



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 9G7G / pdb_00009g7g
Title : Structure of the clippase PaJOS from Pigmentiphaga aceris
Authors : Baumann, U.; Uthoff, M.; Hermanns, T.; Hofmann, K.
Deposited on : 2024-07-21
Resolution : 1.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

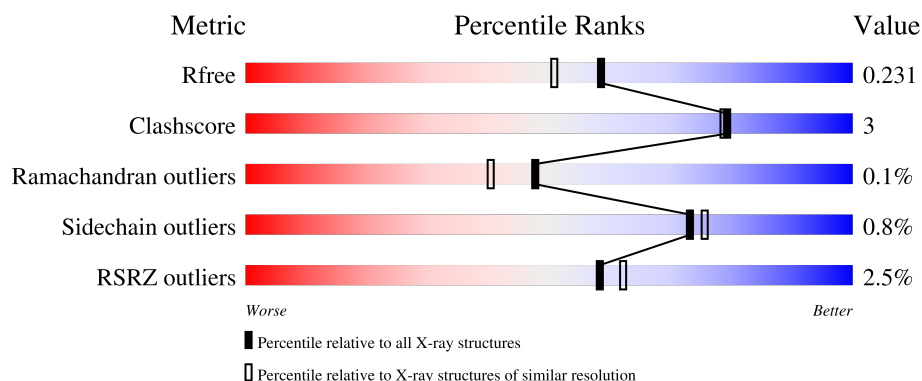
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	2% 82% 6% 11%
1	C	264	3% 83% 5% 12%
1	E	264	2% 83% 5% 12%
1	G	264	0% 84% 6% 11%
1	I	264	0% 85% • 12%

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Mol	Chain	Length	Quality of chain
1	K	264	
1	M	264	
1	O	264	
1	Q	264	
1	S	264	
1	U	264	
1	W	264	
2	B	75	
2	D	75	
2	F	75	
2	H	75	
2	J	75	
2	L	75	
2	N	75	
2	P	75	
2	R	75	
2	T	75	
2	V	75	
2	X	75	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28965 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PaJOS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	2	0
			1762	1106	311	343	2			
1	C	233	Total	C	N	O	S	0	5	0
			1765	1110	309	344	2			
1	E	233	Total	C	N	O	S	0	1	0
			1750	1099	310	339	2			
1	G	236	Total	C	N	O	S	0	1	0
			1768	1109	314	343	2			
1	I	233	Total	C	N	O	S	0	5	0
			1764	1110	307	344	3			
1	K	234	Total	C	N	O	S	0	0	0
			1753	1100	311	340	2			
1	M	236	Total	C	N	O	S	0	0	0
			1759	1105	310	342	2			
1	O	235	Total	C	N	O	S	0	1	0
			1764	1107	313	342	2			
1	Q	236	Total	C	N	O	S	0	1	0
			1770	1110	316	342	2			
1	S	231	Total	C	N	O	S	0	2	0
			1742	1095	308	337	2			
1	U	237	Total	C	N	O	S	0	1	0
			1786	1121	320	343	2			
1	W	236	Total	C	N	O	S	0	1	0
			1767	1110	313	342	2			

- Molecule 2 is a protein called Polyubiquitin-B.

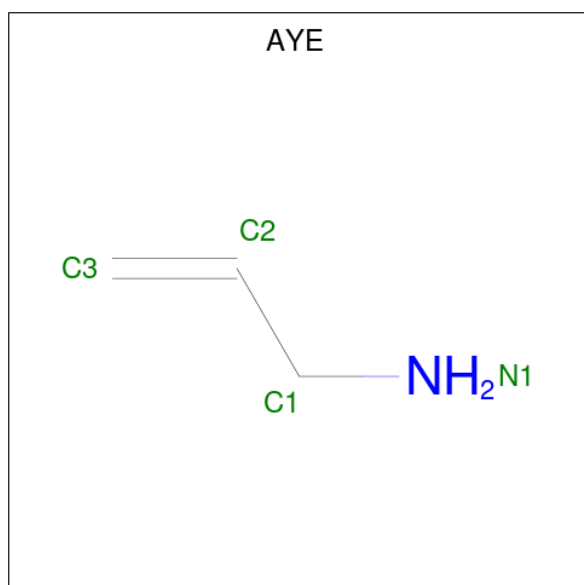
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	D	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	H	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	J	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	L	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	N	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	P	75	Total	C	N	O	S	0	1	0
			602	379	105	117	1			
2	R	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	T	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	V	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	X	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is prop-2-en-1-amine (CCD ID: AYE) (formula: C₃H₇N) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 3	N 1	0	0
3	E	1	Total 4	C 3	N 1	0	0
3	G	1	Total 4	C 3	N 1	0	0
3	I	1	Total 4	C 3	N 1	0	0
3	K	1	Total 4	C 3	N 1	0	0
3	M	1	Total 4	C 3	N 1	0	0
3	O	1	Total 4	C 3	N 1	0	0
3	Q	1	Total 4	C 3	N 1	0	0
3	S	1	Total 4	C 3	N 1	0	0
3	U	1	Total 4	C 3	N 1	0	0
3	W	1	Total 4	C 3	N 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total 60	O 60	0	0
4	B	10	Total 10	O 10	0	0
4	C	47	Total 47	O 47	0	0
4	D	14	Total 14	O 14	0	0
4	E	45	Total 45	O 45	0	0
4	F	20	Total 20	O 20	0	0
4	G	49	Total 49	O 49	0	0
4	H	15	Total 15	O 15	0	0

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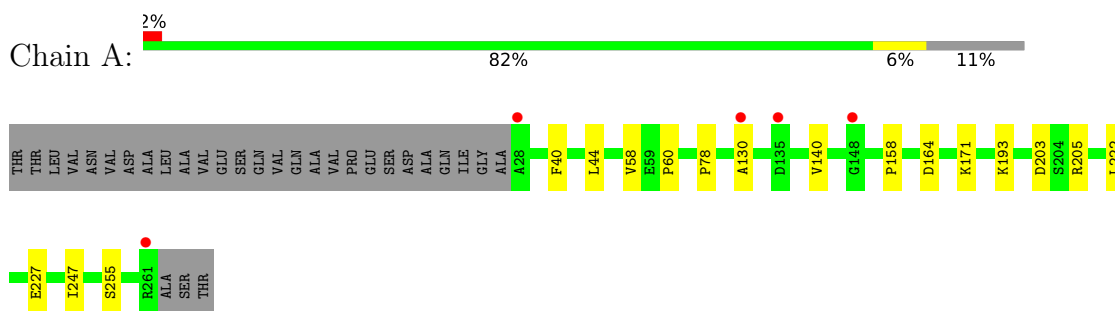
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	54	Total 54	O 54	0	0
4	J	14	Total 14	O 14	0	0
4	K	41	Total 41	O 41	0	0
4	L	20	Total 20	O 20	0	0
4	M	48	Total 48	O 48	0	0
4	N	12	Total 12	O 12	0	0
4	O	32	Total 32	O 32	0	0
4	P	12	Total 12	O 12	0	0
4	Q	12	Total 12	O 12	0	0
4	R	8	Total 8	O 8	0	0
4	S	23	Total 23	O 23	0	0
4	T	9	Total 9	O 9	0	0
4	U	22	Total 22	O 22	0	0
4	V	13	Total 13	O 13	0	0
4	W	12	Total 12	O 12	0	0
4	X	6	Total 6	O 6	0	0

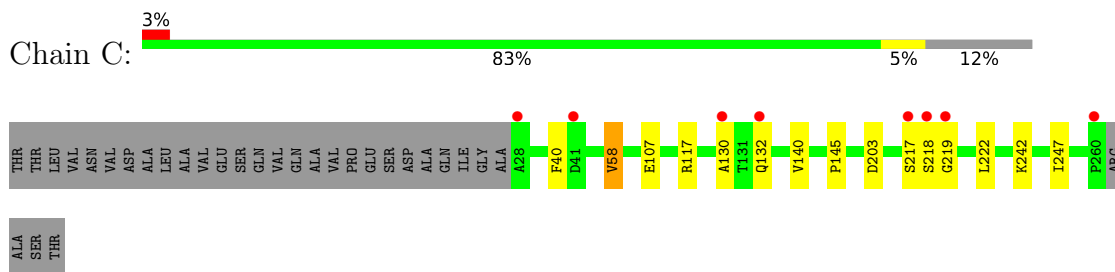
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

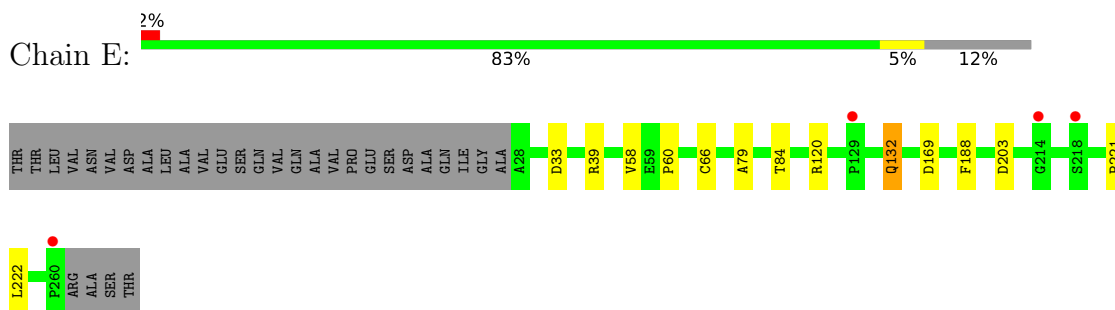
- Molecule 1: PaJOS



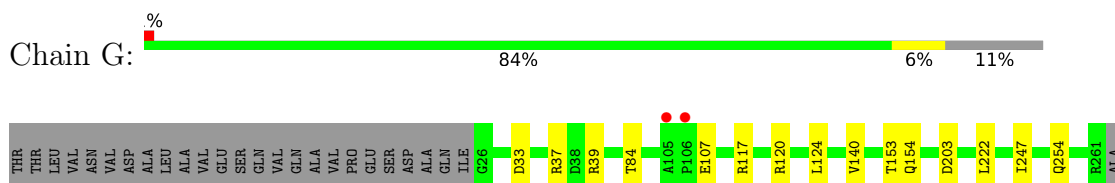
- Molecule 1: PaJOS



- Molecule 1: PaJOS



- Molecule 1: PaJOS



SER
THR

● Molecule 1: PaJOS

Chain I:  %
85% 12%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA ALA GLN ILE GLY ALA A28 P60 R120 P129 Q132 D135 D164 K193 D203 E216 L222 E227 P260 ARG ALA SER THR

