



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 12:18 PM EDT

PDB ID : 6Q1S  
Title : A hypothetical aminotransferase from Mycobacterium tuberculosis, alpha-ketoglutarate and PMP bound form  
Authors : Duan, L.; Sacchettini, J.  
Deposited on : 2019-08-05  
Resolution : 2.30 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4

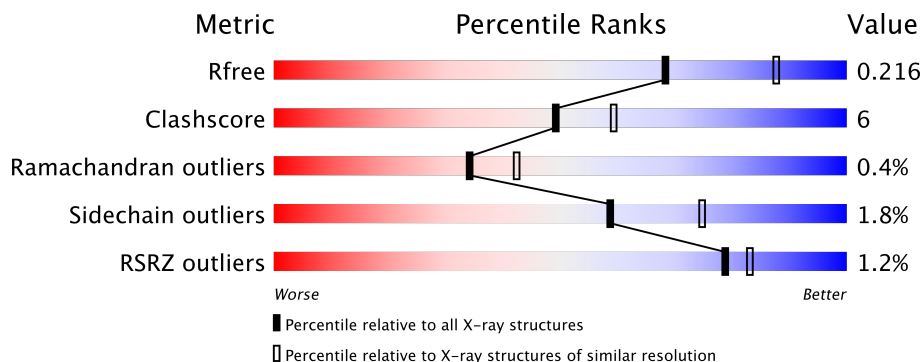
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	291	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	B	291	<div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	C	291	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	D	291	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9014 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.

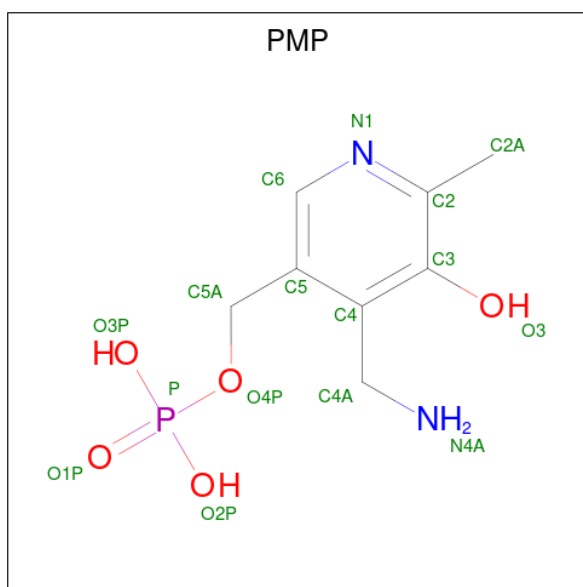
- Molecule 1 is a protein called Probable amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2148	1352	391	396	9			
1	B	284	Total	C	N	O	S	0	0	0
			2149	1353	389	397	10			
1	C	283	Total	C	N	O	S	0	0	0
			2140	1347	390	393	10			
1	D	283	Total	C	N	O	S	0	0	0
			2141	1349	387	395	10			

There are 8 discrepancies between the modelled and reference sequences:

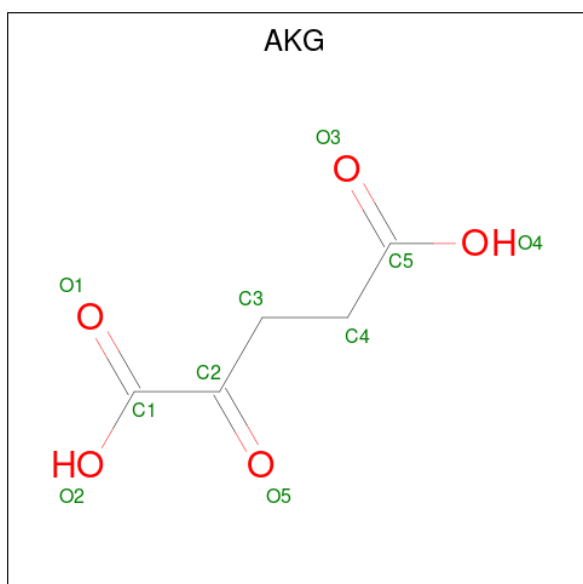
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP Q79FW0
A	0	ALA	-	expression tag	UNP Q79FW0
B	-1	ASN	-	expression tag	UNP Q79FW0
B	0	ALA	-	expression tag	UNP Q79FW0
C	-1	ASN	-	expression tag	UNP Q79FW0
C	0	ALA	-	expression tag	UNP Q79FW0
D	-1	ASN	-	expression tag	UNP Q79FW0
D	0	ALA	-	expression tag	UNP Q79FW0

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P) (labeled as "Ligand of Interest" by author).



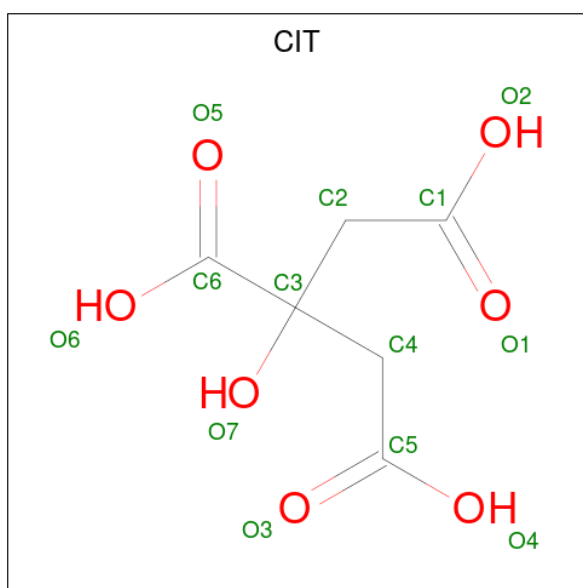
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		

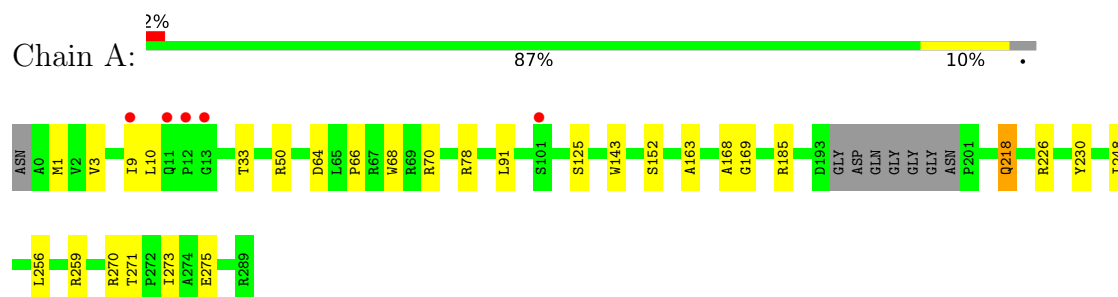
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	53	Total	O	0	0
			53	53		
5	C	94	Total	O	0	0
			94	94		
5	D	49	Total	O	0	0
			49	49		

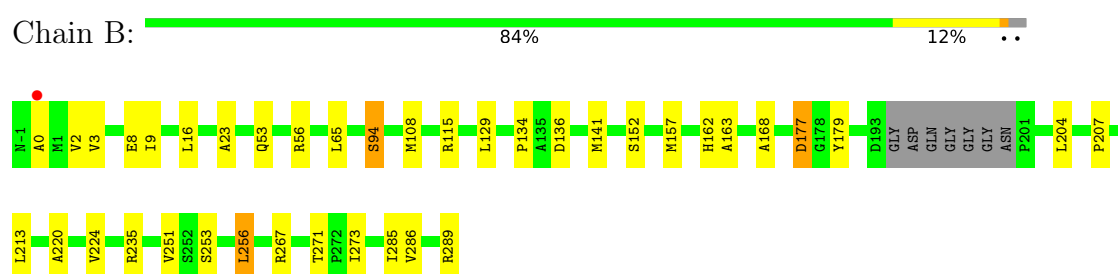
### 3 Residue-property plots [i](#)

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.

