



wwPDB EM Model Validation Summary Report ⓘ

Mar 4, 2020 – 04:53 PM EST

PDB ID : 6PP6
EMDB ID : EMD-20420
Title : ClpX in ClpX-ClpP complex bound to substrate and ATP-gamma-S, class 3
Authors : Fei, X.; Jenni, S.; Harrison, S.C.; Sauer, R.T.
Deposited on : 2019-07-05
Resolution : 4.28 Å (reported)
Based on initial model : 3HWS

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

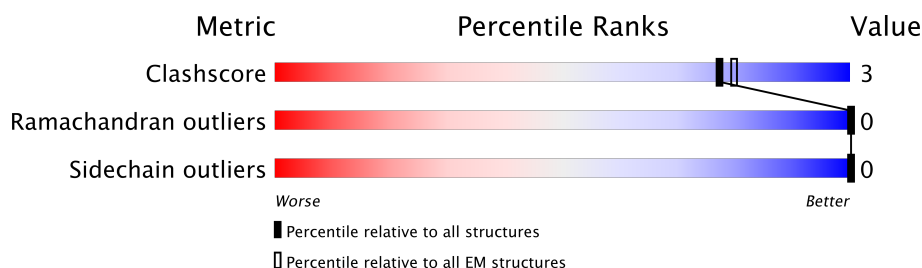
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.28 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	369	87% 6% 7%
1	B	369	86% 7% 6%
1	C	369	86% 8% 6%
1	D	369	89% 5% 5%
1	E	369	86% 8% 7%
1	F	369	81% 8% 10%
2	S	7	86% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32204 atoms, of which 16224 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 ClpX.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	0
			5330	1666	2694	446	519	5		
1	B	346	Total	C	H	N	O	S	0	0
			5353	1674	2706	445	523	5		
1	C	346	Total	C	H	N	O	S	0	0
			5353	1674	2706	445	523	5		
1	D	349	Total	C	H	N	O	S	0	0
			5380	1681	2719	448	527	5		
1	E	345	Total	C	H	N	O	S	0	0
			5336	1669	2698	443	521	5		
1	F	331	Total	C	H	N	O	S	0	0
			5125	1602	2596	425	497	5		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	CYS	conflict	UNP A0A1Q9L861
A	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
A	408	GLU	LYS	conflict	UNP A0A1Q9L861
A	425	GLY	-	expression tag	UNP A0A1Q9L861
A	426	GLY	-	expression tag	UNP A0A1Q9L861
A	427	GLY	-	expression tag	UNP A0A1Q9L861
A	428	THR	-	expression tag	UNP A0A1Q9L861
A	429	SER	-	expression tag	UNP A0A1Q9L861
A	430	GLY	-	expression tag	UNP A0A1Q9L861
B	169	SER	CYS	conflict	UNP A0A1Q9L861
B	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
B	408	GLU	LYS	conflict	UNP A0A1Q9L861
B	425	GLY	-	expression tag	UNP A0A1Q9L861
B	426	GLY	-	expression tag	UNP A0A1Q9L861
B	427	GLY	-	expression tag	UNP A0A1Q9L861
B	428	THR	-	expression tag	UNP A0A1Q9L861
B	429	SER	-	expression tag	UNP A0A1Q9L861
B	430	GLY	-	expression tag	UNP A0A1Q9L861

