



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:40 AM BST

PDB ID : 6JC8  
Title : Crystal structure of aminotransferase CrmG from Actinoalloteichus sp. WH1-2216-6 in complex with amino donor L-Glu  
Authors : Xu, J.; Liu, J.  
Deposited on : 2019-01-28  
Resolution : 2.25 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.dev1  
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.dev1

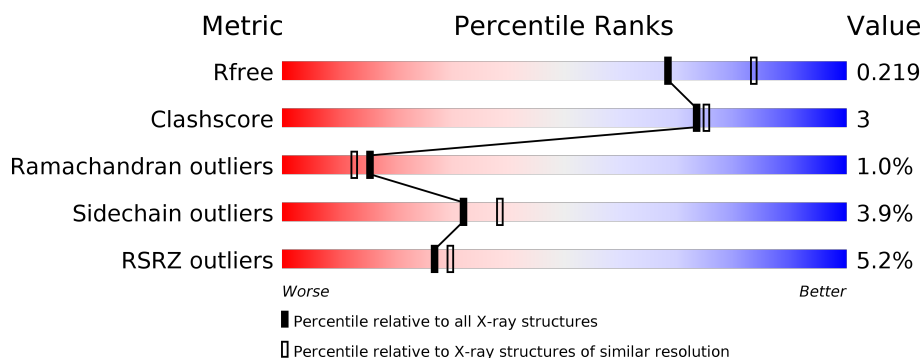
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	523	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	523	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	523	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
1	D	523	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>

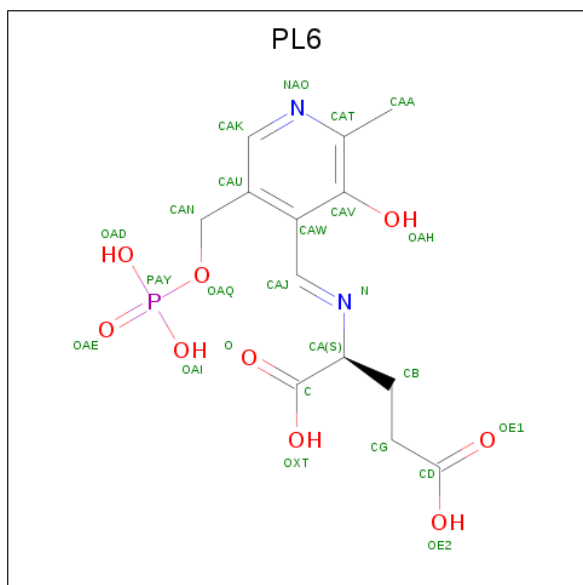


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CrmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total 3958	C 2476	N 716	O 755	S 11	0	0	0
1	B	512	Total 3958	C 2476	N 716	O 755	S 11	0	0	0
1	C	512	Total 3958	C 2476	N 716	O 755	S 11	0	0	0
1	D	512	Total 3958	C 2476	N 716	O 755	S 11	0	0	0

- Molecule 2 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylidene)-L-glutamic acid (three-letter code: PL6) (formula: C<sub>13</sub>H<sub>17</sub>N<sub>2</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 13	N 2	O 9	P 1	0	0
2	B	1	Total 25	C 13	N 2	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

