



## wwPDB EM Validation Summary Report

Nov 21, 2022 – 02:21 AM EST

PDB ID : 7UIX  
EMDB ID : EMD-26556  
Title : ClpAP complex bound to ClpS N-terminal extension, class I  
Authors : Kim, S.; Fei, X.; Sauer, R.T.; Baker, T.A.  
Deposited on : 2022-03-29  
Resolution : 3.24 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

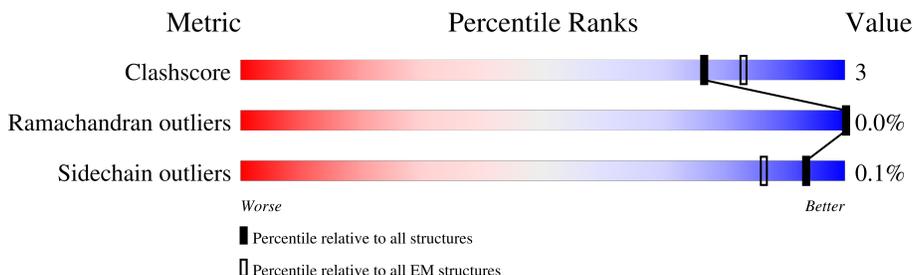
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	758	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>44%</p> </div> <div style="text-align: center;"> </div> </div>
1	B	758	<div style="text-align: center;"> <p>22%</p> </div>
1	C	758	<div style="text-align: center;"> <p>5%</p> </div>
1	D	758	<div style="text-align: center;"> <p>.</p> </div>
1	E	758	<div style="text-align: center;"> <p>10%</p> </div>
1	F	758	<div style="text-align: center;"> <p>32%</p> </div>
2	H	201	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>54%</p> </div> <div style="text-align: center;"> </div> </div>
2	I	201	<div style="text-align: center;"> <p>27%</p> </div>

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Mol	Chain	Length	Quality of chain
2	J	201	
2	K	201	
2	L	201	
2	M	201	
2	N	201	
3	S	106	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 76451 atoms, of which 38430 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 ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	577	9101	2835	4601	804	848	13	0	0
1	B	571	9042	2818	4571	798	842	13	0	0
1	C	580	9140	2847	4618	808	854	13	0	0
1	D	581	9152	2851	4623	809	856	13	0	0
1	E	580	9123	2848	4599	808	855	13	0	0
1	F	571	9022	2811	4563	796	839	13	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	THR	MET	conflict	UNP A0A836NDF2
B	169	THR	MET	conflict	UNP A0A836NDF2
C	169	THR	MET	conflict	UNP A0A836NDF2
D	169	THR	MET	conflict	UNP A0A836NDF2
E	169	THR	MET	conflict	UNP A0A836NDF2
F	169	THR	MET	conflict	UNP A0A836NDF2

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	H	191	3001	943	1506	259	281	12	0	0
2	I	191	3001	943	1506	259	281	12	0	0
2	J	191	3001	943	1506	259	281	12	0	0
2	K	191	3001	943	1506	259	281	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	L	190	2977	937	1493	255	280	12	0	0
2	M	191	3001	943	1506	259	281	12	0	0
2	N	190	2978	937	1494	255	280	12	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	194	ARG	-	expression tag	UNP A0A0K4NM46
H	195	SER	-	expression tag	UNP A0A0K4NM46
H	196	HIS	-	expression tag	UNP A0A0K4NM46
H	197	HIS	-	expression tag	UNP A0A0K4NM46
H	198	HIS	-	expression tag	UNP A0A0K4NM46
H	199	HIS	-	expression tag	UNP A0A0K4NM46
H	200	HIS	-	expression tag	UNP A0A0K4NM46
H	201	HIS	-	expression tag	UNP A0A0K4NM46
I	194	ARG	-	expression tag	UNP A0A0K4NM46
I	195	SER	-	expression tag	UNP A0A0K4NM46
I	196	HIS	-	expression tag	UNP A0A0K4NM46
I	197	HIS	-	expression tag	UNP A0A0K4NM46
I	198	HIS	-	expression tag	UNP A0A0K4NM46
I	199	HIS	-	expression tag	UNP A0A0K4NM46
I	200	HIS	-	expression tag	UNP A0A0K4NM46
I	201	HIS	-	expression tag	UNP A0A0K4NM46
J	194	ARG	-	expression tag	UNP A0A0K4NM46
J	195	SER	-	expression tag	UNP A0A0K4NM46
J	196	HIS	-	expression tag	UNP A0A0K4NM46
J	197	HIS	-	expression tag	UNP A0A0K4NM46
J	198	HIS	-	expression tag	UNP A0A0K4NM46
J	199	HIS	-	expression tag	UNP A0A0K4NM46
J	200	HIS	-	expression tag	UNP A0A0K4NM46
J	201	HIS	-	expression tag	UNP A0A0K4NM46
K	194	ARG	-	expression tag	UNP A0A0K4NM46
K	195	SER	-	expression tag	UNP A0A0K4NM46
K	196	HIS	-	expression tag	UNP A0A0K4NM46
K	197	HIS	-	expression tag	UNP A0A0K4NM46
K	198	HIS	-	expression tag	UNP A0A0K4NM46
K	199	HIS	-	expression tag	UNP A0A0K4NM46
K	200	HIS	-	expression tag	UNP A0A0K4NM46
K	201	HIS	-	expression tag	UNP A0A0K4NM46

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Chain	Residue	Modelled	Actual	Comment	Reference
L	194	ARG	-	expression tag	UNP A0A0K4NM46
L	195	SER	-	expression tag	UNP A0A0K4NM46
L	196	HIS	-	expression tag	UNP A0A0K4NM46
L	197	HIS	-	expression tag	UNP A0A0K4NM46
L	198	HIS	-	expression tag	UNP A0A0K4NM46
L	199	HIS	-	expression tag	UNP A0A0K4NM46
L	200	HIS	-	expression tag	UNP A0A0K4NM46
L	201	HIS	-	expression tag	UNP A0A0K4NM46
M	194	ARG	-	expression tag	UNP A0A0K4NM46
M	195	SER	-	expression tag	UNP A0A0K4NM46
M	196	HIS	-	expression tag	UNP A0A0K4NM46
M	197	HIS	-	expression tag	UNP A0A0K4NM46
M	198	HIS	-	expression tag	UNP A0A0K4NM46
M	199	HIS	-	expression tag	UNP A0A0K4NM46
M	200	HIS	-	expression tag	UNP A0A0K4NM46
M	201	HIS	-	expression tag	UNP A0A0K4NM46
N	194	ARG	-	expression tag	UNP A0A0K4NM46
N	195	SER	-	expression tag	UNP A0A0K4NM46
N	196	HIS	-	expression tag	UNP A0A0K4NM46
N	197	HIS	-	expression tag	UNP A0A0K4NM46
N	198	HIS	-	expression tag	UNP A0A0K4NM46
N	199	HIS	-	expression tag	UNP A0A0K4NM46
N	200	HIS	-	expression tag	UNP A0A0K4NM46
N	201	HIS	-	expression tag	UNP A0A0K4NM46

- Molecule 3 is a protein called ATP-dependent Clp protease adapter protein ClpS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	S	25	396	127	194	34	41	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

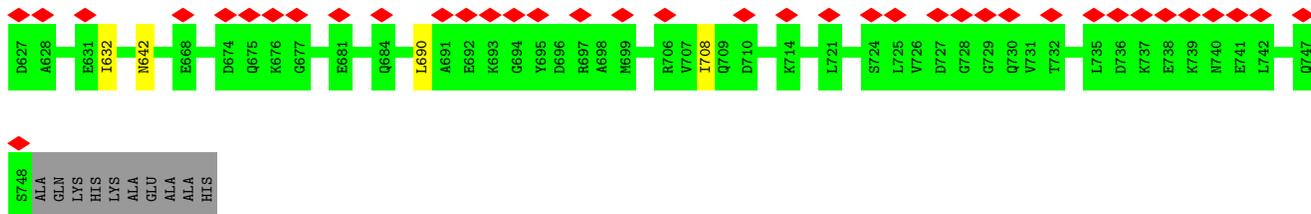




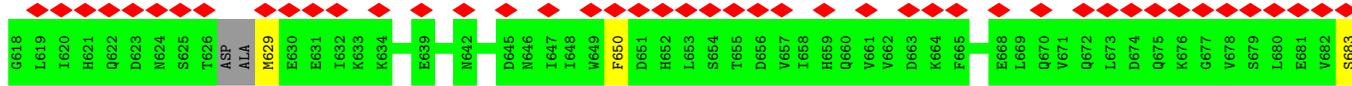
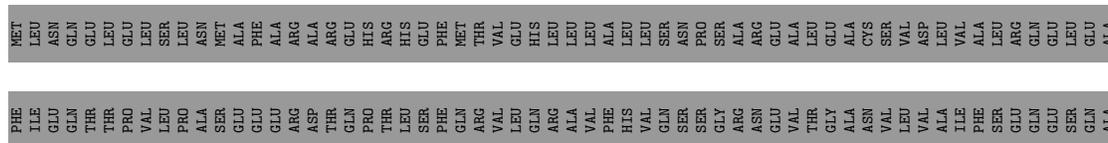