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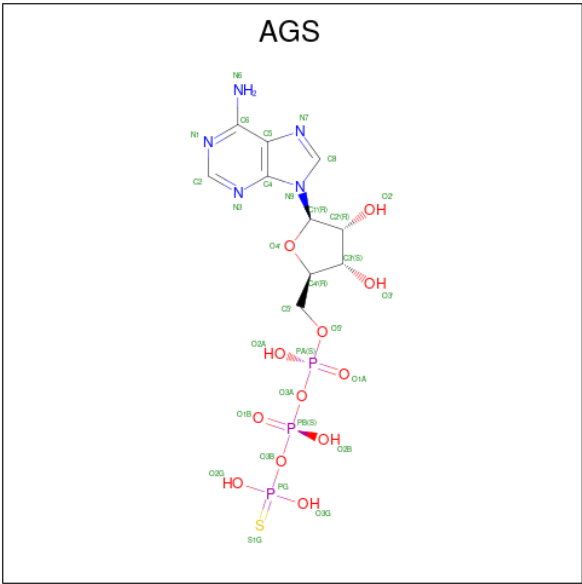
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Chain	Residue	Modelled	Actual	Comment	Reference
C	169	SER	CYS	conflict	UNP A0A1Q9L861
C	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
C	408	GLU	LYS	conflict	UNP A0A1Q9L861
C	425	GLY	-	expression tag	UNP A0A1Q9L861
C	426	GLY	-	expression tag	UNP A0A1Q9L861
C	427	GLY	-	expression tag	UNP A0A1Q9L861
C	428	THR	-	expression tag	UNP A0A1Q9L861
C	429	SER	-	expression tag	UNP A0A1Q9L861
C	430	GLY	-	expression tag	UNP A0A1Q9L861
D	169	SER	CYS	conflict	UNP A0A1Q9L861
D	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
D	408	GLU	LYS	conflict	UNP A0A1Q9L861
D	425	GLY	-	expression tag	UNP A0A1Q9L861
D	426	GLY	-	expression tag	UNP A0A1Q9L861
D	427	GLY	-	expression tag	UNP A0A1Q9L861
D	428	THR	-	expression tag	UNP A0A1Q9L861
D	429	SER	-	expression tag	UNP A0A1Q9L861
D	430	GLY	-	expression tag	UNP A0A1Q9L861
E	169	SER	CYS	conflict	UNP A0A1Q9L861
E	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
E	408	GLU	LYS	conflict	UNP A0A1Q9L861
E	425	GLY	-	expression tag	UNP A0A1Q9L861
E	426	GLY	-	expression tag	UNP A0A1Q9L861
E	427	GLY	-	expression tag	UNP A0A1Q9L861
E	428	THR	-	expression tag	UNP A0A1Q9L861
E	429	SER	-	expression tag	UNP A0A1Q9L861
E	430	GLY	-	expression tag	UNP A0A1Q9L861
F	169	SER	CYS	conflict	UNP A0A1Q9L861
F	185	GLN	GLU	engineered mutation	UNP A0A1Q9L861
F	408	GLU	LYS	conflict	UNP A0A1Q9L861
F	425	GLY	-	expression tag	UNP A0A1Q9L861
F	426	GLY	-	expression tag	UNP A0A1Q9L861
F	427	GLY	-	expression tag	UNP A0A1Q9L861
F	428	THR	-	expression tag	UNP A0A1Q9L861
F	429	SER	-	expression tag	UNP A0A1Q9L861
F	430	GLY	-	expression tag	UNP A0A1Q9L861

- Molecule 2 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	7	Total	C	H	N	O	0	0
			73	24	33	9	7		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
3	B	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
3	C	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
3	D	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
3	E	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

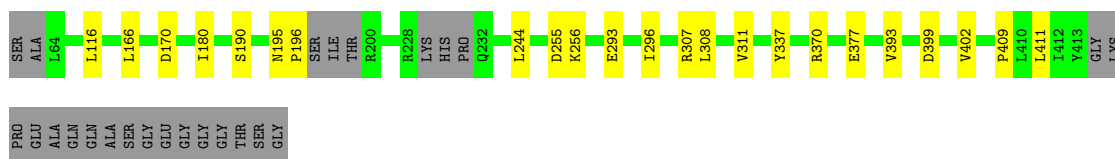


3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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. 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. 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.

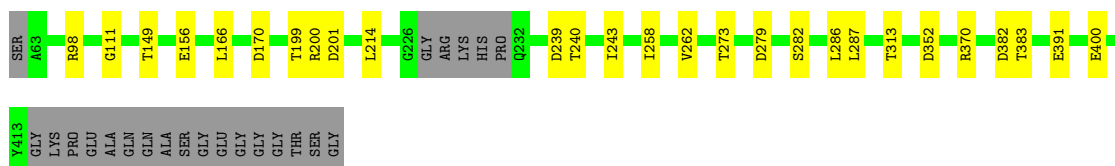
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain A: 




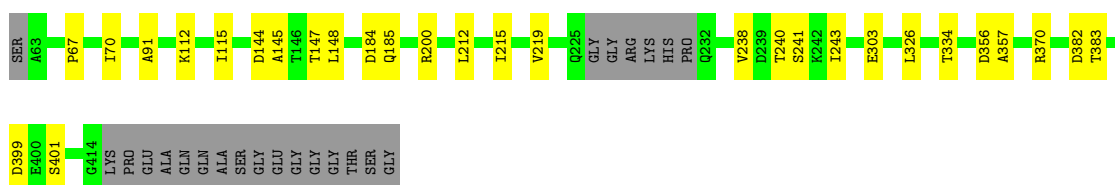
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain B: 




- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain C: 



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain D: 



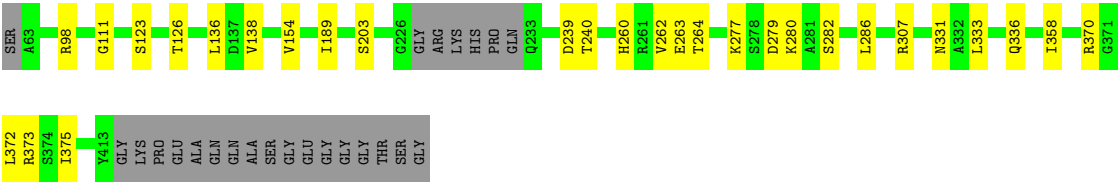
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain E:

86%

8%

7%



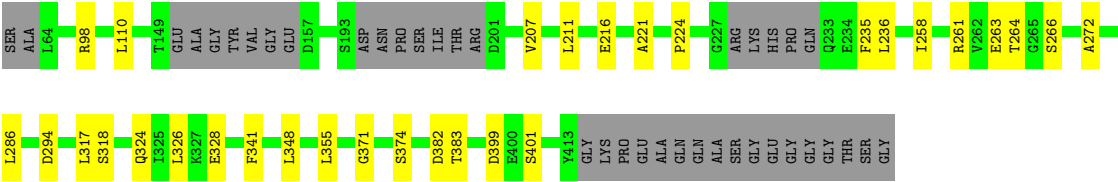
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain F:

81%

8%

10%



- Molecule 2: substrate peptide

Chain S:

86%

14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	115751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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, 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	0.27	0/2668	0.50	0/3604
1	B	0.26	0/2680	0.49	0/3624
1	C	0.27	0/2680	0.51	0/3624
1	D	0.27	0/2694	0.49	0/3642
1	E	0.26	0/2671	0.50	0/3612
1	F	0.26	0/2558	0.48	0/3454
2	S	0.20	0/10	0.27	0/12
All	All	0.26	0/15961	0.50	0/21572

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	2636	2694	2691	17	0
1	B	2647	2706	2704	22	0
1	C	2647	2706	2704	19	0
1	D	2661	2719	2715	12	0
1	E	2638	2698	2696	21	0
1	F	2529	2596	2589	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	40	33	18	1	0
3	A	31	12	12	1	0
3	B	31	12	12	1	0
3	C	31	12	12	2	0
3	D	31	12	12	1	0
3	E	31	12	12	2	0
4	F	27	12	12	0	0
All	All	15980	16224	16189	102	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 102 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:112:LYS:NZ	1:C:241:SER:O	2.28	0.65
1:E:260:HIS:O	1:E:264:THR:N	2.32	0.63
1:A:196:PRO:HD2	1:E:154:VAL:CG2	2.31	0.60
1:A:195:ASN:HB2	1:B:199:THR:HG23	1.86	0.57
1:B:370:ARG:NH1	3:B:600:AGS:S1G	2.76	0.57

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	338/369 (92%)	335 (99%)	3 (1%)	0	100	100
1	B	342/369 (93%)	340 (99%)	2 (1%)	0	100	100
1	C	342/369 (93%)	340 (99%)	2 (1%)	0	100	100
1	D	345/369 (94%)	344 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	341/369 (92%)	339 (99%)	2 (1%)	0	100	100
1	F	323/369 (88%)	320 (99%)	3 (1%)	0	100	100
2	S	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2032/2221 (92%)	2019 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	285/301 (95%)	285 (100%)	0	100	100
1	B	287/301 (95%)	287 (100%)	0	100	100
1	C	287/301 (95%)	287 (100%)	0	100	100
1	D	288/301 (96%)	288 (100%)	0	100	100
1	E	286/301 (95%)	286 (100%)	0	100	100
1	F	274/301 (91%)	274 (100%)	0	100	100
2	S	1/1 (100%)	1 (100%)	0	100	100
All	All	1708/1807 (94%)	1708 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	HIS
1	F	336	GLN
1	C	101	ASN
1	A	225	GLN
1	F	331	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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
3	AGS	A	600	-	25,33,33	0.75	1 (4%)	24,52,52	1.12	2 (8%)
3	AGS	B	600	-	25,33,33	0.74	1 (4%)	24,52,52	1.16	2 (8%)
3	AGS	C	600	-	25,33,33	0.75	1 (4%)	24,52,52	1.17	2 (8%)
3	AGS	D	600	-	25,33,33	0.75	1 (4%)	24,52,52	1.17	2 (8%)
3	AGS	E	600	-	25,33,33	0.75	1 (4%)	24,52,52	1.12	2 (8%)
4	ADP	F	600	-	24,29,29	1.01	1 (4%)	25,45,45	1.55	3 (12%)

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
3	AGS	A	600	-	-	3/17/38/38	0/3/3/3
3	AGS	B	600	-	-	3/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	C	600	-	-	5/17/38/38	0/3/3/3
3	AGS	D	600	-	-	5/17/38/38	0/3/3/3
3	AGS	E	600	-	-	3/17/38/38	0/3/3/3
4	ADP	F	600	-	-	2/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	ADP	C5-C4	3.02	1.47	1.40
3	E	600	AGS	PG-S1G	2.47	1.95	1.90
3	A	600	AGS	PG-S1G	2.46	1.95	1.90
3	D	600	AGS	PG-S1G	2.45	1.95	1.90
3	C	600	AGS	PG-S1G	2.39	1.95	1.90