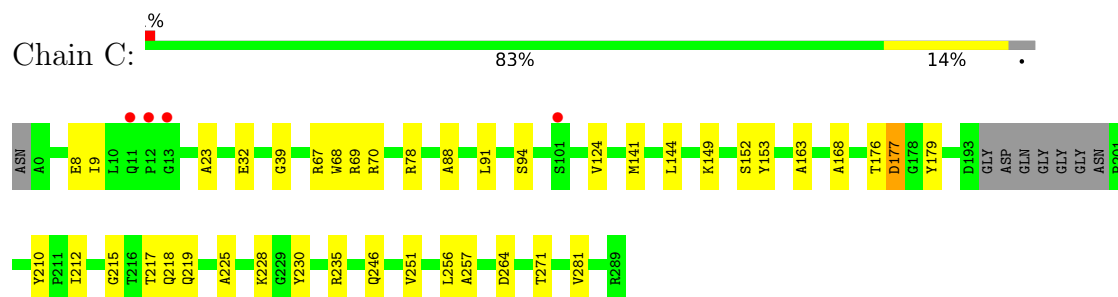
- Molecule 1: Probable amino acid aminotransferase



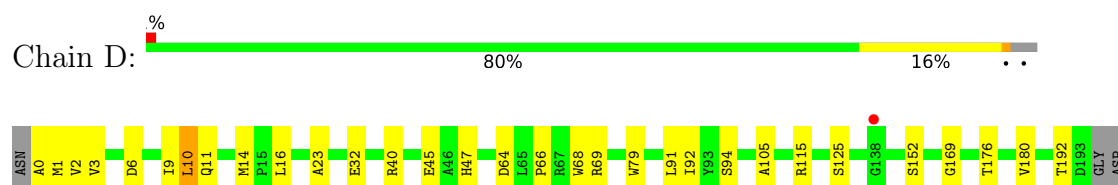
- Molecule 1: Probable amino acid aminotransferase

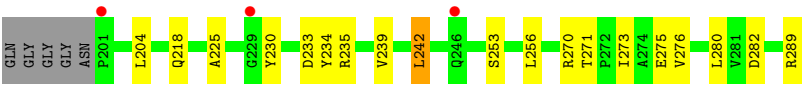


- Molecule 1: Probable amino acid aminotransferase



- Molecule 1: Probable amino acid aminotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.55Å 202.26Å 48.12Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	48.12 – 2.30 48.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.12-2.30) 97.3 (48.12-2.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.205 , 0.227 0.198 , 0.216	Depositor DCC
$R_{free}$ test set	4292 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 21.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
Reported twinning fraction	0.360 for -h,-k,l	Depositor
Outliers	0 of 83076 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, PMP, CIT

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	0.24	0/2190	0.44	0/2987
1	B	0.24	0/2191	0.46	0/2989
1	C	0.25	0/2182	0.46	0/2976
1	D	0.24	0/2183	0.45	0/2978
All	All	0.24	0/8746	0.45	0/11930

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	2148	0	2169	19	0
1	B	2149	0	2165	27	0
1	C	2140	0	2157	26	0
1	D	2141	0	2159	29	0
2	A	16	0	10	2	0
2	B	16	0	10	2	0
2	C	16	0	10	3	0
2	D	16	0	11	3	0
3	A	10	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	1	0
3	C	10	0	4	0	0
3	D	10	0	4	1	0
4	C	26	0	10	1	0
5	A	110	0	0	6	0
5	B	53	0	0	5	0
5	C	94	0	0	8	0
5	D	49	0	0	5	0
All	All	9014	0	8717	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ARG:HH21	1:D:289:ARG:HD3	1.55	0.72
1:A:50:ARG:NH2	5:A:404:HOH:O	2.26	0.68
1:C:9:ILE:HD13	1:C:78:ARG:HD2	1.75	0.68
1:B:157:MET:SD	5:B:452:HOH:O	2.53	0.66
1:A:218:GLN:NE2	5:A:407:HOH:O	2.28	0.66
1:A:270:ARG:NH1	1:A:275:GLU:OE1	2.30	0.65
1:D:270:ARG:NH1	1:D:275:GLU:OE1	2.32	0.63
1:B:23:ALA:HB2	1:B:94:SER:HB2	1.80	0.63
1:A:3:VAL:HG22	1:A:9:ILE:HG12	1.81	0.62
1:C:235:ARG:NH2	5:C:405:HOH:O	2.32	0.61
1:B:286:VAL:HG13	1:B:289:ARG:HD2	1.83	0.60
1:C:8:GLU:N	1:C:8:GLU:OE1	2.36	0.59
1:D:235:ARG:NH1	5:D:406:HOH:O	2.34	0.59
1:C:246:GLN:HB3	1:C:271:THR:HG21	1.84	0.58
1:D:125:SER:O	1:D:169:GLY:N	2.33	0.58
1:C:149:LYS:NZ	2:C:301:PMP:O3	2.36	0.58
1:B:56:ARG:NH2	5:B:405:HOH:O	2.38	0.57
1:C:163:ALA:HB1	1:C:168:ALA:HB3	1.87	0.57
1:B:271:THR:HG22	1:B:273:ILE:H	1.68	0.57
1:B:163:ALA:HB1	1:B:168:ALA:HB3	1.86	0.56
1:B:8:GLU:OE1	1:B:8:GLU:N	2.39	0.56
1:C:70:ARG:NH2	5:C:414:HOH:O	2.37	0.56
1:D:1:MET:HE1	1:D:79:TRP:HB2	1.88	0.56
1:B:53:GLN:OE1	1:B:56:ARG:NH2	2.39	0.55
1:C:69:ARG:NE	5:C:417:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:VAL:HG22	1:D:9:ILE:HG12	1.88	0.54
1:D:45:GLU:OE1	1:D:69:ARG:NH1	2.40	0.54
1:D:11:GLN:HB2	1:D:14:MET:HG3	1.90	0.53
1:B:177:ASP:HB3	1:B:179:TYR:HD1	1.74	0.53
1:B:204:LEU:HD22	1:B:235:ARG:HG3	1.90	0.53
1:C:153:TYR:OH	2:C:301:PMP:O3	2.27	0.52
1:D:180:VAL:HG21	1:D:242:LEU:HD11	1.91	0.52
1:D:280:LEU:HD22	5:D:442:HOH:O	2.11	0.51
1:B:115:ARG:NH2	3:B:302:AKG:O3	2.43	0.50
1:C:67:ARG:NE	5:C:423:HOH:O	2.45	0.50
1:C:152:SER:HB3	1:D:152:SER:HB3	1.92	0.50
1:A:125:SER:O	1:A:169:GLY:N	2.42	0.50
1:C:32:GLU:HB2	1:C:91:LEU:HD12	1.94	0.49
1:C:141:MET:HE1	1:C:144:LEU:HD11	1.95	0.49
1:D:68:TRP:CZ3	1:D:91:LEU:HB3	2.47	0.49
2:A:301:PMP:H4A1	5:A:404:HOH:O	2.13	0.49
1:B:213:LEU:HD23	2:B:301:PMP:H2A3	1.93	0.49
1:A:152:SER:HB3	1:B:152:SER:HB3	1.94	0.49
1:B:177:ASP:HB3	1:B:179:TYR:CD1	2.48	0.49
1:A:163:ALA:HB1	1:A:168:ALA:HB3	1.96	0.48
1:D:32:GLU:HG2	1:D:47:HIS:HB3	1.96	0.48
1:D:115:ARG:NH1	5:D:409:HOH:O	2.39	0.48
1:A:70:ARG:NH1	5:A:412:HOH:O	2.34	0.47
1:B:0:ALA:HB1	5:B:435:HOH:O	2.15	0.47
1:D:204:LEU:HD22	1:D:235:ARG:HG3	1.97	0.47
1:D:276:VAL:O	1:D:280:LEU:HG	2.14	0.47
1:D:253:SER:N	2:D:301:PMP:O3P	2.48	0.46
1:A:68:TRP:CZ3	1:A:91:LEU:HB3	2.51	0.46
1:A:78:ARG:HB3	1:A:78:ARG:NH1	2.30	0.46
1:D:10:LEU:HD22	1:D:11:GLN:H	1.80	0.46
1:D:282:ASP:OD2	5:D:401:HOH:O	2.21	0.46
1:A:248:ILE:N	5:A:425:HOH:O	2.49	0.45
1:B:207:PRO:HD3	1:B:235:ARG:O	2.17	0.45
1:C:149:LYS:NZ	2:C:301:PMP:H4A1	2.31	0.45
1:C:228:LYS:NZ	5:C:429:HOH:O	2.48	0.45
1:B:220:ALA:O	1:B:224:VAL:HG22	2.17	0.45
1:C:39:GLY:N	5:C:425:HOH:O	2.46	0.45
1:C:88:ALA:O	5:C:401:HOH:O	2.21	0.45
1:D:45:GLU:OE2	1:D:69:ARG:HD3	2.17	0.45
1:A:226:ARG:HA	1:A:230:TYR:O	2.17	0.44
1:B:253:SER:N	2:B:301:PMP:O1P	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HA	1:B:256:LEU:O	2.18	0.44
1:B:3:VAL:HG22	1:B:9:ILE:HG13	2.00	0.44
1:A:185:ARG:O	2:A:301:PMP:N4A	2.51	0.44
2:D:301:PMP:N4A	3:D:302:AKG:O5	2.50	0.44
1:B:162:HIS:ND1	5:B:416:HOH:O	2.36	0.44
1:D:225:ALA:HB1	1:D:230:TYR:HB2	2.00	0.44
2:D:301:PMP:O3	2:D:301:PMP:N4A	2.44	0.43
1:C:23:ALA:HB2	1:C:94:SER:CB	2.48	0.43
1:A:64:ASP:OD2	1:A:66:PRO:HD2	2.18	0.43
1:C:177:ASP:OD1	1:C:179:TYR:HD2	2.01	0.43
1:D:64:ASP:OD2	1:D:66:PRO:HD2	2.18	0.43
1:B:2:VAL:HG11	1:B:16:LEU:HD22	2.00	0.42
1:A:271:THR:HG22	1:A:273:ILE:H	1.84	0.42
1:C:264:ASP:O	5:C:402:HOH:O	2.21	0.42
1:A:143:TRP:CE2	1:B:129:LEU:HG	2.54	0.42
1:C:210:TYR:O	1:C:212:ILE:N	2.51	0.42
1:D:92:ILE:O	1:D:105:ALA:HA	2.19	0.42
1:B:108:MET:HG3	5:B:435:HOH:O	2.19	0.42
1:C:217:THR:HB	1:C:251:VAL:HG12	2.00	0.42
1:D:23:ALA:HB2	1:D:94:SER:HB2	2.02	0.42
1:C:257:ALA:HB2	1:C:281:VAL:HG21	2.02	0.41
1:C:215:GLY:O	1:C:219:GLN:HG3	2.20	0.41
4:C:304:CIT:O2	4:C:304:CIT:O7	2.32	0.41
1:D:239:VAL:HA	1:D:242:LEU:HD22	2.01	0.41
1:D:271:THR:HB	1:D:273:ILE:HG22	2.02	0.41
1:A:259:ARG:HG3	5:A:425:HOH:O	2.20	0.41
1:C:68:TRP:CZ3	1:C:91:LEU:HB3	2.56	0.41
1:A:33:THR:HG21	3:A:302:AKG:H41	2.02	0.41
1:B:134:PRO:HG2	1:B:136:ASP:OD1	2.21	0.41
1:B:285:ILE:HG13	1:B:286:VAL:HG23	2.03	0.41
1:D:2:VAL:HG11	1:D:16:LEU:HD22	2.03	0.41
1:A:1:MET:SD	1:A:78:ARG:NH1	2.93	0.41
1:D:0:ALA:O	5:D:402:HOH:O	2.22	0.40
1:D:233:ASP:OD1	1:D:234:TYR:N	2.52	0.40
1:C:225:ALA:HB1	1:C:230:TYR:HB2	2.02	0.40
1:B:141:MET:HB2	1:B:141:MET:HE2	1.91	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	279/291 (96%)	274 (98%)	4 (1%)	1 (0%)	34	42
1	B	280/291 (96%)	276 (99%)	3 (1%)	1 (0%)	34	42
1	C	279/291 (96%)	273 (98%)	5 (2%)	1 (0%)	34	42
1	D	279/291 (96%)	273 (98%)	5 (2%)	1 (0%)	34	42
All	All	1117/1164 (96%)	1096 (98%)	17 (2%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	LEU
1	A	256	LEU
1	B	256	LEU
1	C	256	LEU

