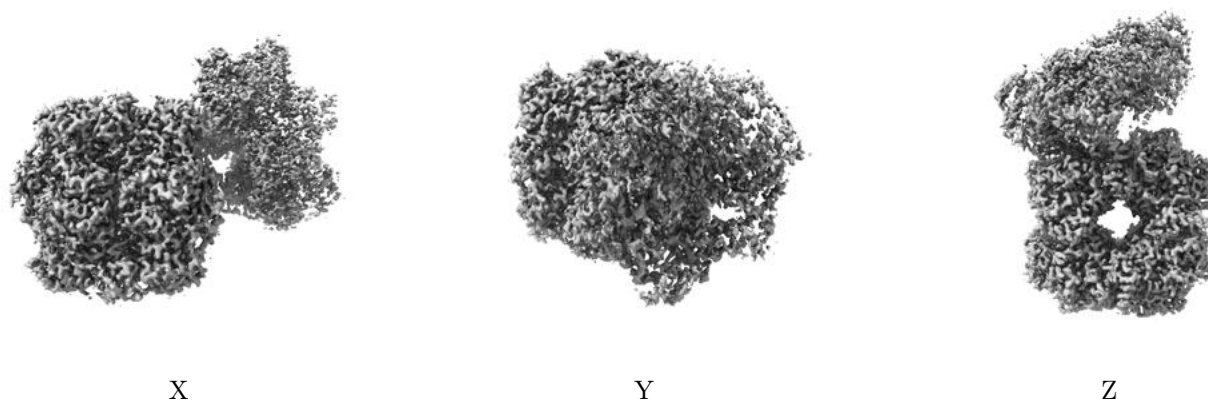


Z

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

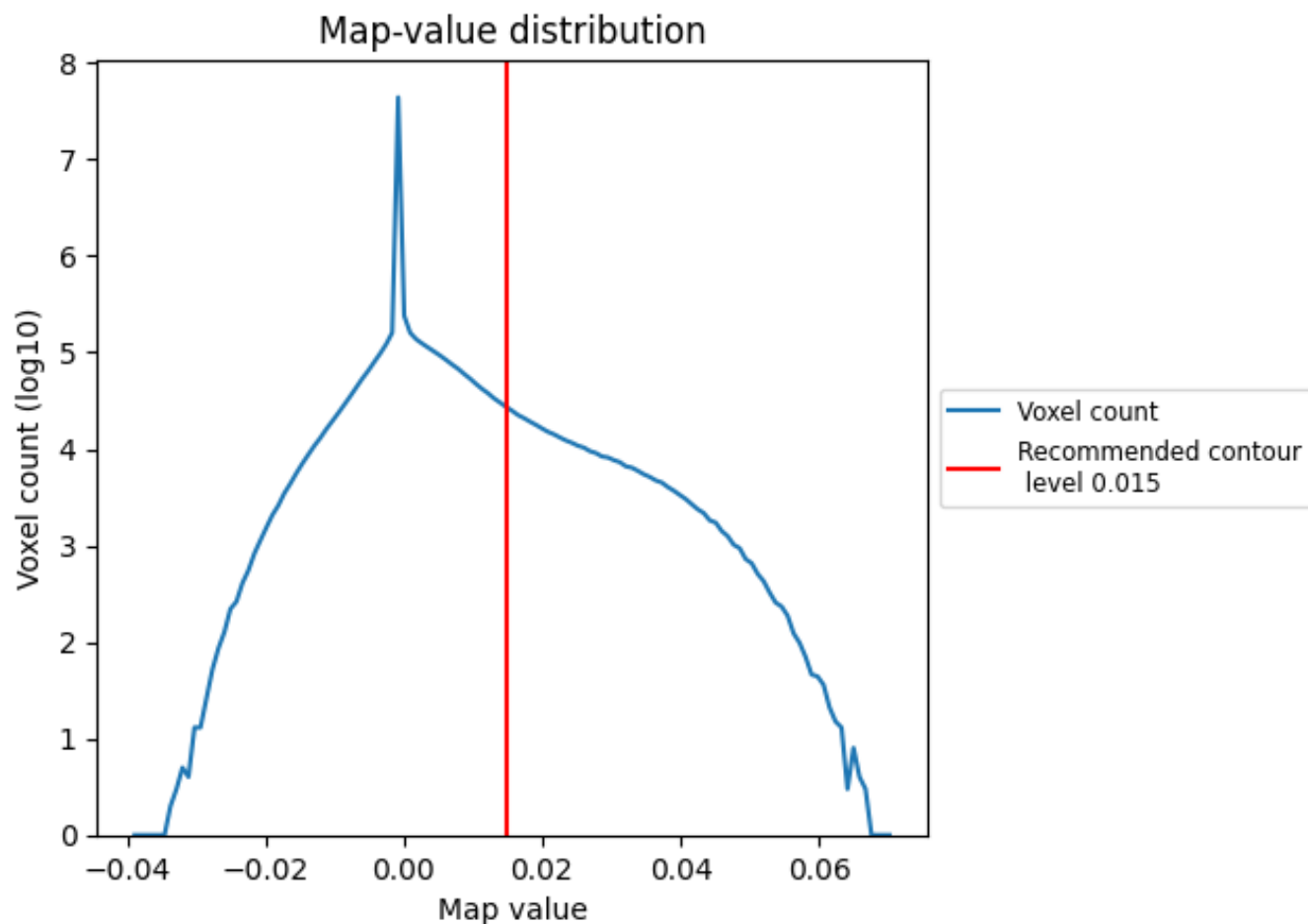
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