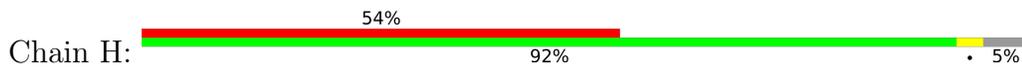


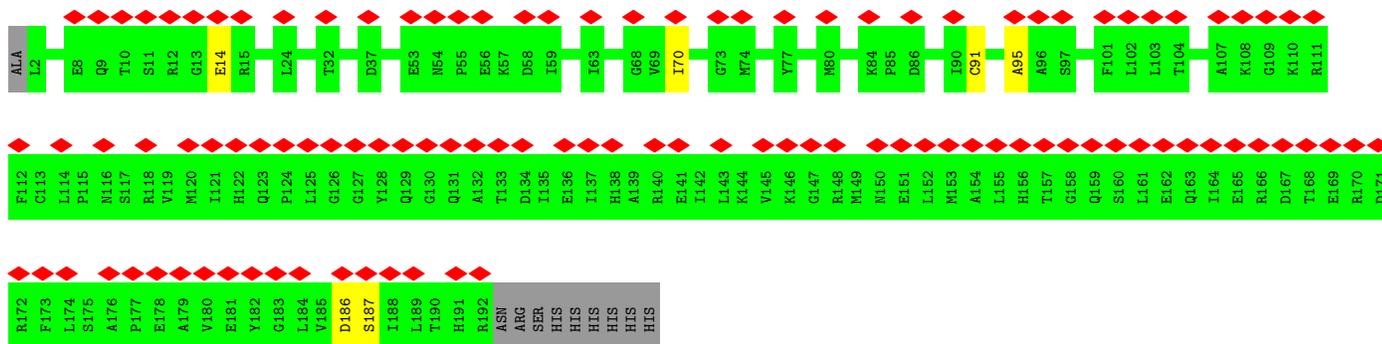


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

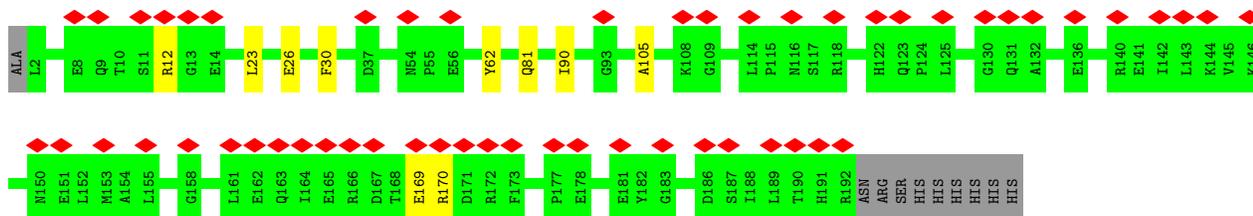
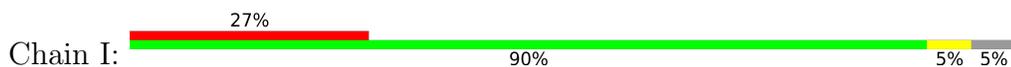


• Molecule 2: ATP-dependent Clp protease proteolytic subunit

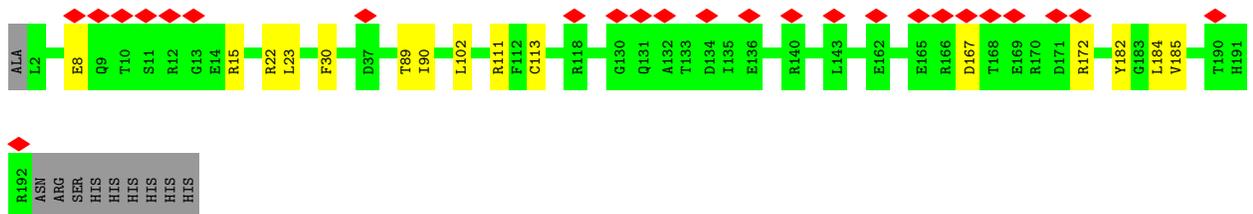
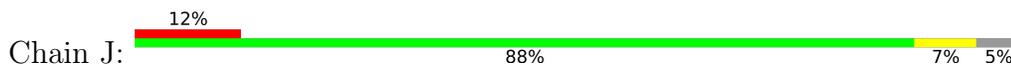




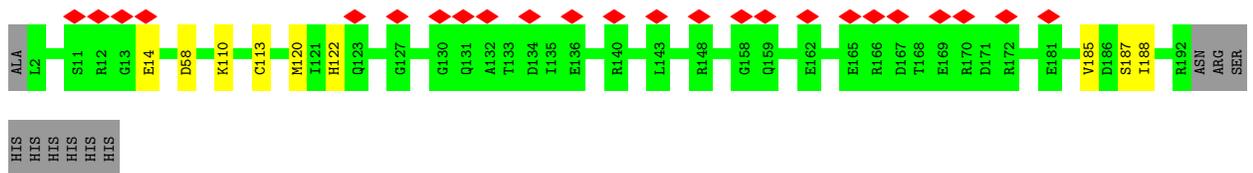
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



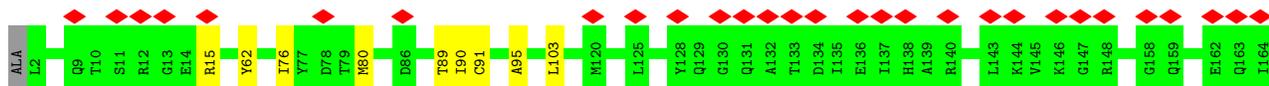
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

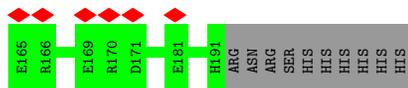


- Molecule 2: ATP-dependent Clp protease proteolytic subunit

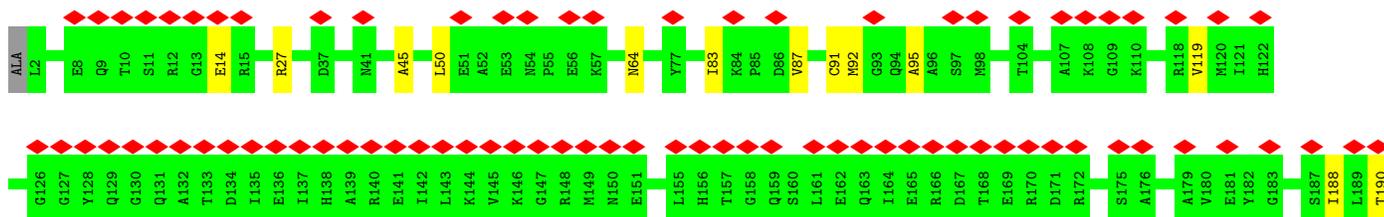
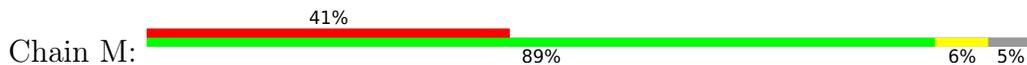


- Molecule 2: ATP-dependent Clp protease proteolytic subunit

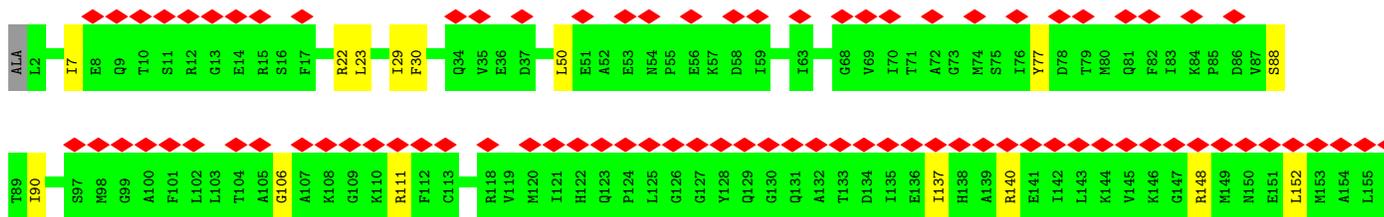
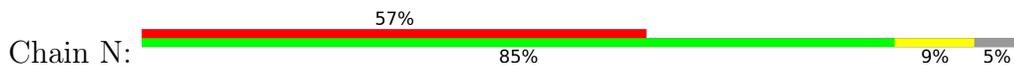




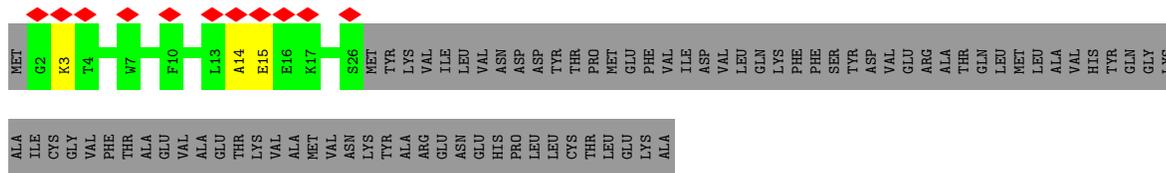
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



• Molecule 2: ATP-dependent Clp protease proteolytic subunit



• Molecule 3: ATP-dependent Clp protease adapter protein ClpS



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51750	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 ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.429	Depositor
Minimum map value	-7.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.98	Depositor
Map size (Å)	152.25, 147.9, 182.7	wwPDB
Map dimensions	210, 170, 175	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.86999995, 0.87	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	A	0.26	0/4566	0.52	0/6162
1	B	0.25	0/4535	0.50	0/6117
1	C	0.25	0/4587	0.50	0/6189
1	D	0.25	0/4595	0.51	0/6202
1	E	0.27	0/4590	0.51	0/6195
1	F	0.26	0/4523	0.53	0/6101
2	H	0.27	0/1519	0.52	0/2047
2	I	0.27	0/1519	0.50	0/2047
2	J	0.27	0/1519	0.51	0/2047
2	K	0.27	0/1519	0.52	0/2047
2	L	0.27	0/1508	0.51	0/2033
2	M	0.27	0/1519	0.51	0/2047
2	N	0.27	0/1508	0.52	0/2033
3	S	0.27	0/206	0.53	0/278
All	All	0.26	0/38213	0.51	0/51545

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 [i](#)

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	4500	4601	4600	36	0
1	B	4471	4571	4571	30	0
1	C	4522	4618	4615	32	0
1	D	4529	4623	4623	37	0
1	E	4524	4599	4619	31	0
1	F	4459	4563	4559	29	0
2	H	1495	1506	1507	4	0
2	I	1495	1506	1507	9	0
2	J	1495	1506	1507	9	0
2	K	1495	1506	1507	6	0
2	L	1484	1493	1494	7	0
2	M	1495	1506	1507	9	0
2	N	1484	1494	1494	11	0
3	S	202	194	193	3	0
4	A	54	24	24	0	0
4	F	27	12	12	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	B	62	24	24	3	0
6	C	62	24	24	2	0
6	D	62	24	24	1	0
6	E	62	24	24	2	0
6	F	31	12	12	2	0
All	All	38021	38430	38447	226	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 226 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:A:460:VAL:HG11	1:A:504:VAL:HG12	1.56	0.86
6:C:802:AGS:O3G	1:D:643:ARG:NH2	2.21	0.73
1:D:400:ASP:OD1	1:E:204:ARG:NH1	2.23	0.71
1:A:404:GLU:OE2	1:B:197:ARG:NH1	2.25	0.70
1:D:229:TRP:O	1:D:233:GLN:NE2	2.23	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/758 (76%)	573 (100%)	2 (0%)	0	100	100
1	B	565/758 (74%)	565 (100%)	0	0	100	100
1	C	576/758 (76%)	576 (100%)	0	0	100	100
1	D	579/758 (76%)	579 (100%)	0	0	100	100
1	E	578/758 (76%)	577 (100%)	0	1 (0%)	47	78
1	F	565/758 (74%)	564 (100%)	1 (0%)	0	100	100
2	H	189/201 (94%)	189 (100%)	0	0	100	100
2	I	189/201 (94%)	189 (100%)	0	0	100	100
2	J	189/201 (94%)	189 (100%)	0	0	100	100
2	K	189/201 (94%)	189 (100%)	0	0	100	100
2	L	188/201 (94%)	188 (100%)	0	0	100	100
2	M	189/201 (94%)	189 (100%)	0	0	100	100
2	N	188/201 (94%)	188 (100%)	0	0	100	100
3	S	23/106 (22%)	23 (100%)	0	0	100	100
All	All	4782/6061 (79%)	4778 (100%)	3 (0%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	442	SER