### 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	222/227 (98%)	220 (99%)	2 (1%)	78	89
1	B	222/227 (98%)	218 (98%)	4 (2%)	59	75
1	C	220/227 (97%)	216 (98%)	4 (2%)	59	75
1	D	221/227 (97%)	215 (97%)	6 (3%)	44	61
All	All	885/908 (98%)	869 (98%)	16 (2%)	59	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	218	GLN
1	B	65	LEU
1	B	94	SER
1	B	177	ASP
1	B	267	ARG
1	C	124	VAL
1	C	176	THR
1	C	177	ASP
1	C	218	GLN
1	D	6	ASP
1	D	10	LEU
1	D	176	THR
1	D	192	THR
1	D	218	GLN
1	D	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

10 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	AKG	D	302	-	3,9,9	0.26	0	4,11,11	1.19	0
4	CIT	C	304	-	3,12,12	1.14	0	3,17,17	2.25	2 (66%)
2	PMP	C	301	-	16,16,16	2.88	3 (18%)	21,23,23	1.05	1 (4%)
2	PMP	B	301	-	16,16,16	2.88	3 (18%)	21,23,23	1.11	1 (4%)
2	PMP	D	301	-	16,16,16	2.92	3 (18%)	21,23,23	1.10	1 (4%)
3	AKG	A	302	-	3,9,9	0.24	0	4,11,11	1.27	0
2	PMP	A	301	-	16,16,16	2.80	3 (18%)	21,23,23	1.09	1 (4%)
4	CIT	C	303	-	3,12,12	0.99	0	3,17,17	1.51	1 (33%)
3	AKG	B	302	-	3,9,9	0.24	0	4,11,11	1.20	0
3	AKG	C	302	-	3,9,9	0.15	0	4,11,11	1.50	1 (25%)

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	AKG	D	302	-	-	1/3/9/9	-
4	CIT	C	304	-	-	0/6/16/16	-
2	PMP	C	301	-	-	2/8/8/8	0/1/1/1
2	PMP	B	301	-	-	1/8/8/8	0/1/1/1
2	PMP	D	301	-	-	2/8/8/8	0/1/1/1
3	AKG	A	302	-	-	0/3/9/9	-
2	PMP	A	301	-	-	4/8/8/8	0/1/1/1
4	CIT	C	303	-	-	1/6/16/16	-
3	AKG	B	302	-	-	3/3/9/9	-
3	AKG	C	302	-	-	1/3/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	PMP	C3-C2	8.14	1.49	1.40
2	B	301	PMP	C3-C2	8.02	1.48	1.40
2	C	301	PMP	C3-C2	7.80	1.48	1.40
2	A	301	PMP	C3-C2	7.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	PMP	C5-C4	6.18	1.49	1.40
2	D	301	PMP	C5-C4	5.93	1.48	1.40
2	B	301	PMP	C5-C4	5.85	1.48	1.40
2	A	301	PMP	C5-C4	5.71	1.48	1.40
2	D	301	PMP	C3-C4	5.50	1.48	1.40
2	B	301	PMP	C3-C4	5.47	1.48	1.40
2	C	301	PMP	C3-C4	5.44	1.48	1.40
2	A	301	PMP	C3-C4	5.44	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	CIT	C3-C2-C1	-3.15	109.94	114.98
4	C	303	CIT	C3-C2-C1	-2.40	111.14	114.98
2	A	301	PMP	C6-N1-C2	2.28	123.39	119.17
3	C	302	AKG	C3-C4-C5	-2.25	108.89	112.67
4	C	304	CIT	C3-C4-C5	-2.19	111.47	114.98
2	D	301	PMP	C6-N1-C2	2.19	123.22	119.17
2	B	301	PMP	C6-N1-C2	2.13	123.12	119.17
2	C	301	PMP	C6-N1-C2	2.11	123.08	119.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PMP	C3-C4-C4A-N4A
2	A	301	PMP	C5-C4-C4A-N4A
2	D	301	PMP	C3-C4-C4A-N4A
3	B	302	AKG	C2-C3-C4-C5
3	D	302	AKG	C2-C3-C4-C5
3	C	302	AKG	C2-C3-C4-C5
2	C	301	PMP	C5-C4-C4A-N4A
2	D	301	PMP	C5-C4-C4A-N4A
4	C	303	CIT	O7-C3-C4-C5
2	A	301	PMP	C4-C5-C5A-O4P
2	B	301	PMP	C5-C4-C4A-N4A
2	C	301	PMP	C5A-O4P-P-O1P
3	B	302	AKG	C1-C2-C3-C4
3	B	302	AKG	O5-C2-C3-C4
2	A	301	PMP	C6-C5-C5A-O4P