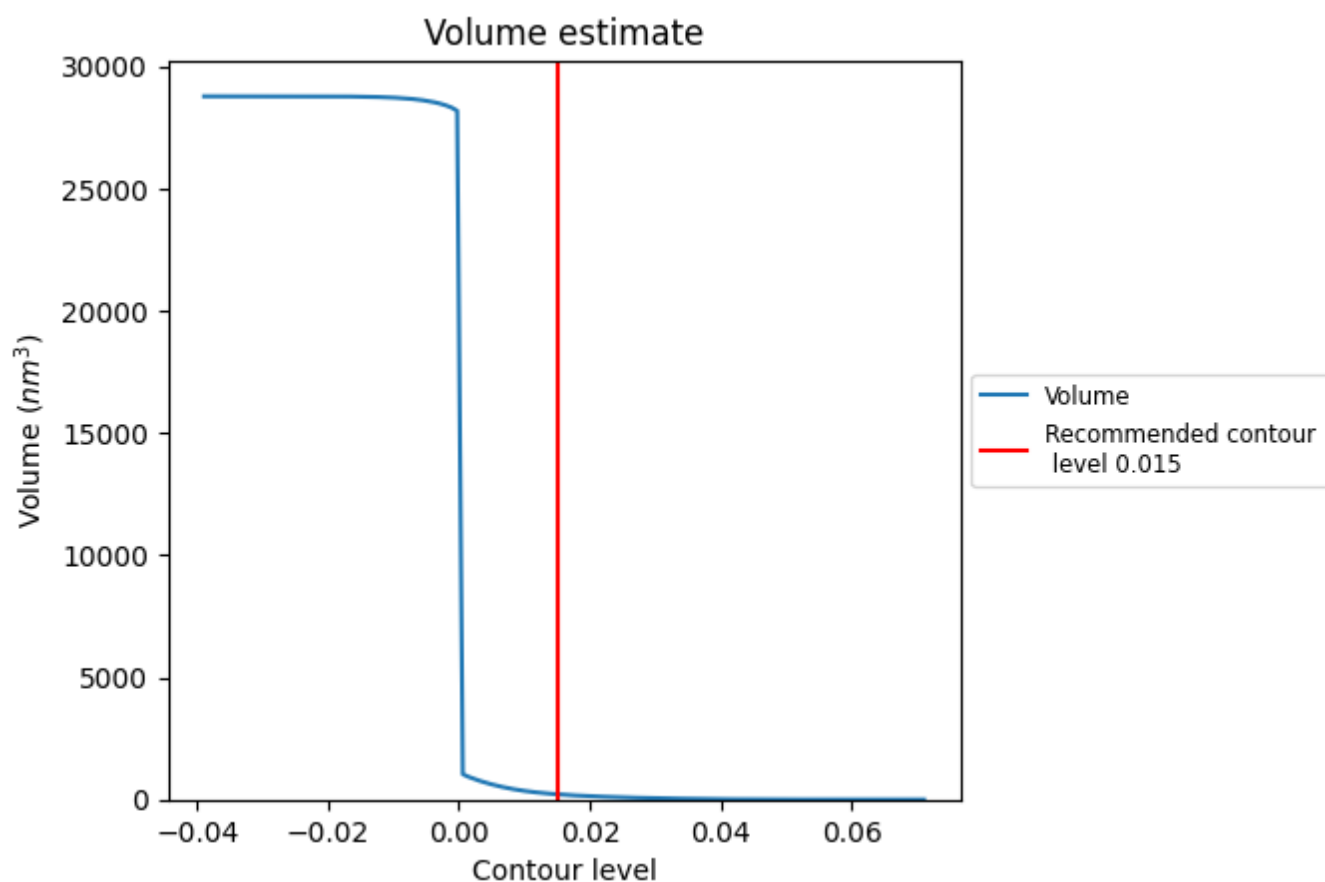
This section contains the results of statistical analysis of the map.