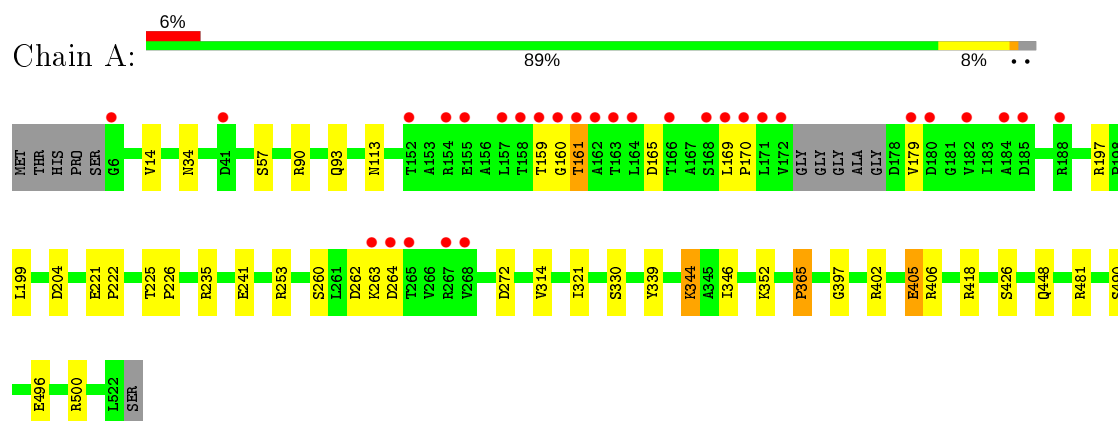
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	152	Total	O	0	0
			152	152		
4	C	130	Total	O	0	0
			130	130		
4	D	134	Total	O	0	0
			134	134		

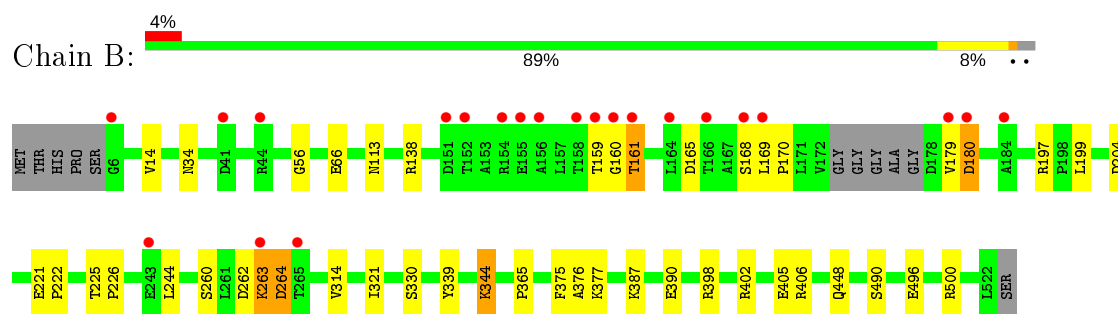
### 3 Residue-property plots [i](#)

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.