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	AGS	PA-O3A-PB	-4.55	118.12	132.57
3	C	600	AGS	PA-O3A-PB	-4.48	118.33	132.57
3	B	600	AGS	PA-O3A-PB	-4.47	118.36	132.57
3	E	600	AGS	PA-O3A-PB	-4.27	118.99	132.57
3	A	600	AGS	PA-O3A-PB	-4.18	119.28	132.57

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	AGS	C5'-O5'-PA-O1A
3	C	600	AGS	PB-O3B-PG-O2G
3	C	600	AGS	PB-O3B-PG-O3G
3	C	600	AGS	C5'-O5'-PA-O1A
3	E	600	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

5 monomers are involved in 7 short contacts:

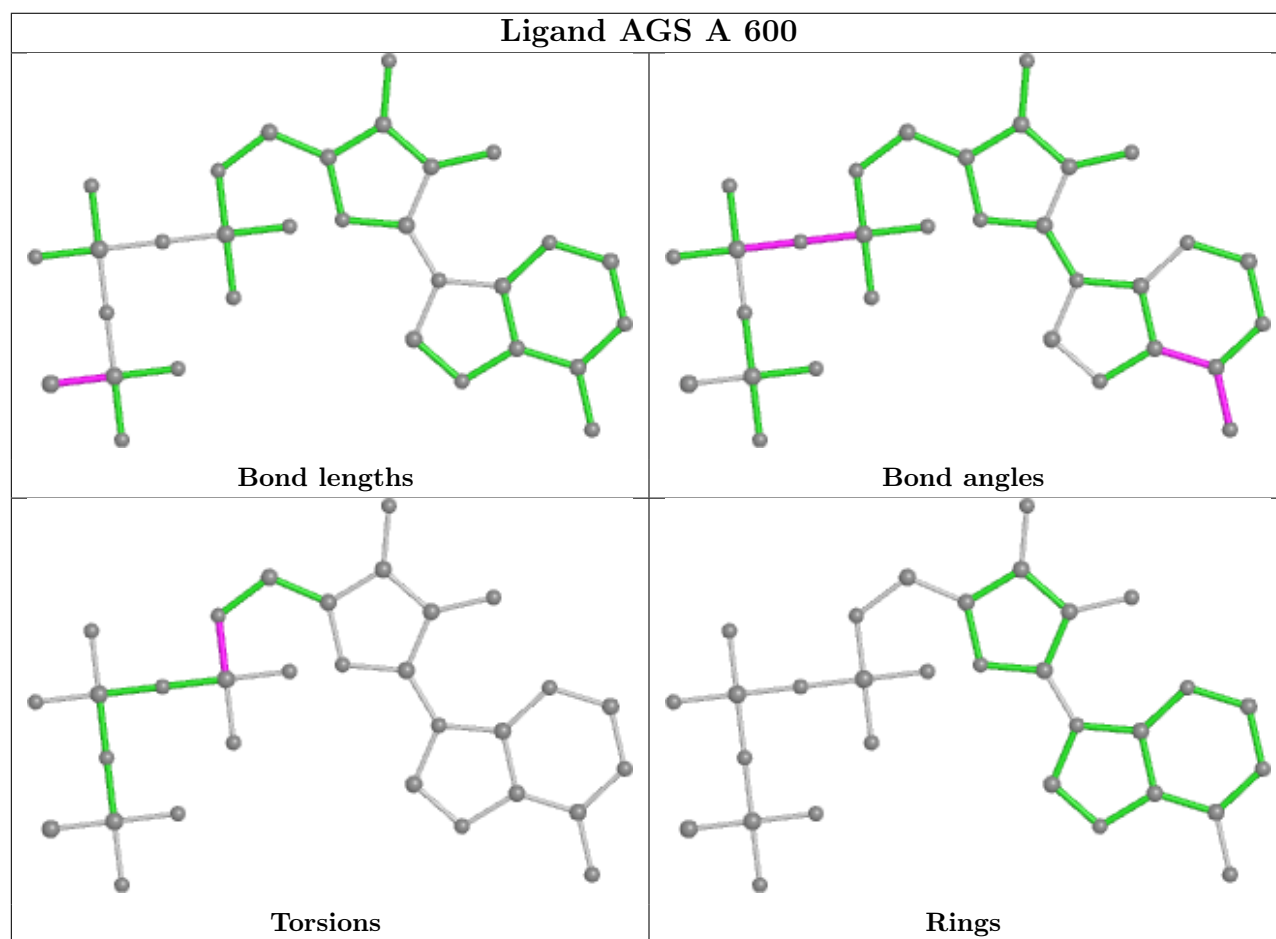
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	AGS	1	0
3	B	600	AGS	1	0
3	C	600	AGS	2	0

