



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:16 pm BST

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 Full wwPDB X-ray Structure Validation 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/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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

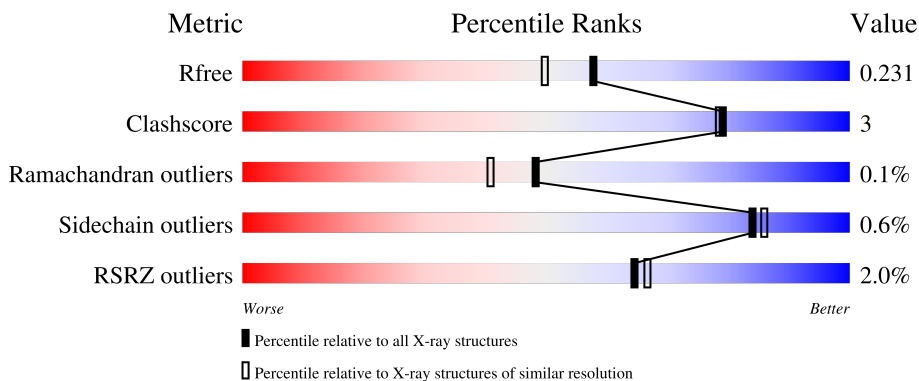
# 1 Overall quality at a glance i

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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      83%      6%      11%</p>
1	C	264	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      83%      5%      12%</p>
1	E	264	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      82%      6%      12%</p>
1	G	264	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      84%      6%      11%</p>
1	I	264	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      85%      •      12%</p>

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Mol	Chain	Length	Quality of chain
1	K	264	<p>3% 79% 9% 11%</p>
1	M	264	<p>86% 11%</p>
1	O	264	<p>81% 8% 11%</p>
1	Q	264	<p>3% 83% 6% 11%</p>
1	S	264	<p>5% 80% 7% 12%</p>
1	U	264	<p>2% 83% 6% 10%</p>
1	W	264	<p>6% 77% 12% 11%</p>
2	B	75	<p>97%</p>
2	D	75	<p>97%</p>
2	F	75	<p>95%</p>
2	H	75	<p>95% 5%</p>
2	J	75	<p>100%</p>
2	L	75	<p>100%</p>
2	N	75	<p>97%</p>
2	P	75	<p>97%</p>
2	R	75	<p>96%</p>
2	T	75	<p>95% 5%</p>
2	V	75	<p>93% 7%</p>
2	X	75	<p>7% 85% 15%</p>

## 2 Entry composition [i](#)

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

- Molecule 2 is a protein called Polyubiquitin-B.

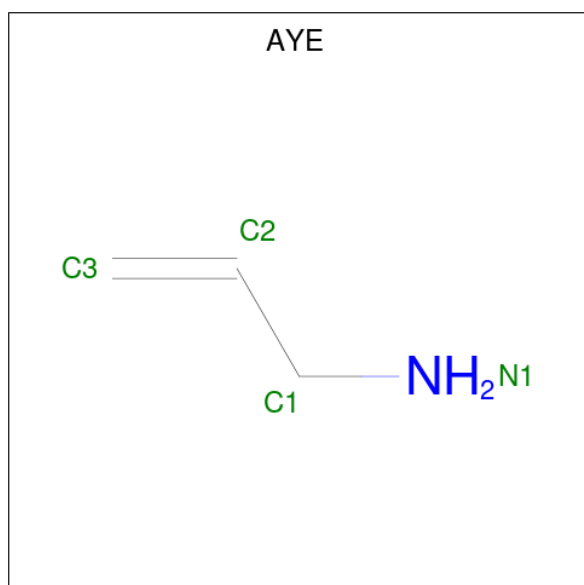
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	75	Total 597	C 376	N 104	O 116	S 1	0	0	0
2	D	75	Total 597	C 376	N 104	O 116	S 1	0	0	0

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

- Molecule 3 is prop-2-en-1-amine (CCD ID: AYE) (formula: C<sub>3</sub>H<sub>7</sub>N) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	N	0	0
			4	3	1		
3	F	1	Total	C	N	0	0
			4	3	1		
3	H	1	Total	C	N	0	0
			4	3	1		
3	J	1	Total	C	N	0	0
			4	3	1		
3	L	1	Total	C	N	0	0
			4	3	1		
3	N	1	Total	C	N	0	0
			4	3	1		
3	P	1	Total	C	N	0	0
			4	3	1		
3	R	1	Total	C	N	0	0
			4	3	1		
3	T	1	Total	C	N	0	0
			4	3	1		
3	V	1	Total	C	N	0	0
			4	3	1		
3	X	1	Total	C	N	0	0
			4	3	1		

- Molecule 4 is water.

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

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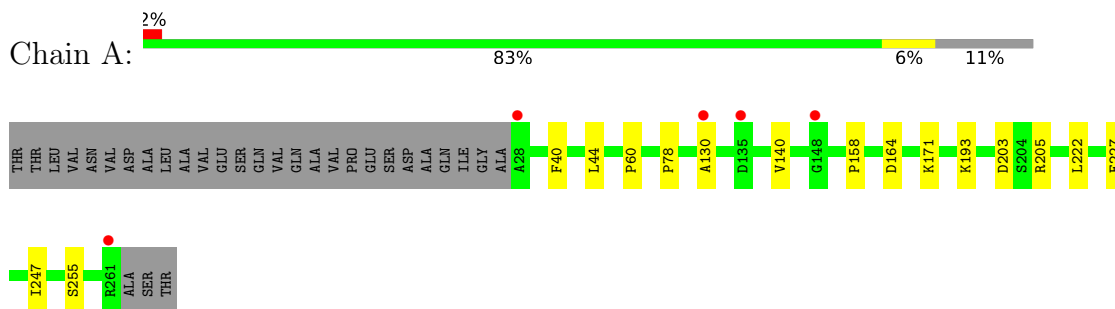
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	54	Total O 54 54	0	0
4	J	14	Total O 14 14	0	0
4	K	41	Total O 41 41	0	0
4	L	20	Total O 20 20	0	0
4	M	48	Total O 48 48	0	0
4	N	12	Total O 12 12	0	0
4	O	32	Total O 32 32	0	0
4	P	12	Total O 12 12	0	0
4	Q	12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

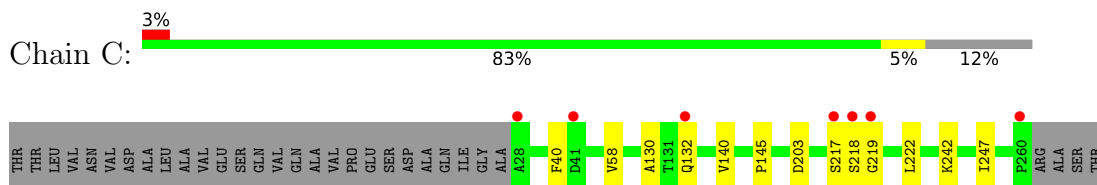
### 3 Residue-property plots [i](#)

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.

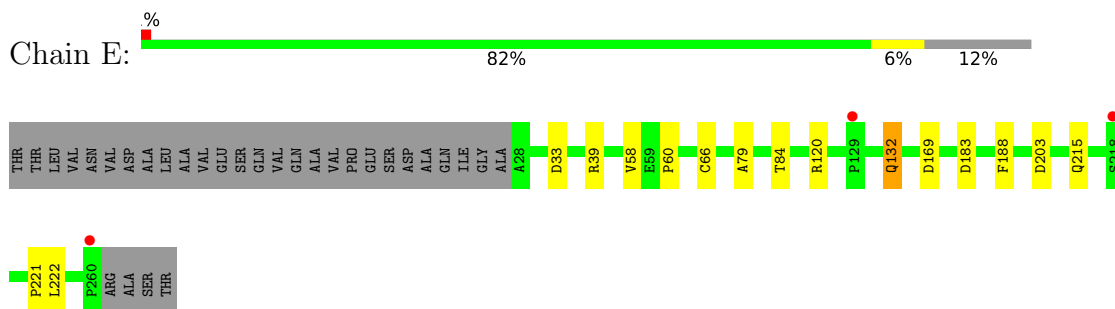
- Molecule 1: PaJOS



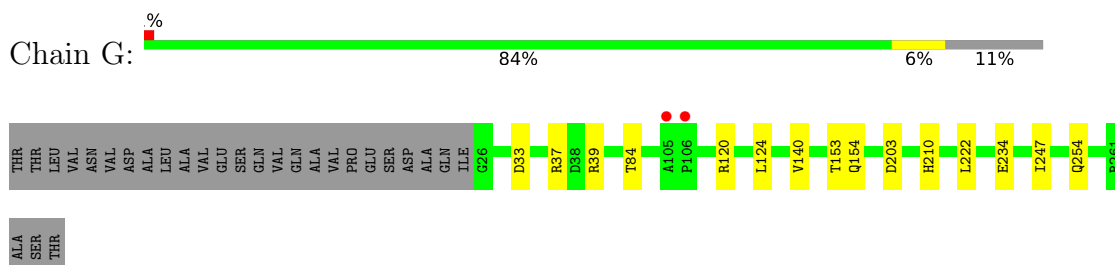
- Molecule 1: PaJOS



- Molecule 1: PaJOS

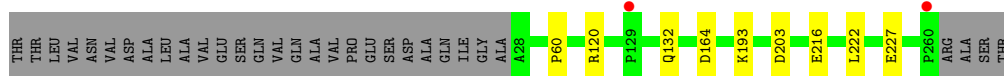
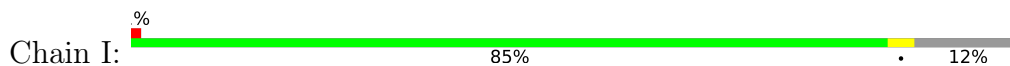


- Molecule 1: PaJOS

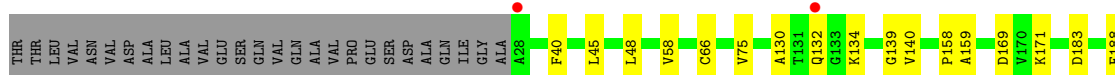
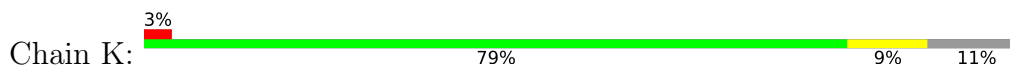




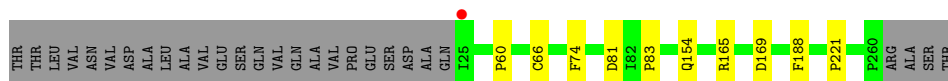
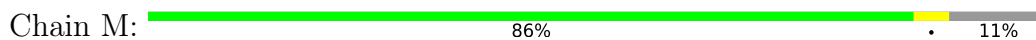
- Molecule 1: PaJOS