● Molecule 1: PaJOS

Chain K:  %
79% 9% 11%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA ALA GLN ILE GLY ALA A28 F40 L45 L48 V58 C66 V75 A130 T131 Q132 G133 K134 G139 V140 V155 P158 A159 D169 V170 K171 D183

F188 D203 S217 S218 G219 L222 E234 T238 I247 I251 S255 P260 R261 ALA SER THR

● Molecule 1: PaJOS

Chain M:  %
84% 5% 11%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA ALA GLN ILE GLY ALA I25 V58 E59 P60 C66 F74 D81 I82 P83 T87 D135 Q154 R165 D169 F188 E216 S217 S218 P221 P260 ARG ALA SER

THR

● Molecule 1: PaJOS

Chain O:  %
81% 8% 11%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA ALA GLN ILE GLY ALA A28 R39 V58 E59 P60 C66 I71 V75 T84 V140 D169 G173 S174 T178 A179 D183 F188 S206 H210

S217 S218 P221 I235 A239 I247 V259 A262 THR

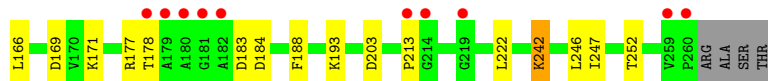
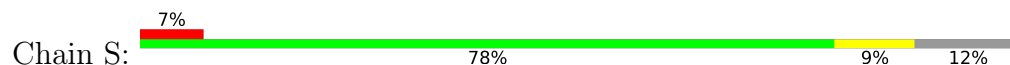
● Molecule 1: PaJOS

Chain Q:  %
83% 6% 11%

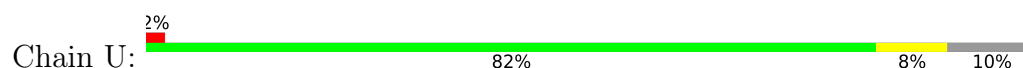
THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA ALA GLN ILE G26 R39 L44 C66 T86 T87 T90 D99 A149 A150 M151 P158 A159 D169 F188 L201 A211 P212 E216 L222



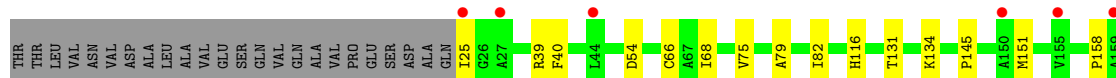
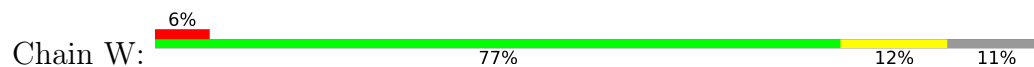
• Molecule 1: PaJOS



• Molecule 1: PaJOS



• Molecule 1: PaJOS



• Molecule 2: Polyubiquitin-B

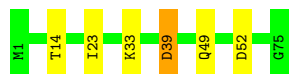


• Molecule 2: Polyubiquitin-B

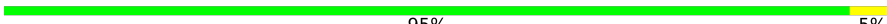


- Molecule 2: Polyubiquitin-B

Chain F:  92% 7%



- Molecule 2: Polyubiquitin-B

Chain H:  95% 5%

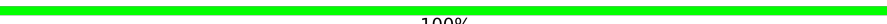


- Molecule 2: Polyubiquitin-B

Chain J:  100%

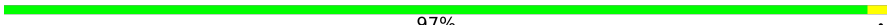
There are no outlier residues recorded for this chain.

- Molecule 2: Polyubiquitin-B

Chain L:  100%

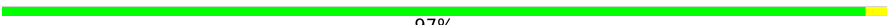
There are no outlier residues recorded for this chain.

- Molecule 2: Polyubiquitin-B

Chain N:  97%

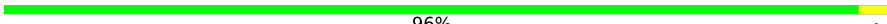


- Molecule 2: Polyubiquitin-B

Chain P:  97%

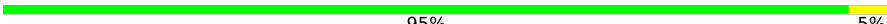


- Molecule 2: Polyubiquitin-B

Chain R:  96%

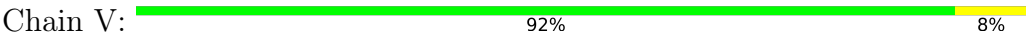


- Molecule 2: Polyubiquitin-B

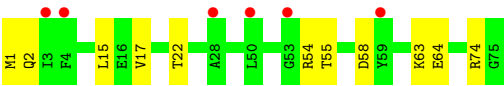
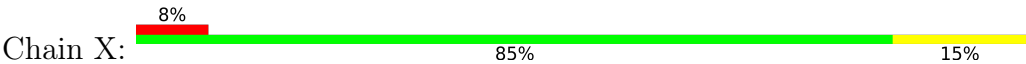
Chain T:  95% 5%



● Molecule 2: Polyubiquitin-B



● Molecule 2: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.95Å 81.32Å 167.39Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	49.03 – 1.89 49.03 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.03-1.89) 95.7 (49.03-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX (dev_5407: ???)	Depositor
R, R_{free}	0.204 , 0.231 0.204 , 0.231	Depositor DCC
R_{free} test set	2124 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28965	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0274e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYE

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	0.36	0/1814	0.53	0/2484
1	C	0.39	0/1826	0.53	0/2502
1	E	0.38	0/1799	0.55	0/2464
1	G	0.36	0/1817	0.55	0/2488
1	I	0.38	0/1825	0.55	0/2500
1	K	0.38	0/1799	0.54	0/2464
1	M	0.38	0/1805	0.57	0/2473
1	O	0.36	0/1813	0.53	0/2483
1	Q	0.32	0/1819	0.48	0/2490
1	S	0.33	0/1793	0.50	0/2454
1	U	0.31	0/1838	0.49	0/2515
1	W	0.30	0/1816	0.48	0/2487
2	B	0.36	0/603	0.52	0/811
2	D	0.37	0/603	0.54	0/811
2	F	0.41	0/603	0.56	0/811
2	H	0.37	0/603	0.58	0/811
2	J	0.38	0/603	0.55	0/811
2	L	0.41	0/603	0.54	0/811
2	N	0.37	0/603	0.55	0/811
2	P	0.36	0/611	0.55	0/822
2	R	0.33	0/603	0.53	0/811
2	T	0.35	0/603	0.56	0/811
2	V	0.33	0/603	0.50	0/811
2	X	0.32	0/603	0.51	0/811
All	All	0.36	0/29008	0.53	0/39547

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	A	1762	0	1701	9	0
1	C	1765	0	1709	8	0
1	E	1750	0	1690	11	0
1	G	1768	0	1706	7	0
1	I	1764	0	1708	7	0
1	K	1753	0	1690	16	0
1	M	1759	0	1696	8	0
1	O	1764	0	1703	14	0
1	Q	1770	0	1711	9	0
1	S	1742	0	1684	12	0
1	U	1786	0	1735	10	0
1	W	1767	0	1709	23	0
2	B	597	0	626	1	0
2	D	597	0	626	1	0
2	F	597	0	626	4	0
2	H	597	0	626	2	0
2	J	597	0	626	0	0
2	L	597	0	626	0	0
2	N	597	0	626	1	0
2	P	602	0	632	1	0
2	R	597	0	626	3	0
2	T	597	0	626	3	0
2	V	597	0	626	2	0
2	X	597	0	626	7	0
3	A	4	0	4	0	0
3	C	4	0	4	0	0
3	E	4	0	4	1	0
3	G	4	0	4	0	0
3	I	4	0	4	0	0
3	K	4	0	4	1	0
3	M	4	0	4	1	0
3	O	4	0	4	1	0
3	Q	4	0	4	1	0
3	S	4	0	4	1	0
3	U	4	0	4	1	0
3	W	4	0	4	1	0
4	A	60	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	47	0	0	0	0
4	D	14	0	0	1	0
4	E	45	0	0	0	0
4	F	20	0	0	1	0
4	G	49	0	0	0	0
4	H	15	0	0	0	0
4	I	54	0	0	2	0
4	J	14	0	0	0	0
4	K	41	0	0	0	0
4	L	20	0	0	0	0
4	M	48	0	0	0	0
4	N	12	0	0	0	0
4	O	32	0	0	1	0
4	P	12	0	0	0	0
4	Q	12	0	0	0	0
4	R	8	0	0	0	0
4	S	23	0	0	0	0
4	T	9	0	0	1	0
4	U	22	0	0	0	0
4	V	13	0	0	0	0
4	W	12	0	0	1	0
4	X	6	0	0	1	0
All	All	28965	0	28008	151	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 151 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)
2:T:49:GLN:N	1:W:216:GLU:OE2	2.09	0.82
1:A:227:GLU:OE2	4:A:401:HOH:O	2.00	0.78
1:U:171:LYS:HE2	1:U:184:ASP:HB2	1.66	0.77
1:I:227:GLU:OE2	4:I:401:HOH:O	2.07	0.72
2:T:11:LYS:NZ	4:T:201:HOH:O	2.23	0.70