### 5.3.2 Protein sidechains [i](#)

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	484/639 (76%)	483 (100%)	1 (0%)	93	97
1	B	483/639 (76%)	483 (100%)	0	100	100
1	C	486/639 (76%)	486 (100%)	0	100	100
1	D	487/639 (76%)	487 (100%)	0	100	100
1	E	487/639 (76%)	486 (100%)	1 (0%)	93	97
1	F	481/639 (75%)	481 (100%)	0	100	100
2	H	162/171 (95%)	162 (100%)	0	100	100
2	I	162/171 (95%)	162 (100%)	0	100	100
2	J	162/171 (95%)	162 (100%)	0	100	100
2	K	162/171 (95%)	162 (100%)	0	100	100
2	L	161/171 (94%)	161 (100%)	0	100	100
2	M	162/171 (95%)	162 (100%)	0	100	100
2	N	161/171 (94%)	160 (99%)	1 (1%)	86	93
3	S	22/93 (24%)	22 (100%)	0	100	100
All	All	4062/5124 (79%)	4059 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	LYS
1	E	442	SER
2	N	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	163	GLN
2	I	150	ASN
1	F	579	GLN
2	H	41	ASN
1	E	329	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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	AGS	B	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.88	1 (3%)
6	AGS	E	802	5	26,33,33	0.82	1 (3%)	26,52,52	0.79	1 (3%)
4	ADP	A	801	5	24,29,29	0.65	0	29,45,45	0.79	1 (3%)
6	AGS	F	802	-	26,33,33	0.82	1 (3%)	26,52,52	0.88	1 (3%)
6	AGS	C	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.80	1 (3%)
6	AGS	B	802	5	26,33,33	0.82	1 (3%)	26,52,52	0.74	1 (3%)
4	ADP	A	802	-	24,29,29	0.66	0	29,45,45	0.75	1 (3%)
6	AGS	D	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.93	1 (3%)
6	AGS	C	802	5	26,33,33	0.83	1 (3%)	26,52,52	0.74	1 (3%)
4	ADP	F	801	5	24,29,29	0.66	0	29,45,45	0.83	1 (3%)
6	AGS	D	802	5	26,33,33	0.81	1 (3%)	26,52,52	0.86	1 (3%)
6	AGS	E	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.74	1 (3%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGS	B	801	5	-	3/17/38/38	0/3/3/3
6	AGS	E	802	5	-	2/17/38/38	0/3/3/3
4	ADP	A	801	5	-	2/12/32/32	0/3/3/3
6	AGS	F	802	-	-	3/17/38/38	0/3/3/3
6	AGS	C	801	5	-	1/17/38/38	0/3/3/3
6	AGS	B	802	5	-	0/17/38/38	0/3/3/3
4	ADP	A	802	-	-	5/12/32/32	0/3/3/3
6	AGS	D	801	5	-	2/17/38/38	0/3/3/3
6	AGS	C	802	5	-	0/17/38/38	0/3/3/3
4	ADP	F	801	5	-	5/12/32/32	0/3/3/3
6	AGS	D	802	5	-	0/17/38/38	0/3/3/3
6	AGS	E	801	5	-	1/17/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	802	AGS	PG-S1G	2.19	1.95	1.90
6	E	802	AGS	PG-S1G	2.15	1.95	1.90
6	D	801	AGS	PG-S1G	2.15	1.95	1.90
6	B	801	AGS	PG-S1G	2.14	1.95	1.90
6	C	802	AGS	PG-S1G	2.13	1.95	1.90

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ADP	C5-C6-N6	2.26	123.78	120.35
6	B	801	AGS	C5-C6-N6	2.20	123.69	120.35
4	A	802	ADP	C5-C6-N6	2.19	123.68	120.35
4	F	801	ADP	C5-C6-N6	2.19	123.68	120.35
6	E	802	AGS	C5-C6-N6	2.18	123.67	120.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

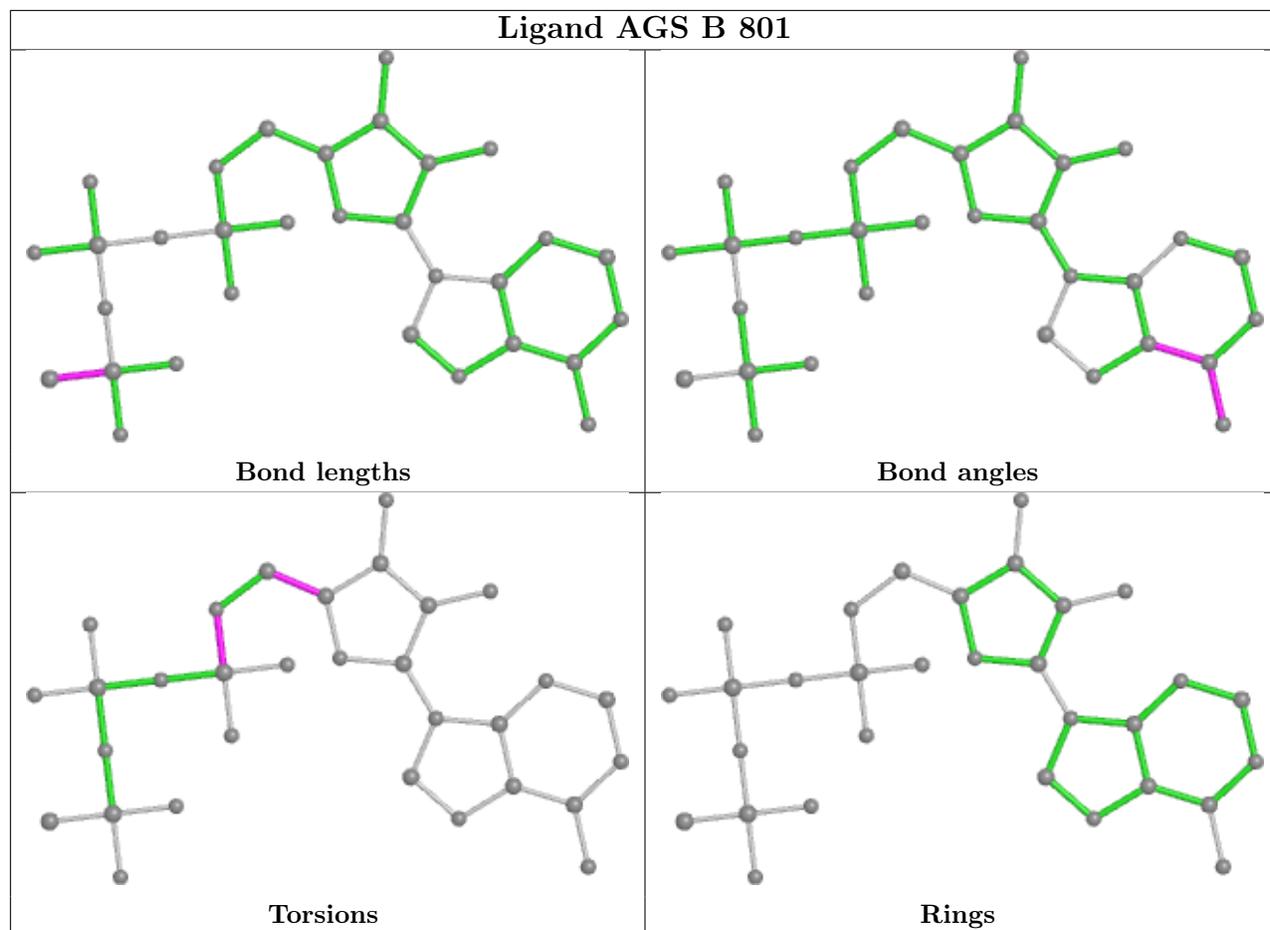
Mol	Chain	Res	Type	Atoms
4	A	801	ADP	C5'-O5'-PA-O1A
4	F	801	ADP	C4'-C5'-O5'-PA
6	D	801	AGS	C5'-O5'-PA-O1A
6	D	801	AGS	C4'-C5'-O5'-PA
6	F	802	AGS	C5'-O5'-PA-O1A