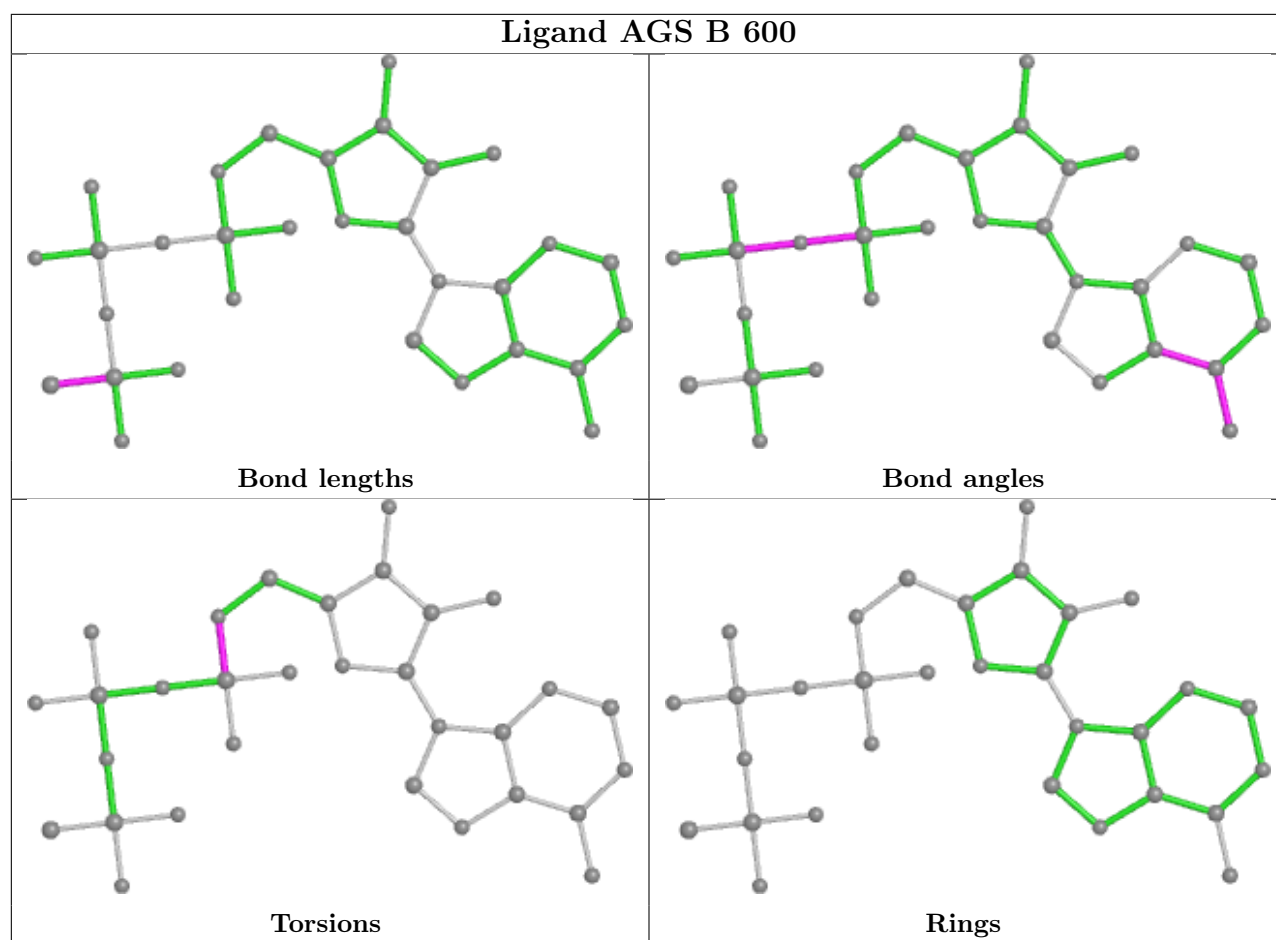
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