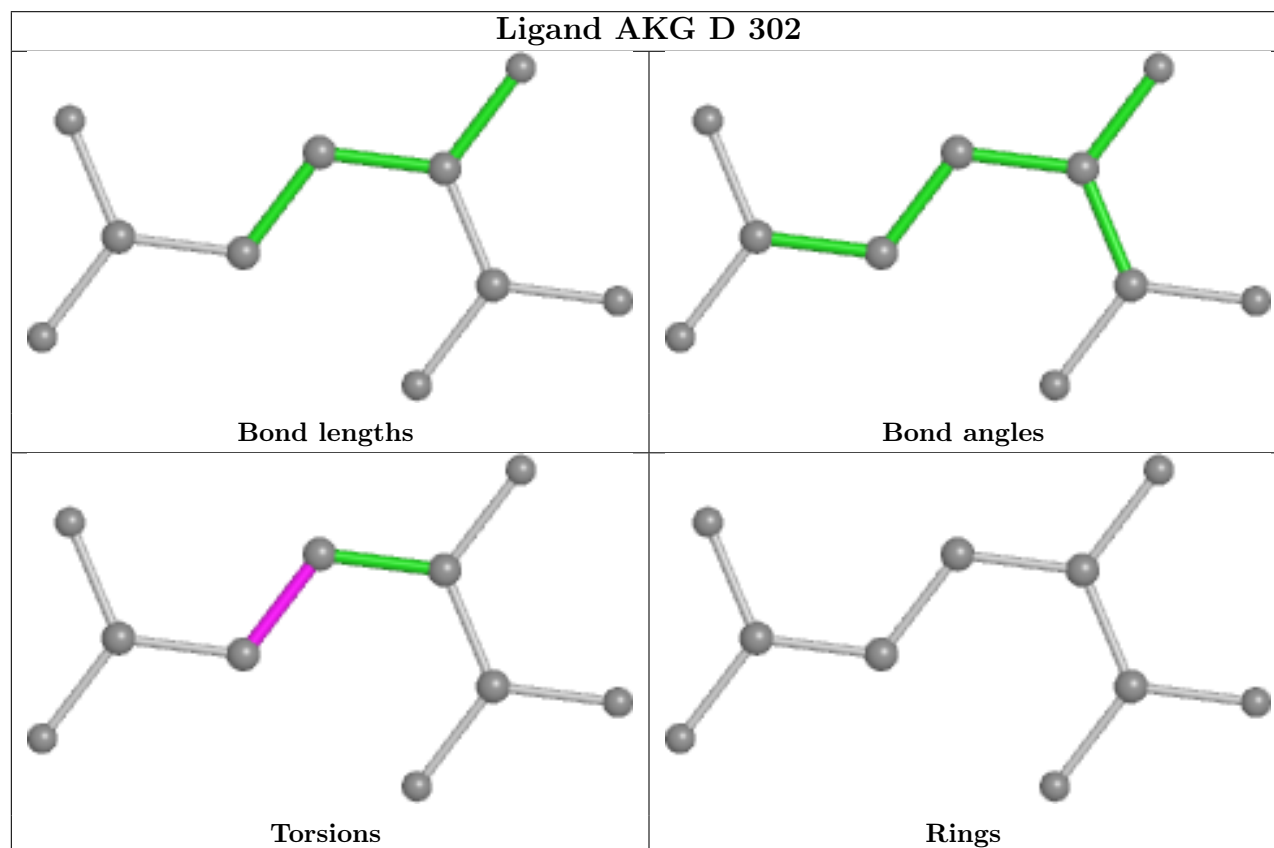
There are no ring outliers.

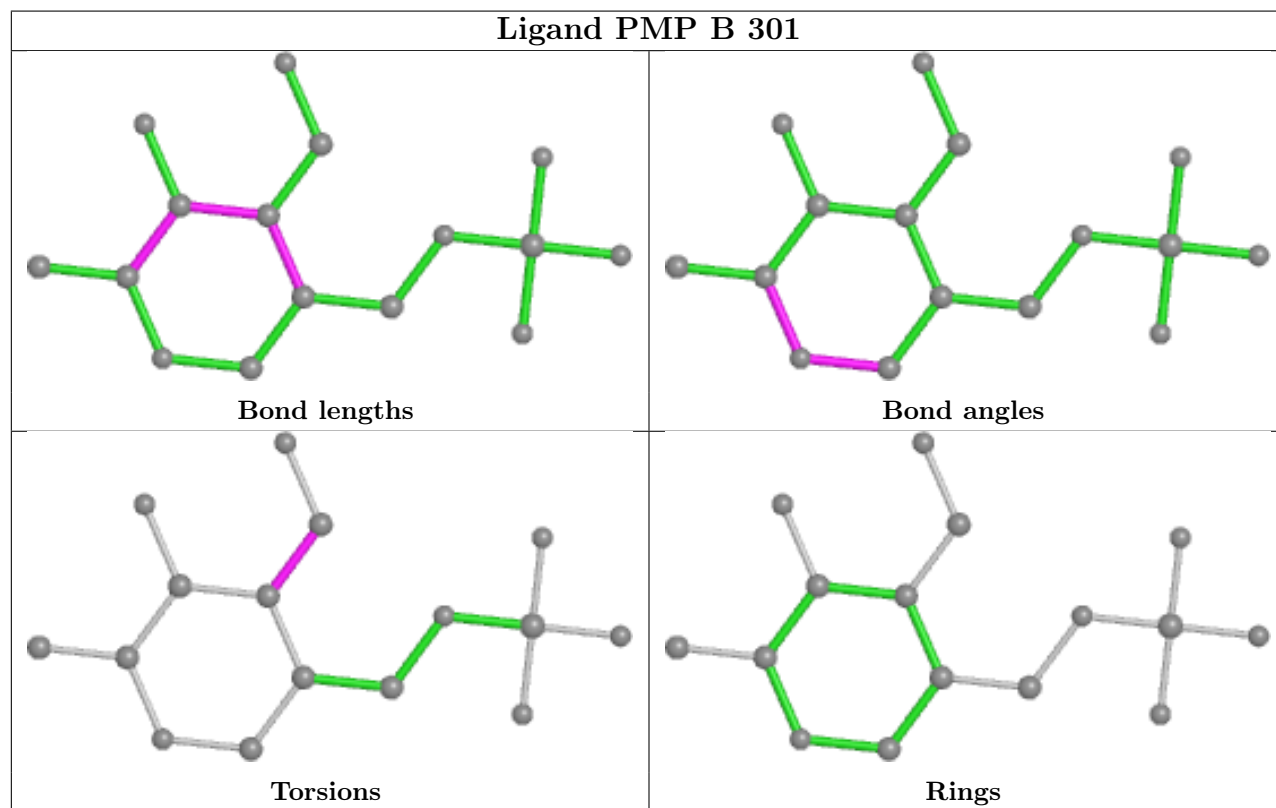
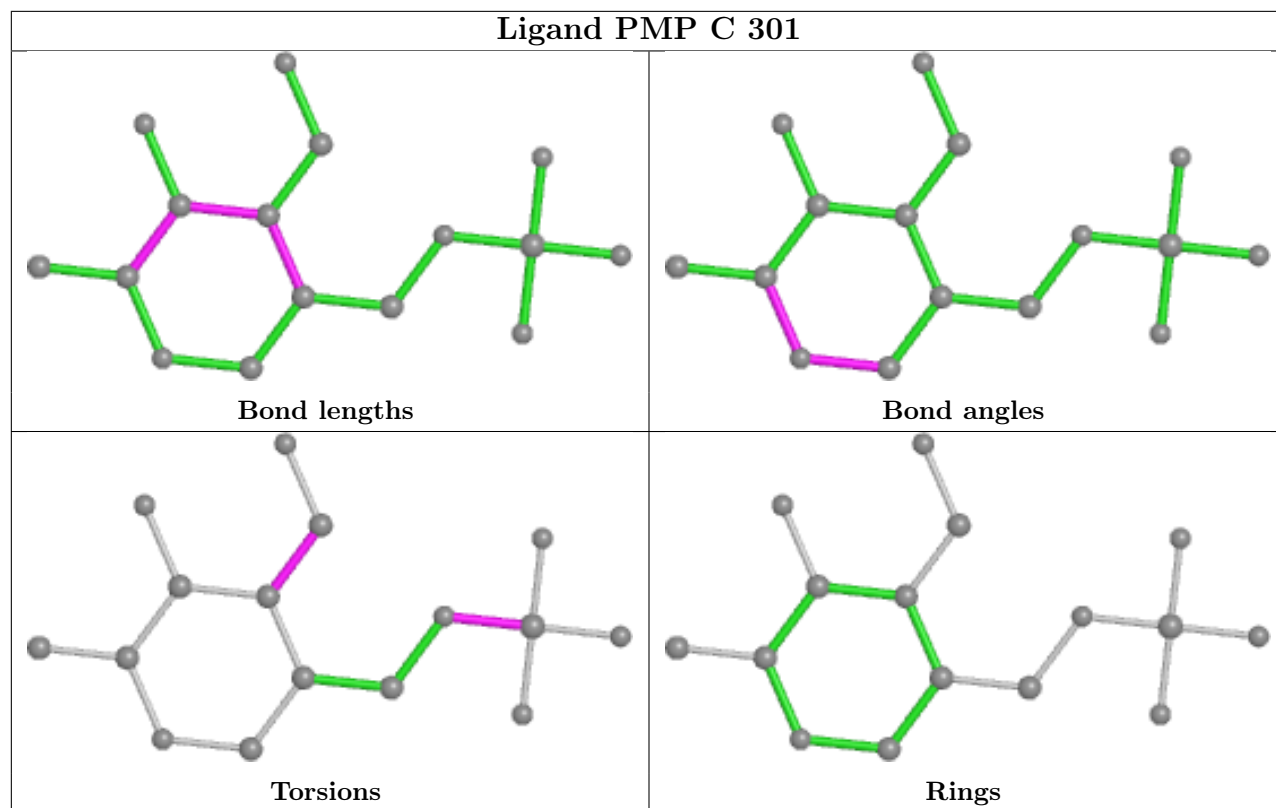