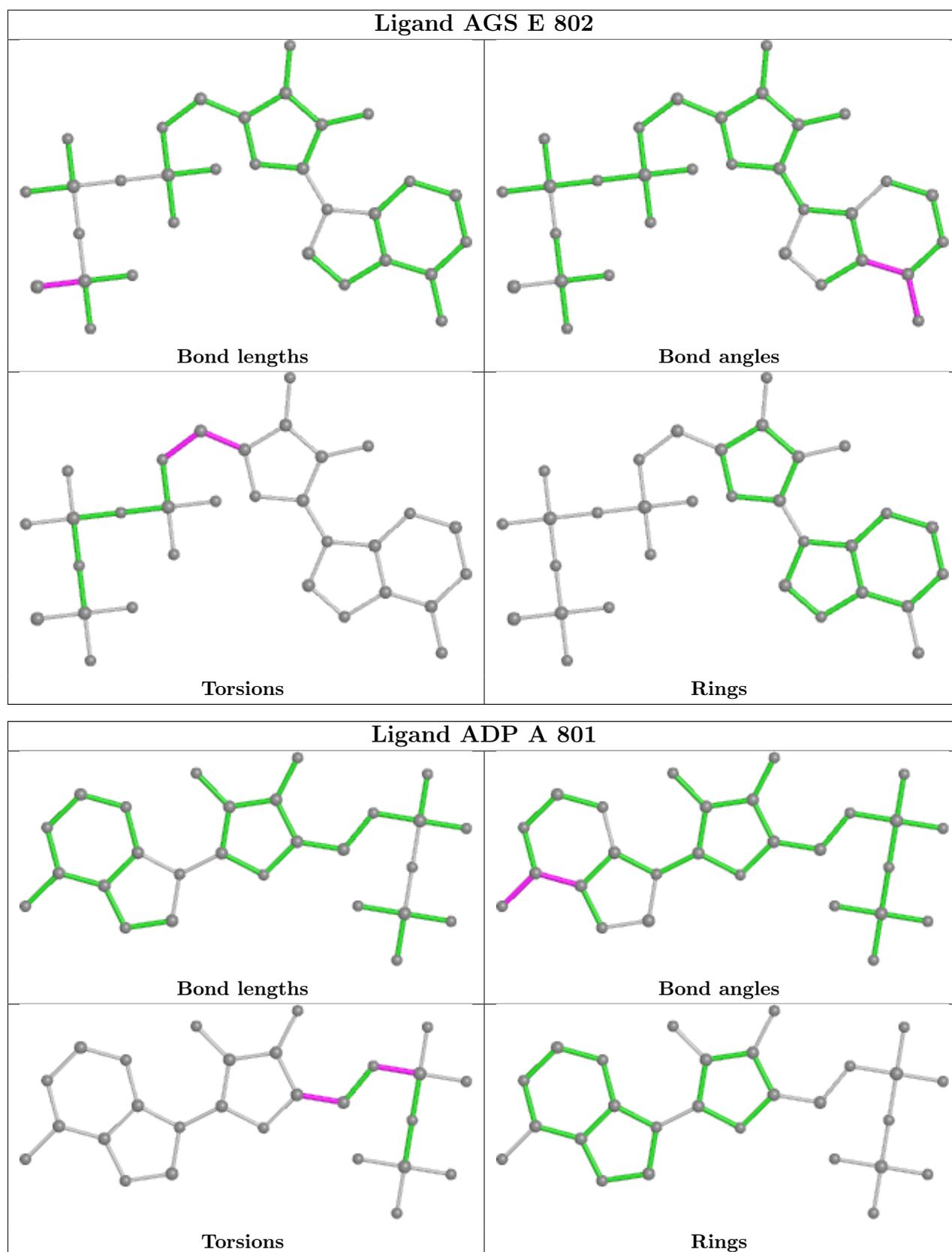
There are no ring outliers.

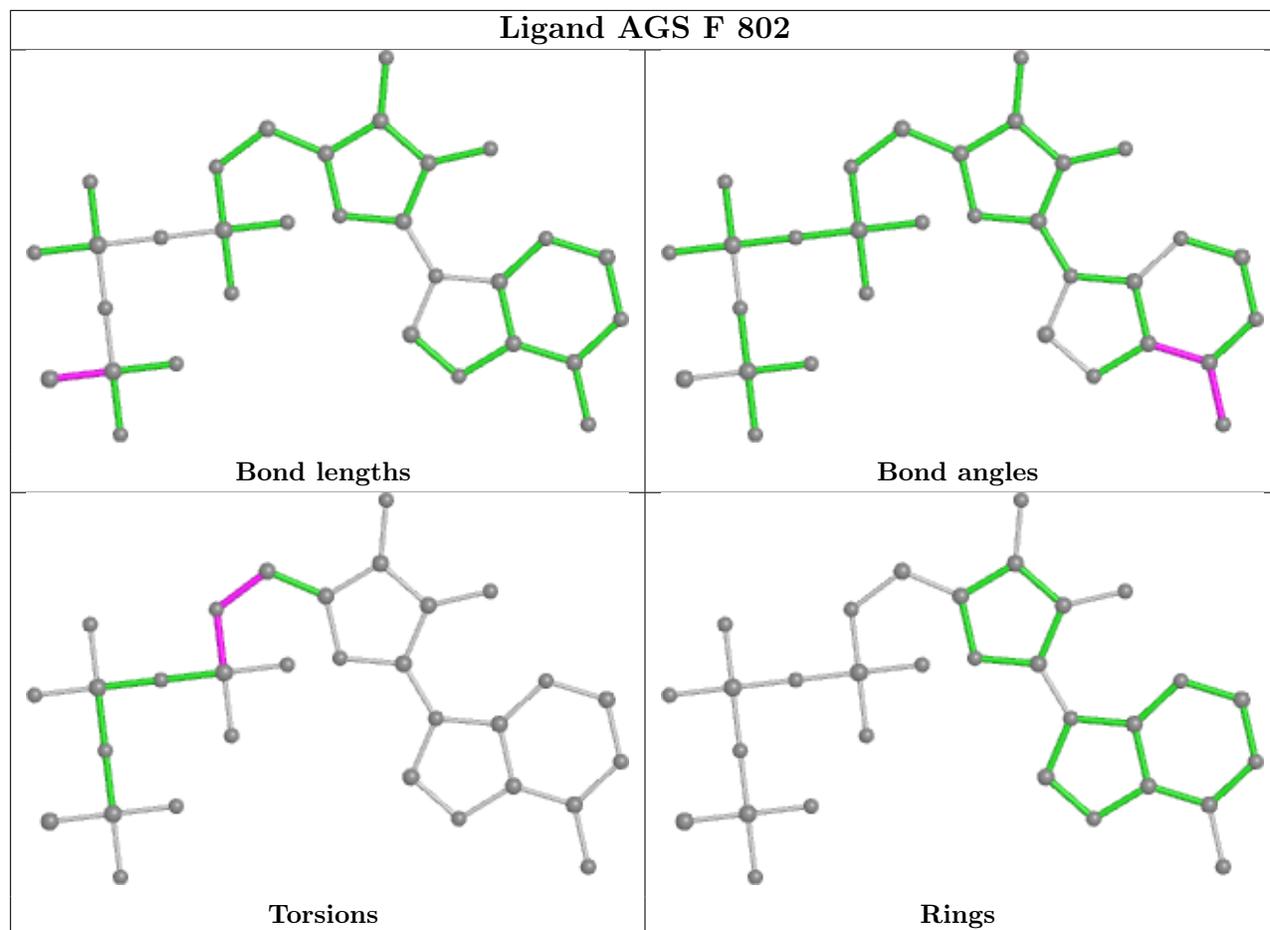
7 monomers are involved in 10 short contacts:

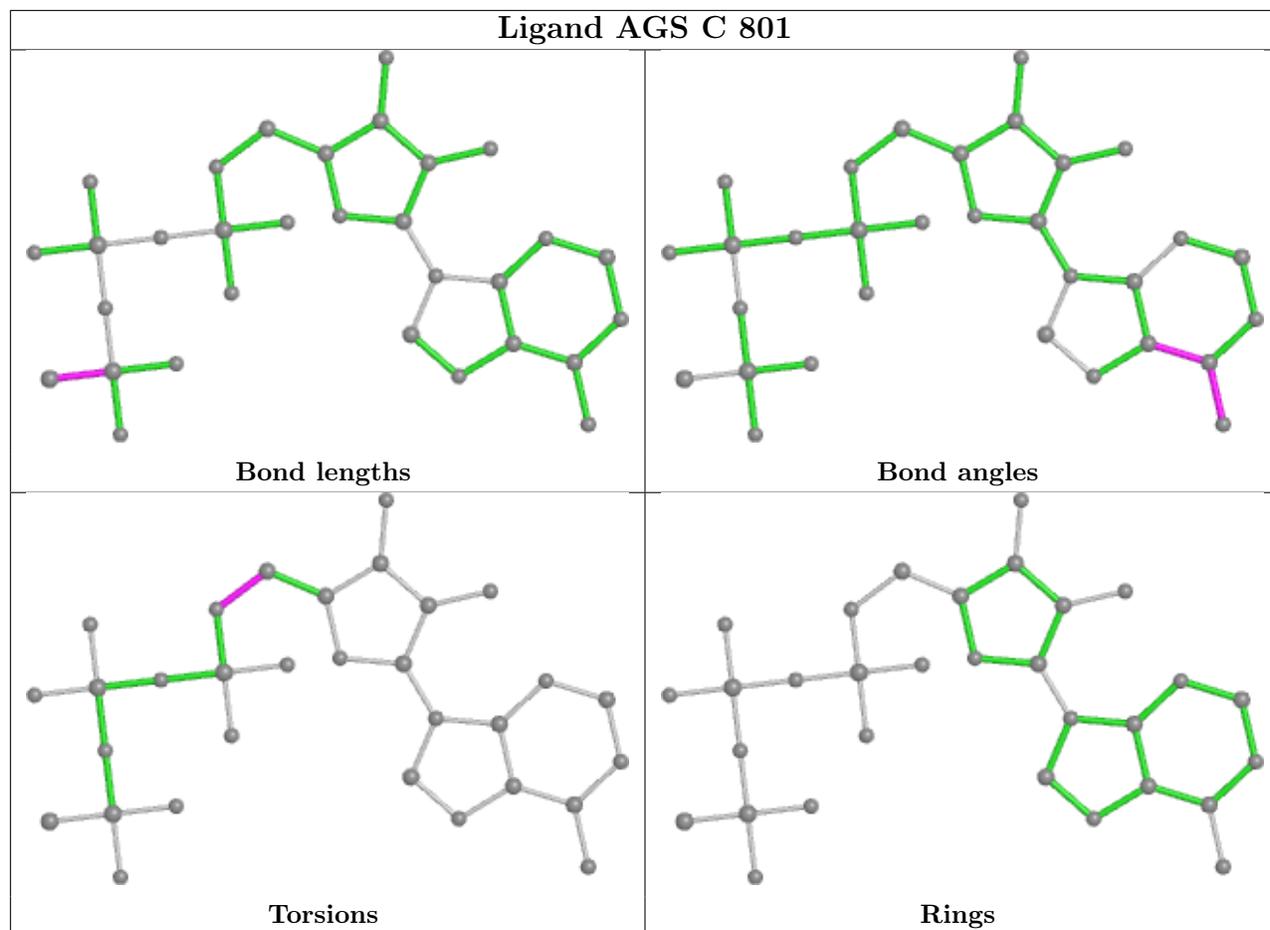
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	AGS	1	0
6	F	802	AGS	2	0
6	C	801	AGS	1	0
6	B	802	AGS	2	0
6	D	801	AGS	1	0
6	C	802	AGS	1	0
6	E	801	AGS	2	0