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	234/264 (89%)	231 (99%)	3 (1%)	0	100	100
1	C	236/264 (89%)	232 (98%)	3 (1%)	1 (0%)	30	22
1	E	232/264 (88%)	229 (99%)	3 (1%)	0	100	100
1	G	235/264 (89%)	229 (97%)	6 (3%)	0	100	100
1	I	236/264 (89%)	233 (99%)	3 (1%)	0	100	100
1	K	232/264 (88%)	228 (98%)	4 (2%)	0	100	100
1	M	234/264 (89%)	229 (98%)	5 (2%)	0	100	100
1	O	234/264 (89%)	232 (99%)	2 (1%)	0	100	100
1	Q	235/264 (89%)	230 (98%)	5 (2%)	0	100	100
1	S	229/264 (87%)	226 (99%)	3 (1%)	0	100	100
1	U	237/264 (90%)	231 (98%)	6 (2%)	0	100	100
1	W	235/264 (89%)	229 (97%)	5 (2%)	1 (0%)	30	22
2	B	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	D	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	F	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	H	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	J	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	L	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	N	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	P	74/75 (99%)	73 (99%)	1 (1%)	0	100	100
2	R	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	T	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	V	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	X	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
All	All	3686/4068 (91%)	3624 (98%)	60 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	216	GLU
1	C	218	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	185/206 (90%)	183 (99%)	2 (1%)	65	67
1	C	187/206 (91%)	186 (100%)	1 (0%)	81	84
1	E	183/206 (89%)	182 (100%)	1 (0%)	81	84
1	G	184/206 (89%)	183 (100%)	1 (0%)	81	84
1	I	187/206 (91%)	187 (100%)	0	100	100
1	K	183/206 (89%)	180 (98%)	3 (2%)	55	54
1	M	183/206 (89%)	181 (99%)	2 (1%)	65	67
1	O	184/206 (89%)	183 (100%)	1 (0%)	81	84
1	Q	184/206 (89%)	182 (99%)	2 (1%)	65	67
1	S	183/206 (89%)	178 (97%)	5 (3%)	39	34
1	U	186/206 (90%)	184 (99%)	2 (1%)	65	67
1	W	184/206 (89%)	183 (100%)	1 (0%)	81	84
2	B	68/68 (100%)	68 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100
2	F	68/68 (100%)	67 (98%)	1 (2%)	57	56
2	H	68/68 (100%)	68 (100%)	0	100	100
2	J	68/68 (100%)	68 (100%)	0	100	100
2	L	68/68 (100%)	68 (100%)	0	100	100
2	N	68/68 (100%)	68 (100%)	0	100	100
2	P	69/68 (102%)	69 (100%)	0	100	100
2	R	68/68 (100%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	68/68 (100%)	68 (100%)	0	100	100
2	V	68/68 (100%)	66 (97%)	2 (3%)	37	31
2	X	68/68 (100%)	67 (98%)	1 (2%)	57	56
All	All	3030/3288 (92%)	3005 (99%)	25 (1%)	73	75

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	58	VAL
1	S	178	THR
2	X	74	ARG
1	S	151	MET
1	S	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	154	GLN
1	U	225	GLN
2	X	68	HIS
1	W	116	HIS
1	Q	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	AYE	W	301	2,1	3,3,3	0.40	0	2,2,2	0.32	0
3	AYE	G	301	2,1	3,3,3	0.14	0	2,2,2	0.79	0
3	AYE	E	301	2,1	3,3,3	0.28	0	2,2,2	0.57	0
3	AYE	I	301	2,1	3,3,3	0.33	0	2,2,2	0.96	0
3	AYE	S	301	2,1	3,3,3	0.21	0	2,2,2	0.66	0
3	AYE	A	301	2,1	3,3,3	0.30	0	2,2,2	0.58	0
3	AYE	O	301	2,1	3,3,3	0.24	0	2,2,2	0.66	0
3	AYE	U	301	2,1	3,3,3	0.13	0	2,2,2	0.67	0
3	AYE	K	301	2,1	3,3,3	0.31	0	2,2,2	0.84	0
3	AYE	M	301	2,1	3,3,3	0.29	0	2,2,2	0.71	0
3	AYE	Q	301	2,1	3,3,3	0.19	0	2,2,2	0.64	0
3	AYE	C	301	2,1	3,3,3	0.23	0	2,2,2	1.32	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
3	AYE	W	301	2,1	-	0/1/1/1	-
3	AYE	G	301	2,1	-	0/1/1/1	-
3	AYE	E	301	2,1	-	0/1/1/1	-
3	AYE	I	301	2,1	-	0/1/1/1	-
3	AYE	S	301	2,1	-	0/1/1/1	-
3	AYE	A	301	2,1	-	0/1/1/1	-
3	AYE	O	301	2,1	-	0/1/1/1	-
3	AYE	U	301	2,1	-	0/1/1/1	-
3	AYE	K	301	2,1	-	0/1/1/1	-
3	AYE	M	301	2,1	-	0/1/1/1	-
3	AYE	Q	301	2,1	-	0/1/1/1	-
3	AYE	C	301	2,1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

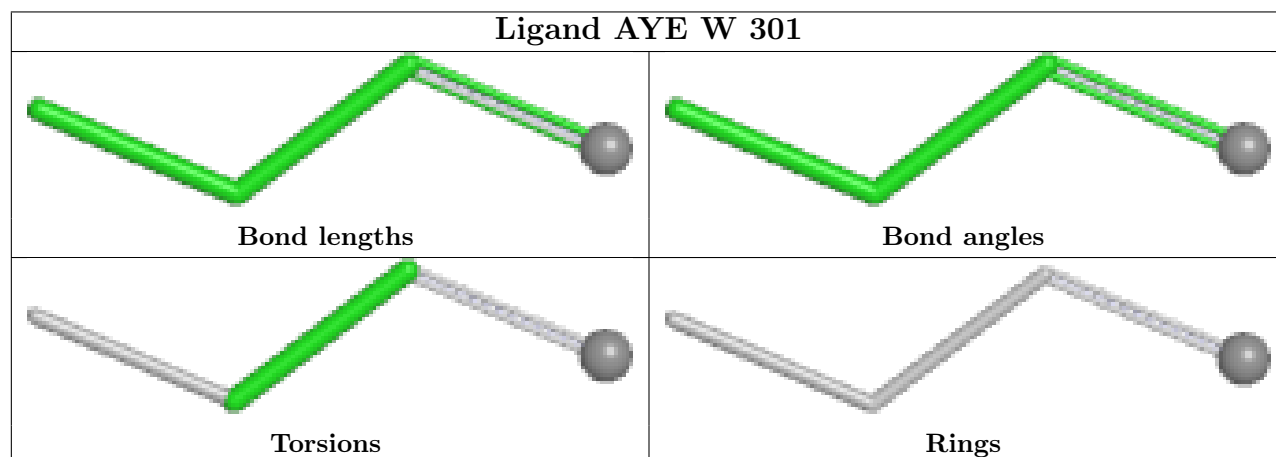
There are no torsion outliers.

There are no ring outliers.

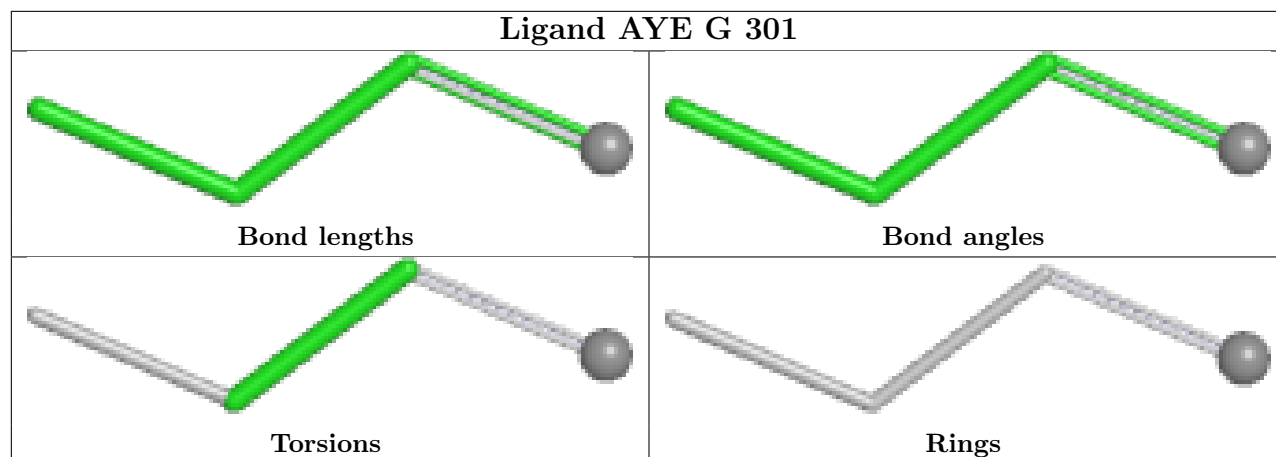
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	301	AYE	1	0
3	E	301	AYE	1	0
3	S	301	AYE	1	0
3	O	301	AYE	1	0
3	U	301	AYE	1	0
3	K	301	AYE	1	0
3	M	301	AYE	1	0
3	Q	301	AYE	1	0