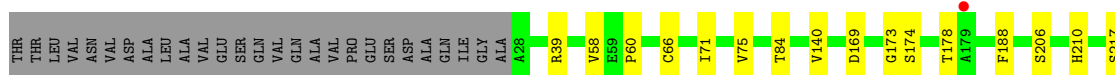
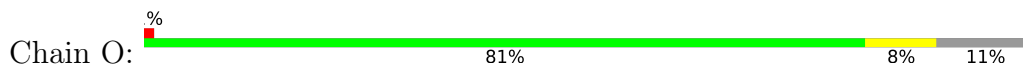
- Molecule 1: PaJOS



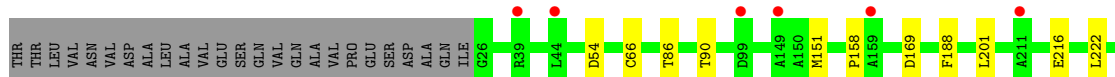
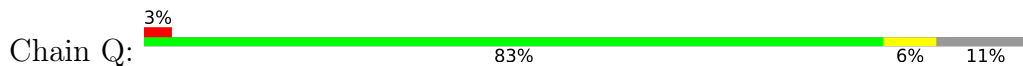
- Molecule 1: PaJOS



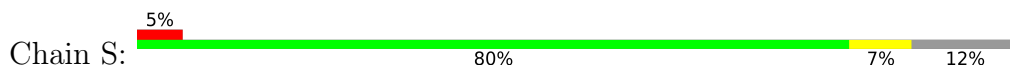
- Molecule 1: PaJOS

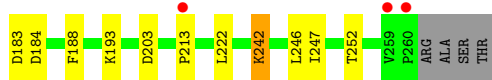


- Molecule 1: PaJOS

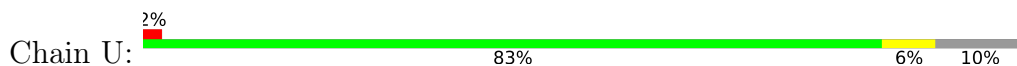


- Molecule 1: PaJOS

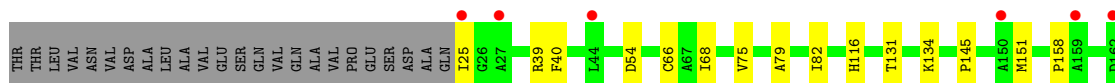
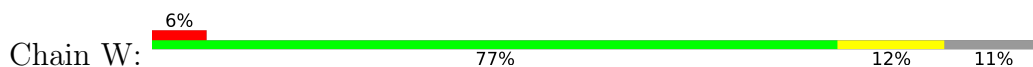




● Molecule 1: PaJOS



● Molecule 1: PaJOS



● Molecule 2: Polyubiquitin-B



● Molecule 2: Polyubiquitin-B

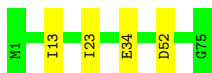


● Molecule 2: Polyubiquitin-B



● 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%

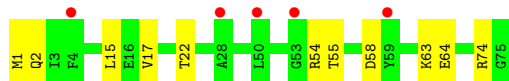
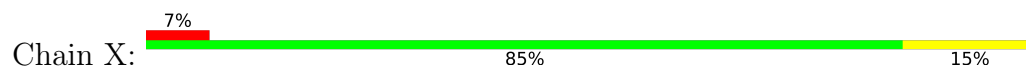


- Molecule 2: Polyubiquitin-B

Chain V:  93% 7%



- Molecule 2: Polyubiquitin-B



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (dev_5407: ???)	Depositor
R, $R_{free}$	0.204 , 0.231 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	270105 reflections (0.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	28965	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.41	0/1814	0.62	0/2484
1	C	0.43	0/1826	0.62	0/2502
1	E	0.42	0/1799	0.63	0/2464
1	G	0.40	0/1817	0.64	0/2488
1	I	0.43	0/1825	0.63	0/2500
1	K	0.42	0/1799	0.64	0/2464
1	M	0.44	0/1805	0.64	0/2473
1	O	0.41	0/1813	0.62	0/2483
1	Q	0.38	0/1819	0.61	0/2490
1	S	0.38	0/1793	0.61	0/2454
1	U	0.36	0/1838	0.62	0/2515
1	W	0.37	0/1816	0.60	0/2487
2	B	0.40	0/603	0.63	0/811
2	D	0.42	0/603	0.65	0/811
2	F	0.44	0/603	0.65	0/811
2	H	0.38	0/603	0.68	0/811
2	J	0.41	0/603	0.65	0/811
2	L	0.44	0/603	0.62	0/811
2	N	0.39	0/603	0.66	0/811
2	P	0.39	0/611	0.66	0/822
2	R	0.36	0/603	0.63	0/811
2	T	0.38	0/603	0.67	0/811
2	V	0.38	0/603	0.63	0/811
2	X	0.34	0/603	0.63	0/811
All	All	0.40	0/29008	0.63	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 [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	1762	0	1701	9	0
1	C	1765	0	1709	7	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	7	0
1	O	1764	0	1703	14	0
1	Q	1770	0	1711	9	0
1	S	1742	0	1684	11	0
1	U	1786	0	1735	8	0
1	W	1767	0	1709	22	0
2	B	597	0	626	1	0
2	D	597	0	626	1	0
2	F	597	0	626	3	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	B	4	0	4	0	0
3	D	4	0	4	0	0
3	F	4	0	4	1	0
3	H	4	0	4	0	0
3	J	4	0	4	0	0
3	L	4	0	4	1	0
3	N	4	0	4	1	0
3	P	4	0	4	1	0
3	R	4	0	4	1	0
3	T	4	0	4	1	0
3	V	4	0	4	1	0
3	X	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	144	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.