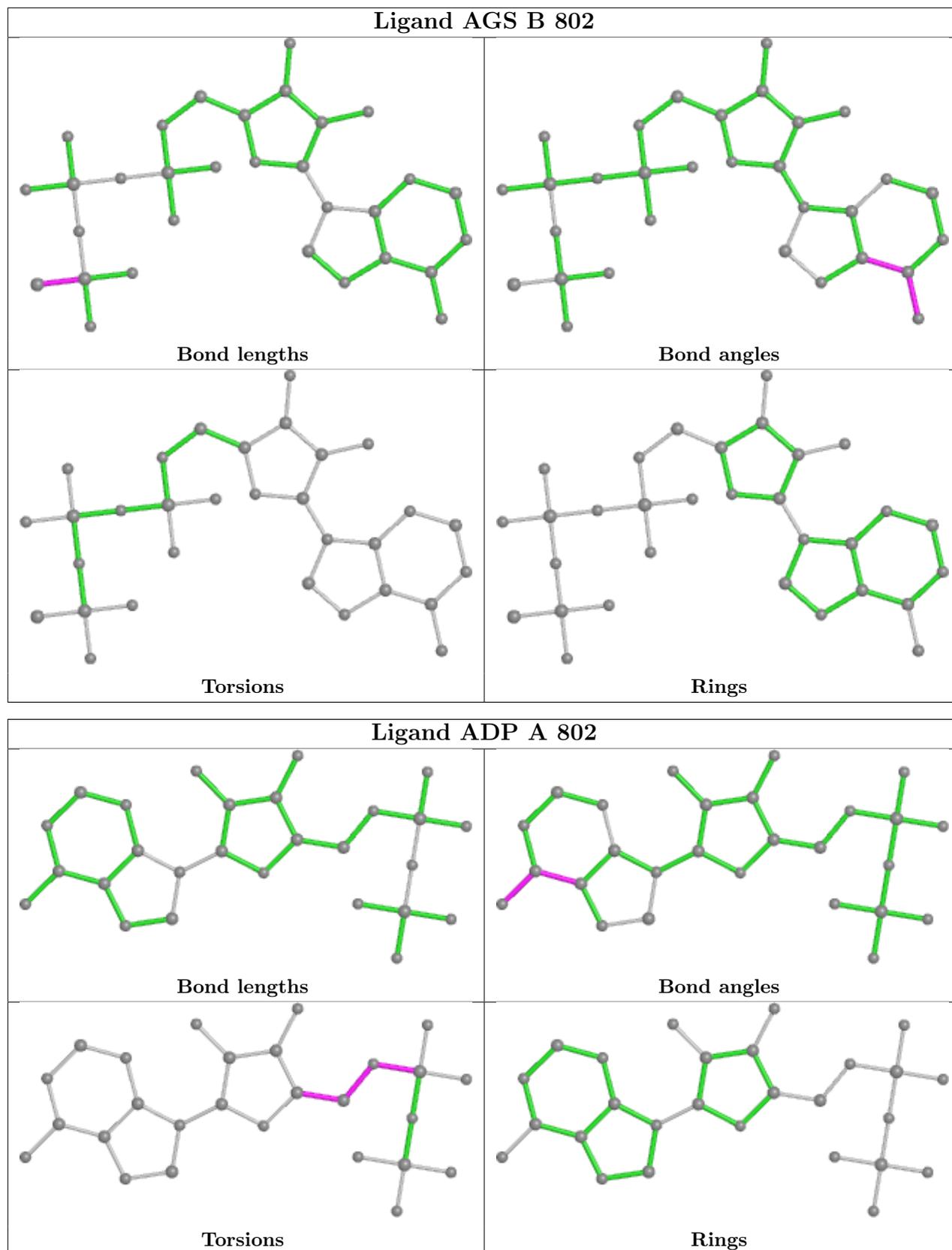
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