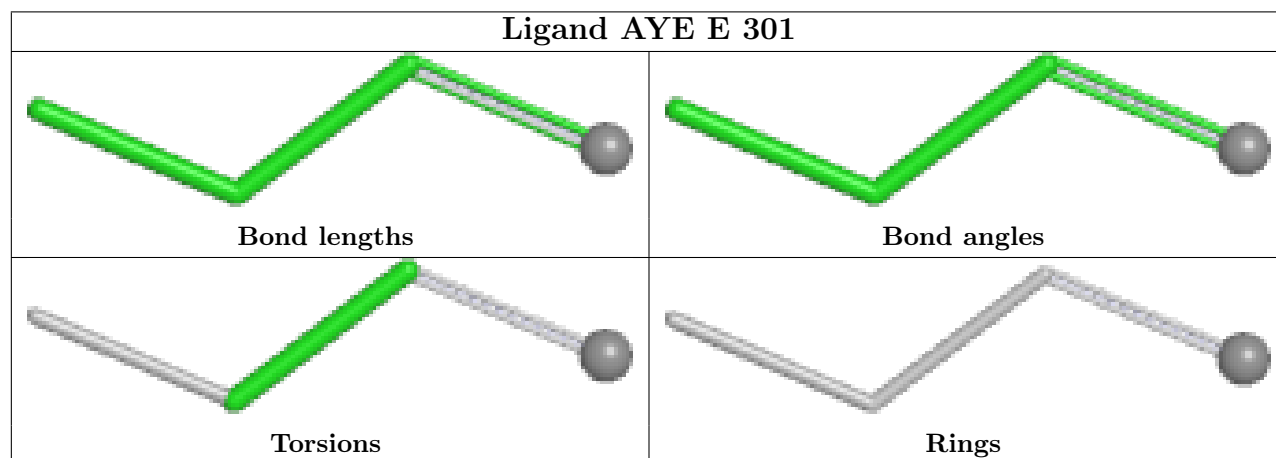
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



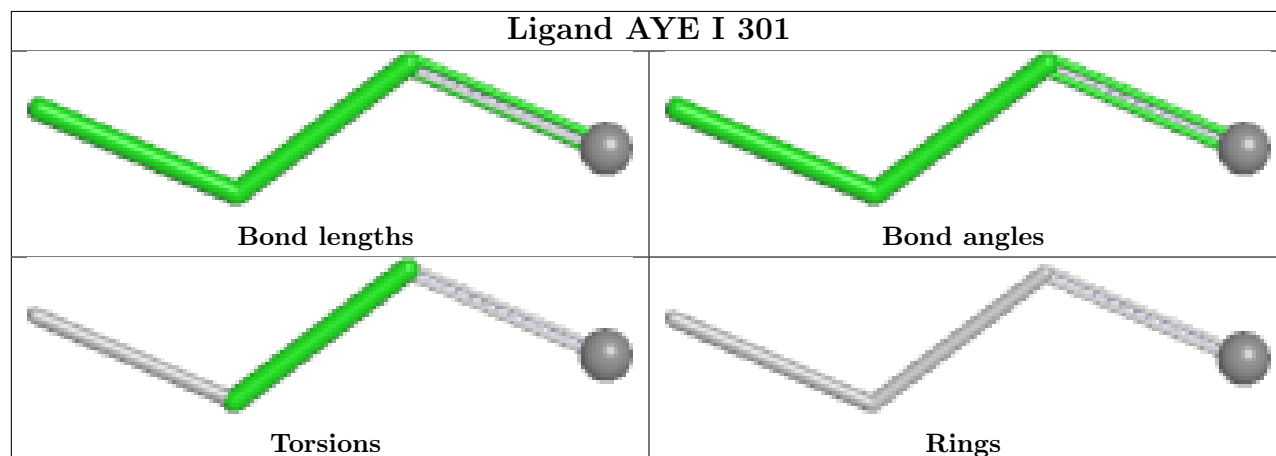
Ligand AYE G 301

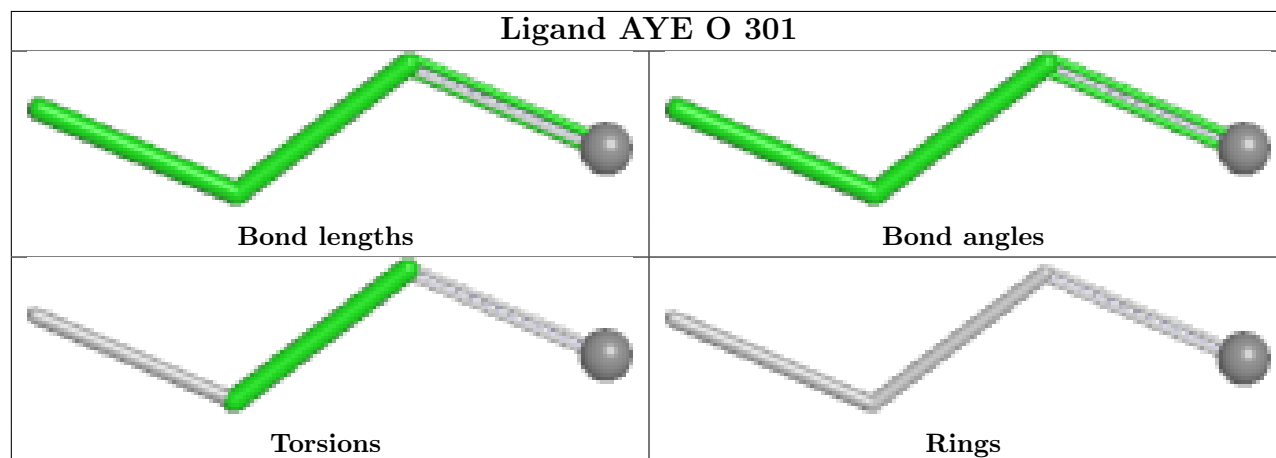
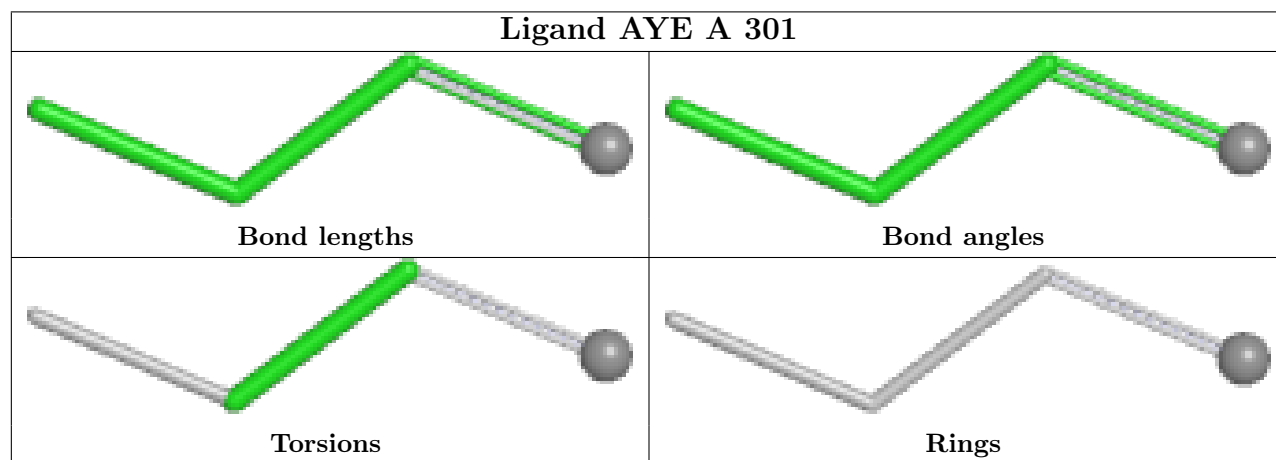
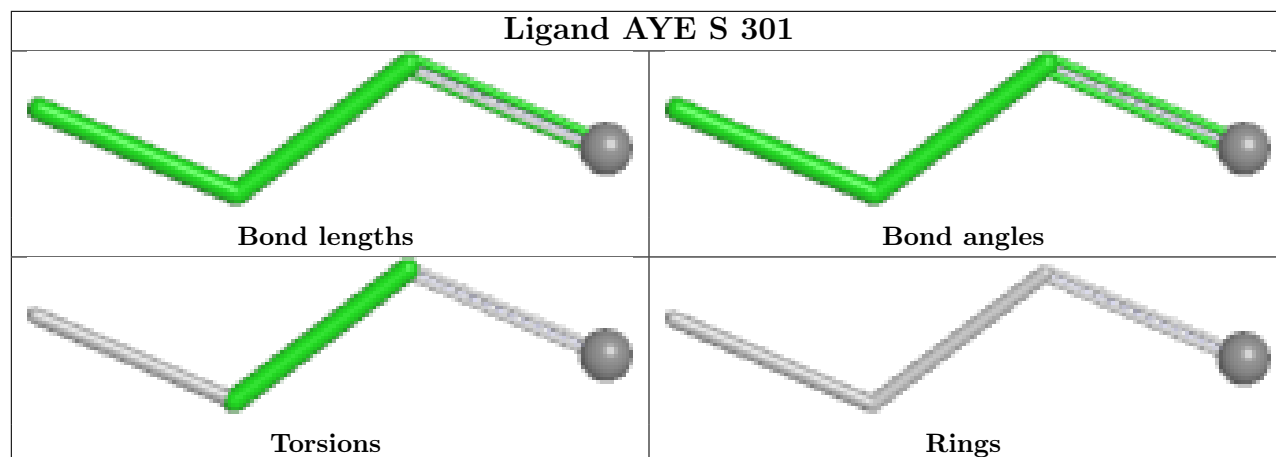