All (144) 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:301: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:301:HOH:O	2.07	0.72
2:T:11:LYS:NZ	4:T:201:HOH:O	2.23	0.70
1:O:140:VAL:HG22	1:O:247:ILE:HG12	1.73	0.70
1:W:205[B]:ARG:NH2	1:W:207:SER:O	2.25	0.69
2:T:39:ASP:O	2:T:72:ARG:NE	2.19	0.67
1:E:132:GLN:OE1	1:E:132:GLN:N	2.31	0.64
2:X:54:ARG:HH21	2:X:58:ASP:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:HB3	1:A:222:LEU:HB2	1.79	0.63
1:K:159:ALA:HB2	1:K:261:ARG:HH22	1.64	0.62
1:C:140:VAL:HG22	1:C:247:ILE:HG12	1.80	0.62
2:V:63:LYS:HG3	2:V:64:GLU:HG2	1.82	0.62
1:O:174:SER:O	1:O:178:THR:HG23	2.00	0.61
1:Q:151:MET:HE3	1:Q:240:HIS:HA	1.84	0.60
1:K:40:PHE:HE1	1:K:75:VAL:HG11	1.66	0.60
2:D:32:ASP:OD2	4:D:201:HOH:O	2.17	0.58
1:I:203:ASP:HB3	1:I:222:LEU:HB2	1.84	0.58
1:G:140:VAL:HG22	1:G:247:ILE:HG12	1.83	0.58
1:K:132:GLN:N	1:K:132:GLN:OE1	2.36	0.58
1:E:60:PRO:HD3	1:O:60:PRO:HD3	1.86	0.57
1:G:153:THR:OG1	1:G:154:GLN:OE1	2.08	0.57
1:I:132:GLN:OE1	1:I:132:GLN:N	2.29	0.57
1:K:48:LEU:HG	1:K:134:LYS:HE3	1.86	0.57
1:E:33:ASP:OD2	1:E:120[B]:ARG:NH2	2.38	0.56
1:W:131:THR:HA	1:W:134:LYS:HD2	1.88	0.56
1:W:177:ARG:NH2	1:W:183:ASP:O	2.27	0.56
1:W:187:HIS:CE1	1:W:205[B]:ARG:HD3	2.42	0.55
2:X:63:LYS:HG3	2:X:64:GLU:HG3	1.89	0.55
2:V:13:ILE:HD13	2:V:34:GLU:HG3	1.89	0.55
1:U:151:MET:HE3	1:U:240:HIS:HA	1.89	0.54
1:E:58:VAL:O	1:O:60:PRO:HG2	2.06	0.54
1:K:234:GLU:O	1:K:238:THR:HB	2.07	0.54
1:W:54:ASP:N	1:W:54:ASP:OD1	2.40	0.53
1:Q:158:PRO:HA	1:Q:261:ARG:HH22	1.74	0.53
1:S:140:VAL:HG22	1:S:247:ILE:HG12	1.91	0.53
1:A:60:PRO:HG2	1:C:58:VAL:O	2.09	0.52
1:S:171:LYS:NZ	1:W:183:ASP:OD1	2.22	0.52
1:Q:234:GLU:O	1:Q:238:THR:OG1	2.27	0.52
2:R:63:LYS:HG3	2:R:64:GLU:HG3	1.92	0.52
1:Q:228:PRO:O	1:Q:232:LEU:HD23	2.09	0.51
1:K:140:VAL:HG22	1:K:247:ILE:HG12	1.92	0.51
1:U:86:THR:O	1:U:90:THR:HG23	2.10	0.51
1:K:40:PHE:CE2	1:K:130:ALA:HB3	2.46	0.51
2:X:1:MET:HA	2:X:63:LYS:HZ2	1.75	0.51
1:A:140:VAL:HG22	1:A:247:ILE:HG12	1.93	0.50
1:S:164:ASP:HB2	1:S:193:LYS:HB2	1.94	0.50
1:W:169:ASP:HB2	1:W:188:PHE:CE1	2.47	0.50
1:O:206:SER:OG	1:O:217:SER:HB3	2.12	0.49
2:X:1:MET:N	2:X:17:VAL:O	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1:MET:HA	2:R:63:LYS:HZ3	1.76	0.49
1:W:205[B]:ARG:CZ	1:W:205[B]:ARG:HB2	2.40	0.49
1:W:116:HIS:HD2	4:X:205:HOH:O	1.96	0.49
1:W:151:MET:HE2	1:W:240:HIS:HB3	1.95	0.49
1:C:132:GLN:N	1:C:132:GLN:OE1	2.46	0.49
2:F:49:GLN:NE2	4:F:201:HOH:O	2.26	0.49
1:W:40:PHE:HE1	1:W:75:VAL:HG11	1.78	0.49
1:C:40:PHE:CE2	1:C:130:ALA:HB3	2.48	0.48
1:E:203:ASP:HB3	1:E:222:LEU:HB3	1.94	0.48
1:G:37:ARG:NH1	1:G:124:LEU:O	2.45	0.48
1:W:205[B]:ARG:HB3	1:W:217:SER:HB3	1.95	0.48
1:U:71:ILE:O	1:U:75:VAL:HG22	2.14	0.48
1:S:177:ARG:NH2	1:S:183:ASP:O	2.36	0.48
1:W:158:PRO:HG3	1:W:255:SER:HB3	1.94	0.48
1:E:39:ARG:HG2	1:E:84:THR:HG21	1.96	0.47
1:O:66:CYS:HB3	3:P:101:AYE:H3A	1.69	0.47
1:S:166:LEU:HD22	1:S:246:LEU:HD11	1.97	0.47
1:W:203:ASP:HB3	1:W:222:LEU:HB3	1.96	0.47
1:A:158:PRO:HG3	1:A:255:SER:HB3	1.95	0.47
1:G:203:ASP:HB3	1:G:222:LEU:HB3	1.95	0.47
2:F:39:ASP:OD1	2:F:39:ASP:N	2.47	0.47
1:G:33:ASP:OD2	1:G:120:ARG:NH2	2.48	0.47
1:K:139:GLY:HA3	1:K:251:ILE:O	2.15	0.47
2:R:1:MET:HB2	2:R:63:LYS:HD3	1.97	0.47
1:I:216:GLU:HG3	1:M:154:GLN:OE1	2.15	0.46
1:O:71:ILE:O	1:O:75:VAL:HG22	2.16	0.46
1:K:66:CYS:HB3	3:L:101:AYE:H3A	1.78	0.46
1:W:168:PHE:CE1	1:W:246:LEU:HD13	2.50	0.46
2:X:1:MET:HB2	2:X:63:LYS:HD3	1.97	0.46
1:I:60:PRO:HG3	1:K:58:VAL:O	2.16	0.46
1:S:203:ASP:HB3	1:S:222:LEU:HB3	1.98	0.46
2:X:2:GLN:HA	2:X:15:LEU:O	2.17	0.45
1:E:39:ARG:NH1	1:E:79:ALA:O	2.49	0.45
1:M:81:ASP:CG	1:M:83:PRO:HD2	2.36	0.45
1:Q:86:THR:O	1:Q:90:THR:HG23	2.17	0.45
1:S:169:ASP:HB2	1:S:188:PHE:CE1	2.51	0.44
1:Q:169:ASP:HB2	1:Q:188:PHE:CE1	2.53	0.44
1:W:145:PRO:HD3	1:W:242:LYS:O	2.17	0.44
1:U:164:ASP:HB2	1:U:193:LYS:HB2	2.00	0.44
1:W:66:CYS:HB3	3:X:101:AYE:H3A	1.79	0.44
1:M:66:CYS:HB3	3:N:101:AYE:H3A	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:THR:HA	2:B:55:THR:HA	2.01	0.43
1:K:169:ASP:HB2	1:K:188:PHE:CE1	2.53	0.43
1:S:184:ASP:OD2	1:S:242:LYS:HE2	2.18	0.43
1:C:217:SER:O	1:C:219:GLY:N	2.47	0.43
1:W:164:ASP:HB2	1:W:193:LYS:HB2	2.01	0.43
1:K:158:PRO:HG3	1:K:255:SER:HB3	1.99	0.43
1:Q:66:CYS:HB3	3:R:101:AYE:H3A	1.72	0.43
1:Q:216:GLU:OE1	1:Q:216:GLU:N	2.42	0.43
1:E:66:CYS:HB3	3:F:101:AYE:H3A	1.80	0.43
1:I:164:ASP:HB2	1:I:193:LYS:HB2	2.01	0.43
2:N:22:THR:HA	2:N:55:THR:HA	2.01	0.43
1:O:210:HIS:HD2	1:O:235:ILE:HG12	1.84	0.43
1:U:145:PRO:HD3	1:U:242:LYS:O	2.19	0.43
1:O:239:ALA:HA	4:O:304:HOH:O	2.18	0.43
1:E:169:ASP:HB2	1:E:188:PHE:CE1	2.54	0.42
1:O:169:ASP:HB2	1:O:188:PHE:CE1	2.54	0.42
1:O:173:GLY:O	1:O:239:ALA:HB1	2.19	0.42
1:K:45:LEU:HD22	1:K:75:VAL:HG12	2.02	0.42
1:U:66:CYS:HB3	3:V:101:AYE:H3A	1.80	0.42
1:K:203:ASP:HB3	1:K:222:LEU:HB3	2.01	0.42
1:U:139:GLY:HA3	1:U:251:ILE:O	2.19	0.42
1:W:68:ILE:HD13	1:W:82:ILE:HA	2.01	0.42
1:E:60:PRO:HA	1:E:221:PRO:HG3	2.01	0.42
2:F:23:ILE:HB	2:F:52:ASP:HA	2.01	0.42
1:K:159:ALA:HB2	1:K:261:ARG:HH12	1.85	0.42
1:W:39:ARG:NH1	1:W:79:ALA:O	2.52	0.42
1:A:164:ASP:HB2	1:A:193:LYS:HB2	2.02	0.42
2:H:13:ILE:HD13	2:H:34:GLU:HG3	2.01	0.42
1:W:209:VAL:HG13	4:W:304:HOH:O	2.19	0.42
1:A:205:ARG:HD3	4:A:304:HOH:O	2.19	0.41
1:K:171:LYS:HB3	1:K:171:LYS:HE2	1.97	0.41
1:I:120:ARG:HD2	4:I:304:HOH:O	2.21	0.41
1:S:66:CYS:HB3	3:T:101:AYE:H3A	1.86	0.41
2:X:22:THR:HA	2:X:55:THR:HA	2.03	0.41
1:A:40:PHE:CE2	1:A:130:ALA:HB3	2.54	0.41
1:A:44:LEU:O	1:A:78:PRO:HD2	2.21	0.41
1:M:81:ASP:OD2	1:M:83:PRO:HD2	2.20	0.41
1:C:203:ASP:HB3	1:C:222:LEU:HB3	2.03	0.41
1:G:39:ARG:HG2	1:G:84:THR:HG21	2.02	0.41
2:H:23:ILE:HB	2:H:52:ASP:HA	2.02	0.41
1:O:60:PRO:HG3	1:O:221:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:22:THR:HA	2:P:55:THR:HA	2.03	0.41
1:E:60:PRO:HG3	1:O:58:VAL:O	2.20	0.41
1:Q:201:LEU:HD22	1:Q:222:LEU:HD22	2.03	0.41
1:G:210:HIS:HE2	1:G:234:GLU:HG2	1.86	0.41
1:S:141:SER:HB2	1:S:252:THR:O	2.21	0.40
1:M:169:ASP:HB2	1:M:188:PHE:CE1	2.56	0.40
1:M:74:PHE:CZ	1:M:165:ARG:HG3	2.57	0.40
1:O:39:ARG:HG2	1:O:84:THR:HG21	2.04	0.40
1:S:177:ARG:HG2	1:S:213:PRO:HB3	2.04	0.40
1:C:145:PRO:HD3	1:C:242:LYS:O	2.22	0.40
1:M:60:PRO:HA	1:M:221:PRO:HG3	2.03	0.40

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 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	216	GLU
1	C	218	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 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%)	184 (100%)	1 (0%)	86	88
1	C	187/206 (91%)	187 (100%)	0	100	100
1	E	183/206 (89%)	180 (98%)	3 (2%)	58	56
1	G	184/206 (89%)	183 (100%)	1 (0%)	86	88
1	I	187/206 (91%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	183/206 (89%)	182 (100%)	1 (0%)	86	88
1	M	183/206 (89%)	183 (100%)	0	100	100
1	O	184/206 (89%)	183 (100%)	1 (0%)	86	88
1	Q	184/206 (89%)	183 (100%)	1 (0%)	86	88
1	S	183/206 (89%)	181 (99%)	2 (1%)	70	71
1	U	186/206 (90%)	184 (99%)	2 (1%)	70	71
1	W	184/206 (89%)	183 (100%)	1 (0%)	86	88
2	B	68/68 (100%)	68 (100%)	0	100	100
2	D	68/68 (100%)	67 (98%)	1 (2%)	60	59
2	F	68/68 (100%)	67 (98%)	1 (2%)	60	59
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
2	T	68/68 (100%)	68 (100%)	0	100	100
2	V	68/68 (100%)	67 (98%)	1 (2%)	60	59
2	X	68/68 (100%)	67 (98%)	1 (2%)	60	59
All	All	3030/3288 (92%)	3013 (99%)	17 (1%)	84	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
2	D	48	LYS
1	E	132	GLN
1	E	183	ASP
1	E	215	GLN
2	F	39	ASP
1	G	254	GLN
1	K	183	ASP
1	O	261	ARG
1	Q	54	ASP
1	S	54	ASP

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Mol	Chain	Res	Type
1	S	242	LYS
1	U	54	ASP
1	U	225	GLN
2	V	74	ARG
1	W	25	ILE
2	X	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	34	GLN
1	I	34	GLN
1	I	240	HIS
2	J	68	HIS
1	M	34	GLN
1	Q	240	HIS
1	U	225	GLN
1	W	34	GLN
2	X	62	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	H	101	1,2	3,3,3	0.13	0	1,2,2	0.04	0
3	AYE	F	101	1,2	3,3,3	0.16	0	1,2,2	0.12	0
3	AYE	B	101	1,2	3,3,3	0.19	0	1,2,2	0.13	0
3	AYE	D	101	1,2	3,3,3	0.20	0	1,2,2	0.78	0
3	AYE	L	101	1,2	3,3,3	0.23	0	1,2,2	0.48	0
3	AYE	X	101	1,2	3,3,3	0.33	0	1,2,2	0.17	0
3	AYE	P	101	1,2	3,3,3	0.05	0	1,2,2	0.03	0
3	AYE	J	101	1,2	3,3,3	0.18	0	1,2,2	0.38	0
3	AYE	V	101	1,2	3,3,3	0.09	0	1,2,2	0.05	0
3	AYE	T	101	1,2	3,3,3	0.13	0	1,2,2	0.04	0
3	AYE	N	101	1,2	3,3,3	0.25	0	1,2,2	0.13	0
3	AYE	R	101	1,2	3,3,3	0.16	0	1,2,2	0.24	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	H	101	1,2	-	0/1/1/1	-
3	AYE	F	101	1,2	-	0/1/1/1	-
3	AYE	B	101	1,2	-	0/1/1/1	-
3	AYE	D	101	1,2	-	0/1/1/1	-
3	AYE	L	101	1,2	-	0/1/1/1	-
3	AYE	X	101	1,2	-	0/1/1/1	-
3	AYE	P	101	1,2	-	0/1/1/1	-
3	AYE	J	101	1,2	-	0/1/1/1	-
3	AYE	V	101	1,2	-	0/1/1/1	-
3	AYE	T	101	1,2	-	0/1/1/1	-
3	AYE	N	101	1,2	-	0/1/1/1	-
3	AYE	R	101	1,2	-	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.