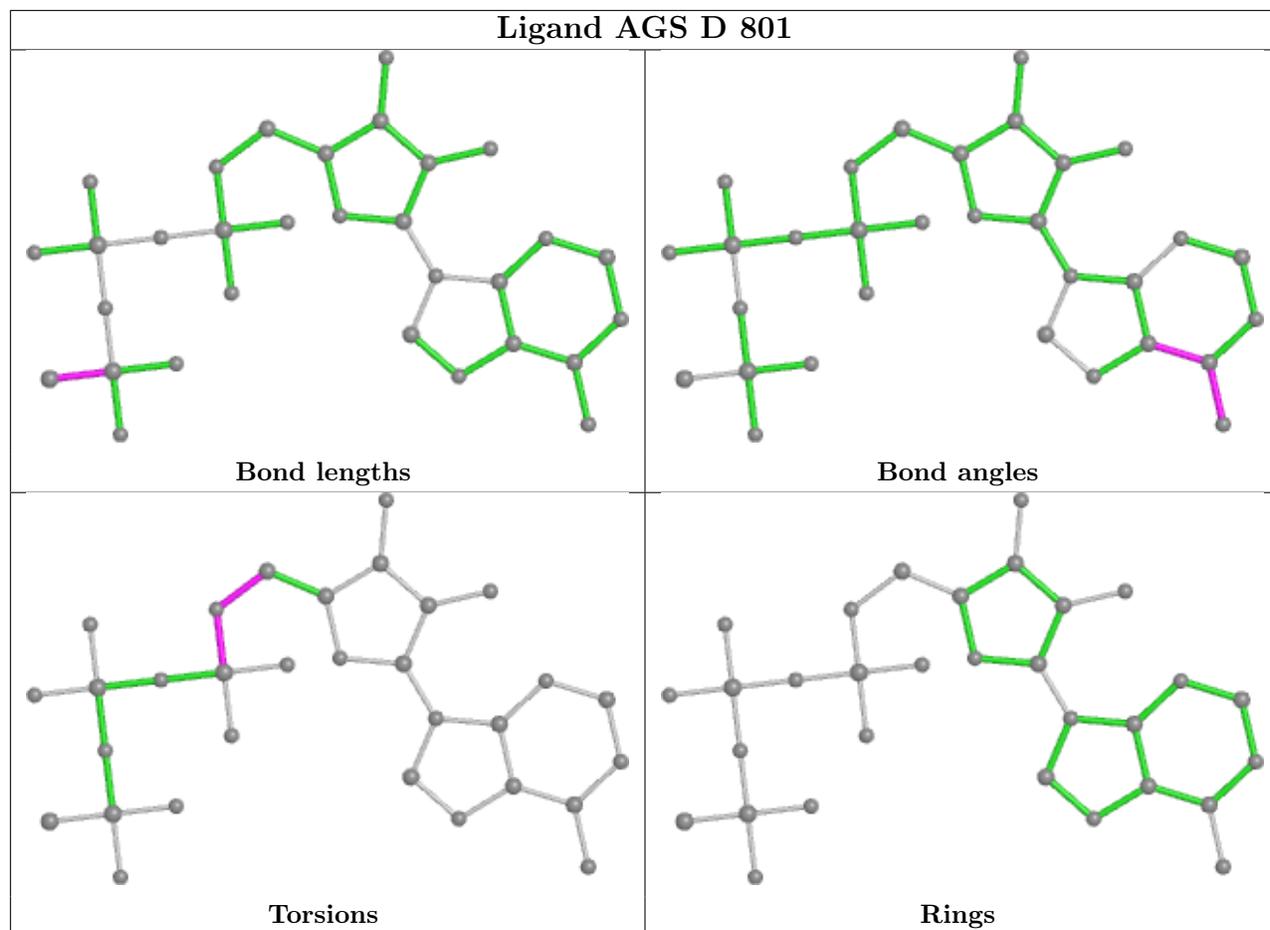


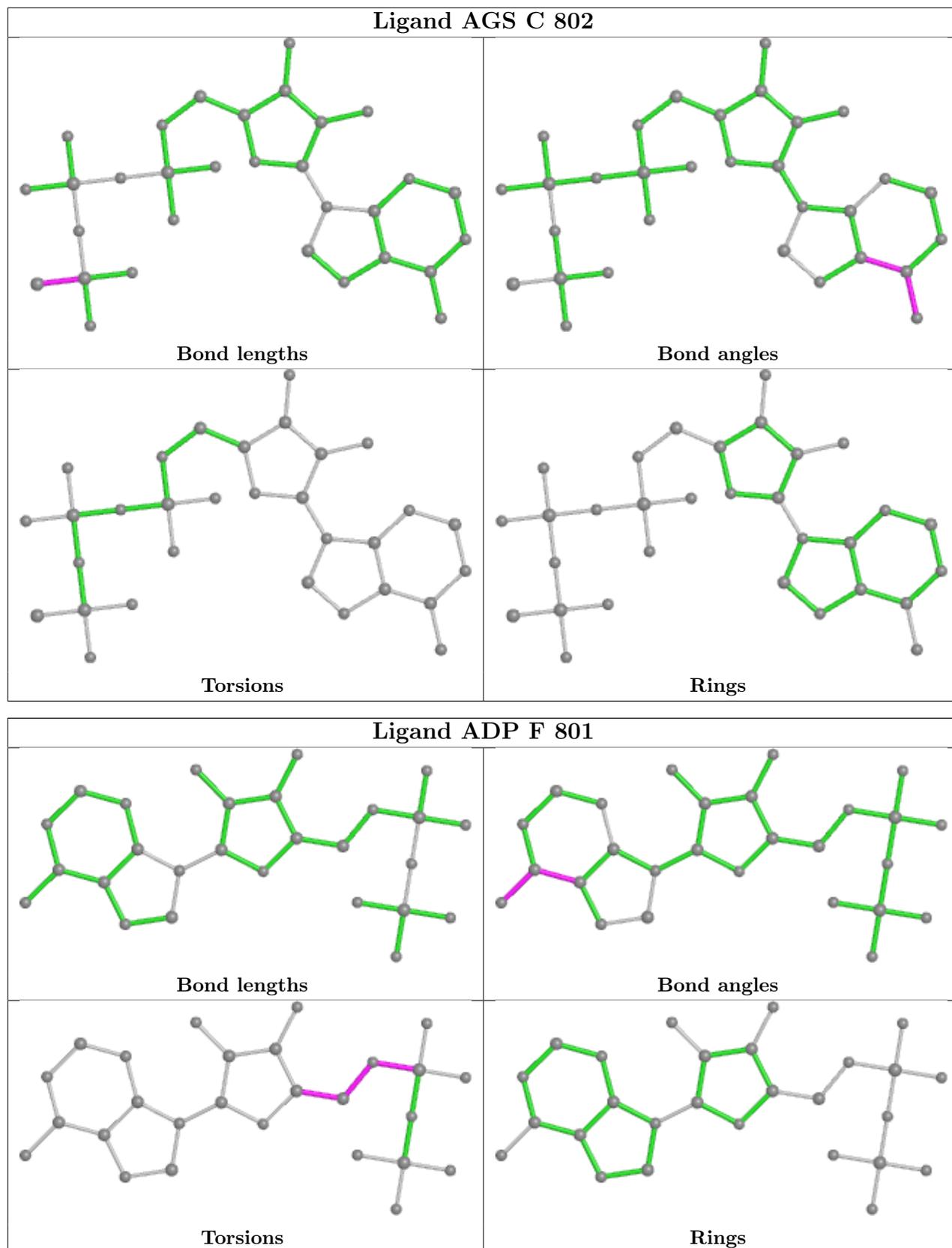


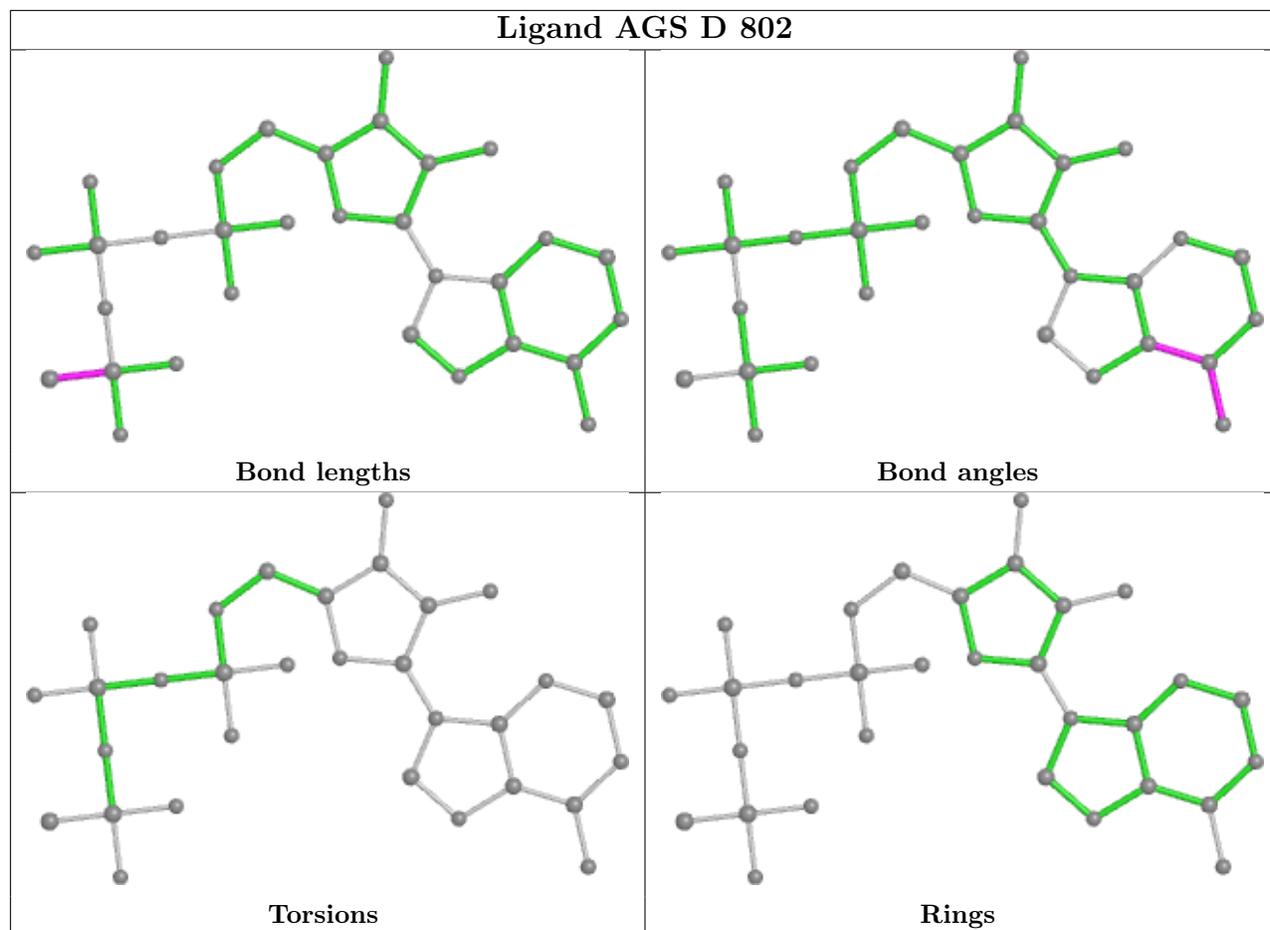


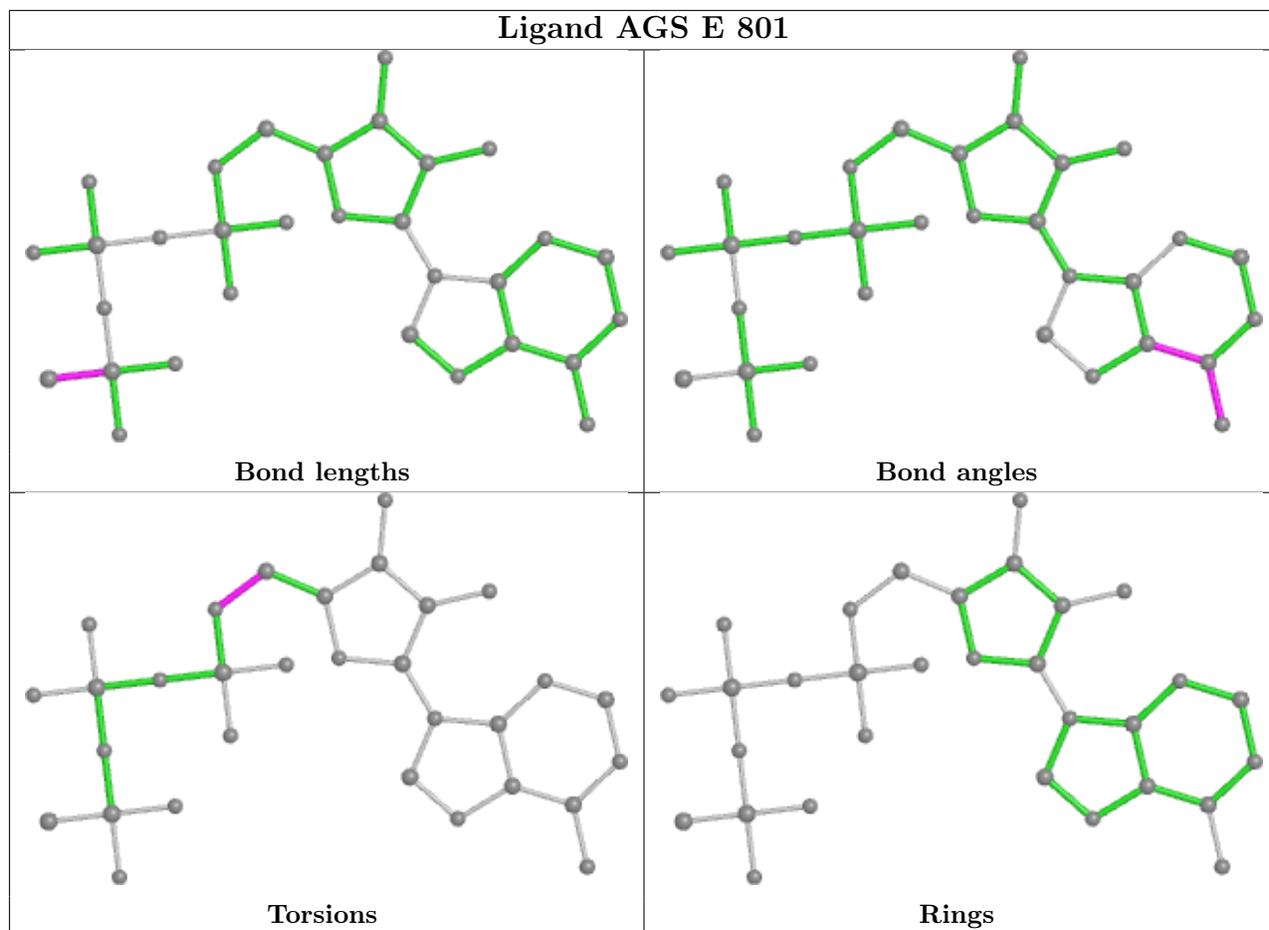












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	746:PHE	C	747:GLN	N	3.15
1	B	746:PHE	C	747:GLN	N	3.14

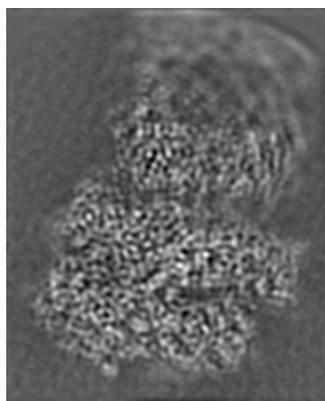
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26556. These allow visual inspection of the internal detail of the map and identification of artifacts.