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.

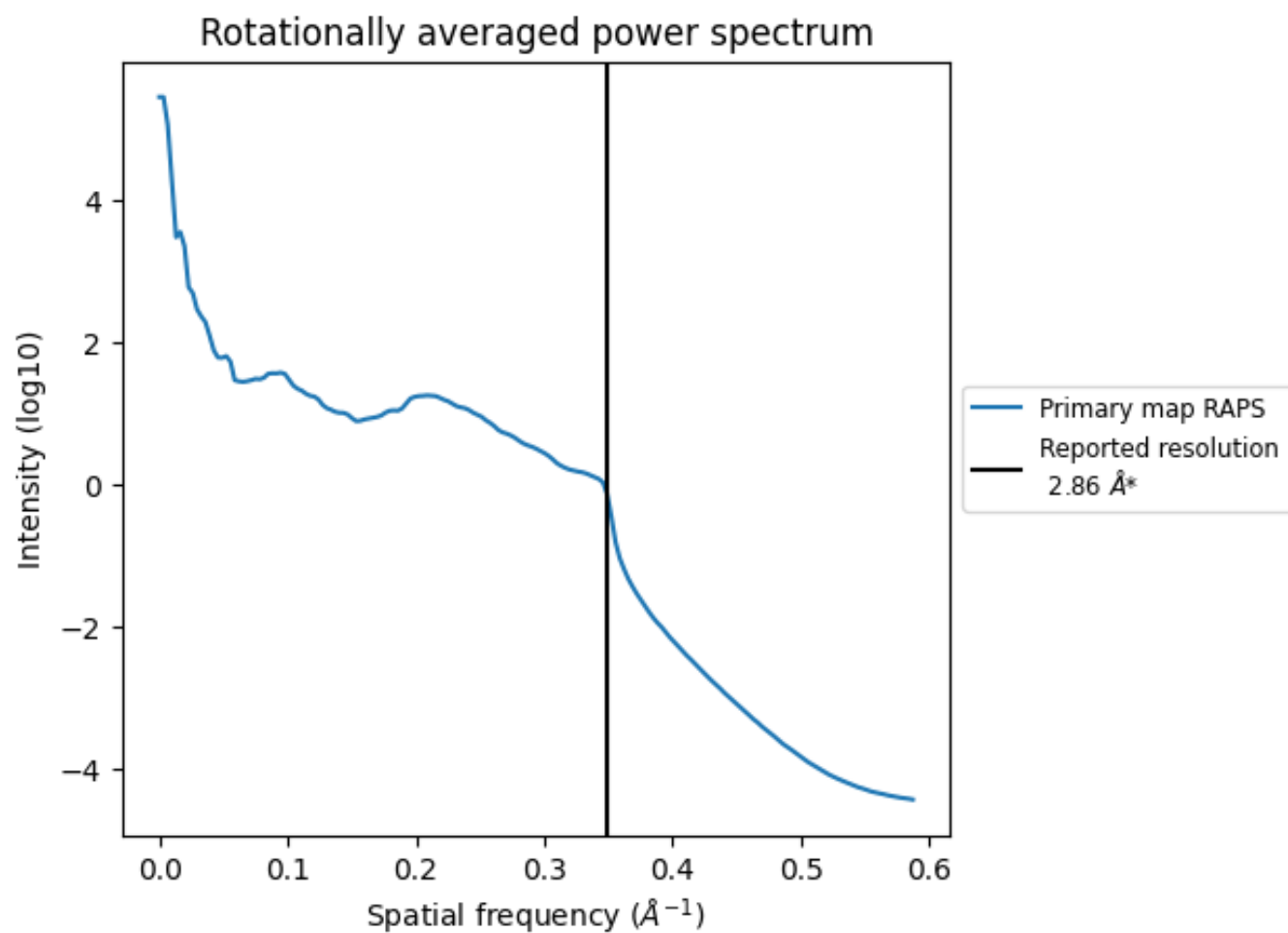
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217 nm³; this corresponds to an approximate mass of 196 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 ⓘ