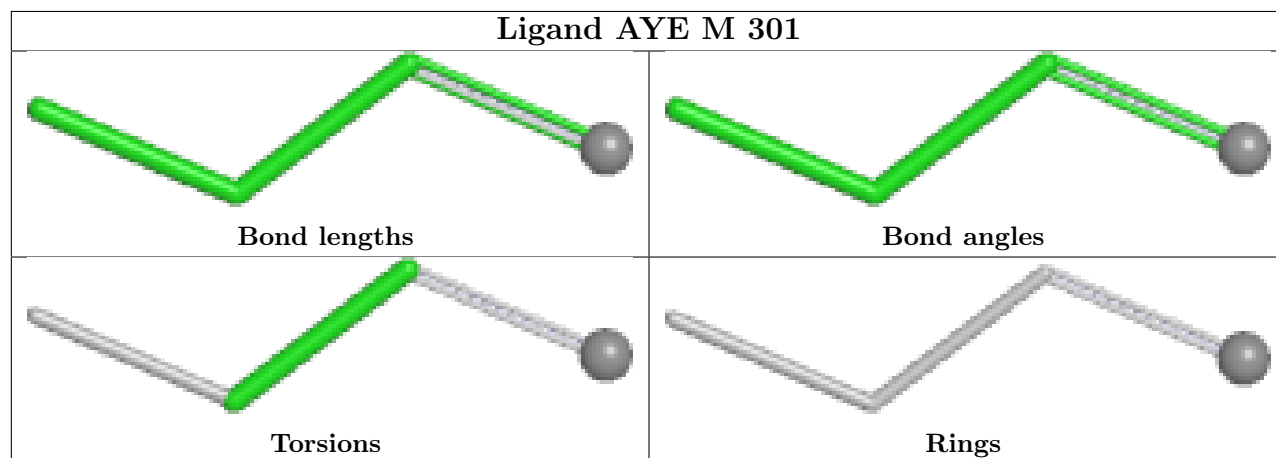
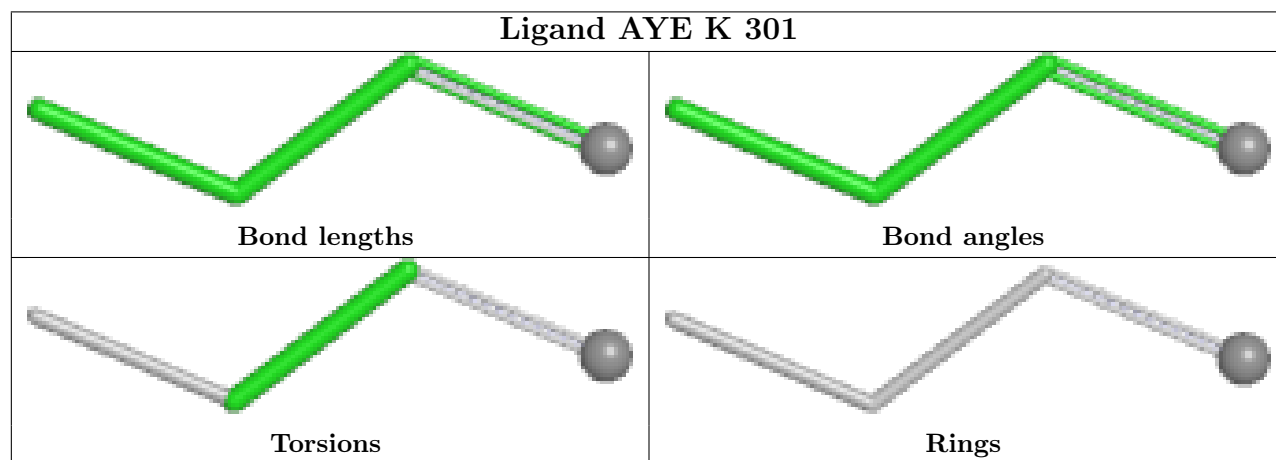
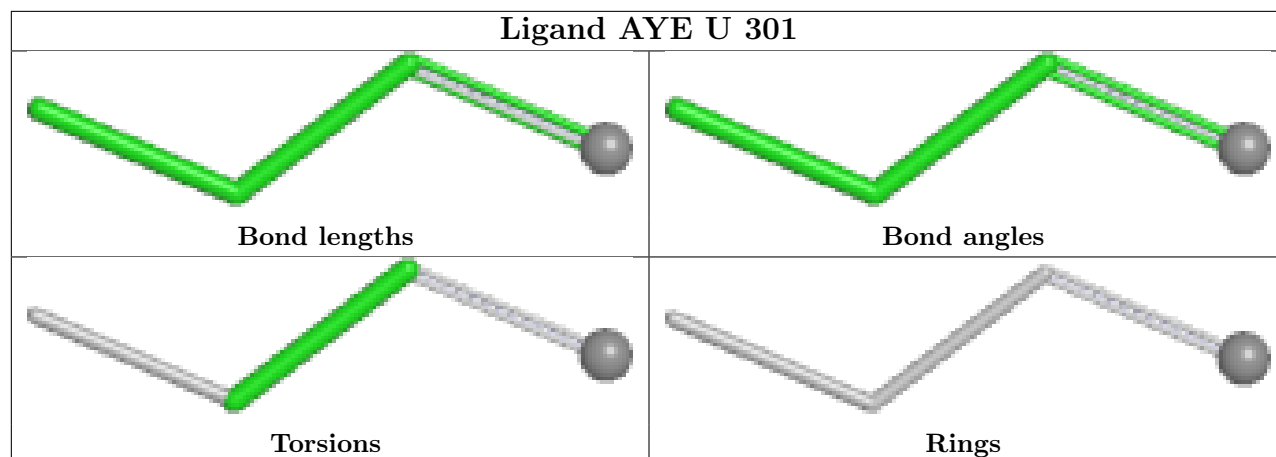
Ligand AYE E 301