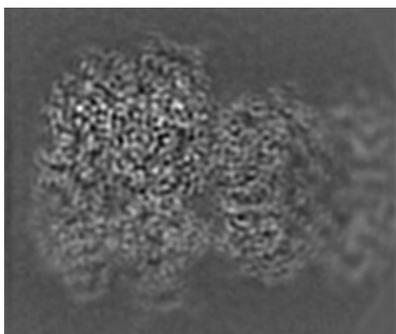
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

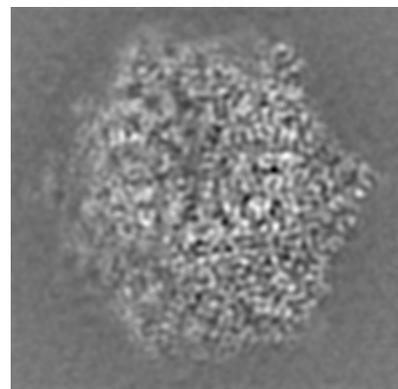
#### 6.1.1 Primary map



X



Y

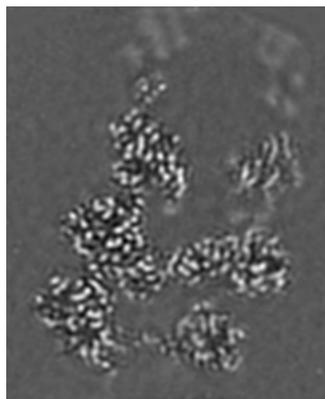


Z

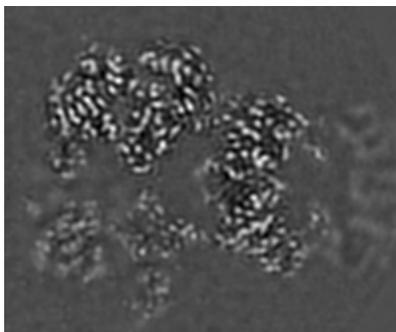
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

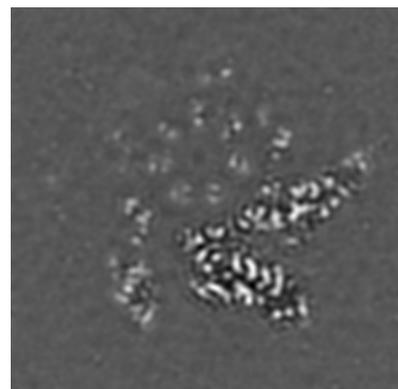
#### 6.2.1 Primary map



X Index: 87



Y Index: 85

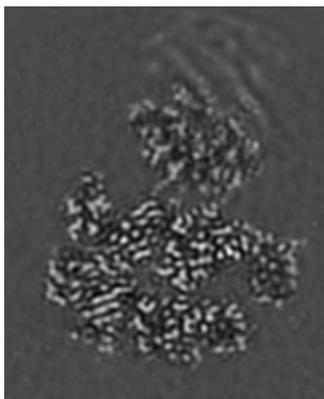


Z Index: 105

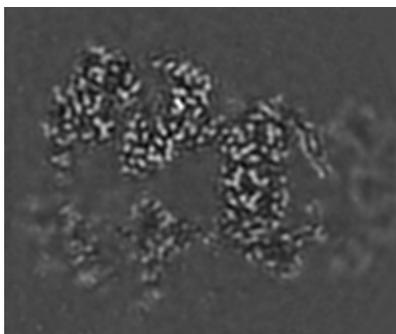
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

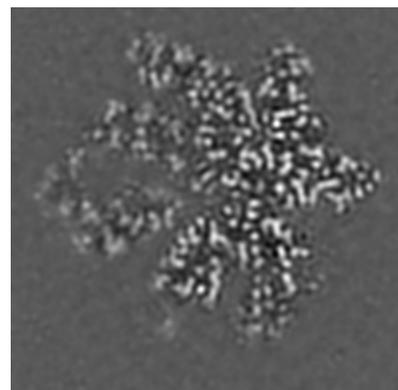
### 6.3.1 Primary map



X Index: 117



Y Index: 81



Z Index: 79

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.98. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

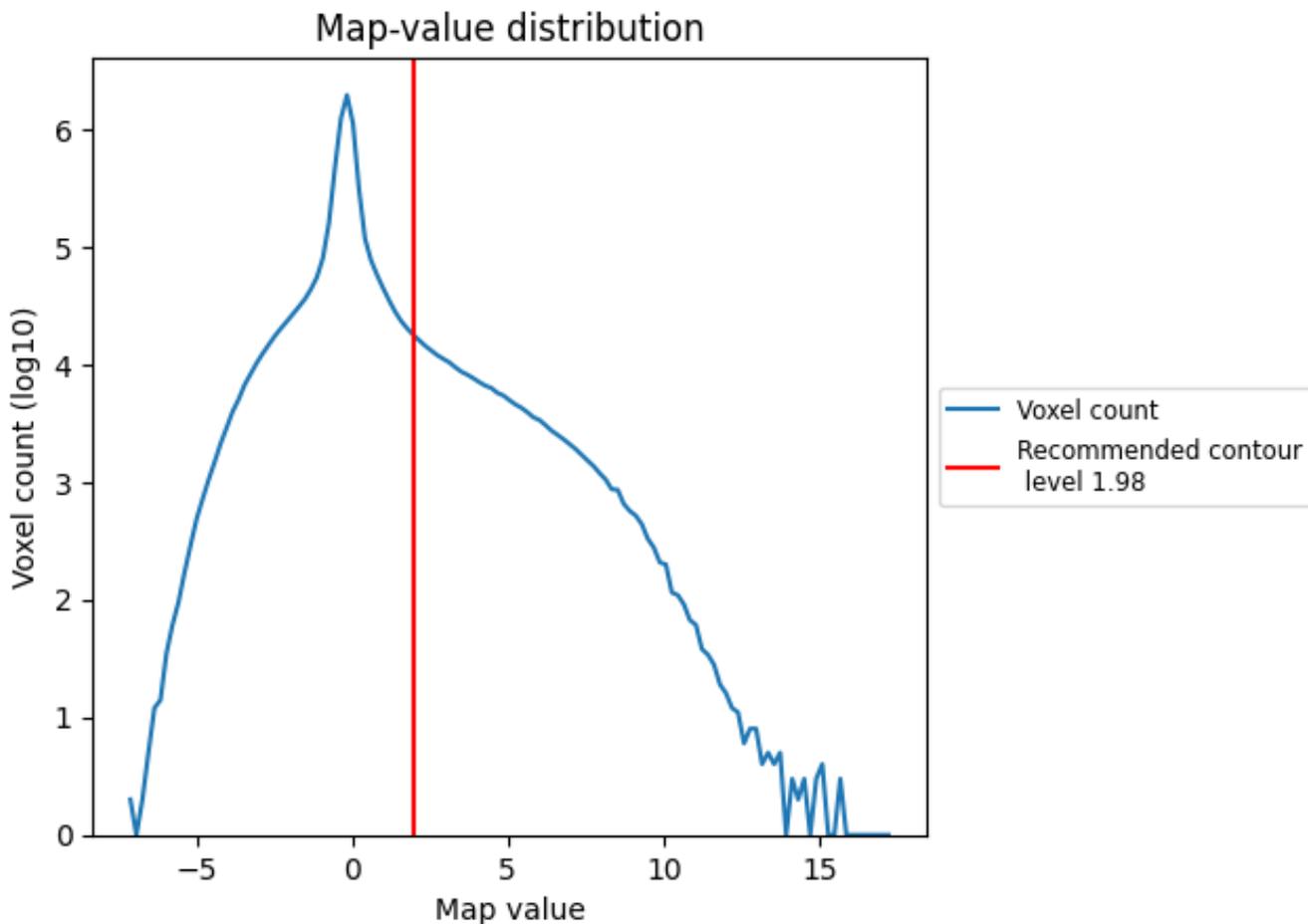
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

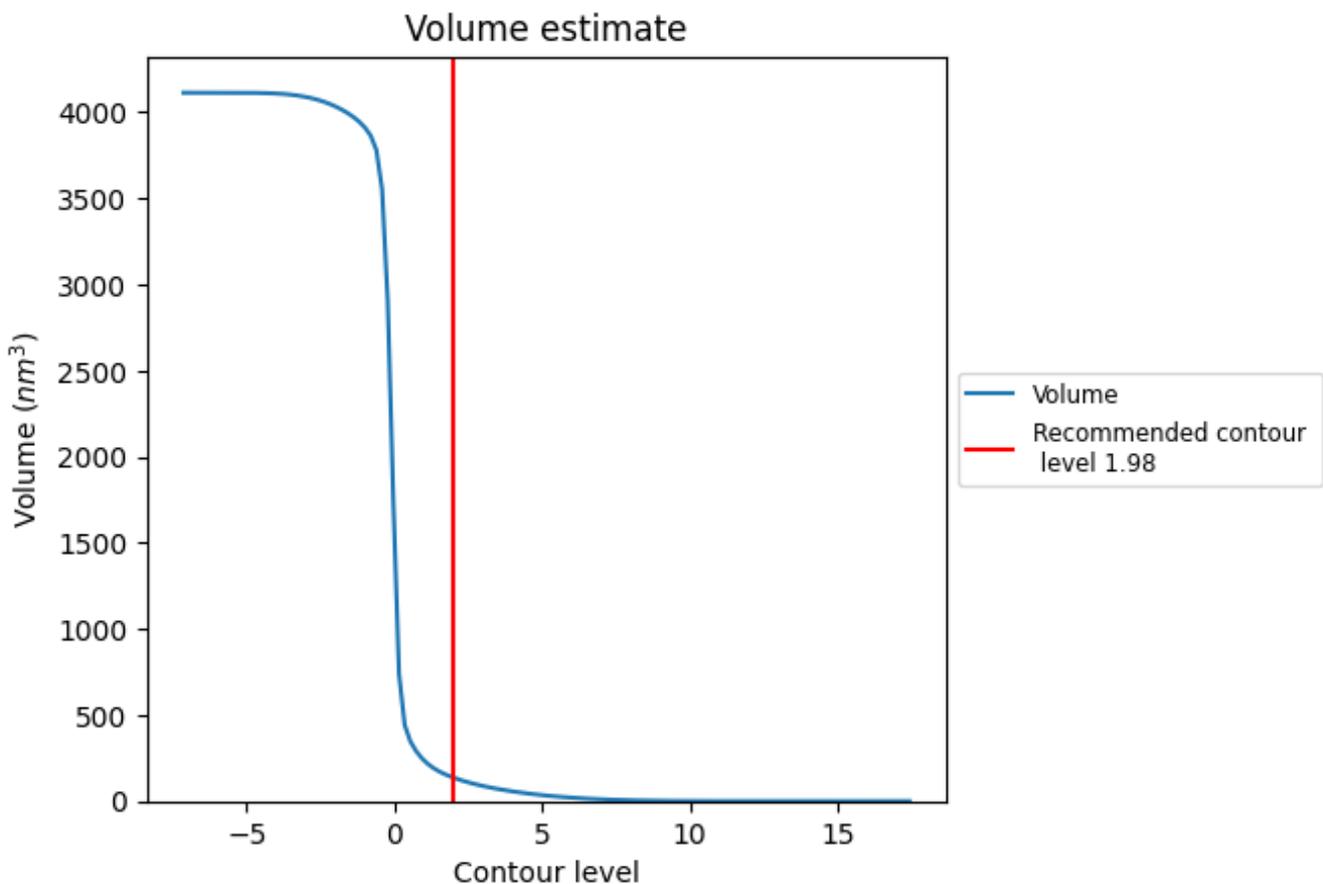
This section contains the results of statistical analysis of the map.