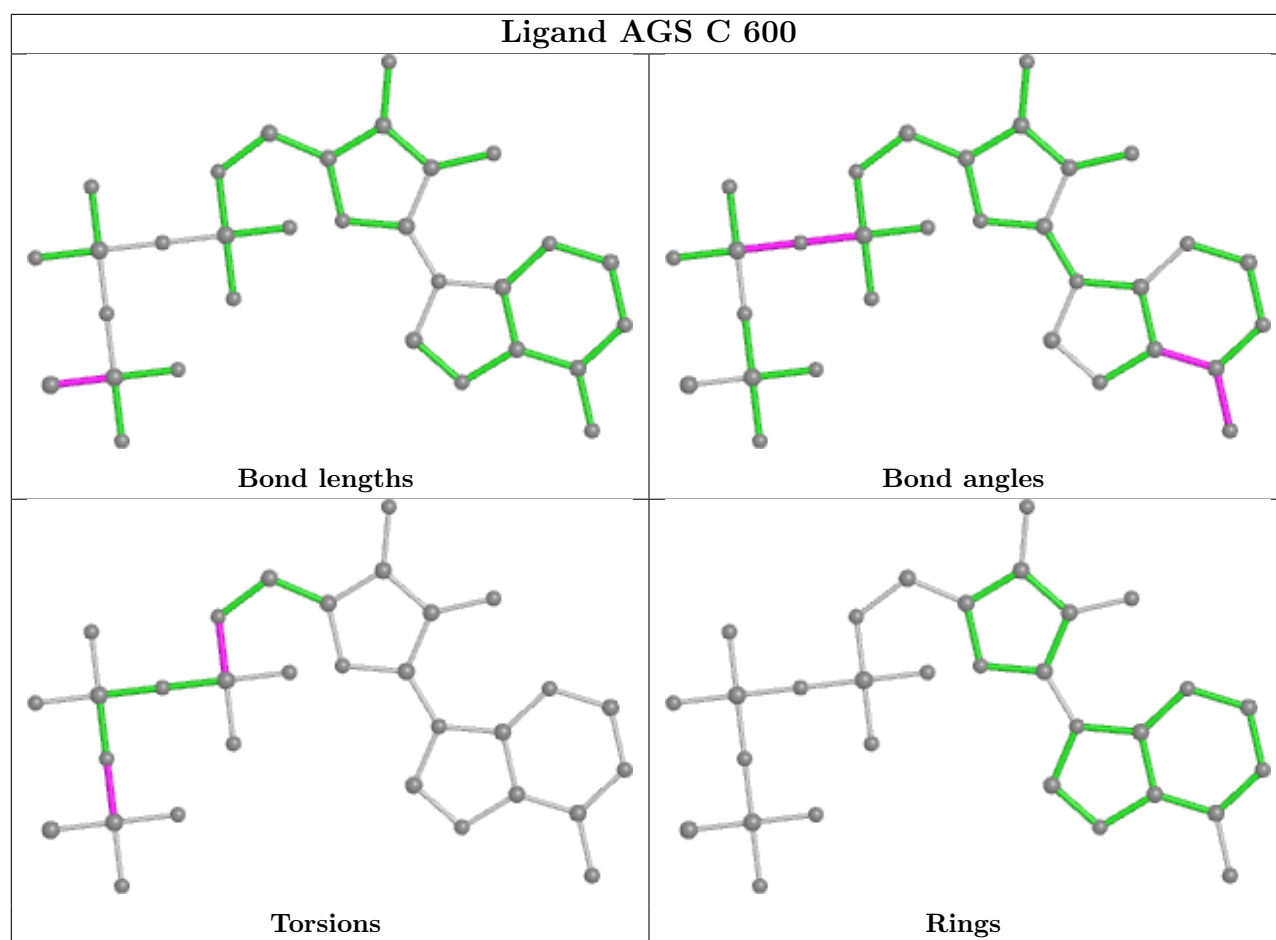
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