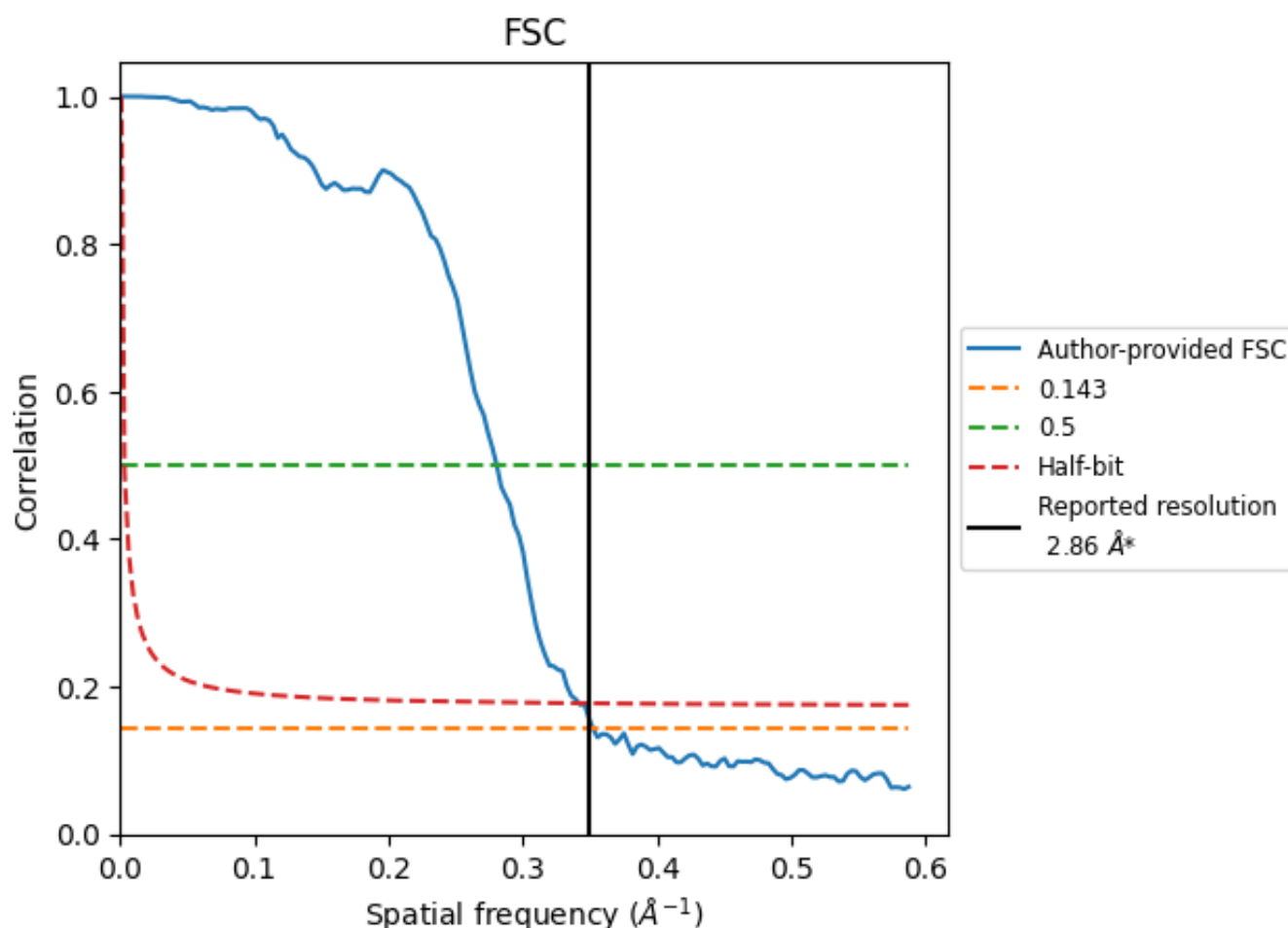


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

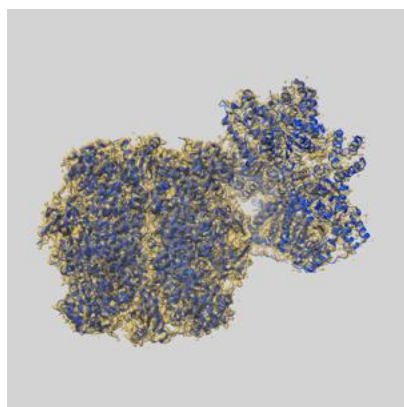
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.84	3.56	2.93
Unmasked-calculated*	-	-	-

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

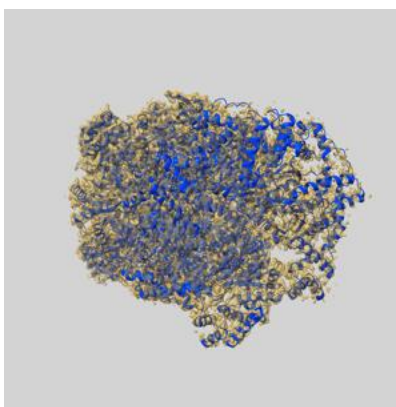
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11028 and PDB model 6Z1F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

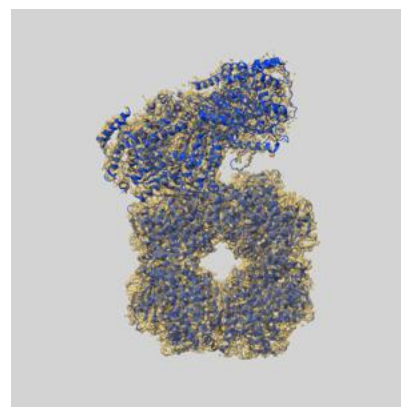
9.1 Map-model overlay [i](#)