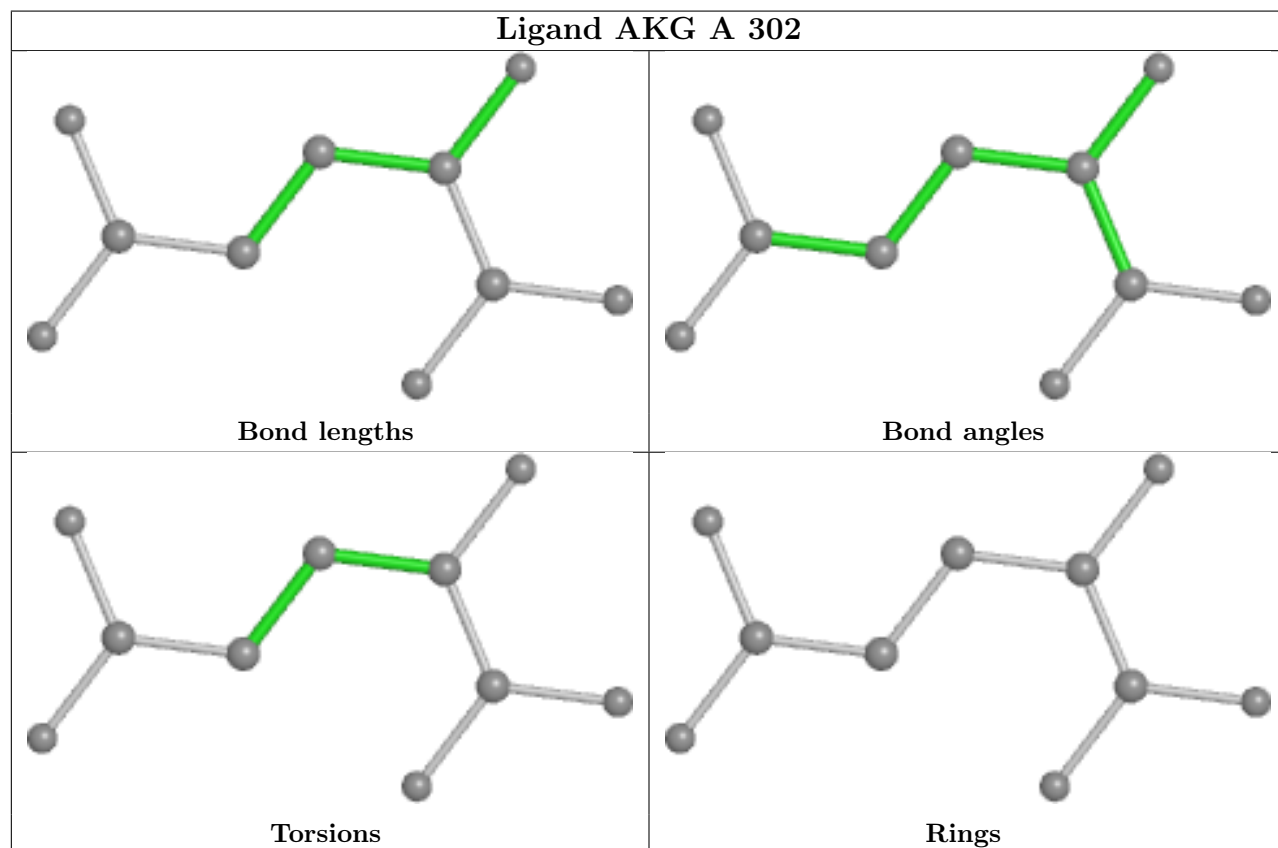
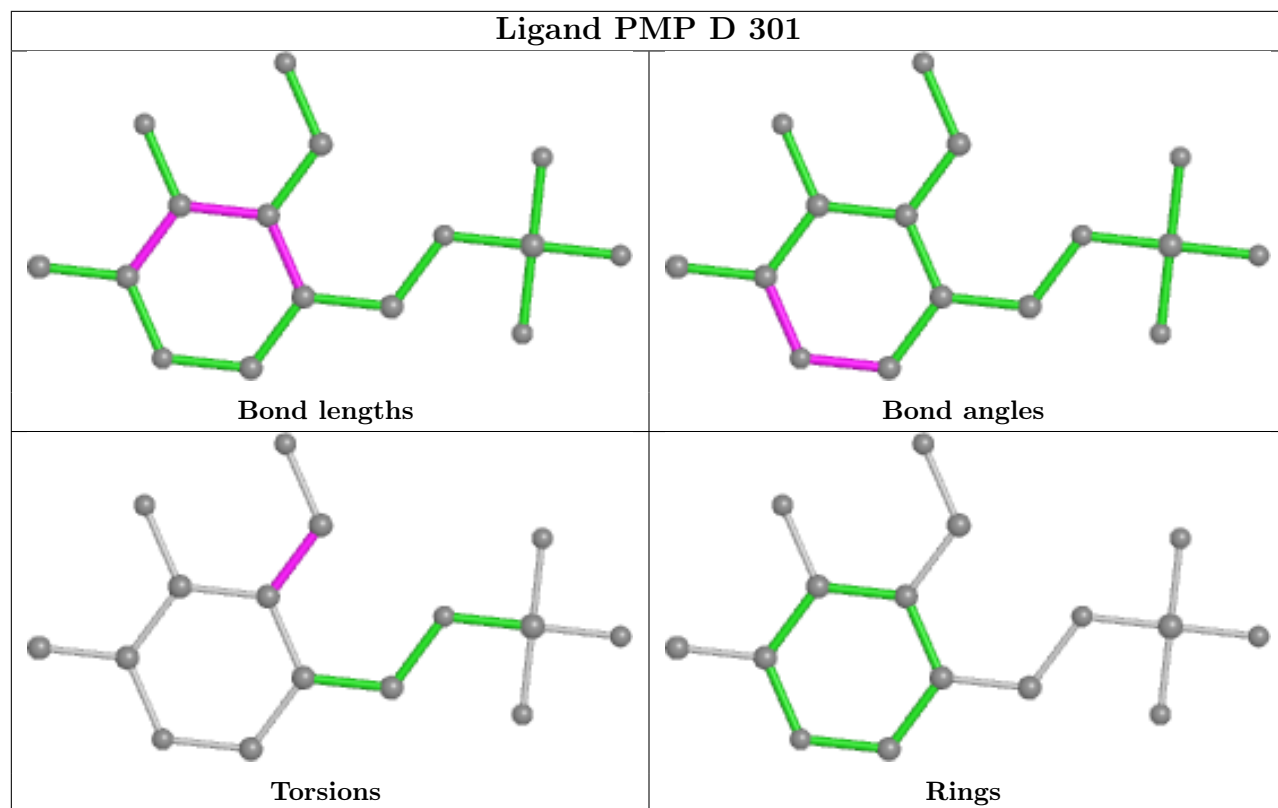
8 monomers are involved in 13 short contacts:

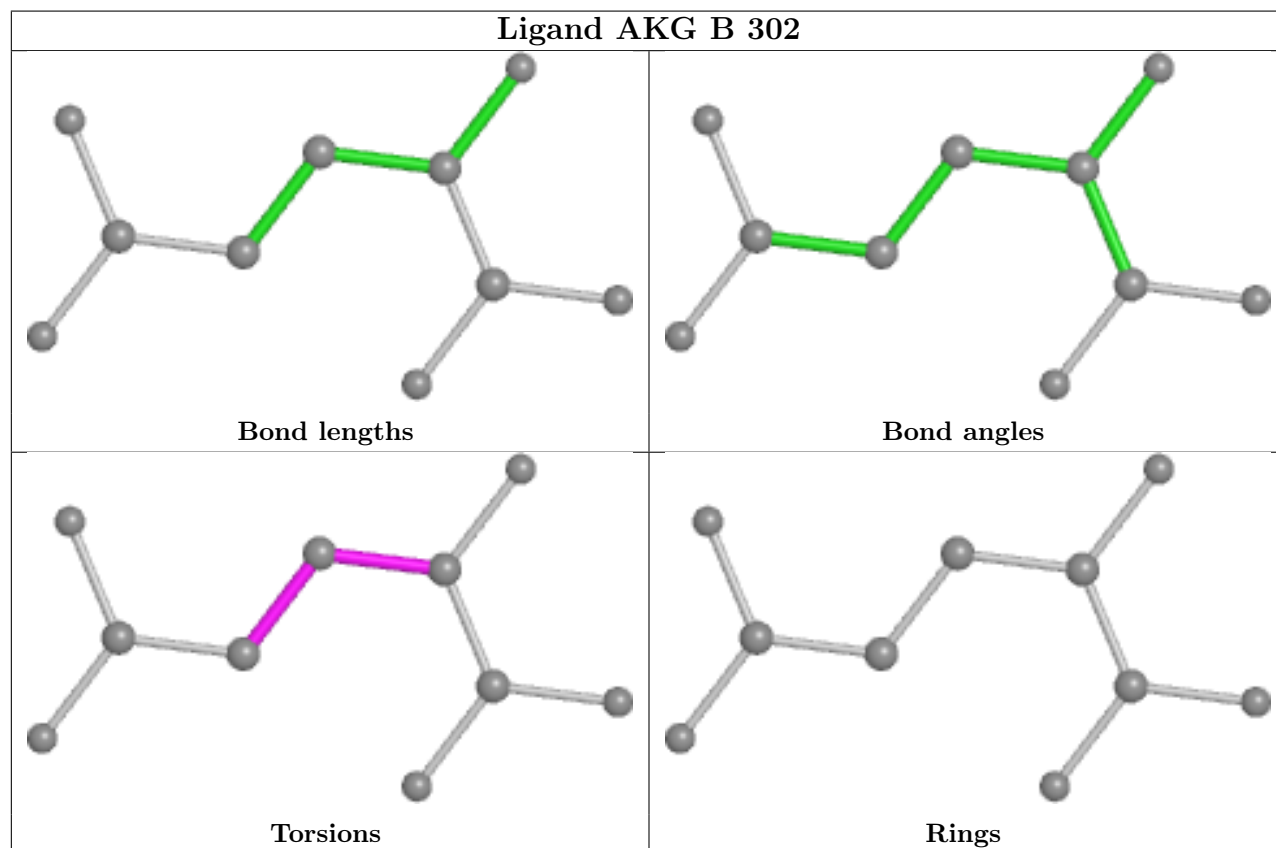
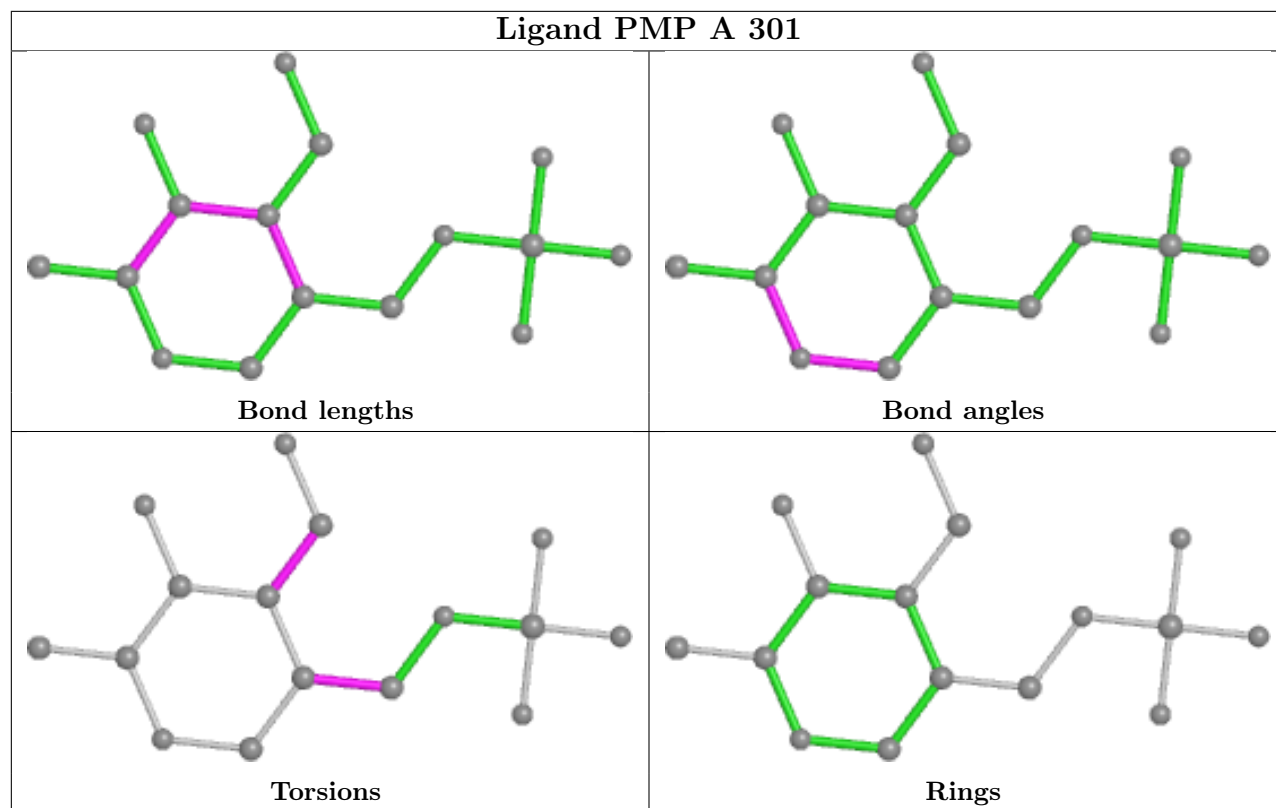
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	AKG	1	0
4	C	304	CIT	1	0
2	C	301	PMP	3	0
2	B	301	PMP	2	0
2	D	301	PMP	3	0
3	A	302	AKG	1	0
2	A	301	PMP	2	0
3	B	302	AKG	1	0