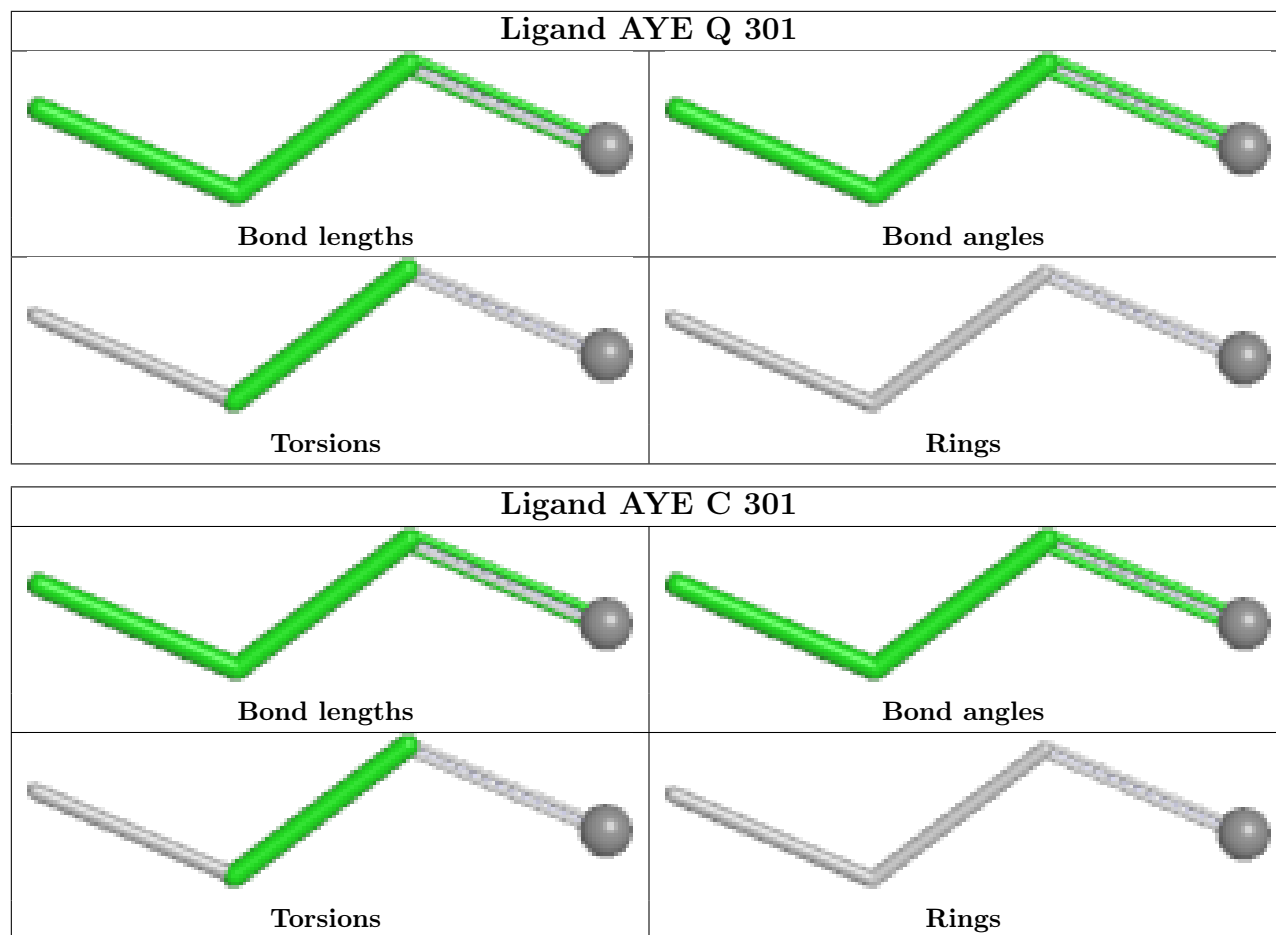


Ligand AYE I 301









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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/264 (88%)	0.02	5 (2%) 63 67	25, 42, 64, 96	2 (0%)
1	C	233/264 (88%)	0.06	8 (3%) 48 51	22, 41, 71, 122	5 (2%)
1	E	233/264 (88%)	0.06	4 (1%) 69 72	25, 42, 72, 90	1 (0%)
1	G	236/264 (89%)	-0.00	2 (0%) 82 85	31, 42, 61, 91	1 (0%)
1	I	233/264 (88%)	0.02	3 (1%) 75 78	25, 40, 61, 85	5 (2%)
1	K	234/264 (88%)	0.07	7 (2%) 52 56	30, 42, 68, 99	0
1	M	236/264 (89%)	0.13	3 (1%) 75 78	29, 44, 66, 105	0
1	O	235/264 (89%)	0.27	4 (1%) 69 72	30, 47, 81, 107	1 (0%)
1	Q	236/264 (89%)	0.60	9 (3%) 44 47	23, 65, 94, 110	1 (0%)
1	S	231/264 (87%)	0.54	18 (7%) 19 20	22, 55, 101, 131	2 (0%)
1	U	237/264 (89%)	0.54	6 (2%) 58 62	22, 57, 82, 111	1 (0%)
1	W	236/264 (89%)	0.72	17 (7%) 21 23	34, 62, 92, 125	1 (0%)
2	B	75/75 (100%)	0.08	0 100 100	33, 50, 65, 68	0
2	D	75/75 (100%)	0.01	0 100 100	33, 47, 62, 72	0
2	F	75/75 (100%)	-0.14	0 100 100	32, 41, 56, 57	0
2	H	75/75 (100%)	0.24	0 100 100	33, 48, 65, 68	0
2	J	75/75 (100%)	0.14	0 100 100	31, 47, 63, 72	0
2	L	75/75 (100%)	-0.02	0 100 100	34, 43, 57, 63	0
2	N	75/75 (100%)	0.12	0 100 100	31, 49, 68, 69	0
2	P	75/75 (100%)	0.12	0 100 100	33, 48, 65, 70	1 (1%)
2	R	75/75 (100%)	0.23	0 100 100	35, 53, 69, 77	0
2	T	75/75 (100%)	0.39	0 100 100	35, 57, 78, 81	0
2	V	75/75 (100%)	0.37	0 100 100	38, 54, 70, 78	0
2	X	75/75 (100%)	1.04	6 (8%) 18 19	42, 78, 101, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3714/4068 (91%)	0.24	92 (2%) 58 62	22, 47, 82, 131	21 (0%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	25	ILE	6.4
1	M	25	ILE	4.4
1	A	148	GLY	3.9
1	I	260	PRO	3.8
1	A	135	ASP	3.7

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

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

6.3 Carbohydrates ⓘ

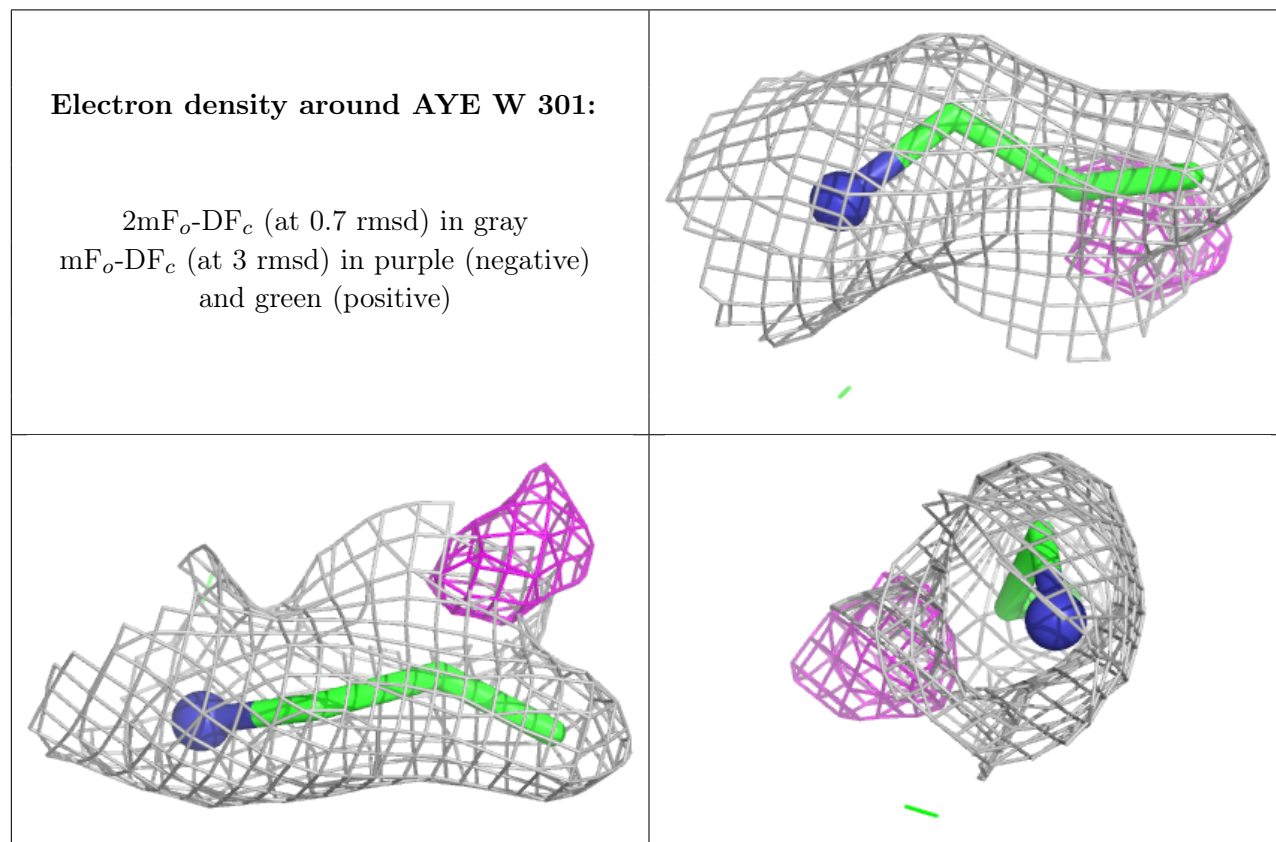
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

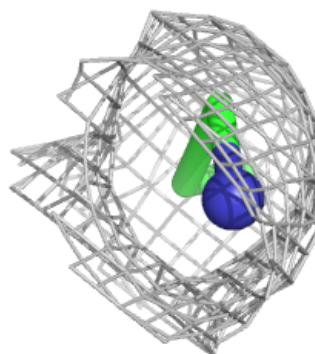
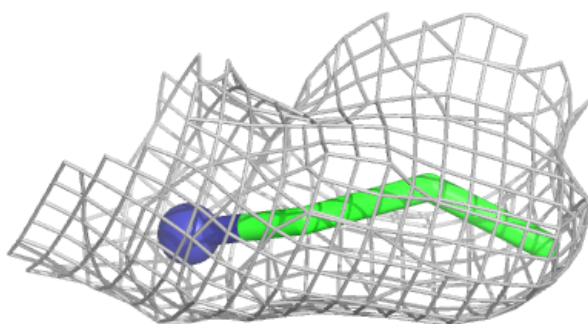
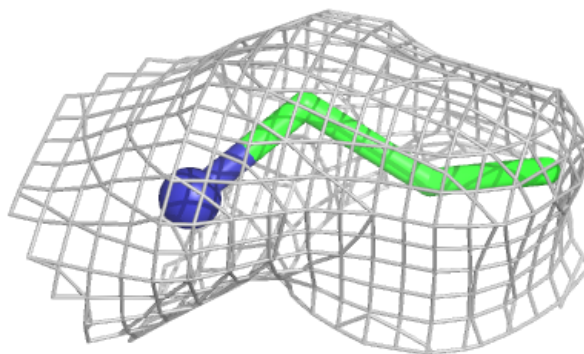
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AYE	W	301	4/4	0.90	0.13	41,42,43,45	0
3	AYE	U	301	4/4	0.93	0.12	44,45,46,49	0
3	AYE	Q	301	4/4	0.94	0.10	44,44,50,51	0
3	AYE	A	301	4/4	0.94	0.08	33,33,34,35	0
3	AYE	I	301	4/4	0.94	0.08	29,30,33,33	0
3	AYE	O	301	4/4	0.95	0.08	37,38,40,40	0
3	AYE	E	301	4/4	0.96	0.06	34,35,35,36	0
3	AYE	S	301	4/4	0.96	0.08	38,39,40,41	0
3	AYE	K	301	4/4	0.97	0.05	31,33,34,34	0
3	AYE	G	301	4/4	0.97	0.06	35,35,36,36	0
3	AYE	M	301	4/4	0.98	0.06	34,36,37,38	0
3	AYE	C	301	4/4	0.98	0.06	33,33,33,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

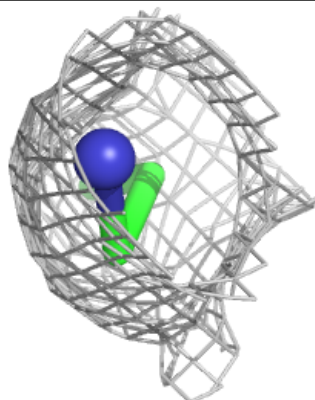
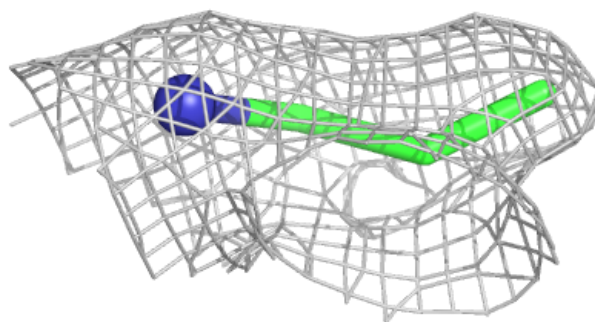
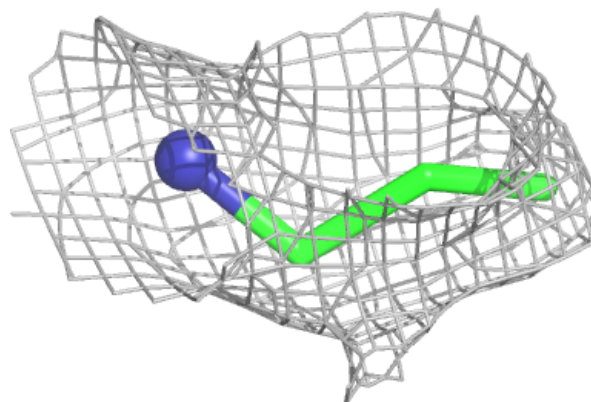