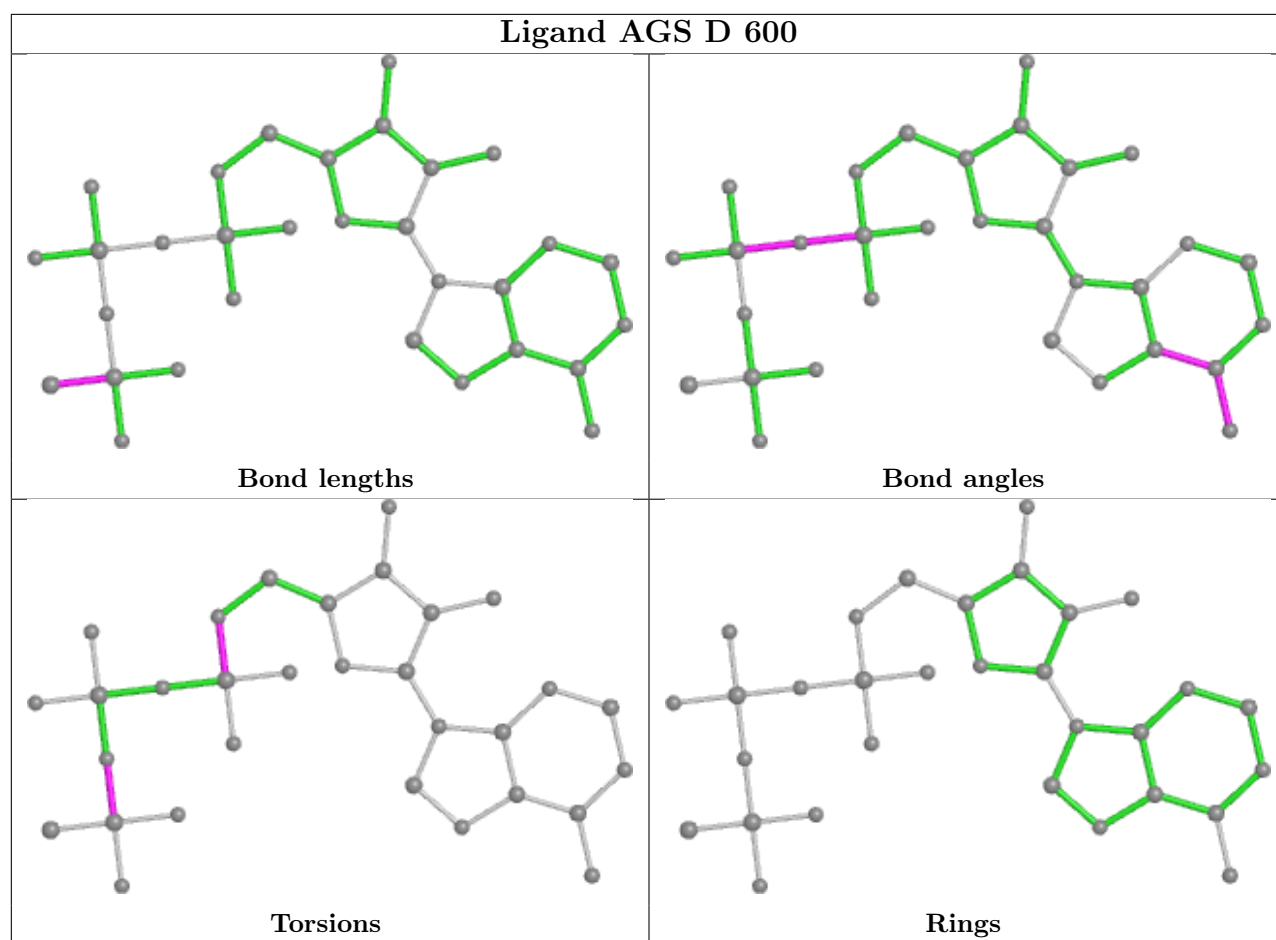
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	AGS	1	0
3	E	600	AGS	2	0