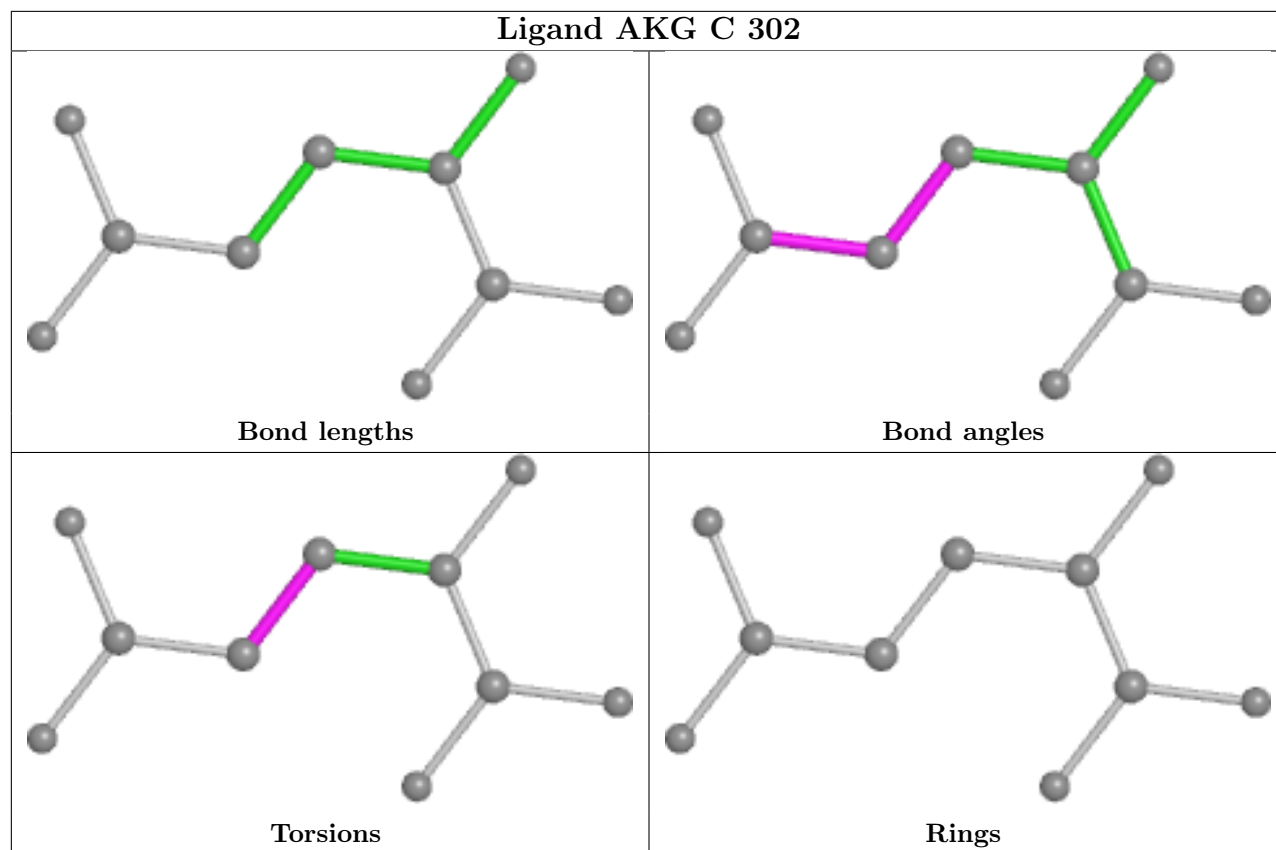
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	283/291 (97%)	-0.25	5 (1%) 68 74	15, 20, 33, 47	0
1	B	284/291 (97%)	-0.24	1 (0%) 92 95	18, 29, 40, 47	0
1	C	283/291 (97%)	-0.27	4 (1%) 75 80	15, 19, 32, 48	0
1	D	283/291 (97%)	-0.16	4 (1%) 75 80	18, 29, 40, 50	0
All	All	1133/1164 (97%)	-0.23	14 (1%) 79 83	15, 24, 39, 50	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	PRO	4.6
1	A	12	PRO	3.7
1	A	101	SER	3.4
1	C	101	SER	3.3
1	A	13	GLY	3.0
1	B	0	ALA	2.9
1	D	201	PRO	2.7
1	C	11	GLN	2.7
1	A	9	ILE	2.5
1	D	138	GLY	2.4
1	D	229	GLY	2.3
1	C	13	GLY	2.2
1	D	246	GLN	2.2
1	A	11	GLN	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](#)

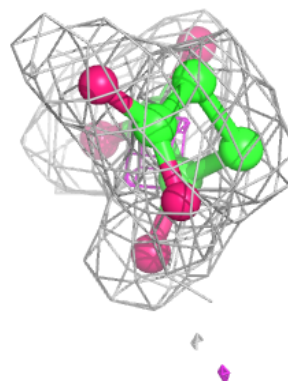
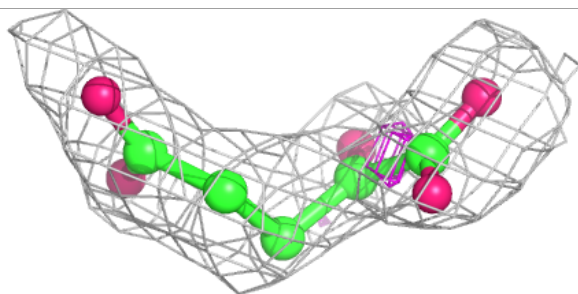
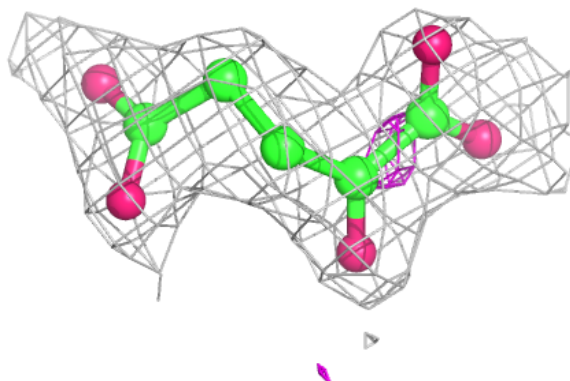
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AKG	D	302	10/10	0.85	0.24	41,42,43,44	0
4	CIT	C	303	13/13	0.88	0.13	22,29,38,40	0
3	AKG	B	302	10/10	0.90	0.15	29,34,38,39	0
3	AKG	A	302	10/10	0.91	0.12	29,36,40,41	0
3	AKG	C	302	10/10	0.92	0.14	22,25,32,32	0
2	PMP	C	301	16/16	0.96	0.11	15,22,26,29	0
4	CIT	C	304	13/13	0.97	0.11	20,21,31,32	0
2	PMP	D	301	16/16	0.97	0.12	21,23,24,25	0
2	PMP	A	301	16/16	0.98	0.10	16,17,22,23	0
2	PMP	B	301	16/16	0.98	0.11	22,24,29,32	0

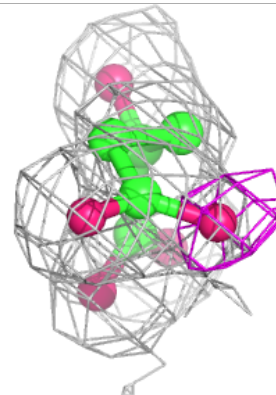
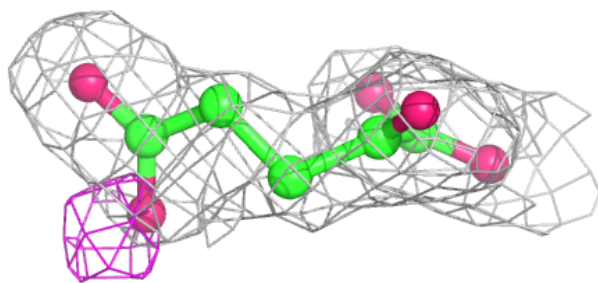
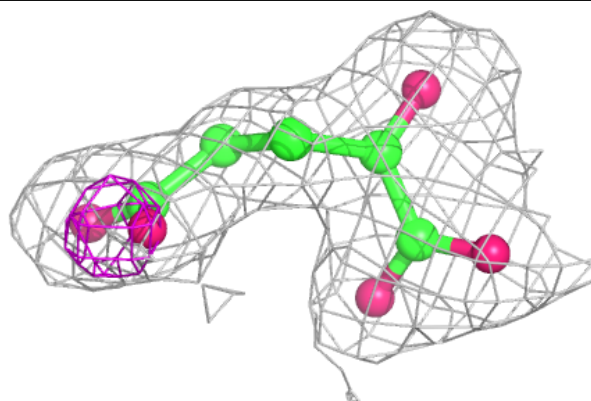
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AKG D 302:**

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

**Electron density around AKG B 302:**

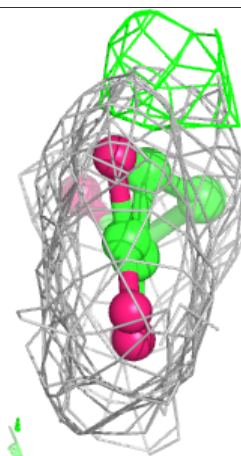
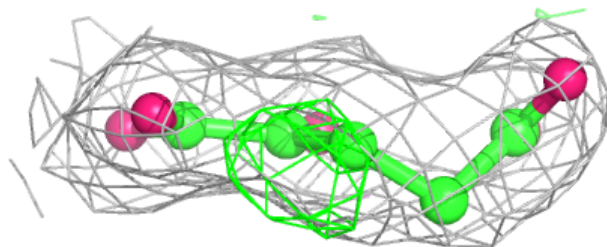
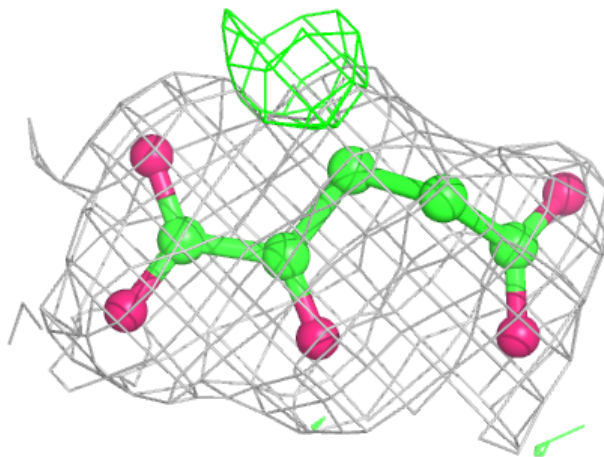
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