Electron density around AYE U 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

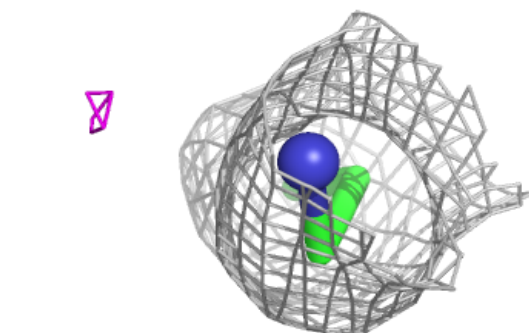
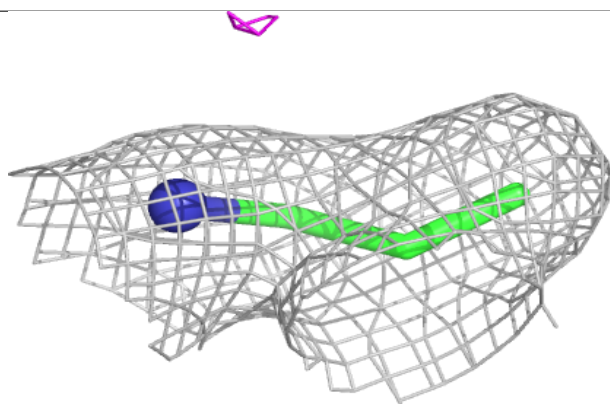
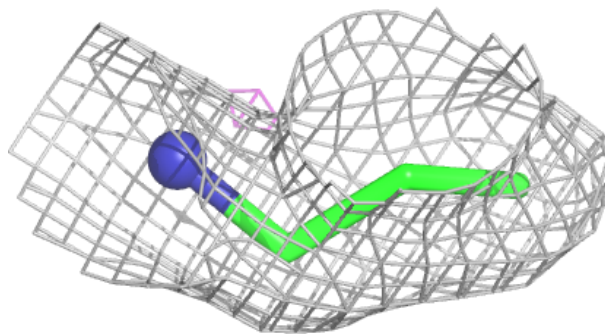
**Electron density around AYE Q 301:**

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and green (positive)

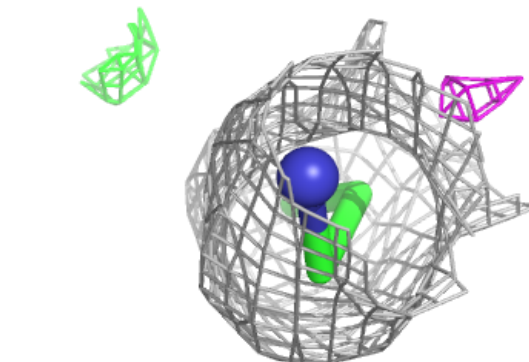
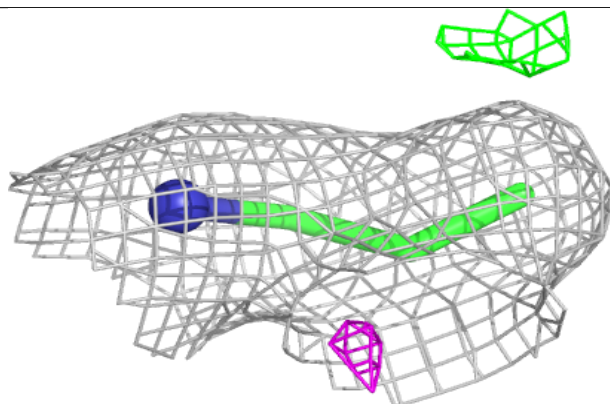
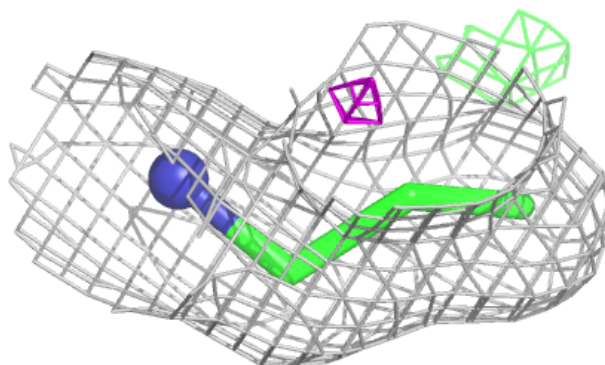


Electron density around AYE A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

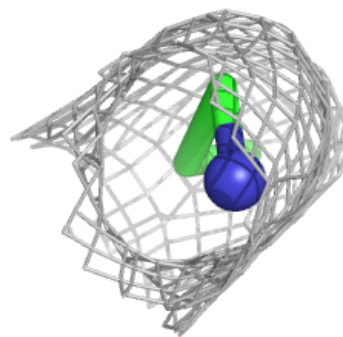
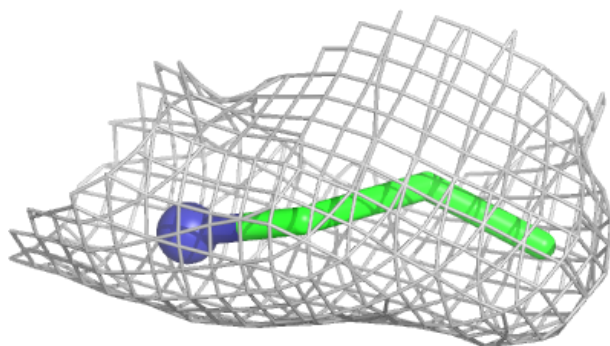
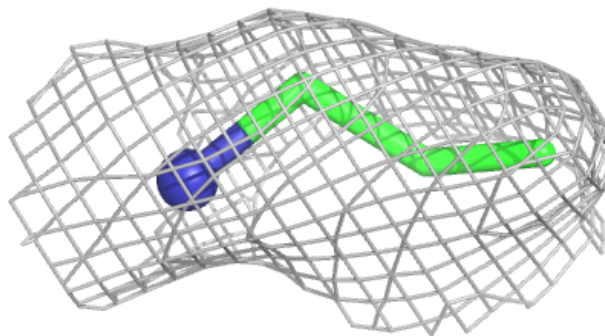
**Electron density around AYE I 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

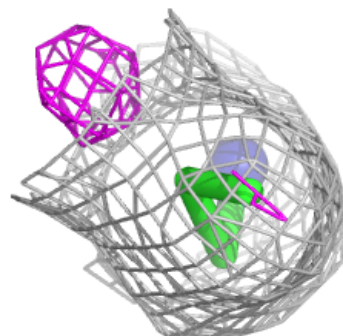
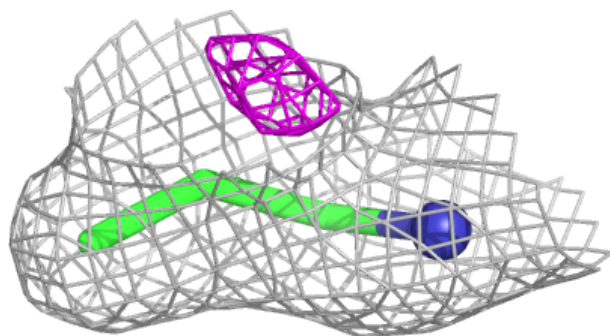
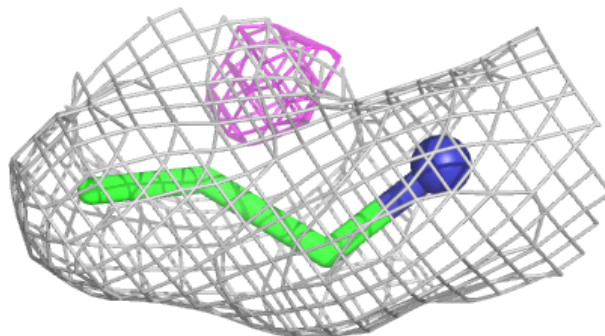


Electron density around AYE O 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

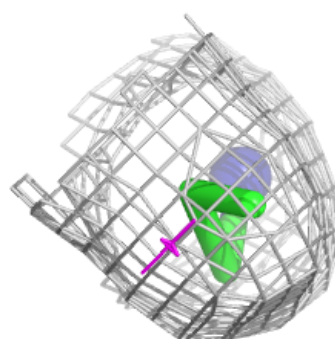
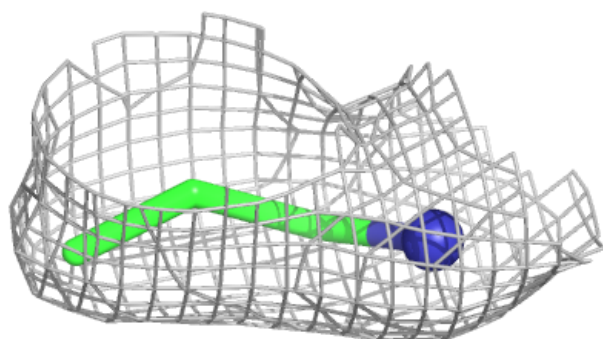
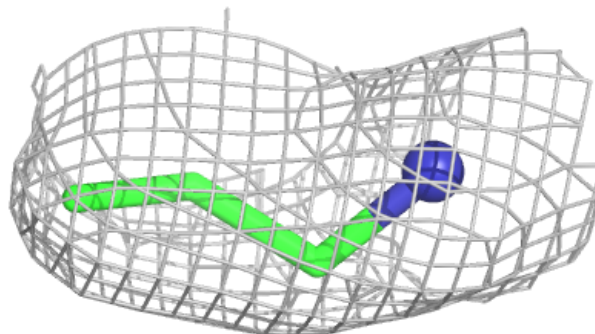
**Electron density around AYE E 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