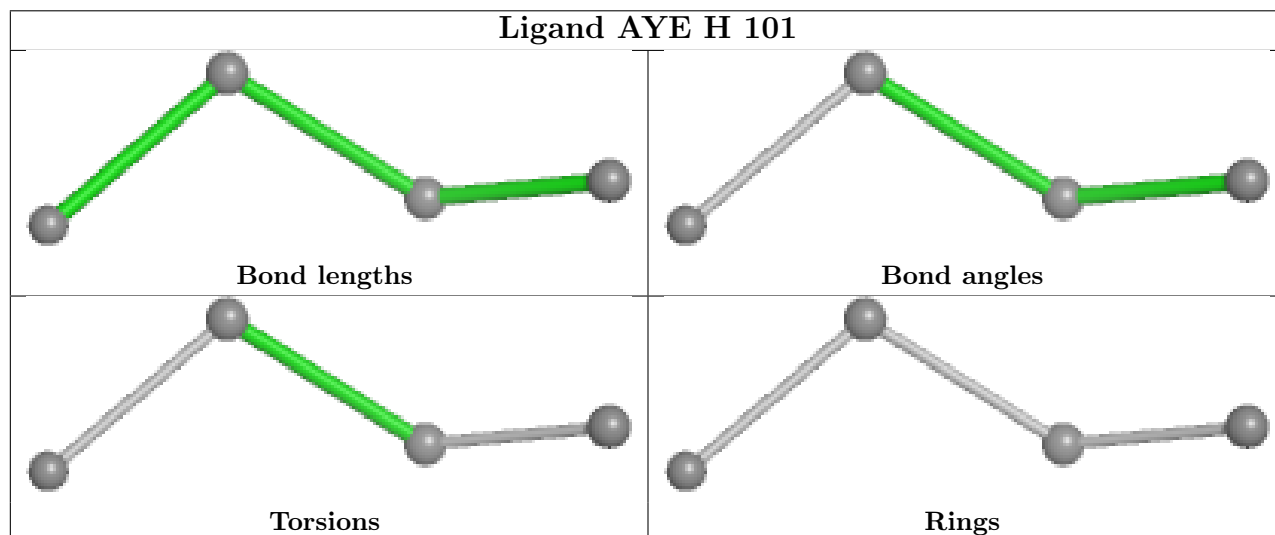


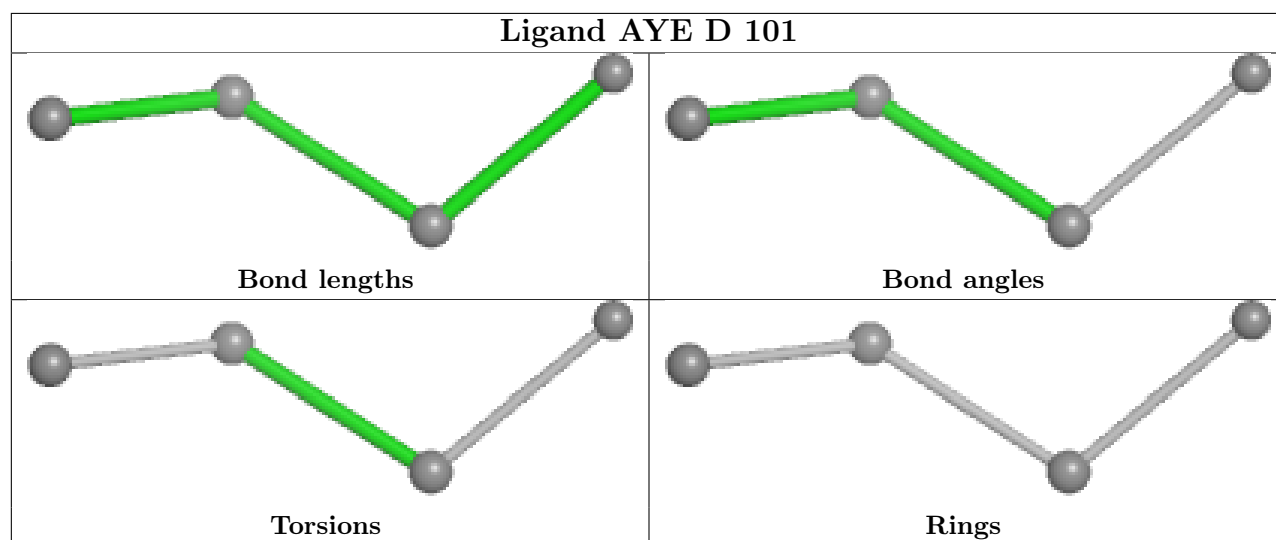
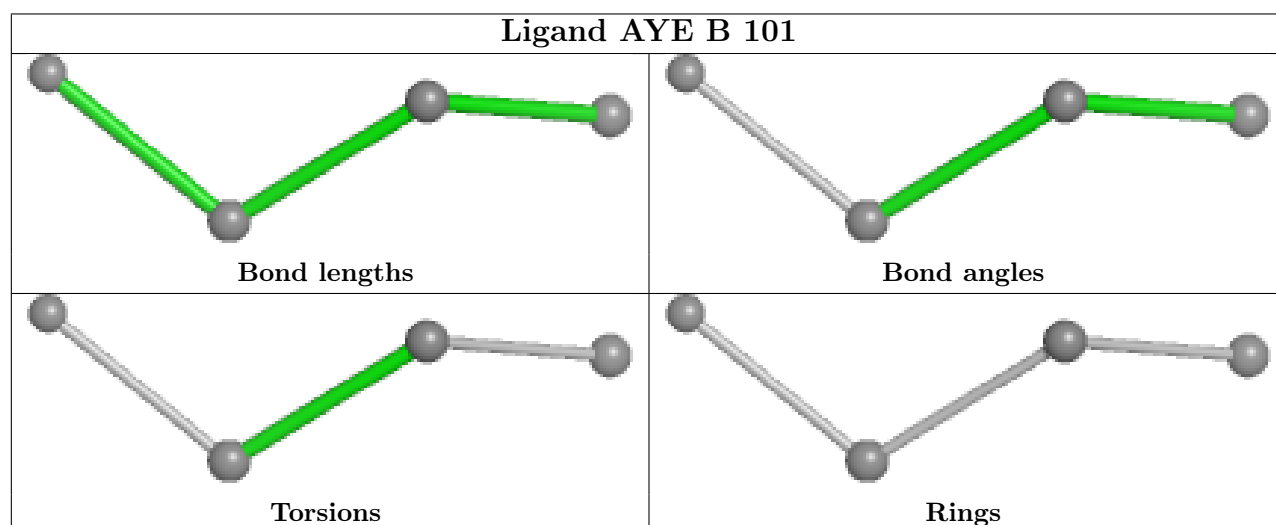
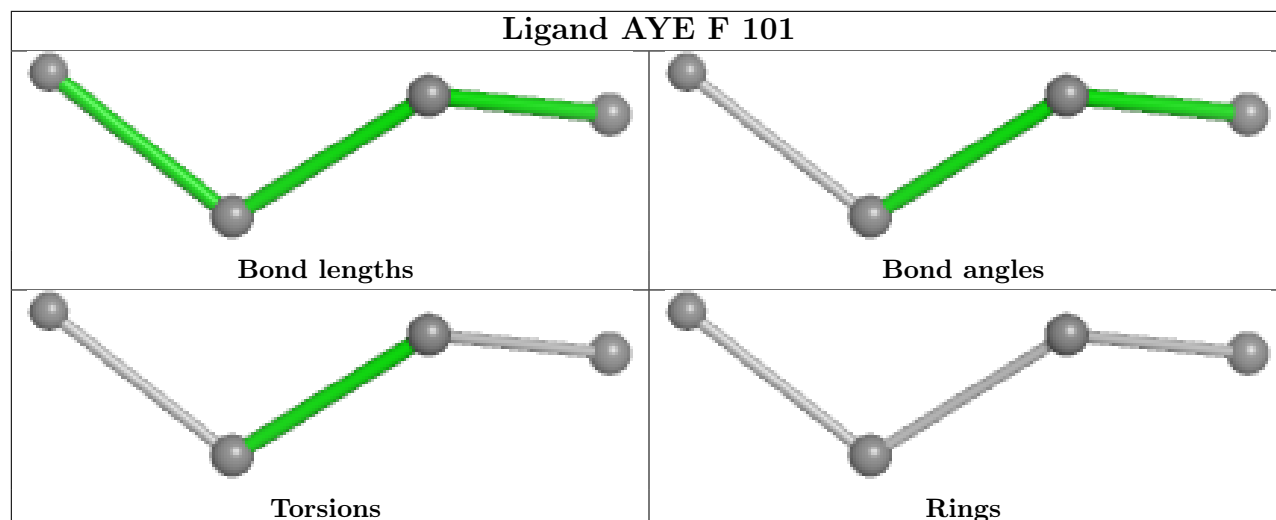
There are no ring outliers.