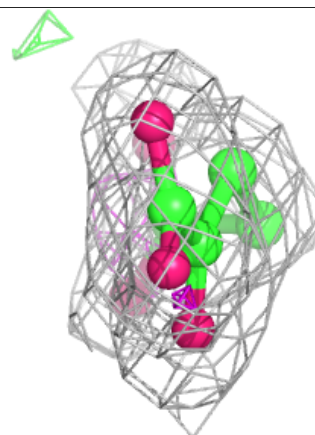
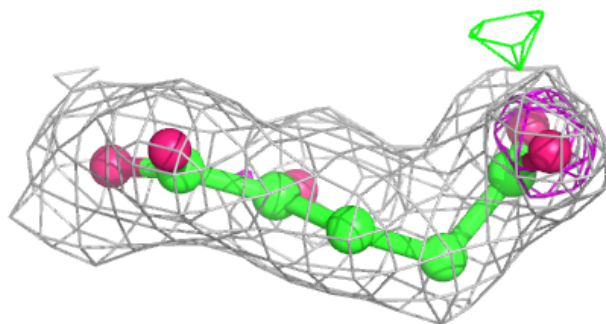
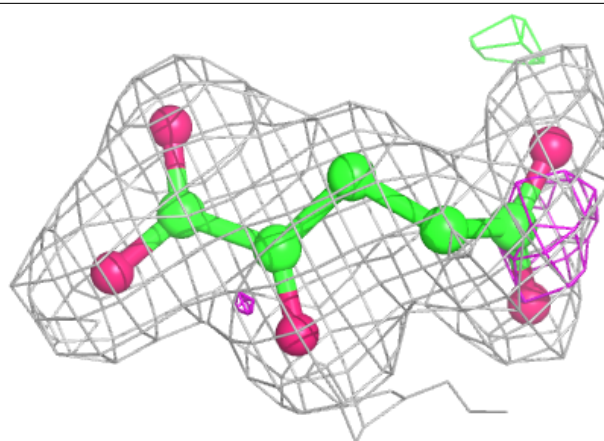
**Electron density around AKG A 302:**

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

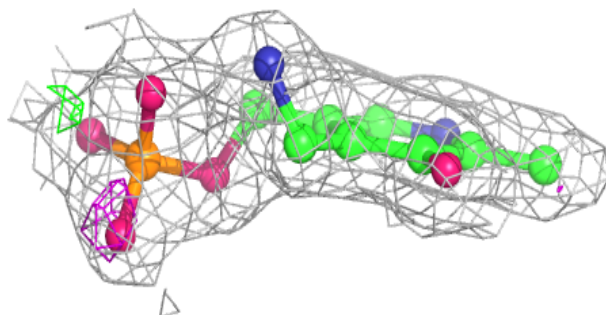
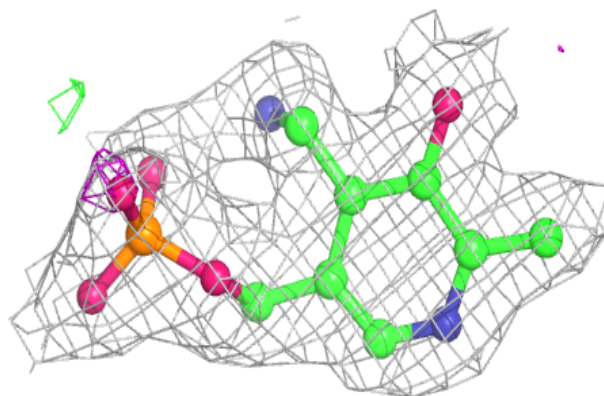


**Electron density around AKG C 302:**

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

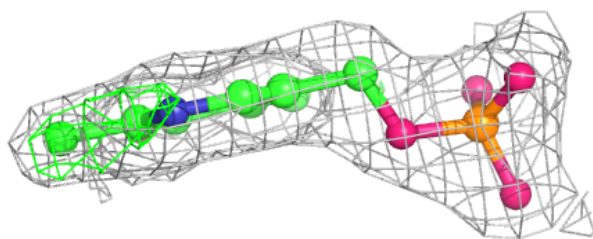
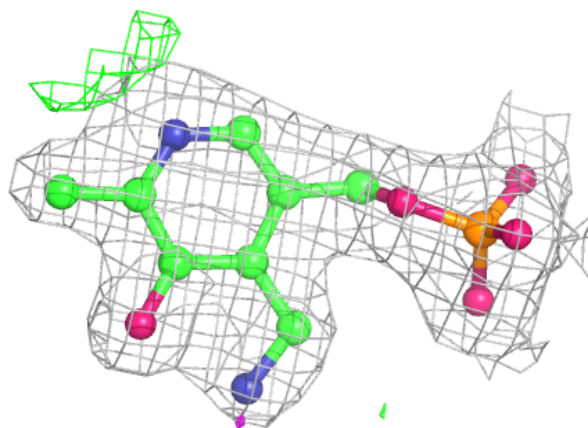
**Electron density around PMP C 301:**

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



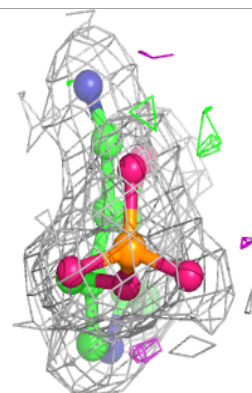
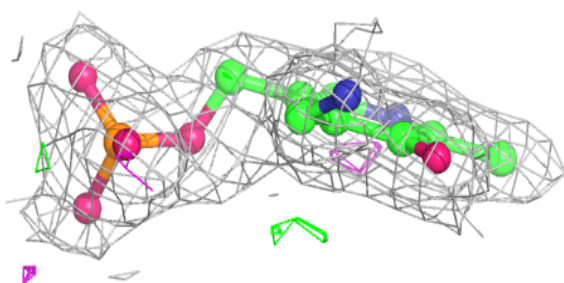
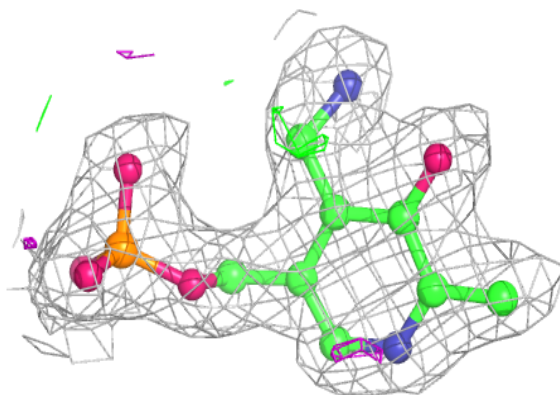
**Electron density around PMP D 301:**

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and green (positive)

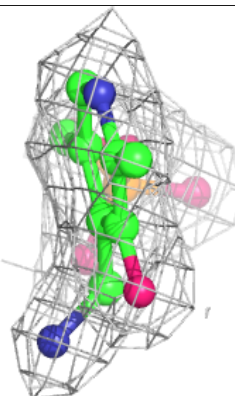
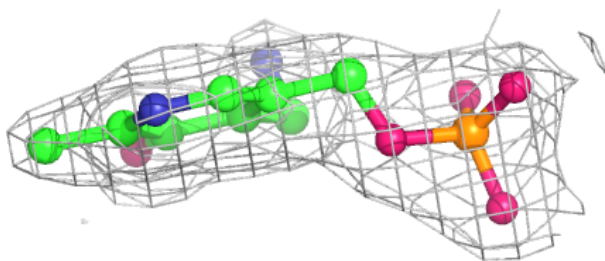
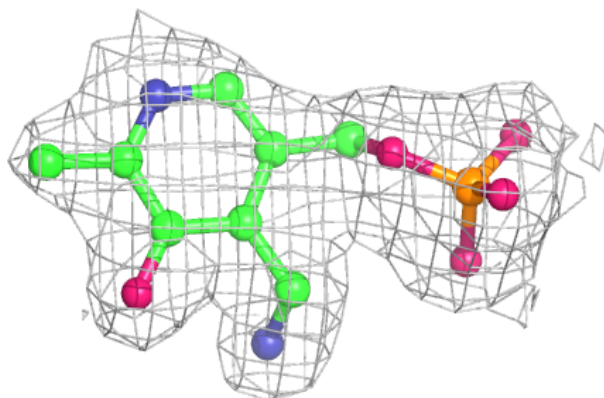


**Electron density around PMP A 301:**

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

**Electron density around PMP B 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 [i](#)

There are no such residues in this entry.