X



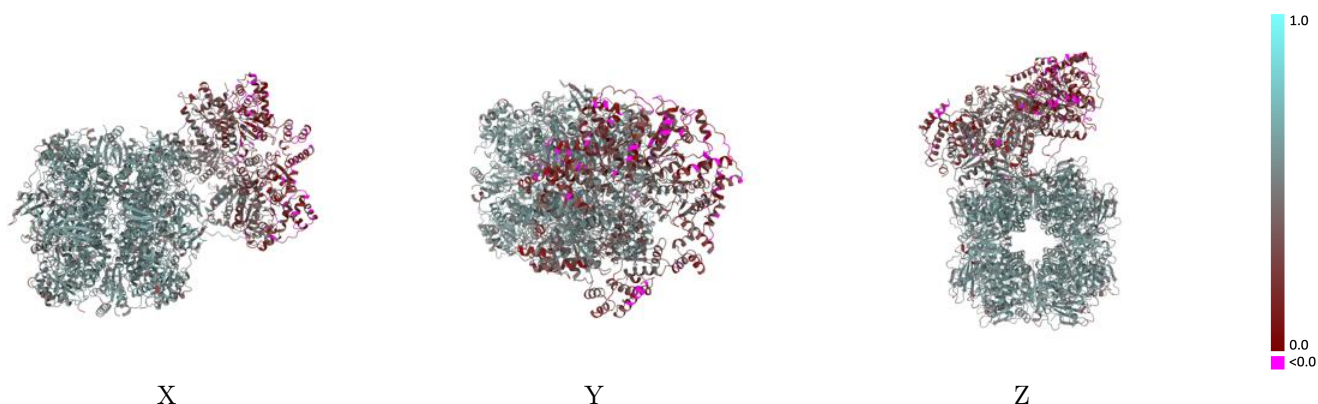
Y



Z

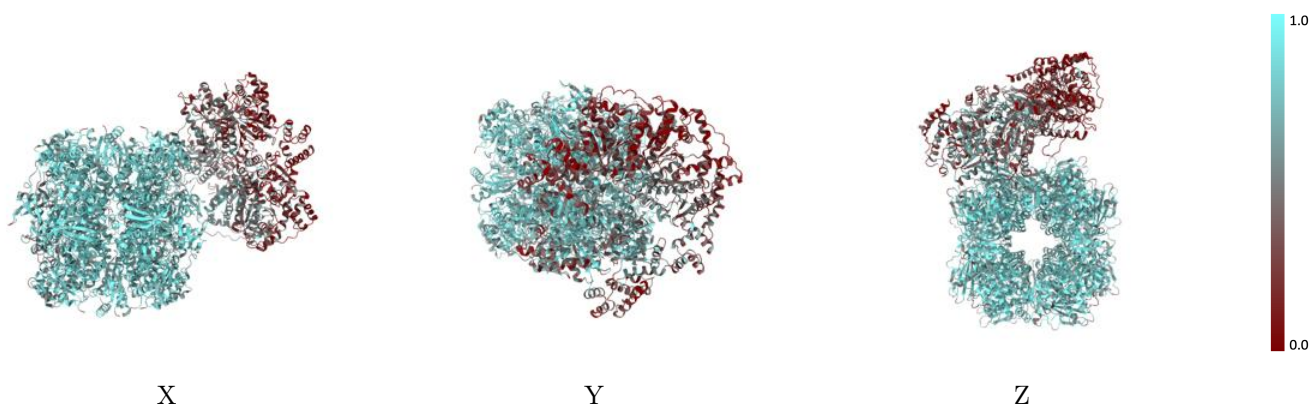
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