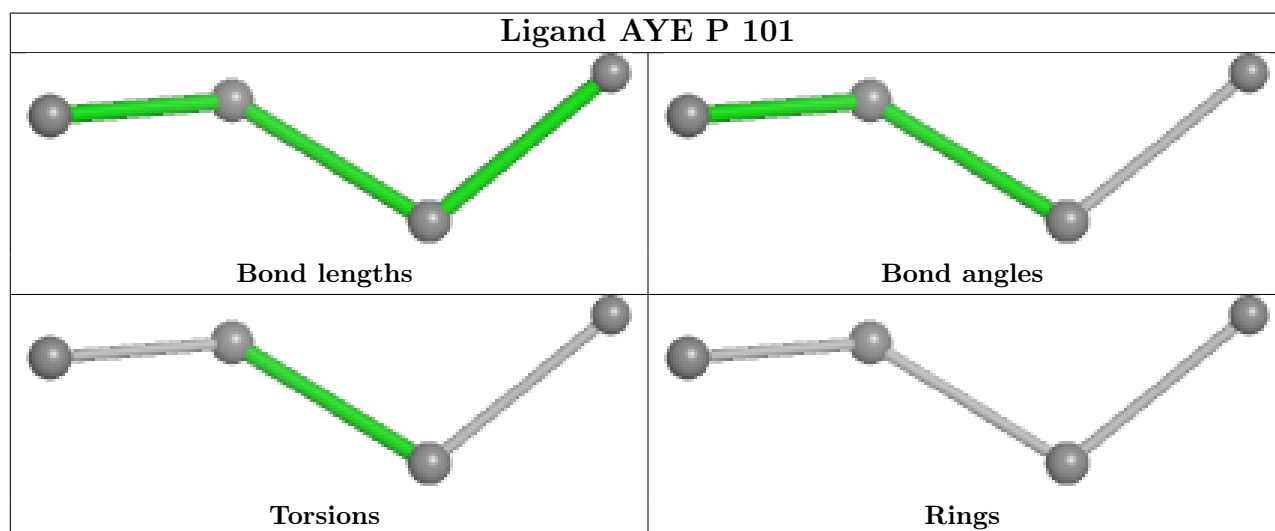
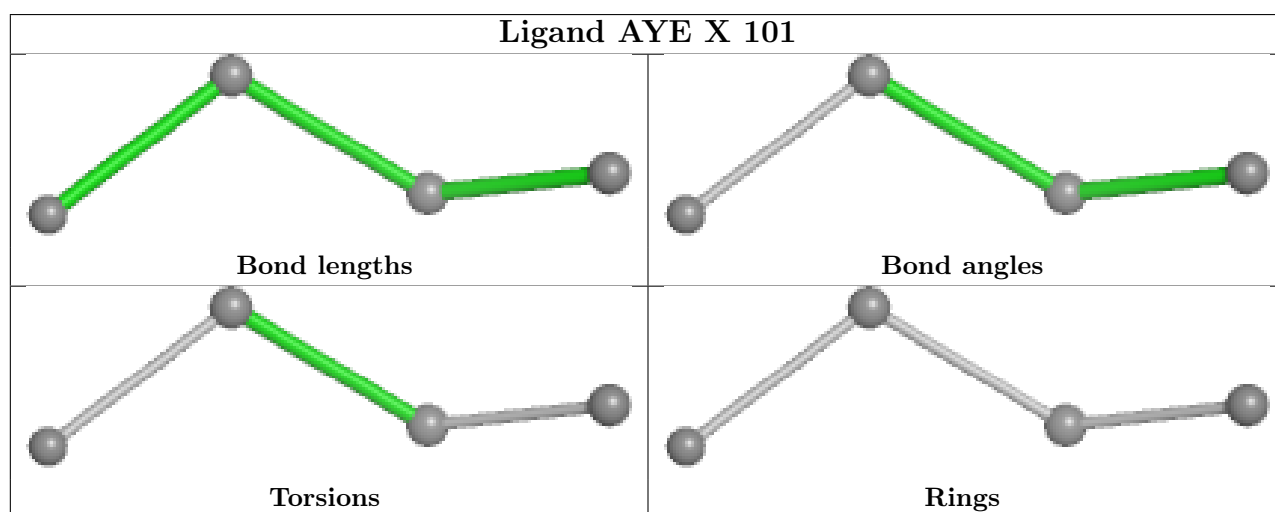
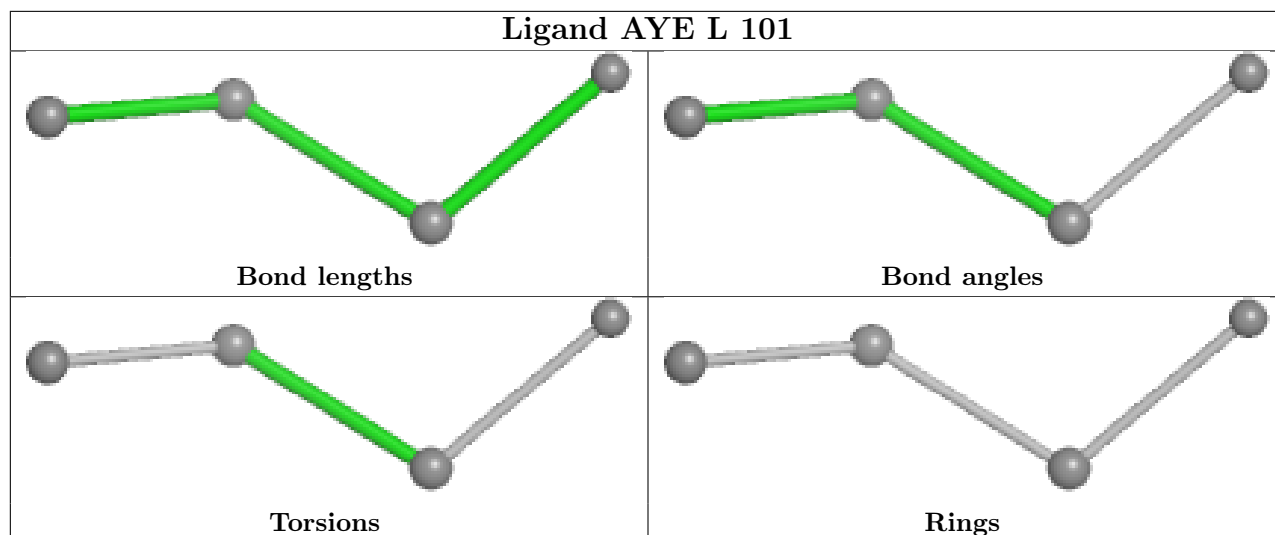
8 monomers are involved in 8 short contacts:

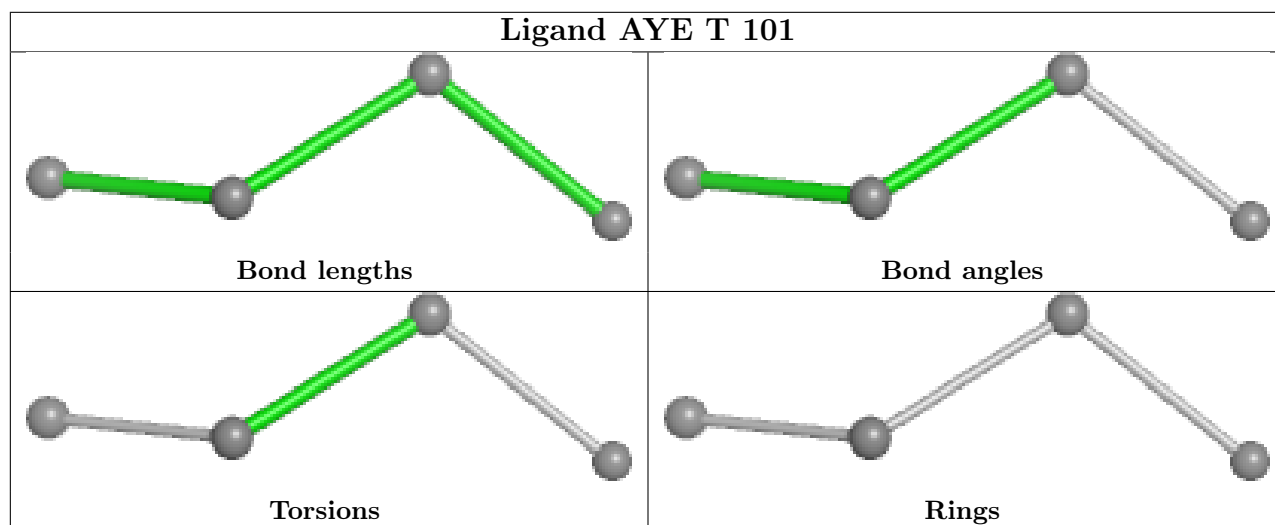
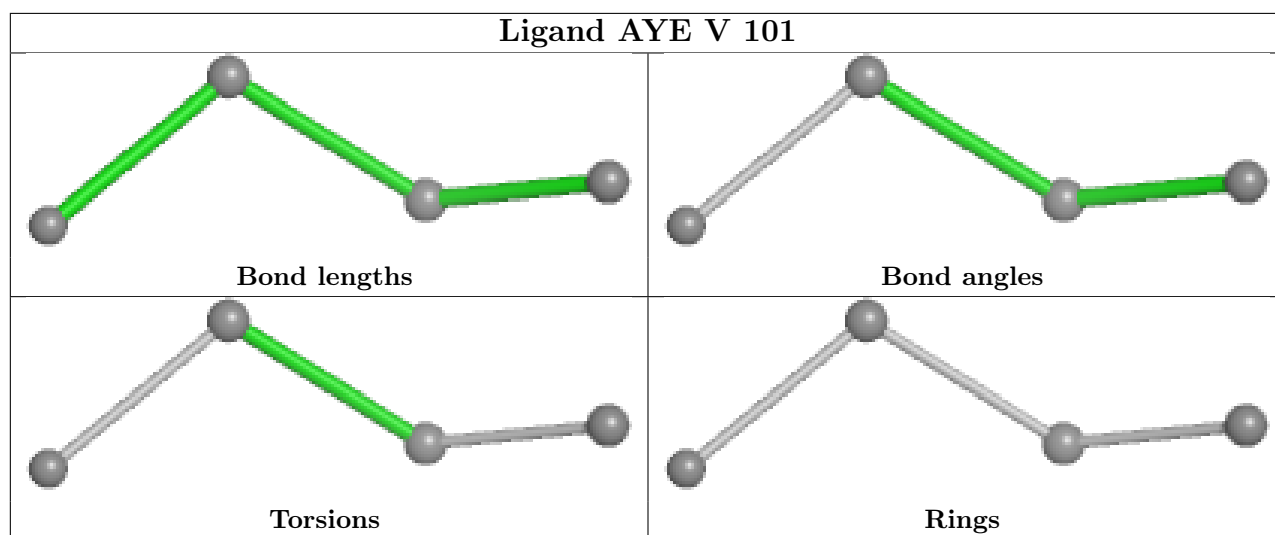
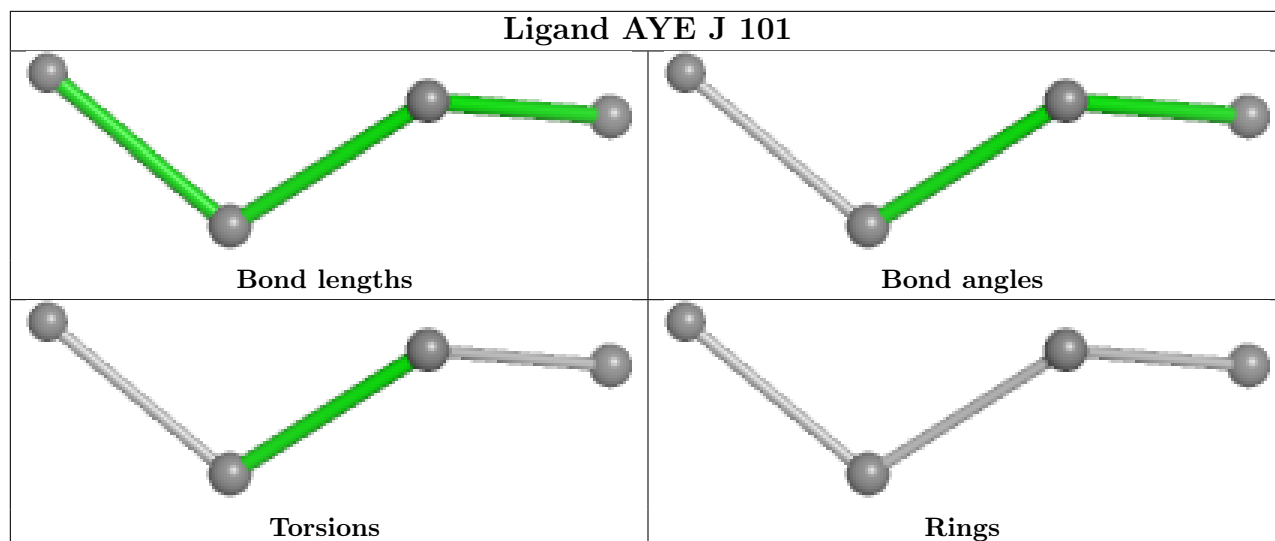
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	101	AYE	1	0
3	L	101	AYE	1	0
3	X	101	AYE	1	0
3	P	101	AYE	1	0
3	V	101	AYE	1	0
3	T	101	AYE	1	0
3	N	101	AYE	1	0
3	R	101	AYE	1	0