### 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  $138 \text{ nm}^3$ ; this corresponds to an approximate mass of 125 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

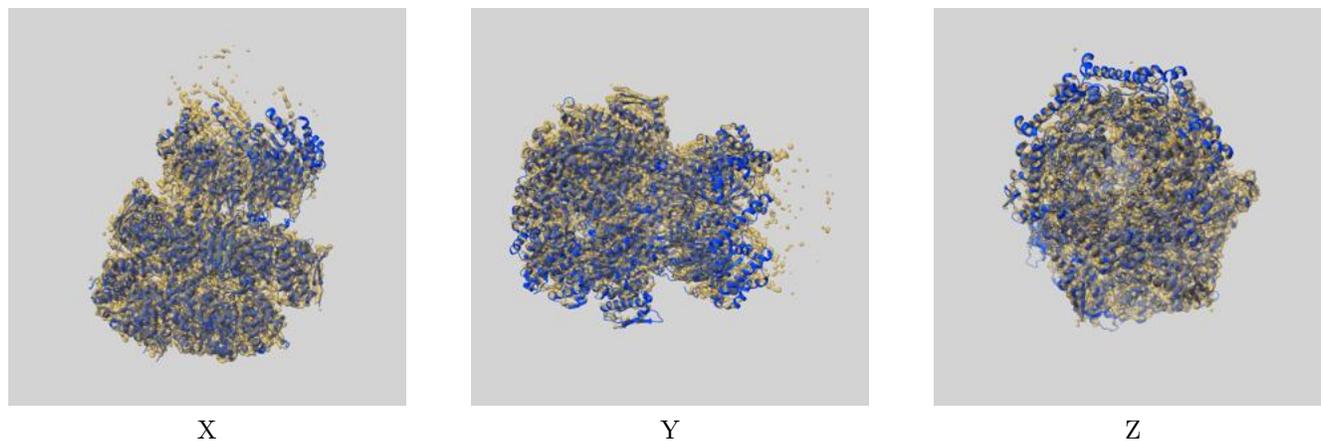
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

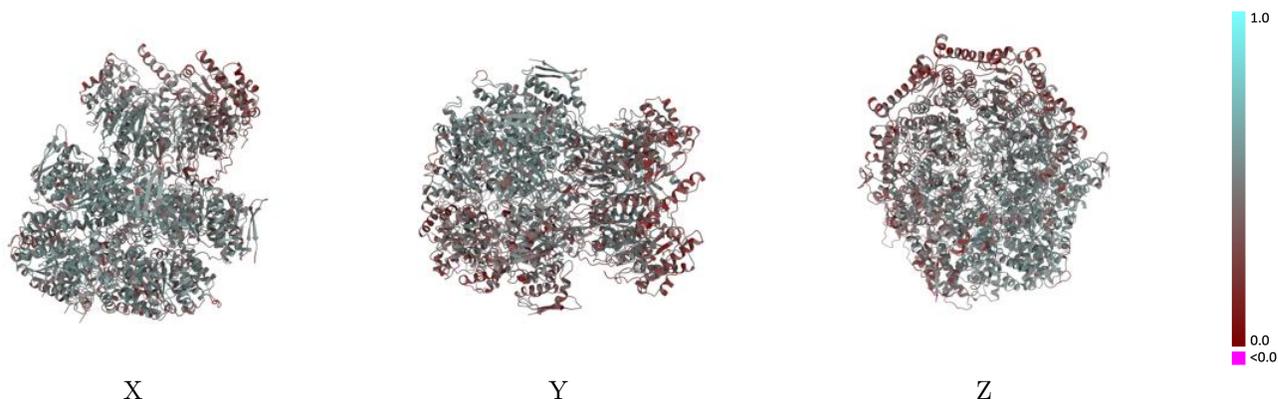
This section contains information regarding the fit between EMDB map EMD-26556 and PDB model 7UIX. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



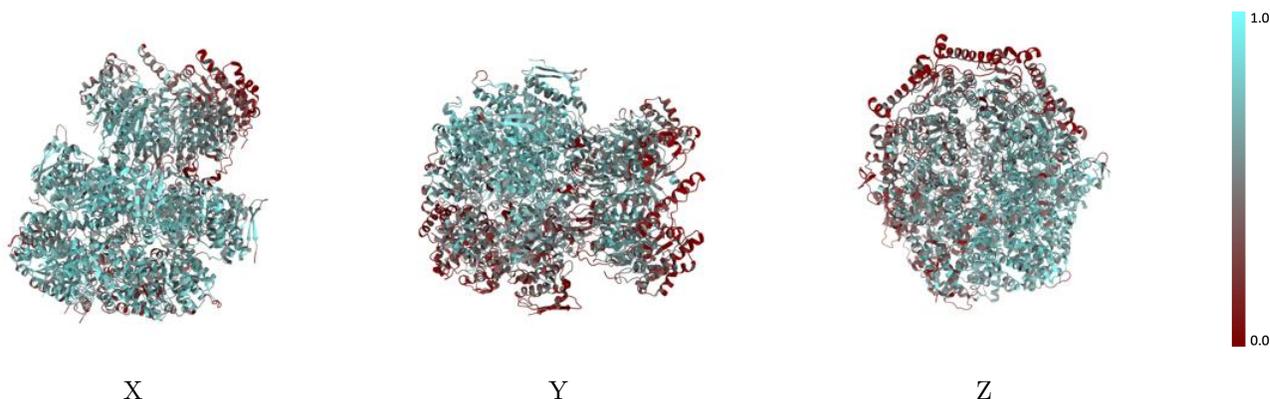
The images above show the 3D surface view of the map at the recommended contour level 1.98 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



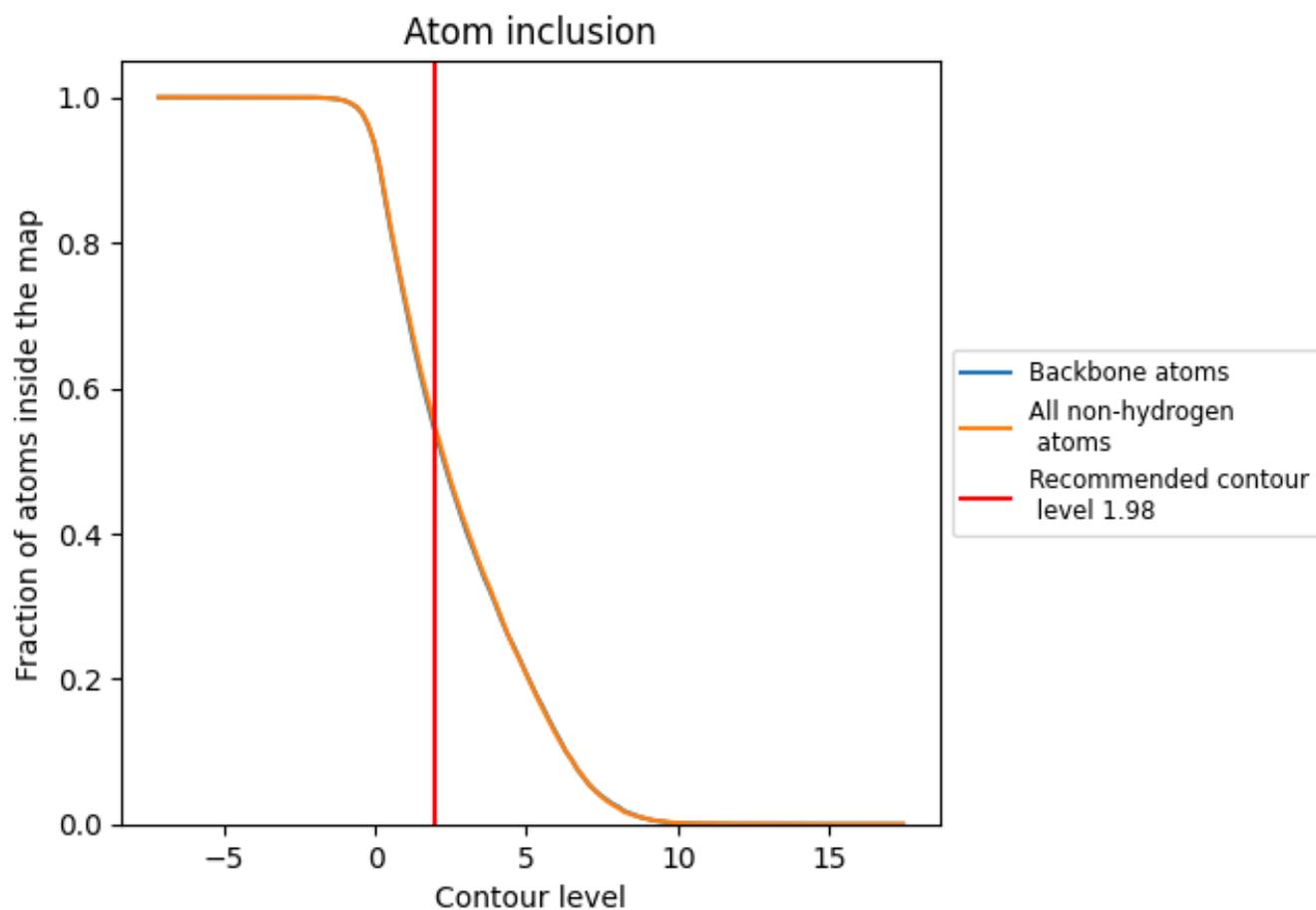
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.98).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 55% 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 (1.98) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5468	 0.4490
A	 0.3564	 0.3720
B	 0.5483	 0.4490
C	 0.7113	 0.5190
D	 0.7170	 0.5220
E	 0.6496	 0.4880
F	 0.4515	 0.4160
H	 0.3577	 0.3490
I	 0.5249	 0.4300
J	 0.6157	 0.4750
K	 0.6259	 0.4670
L	 0.5879	 0.4590
M	 0.4307	 0.3940
N	 0.3249	 0.3370
S	 0.3719	 0.4340