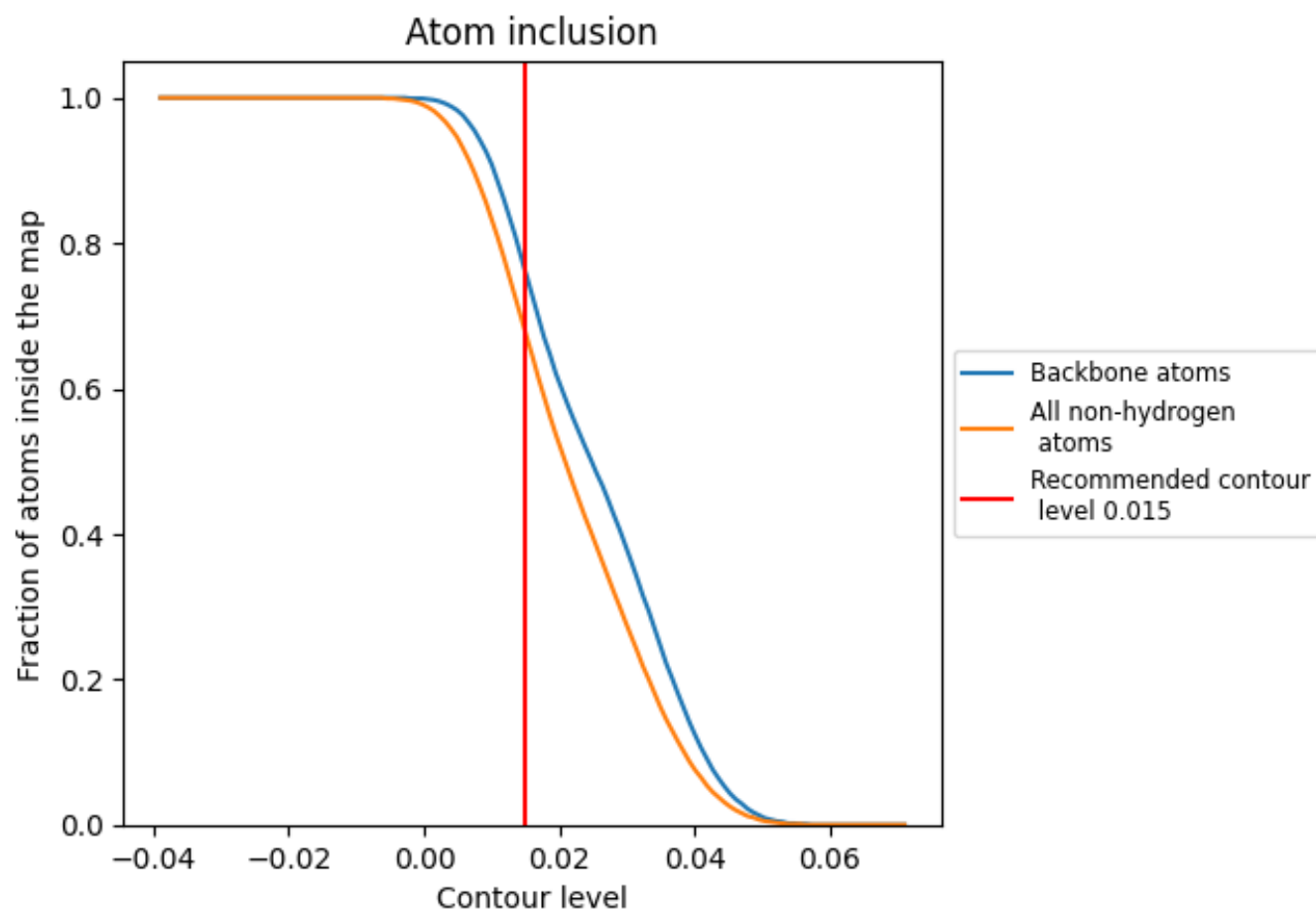
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.4890
1	 0.4390	 0.3410
2	 0.3430	 0.2910
3	 0.2140	 0.2070
4	 0.2410	 0.2270
5	 0.4330	 0.3410
6	 0.4980	 0.3790
A	 0.8150	 0.5730
B	 0.8110	 0.5700
C	 0.8040	 0.5580
D	 0.8130	 0.5700
E	 0.7830	 0.5580
F	 0.7940	 0.5620
G	 0.7970	 0.5660
H	 0.8090	 0.5660
I	 0.7570	 0.5340
J	 0.7790	 0.5450
K	 0.7570	 0.5160
L	 0.7630	 0.5430
M	 0.7630	 0.5370
N	 0.7560	 0.5450
O	 0.7360	 0.5320
P	 0.8010	 0.5450