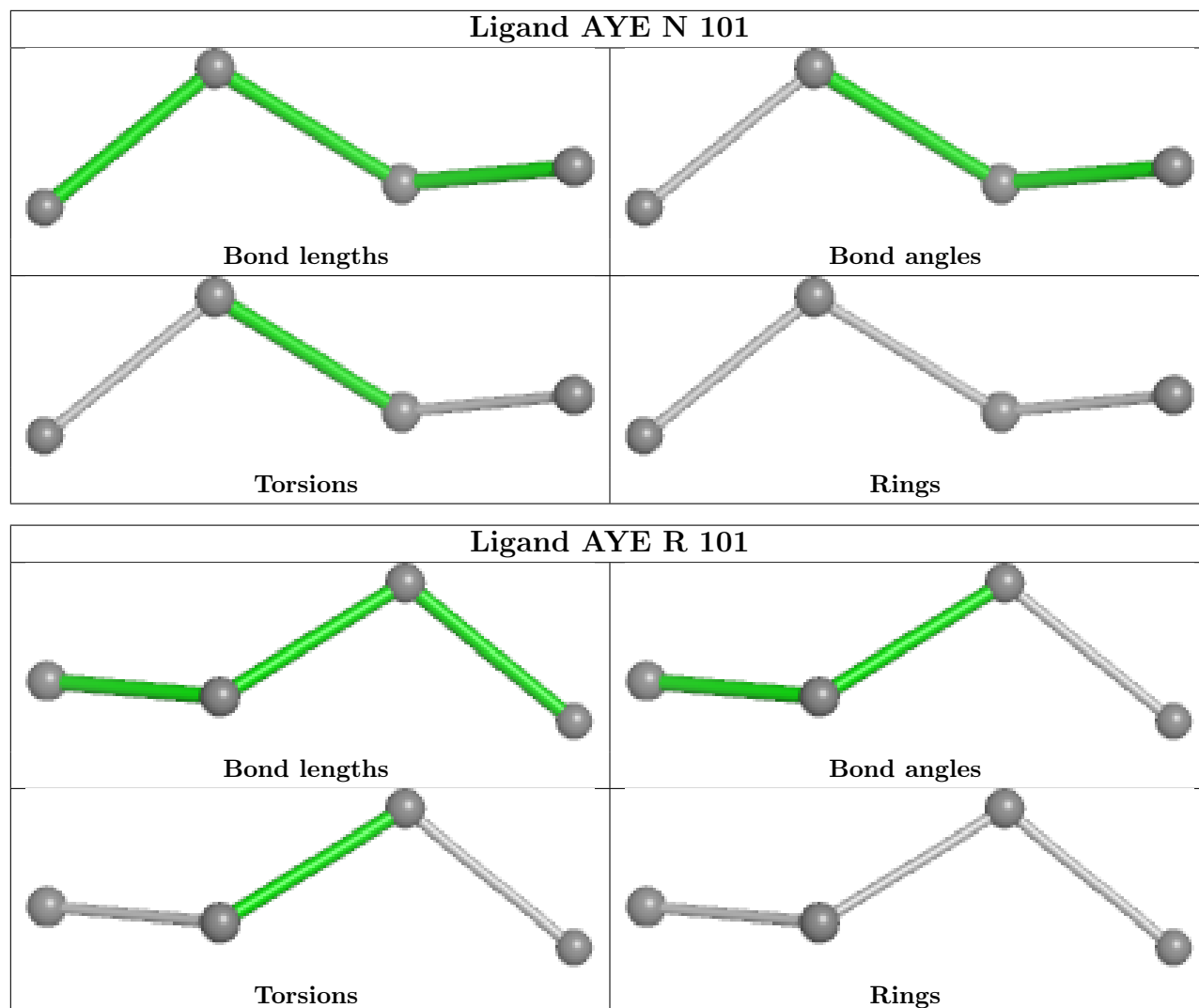
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	234/264 (88%)	-0.08	5 (2%) 63 65	25, 42, 64, 96	2 (0%)
1	C	233/264 (88%)	-0.04	7 (3%) 52 55	22, 41, 71, 122	5 (2%)
1	E	233/264 (88%)	-0.04	3 (1%) 74 76	25, 42, 72, 90	1 (0%)
1	G	236/264 (89%)	-0.11	2 (0%) 82 84	31, 42, 61, 91	1 (0%)
1	I	233/264 (88%)	-0.08	2 (0%) 81 82	25, 40, 61, 85	5 (2%)
1	K	234/264 (88%)	-0.03	7 (2%) 52 55	30, 42, 68, 99	0
1	M	236/264 (89%)	0.02	1 (0%) 89 90	29, 44, 66, 105	0
1	O	235/264 (89%)	0.16	3 (1%) 74 76	30, 47, 81, 107	1 (0%)
1	Q	236/264 (89%)	0.48	8 (3%) 48 50	23, 65, 94, 110	1 (0%)
1	S	231/264 (87%)	0.42	12 (5%) 34 35	22, 55, 101, 131	2 (0%)
1	U	237/264 (89%)	0.43	5 (2%) 63 65	22, 57, 82, 111	1 (0%)
1	W	236/264 (89%)	0.61	15 (6%) 27 28	34, 62, 92, 125	1 (0%)
2	B	75/75 (100%)	-0.02	0 100 100	33, 50, 65, 68	0
2	D	75/75 (100%)	-0.09	0 100 100	33, 47, 62, 72	0
2	F	75/75 (100%)	-0.24	0 100 100	32, 41, 56, 57	0
2	H	75/75 (100%)	0.13	0 100 100	33, 48, 65, 68	0
2	J	75/75 (100%)	0.04	0 100 100	31, 47, 63, 72	0
2	L	75/75 (100%)	-0.12	0 100 100	34, 43, 57, 63	0
2	N	75/75 (100%)	0.02	0 100 100	31, 49, 68, 69	0
2	P	75/75 (100%)	0.02	0 100 100	33, 48, 65, 70	1 (1%)
2	R	75/75 (100%)	0.13	0 100 100	35, 53, 69, 77	0
2	T	75/75 (100%)	0.28	0 100 100	35, 57, 78, 81	0
2	V	75/75 (100%)	0.27	0 100 100	38, 54, 70, 78	0
2	X	75/75 (100%)	0.93	5 (6%) 25 26	42, 78, 101, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3714/4068 (91%)	0.14	75 (2%) 64 67	22, 47, 82, 131	21 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	25	ILE	6.2
1	M	25	ILE	4.2
1	A	148	GLY	3.6
1	I	260	PRO	3.6
1	A	135	ASP	3.6
1	A	261	ARG	3.4
1	W	260	PRO	3.4
1	C	218	SER	3.4
1	E	260	PRO	3.2
1	C	260	PRO	3.2
1	S	179	ALA	3.2
1	W	44	LEU	3.1
1	K	261	ARG	3.0
1	C	219	GLY	3.0
1	S	182	ALA	3.0
2	X	53	GLY	3.0
1	S	259	VAL	3.0
1	S	181	GLY	2.8
1	S	180	ALA	2.7
1	W	27	ALA	2.7
1	W	180	ALA	2.7
1	K	28	ALA	2.7
1	A	130	ALA	2.6
1	O	262	ALA	2.6
1	K	260	PRO	2.5
1	S	152	ILE	2.5
1	A	28	ALA	2.5
1	W	150	ALA	2.5
1	W	259	VAL	2.5
1	C	217	SER	2.4
1	Q	44	LEU	2.4
1	W	159	ALA	2.4
1	G	106	PRO	2.4
1	C	28	ALA	2.3
1	W	162	ASP	2.3
1	S	260	PRO	2.3
1	U	177	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	211	ALA	2.3
1	W	176	ALA	2.3
1	W	219	GLY	2.3
1	C	132	GLN	2.3
1	Q	99	ASP	2.3
1	W	179	ALA	2.2
1	K	218	SER	2.2
1	Q	261	ARG	2.2
1	S	146	ARG	2.2
1	U	150	ALA	2.2
1	U	211	ALA	2.2
2	X	28	ALA	2.2
1	U	25	ILE	2.2
1	W	181	GLY	2.2
1	E	129	PRO	2.2
2	X	59	TYR	2.2
1	E	218	SER	2.1
1	K	132	GLN	2.1
1	W	216	GLU	2.1
1	G	105	ALA	2.1
1	S	44	LEU	2.1
1	W	182	ALA	2.1
1	Q	39	ARG	2.1
1	C	41	ASP	2.1
1	O	179	ALA	2.1
2	X	50	LEU	2.1
1	S	178	THR	2.1
1	S	162	ASP	2.0
1	I	129	PRO	2.0
1	Q	260	PRO	2.0
1	U	176	ALA	2.0
1	K	219	GLY	2.0
1	Q	149	ALA	2.0
1	Q	159	ALA	2.0
1	S	213	PRO	2.0
1	K	217	SER	2.0
1	O	218	SER	2.0
2	X	4	PHE	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

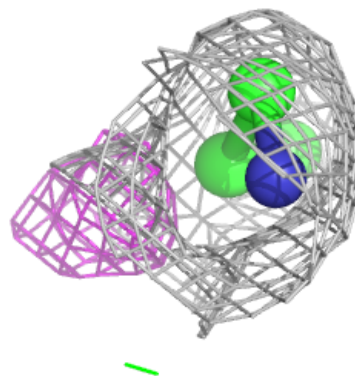
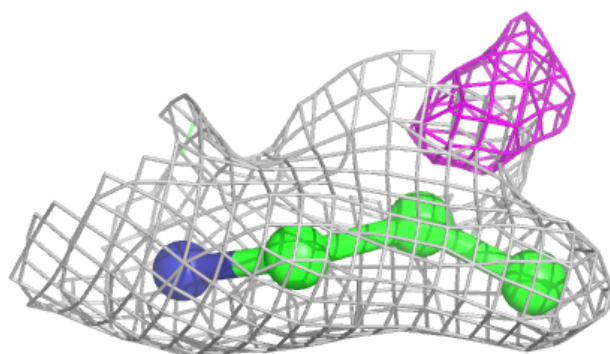
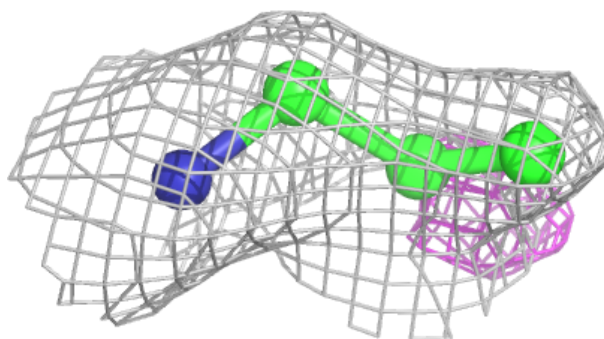
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	AYE	X	101	4/4	0.90	0.13	41,42,43,45	0
3	AYE	V	101	4/4	0.93	0.12	44,45,46,49	0
3	AYE	R	101	4/4	0.94	0.10	44,44,50,51	0
3	AYE	B	101	4/4	0.94	0.08	33,33,34,35	0
3	AYE	J	101	4/4	0.94	0.08	29,30,33,33	0
3	AYE	P	101	4/4	0.95	0.08	37,38,40,40	0
3	AYE	F	101	4/4	0.96	0.06	34,35,35,36	0
3	AYE	T	101	4/4	0.96	0.08	38,39,40,41	0
3	AYE	L	101	4/4	0.97	0.05	31,33,34,34	0
3	AYE	H	101	4/4	0.97	0.06	35,35,36,36	0
3	AYE	N	101	4/4	0.98	0.06	34,36,37,38	0
3	AYE	D	101	4/4	0.98	0.06	33,33,33,34	0