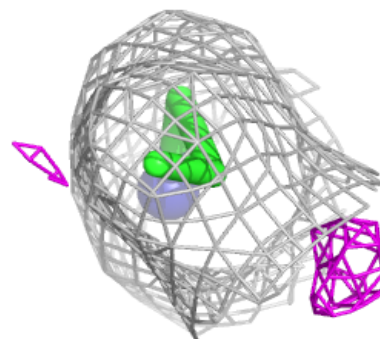
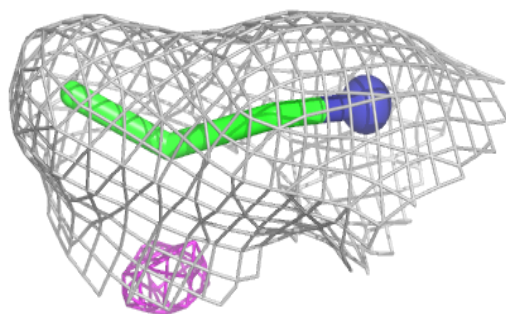
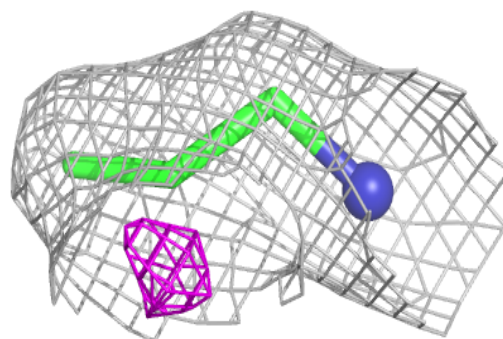


Electron density around AYE S 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

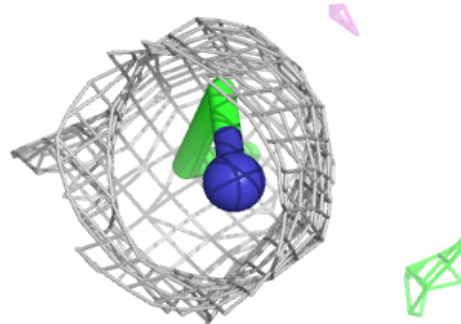
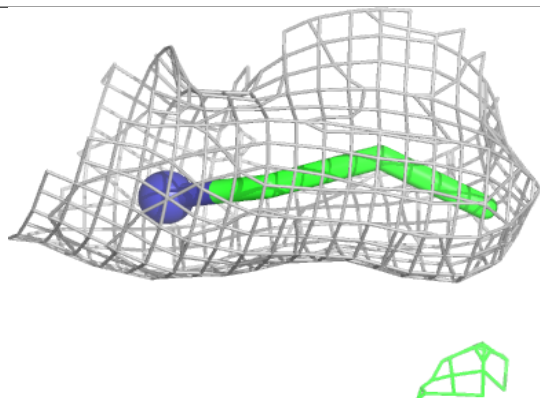
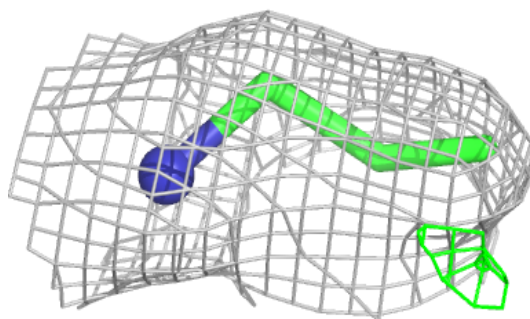
**Electron density around AYE K 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

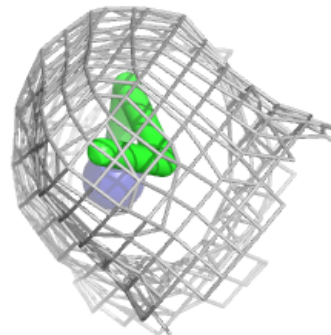
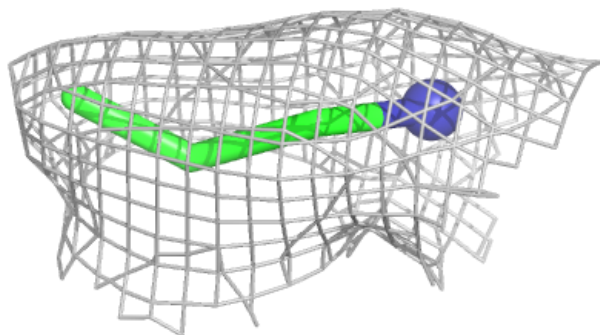
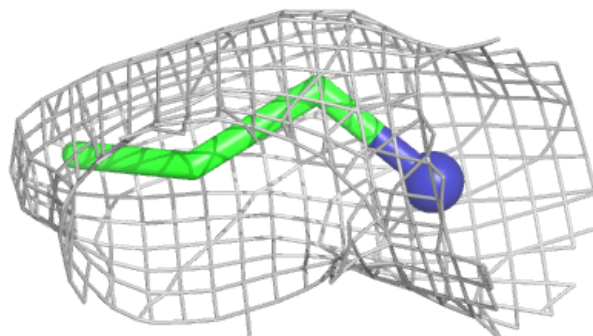


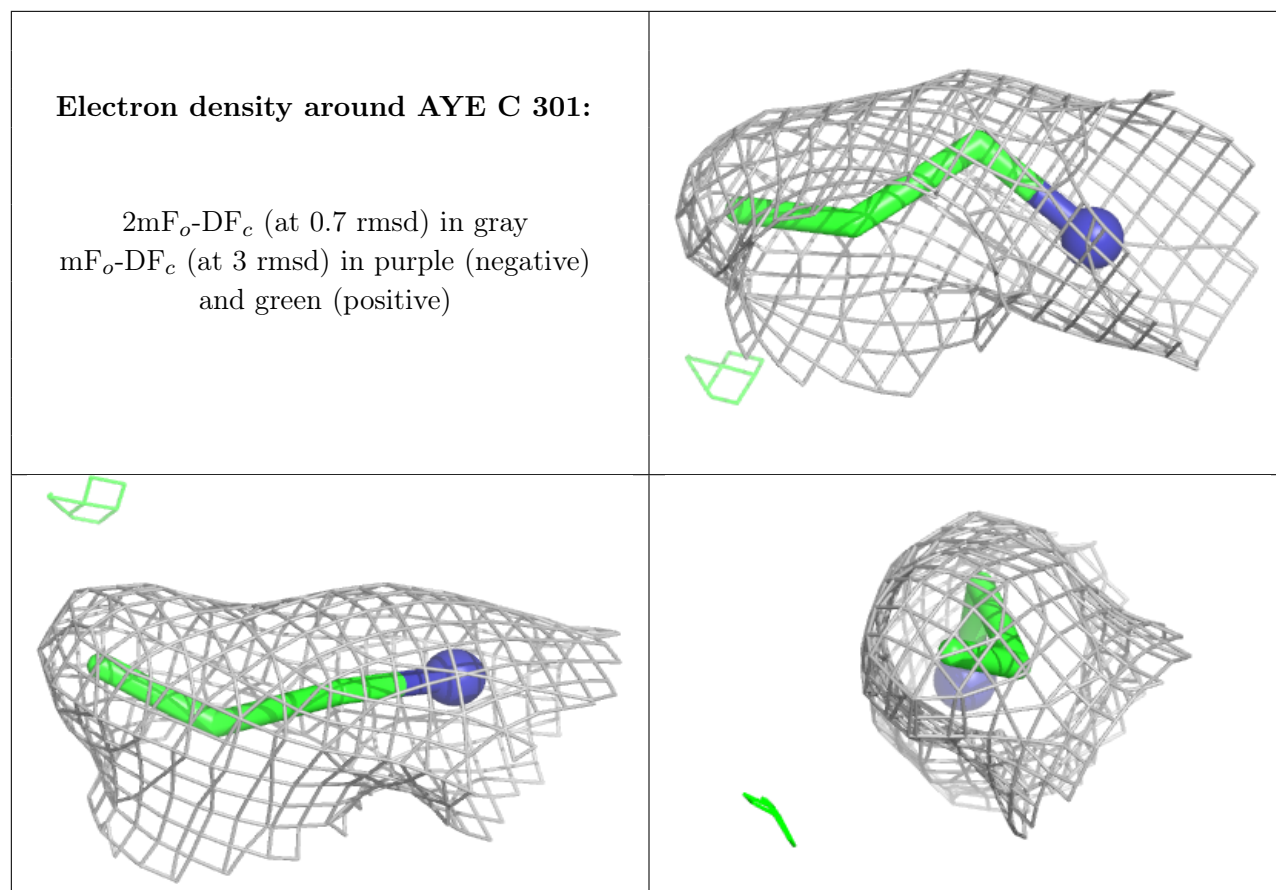
Electron density around AYE G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AYE M 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.