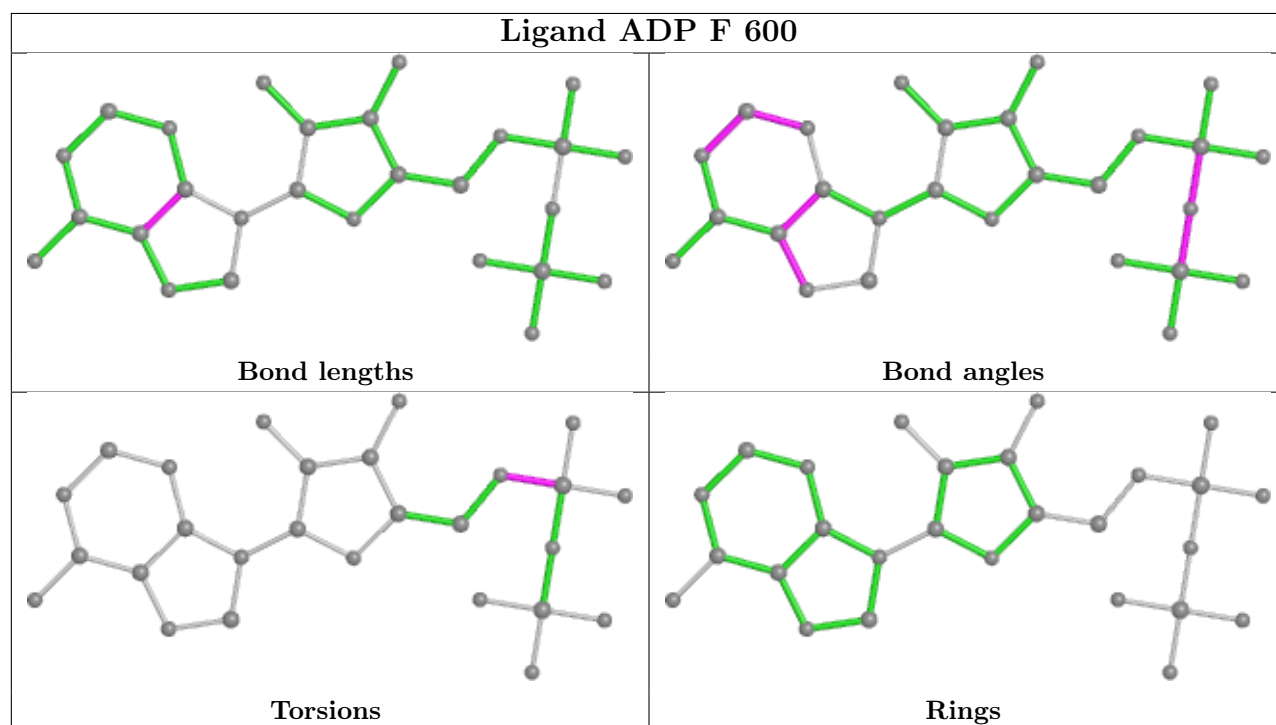
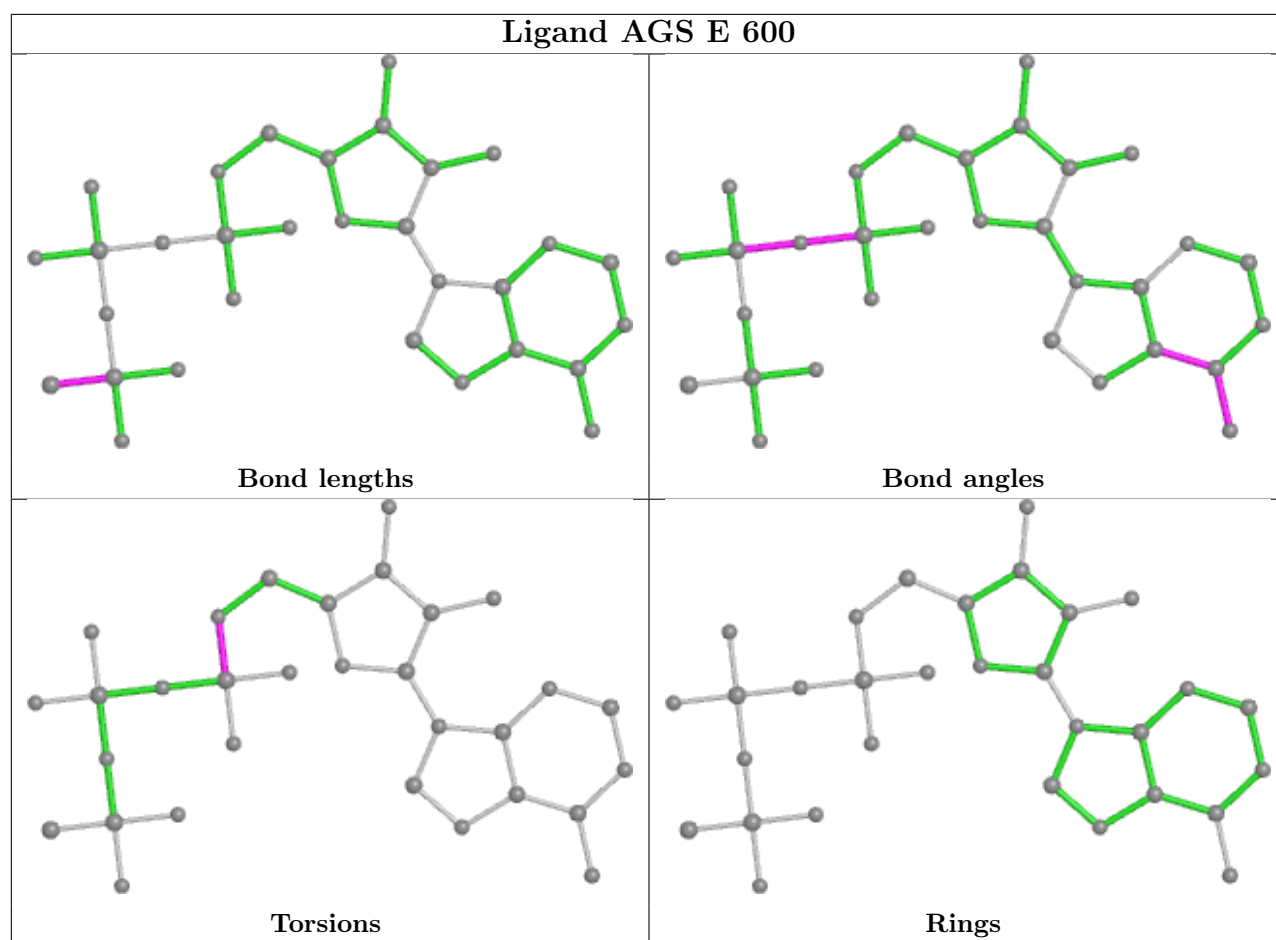
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.