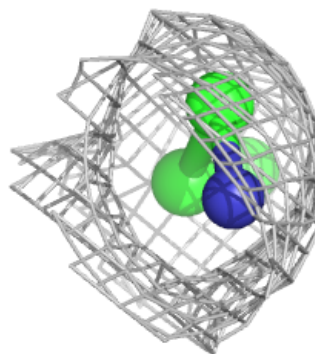
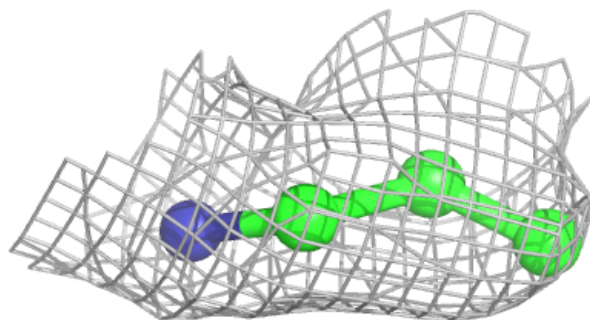
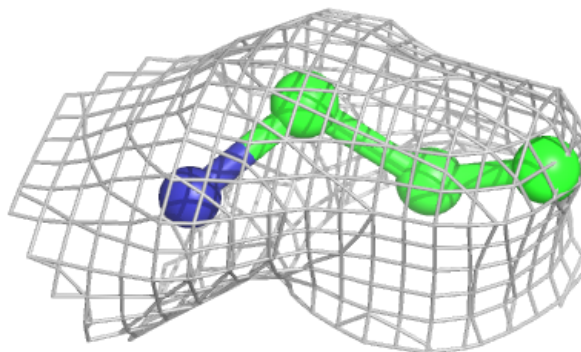
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AYE X 101:**

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

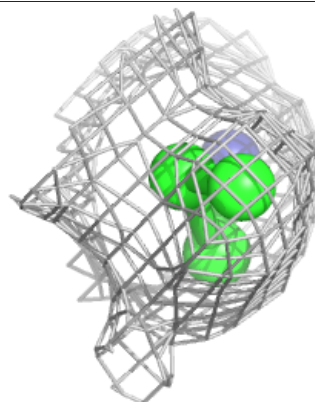
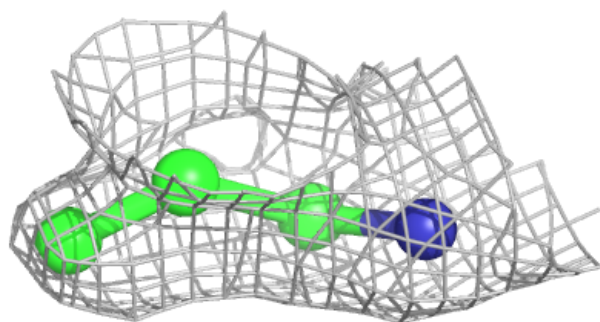
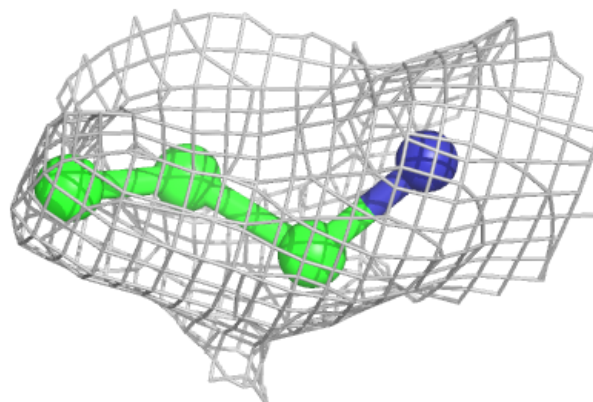
**Electron density around AYE V 101:**

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

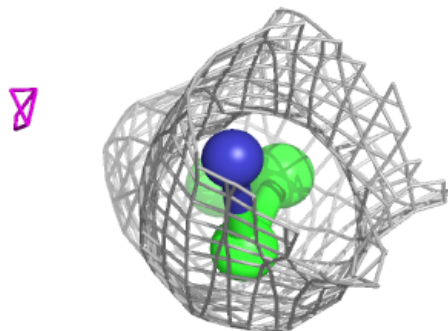
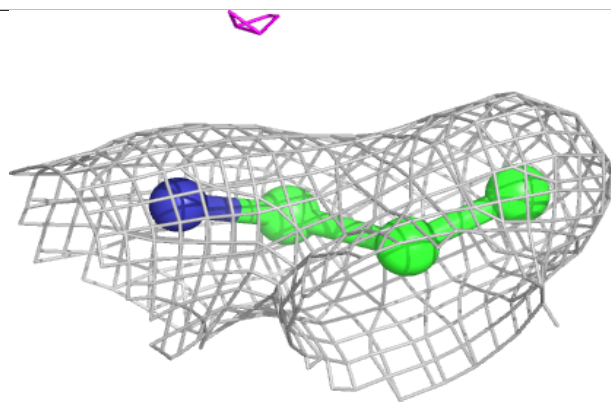
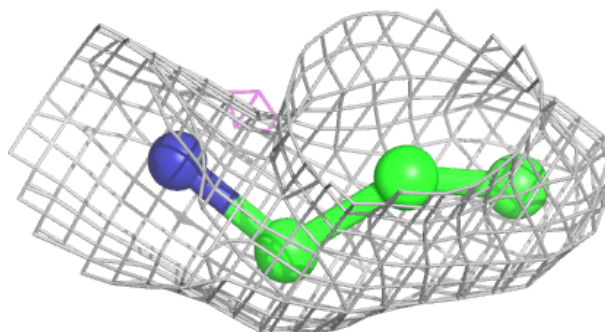


**Electron density around AYE R 101:**

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

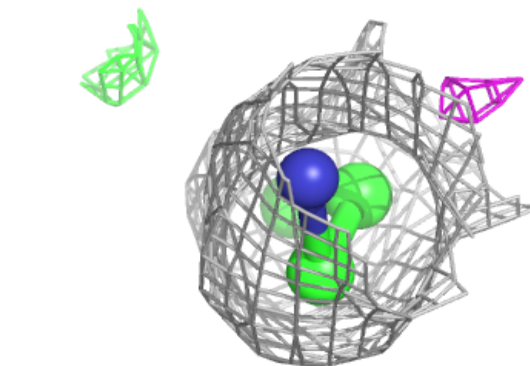
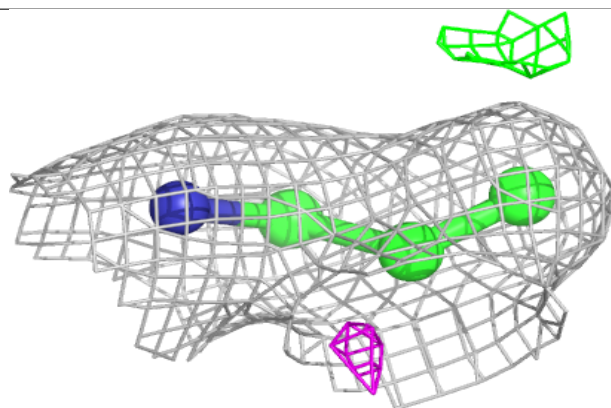
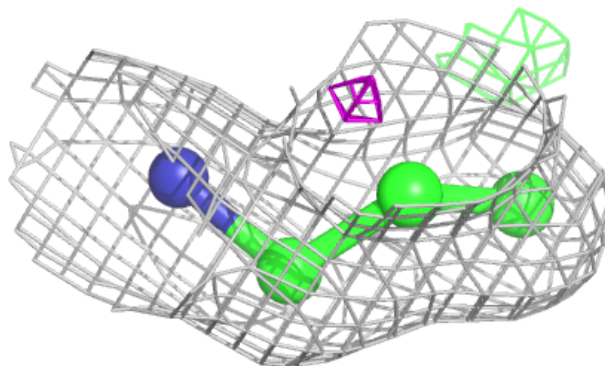
**Electron density around AYE B 101:**

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

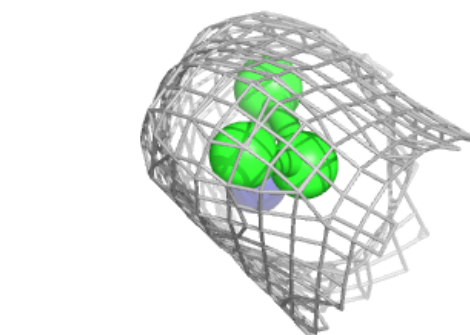
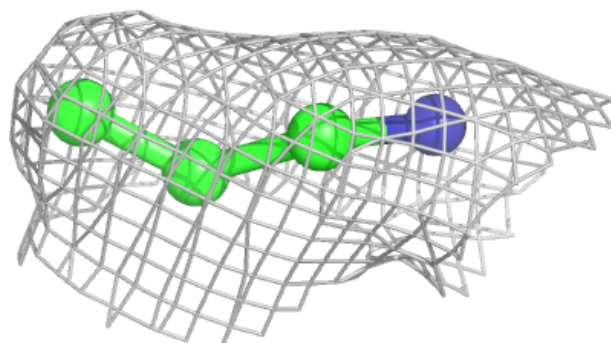
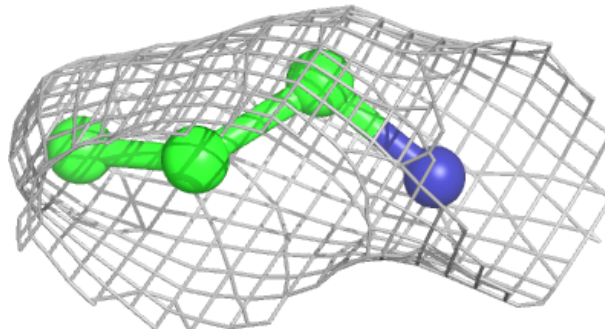


**Electron density around AYE J 101:**

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

**Electron density around AYE P 101:**

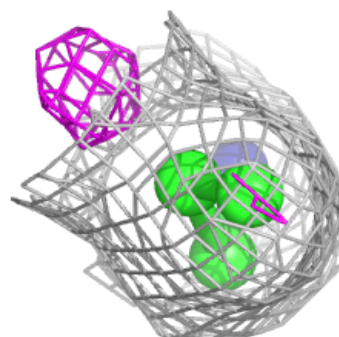
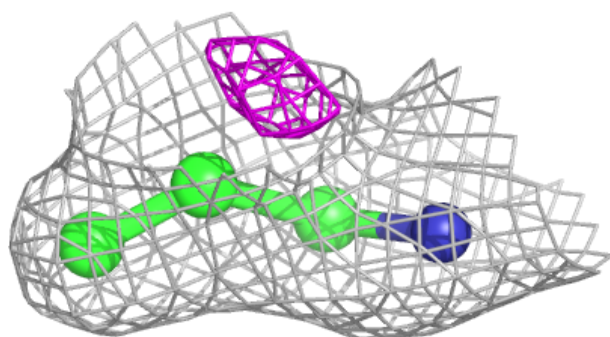
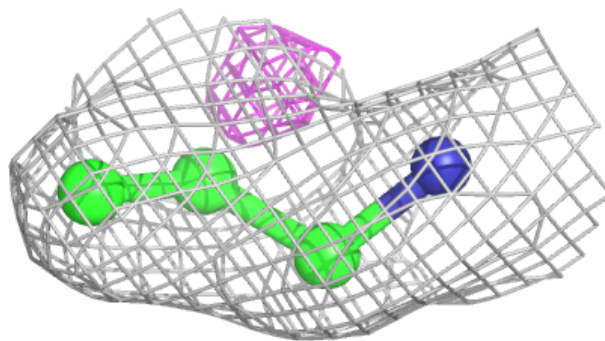
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



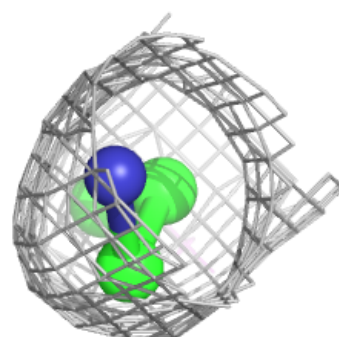
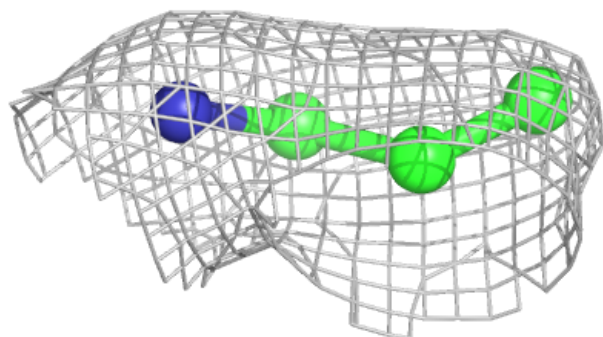
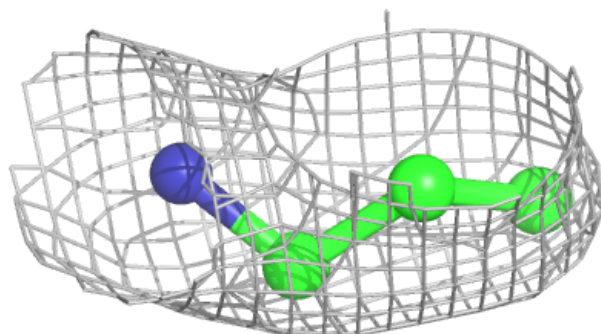


**Electron density around AYE F 101:**

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

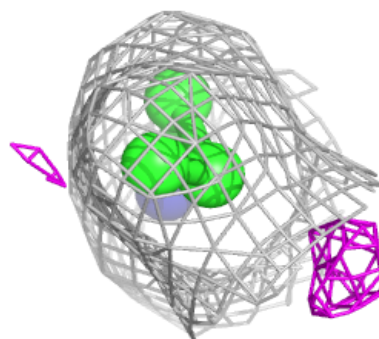
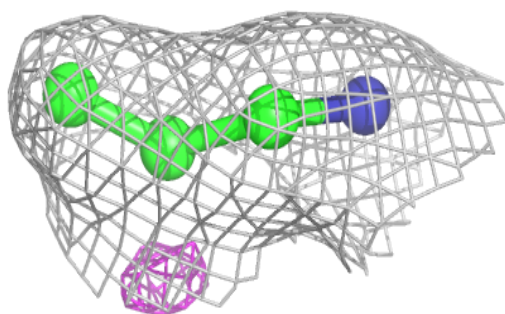
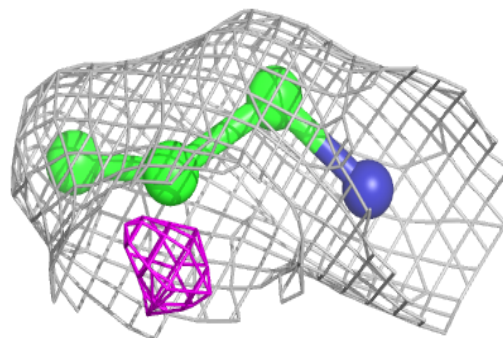
**Electron density around AYE T 101:**

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

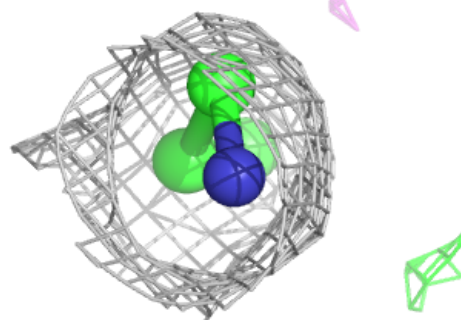
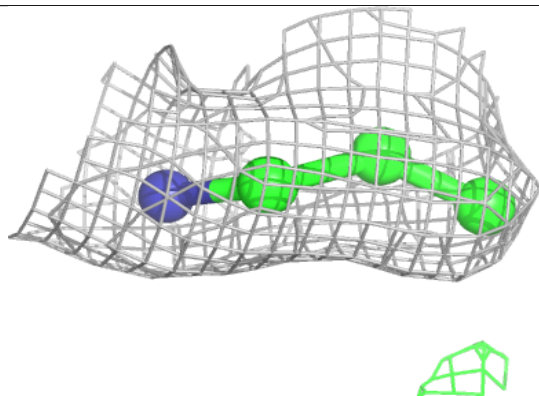
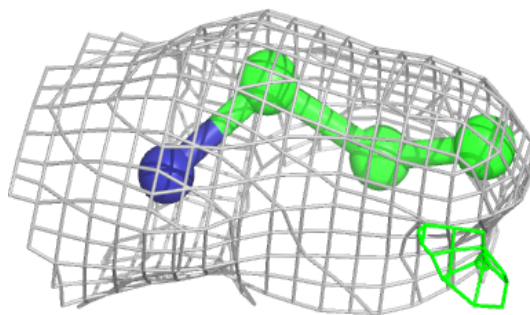


**Electron density around AYE L 101:**

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

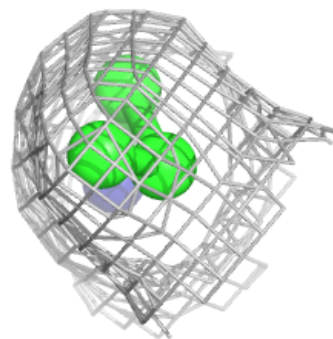
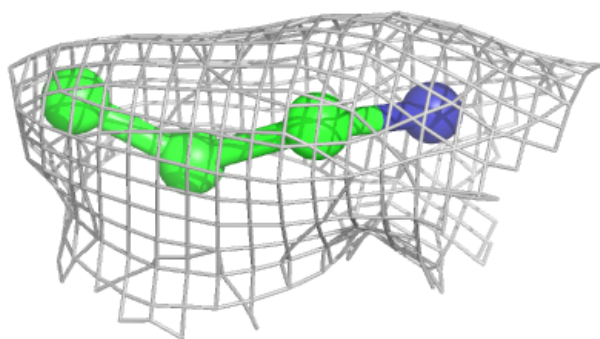
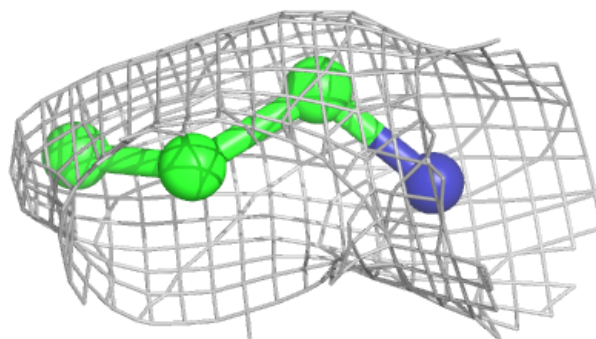
**Electron density around AYE H 101:**

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

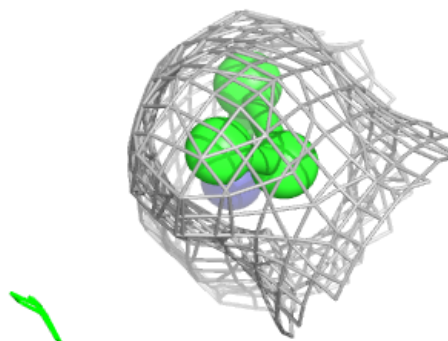
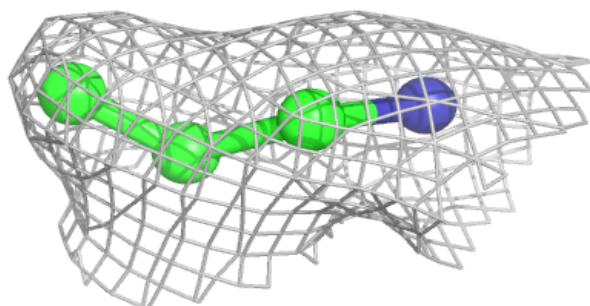
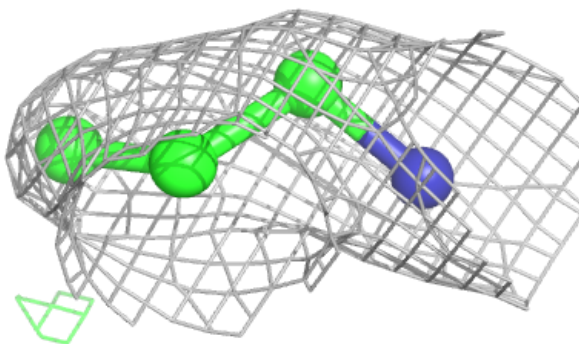


**Electron density around AYE N 101:**

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

**Electron density around AYE D 101:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.