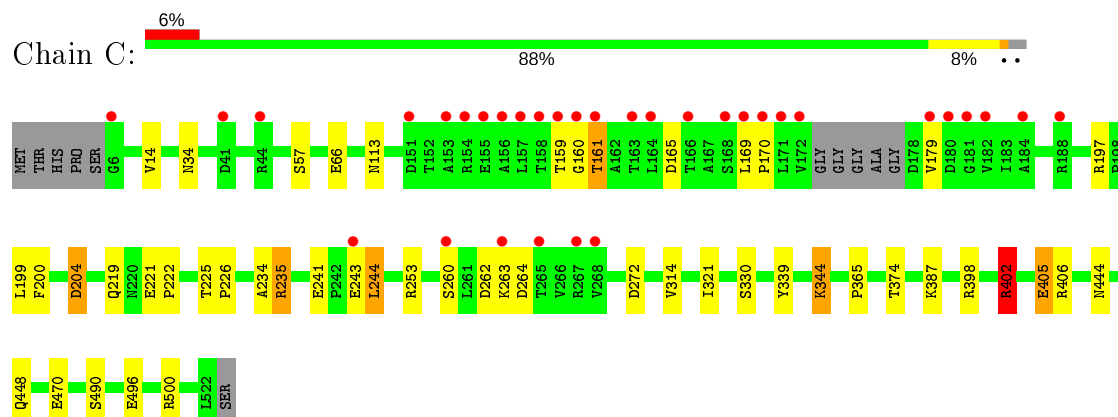
#### • Molecule 1: CrmG



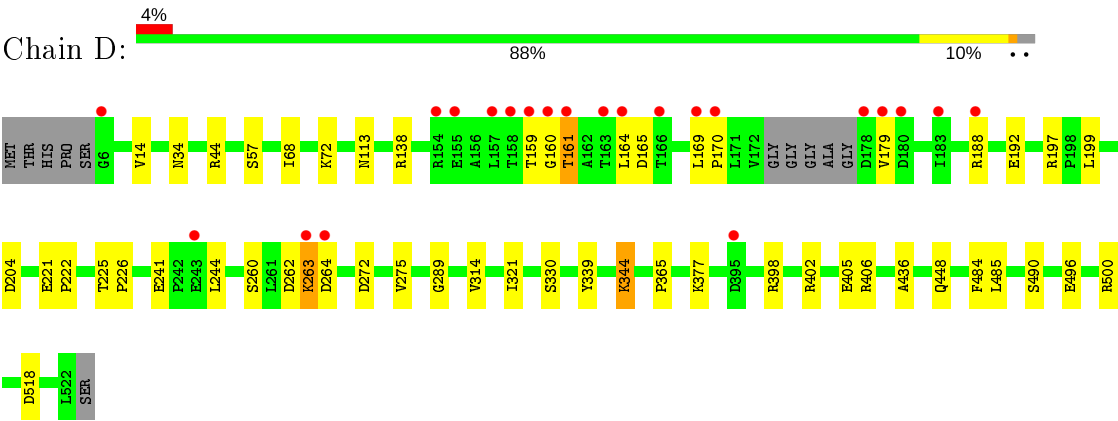
#### • Molecule 1: CrmG



#### • Molecule 1: CrmG



● Molecule 1: CrmG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.09 Å 83.93 Å 88.46 Å 106.60° 109.11° 95.13°	Depositor
Resolution (Å)	49.46 – 2.25 49.46 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.46-2.25) 95.0 (49.46-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.25 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.177 , 0.215 0.184 , 0.219	Depositor DCC
$R_{free}$ test set	4707 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.137 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL6, GOL

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	0.70	0/4025	0.85	1/5453 (0.0%)
1	B	0.72	0/4025	0.86	1/5453 (0.0%)
1	C	0.70	0/4025	0.87	2/5453 (0.0%)
1	D	0.71	0/4025	0.85	1/5453 (0.0%)
All	All	0.71	0/16100	0.86	5/21812 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	TYR	CB-CG-CD1	6.29	124.77	121.00
1	C	339	TYR	CB-CG-CD1	6.25	124.75	121.00
1	B	339	TYR	CB-CG-CD1	6.23	124.74	121.00
1	A	339	TYR	CB-CG-CD1	6.05	124.63	121.00
1	C	402	ARG	CG-CD-NE	5.74	123.86	111.80

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	3958	0	3937	25	0
1	B	3958	0	3937	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3958	0	3937	28	0
1	D	3958	0	3937	24	0
2	A	25	0	12	4	0
2	B	25	0	13	4	0
2	C	25	0	13	3	0
2	D	25	0	13	6	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
4	A	132	0	0	7	0
4	B	152	0	0	5	0
4	C	130	0	0	4	0
4	D	134	0	0	3	0
All	All	16492	0	15815	105	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 (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:O	4:A:701:HOH:O	2.04	0.76
2:D:601:PL6:OAH	2:D:601:PL6:N	2.16	0.73
1:A:496:GLU:OE1	1:A:500:ARG:NH2	2.23	0.72
2:C:601:PL6:OAH	2:C:601:PL6:N	2.17	0.71
1:B:496:GLU:OE1	1:B:500:ARG:NH2	2.24	0.71
2:A:601:PL6:N	2:A:601:PL6:OAH	2.21	0.70
1:C:496:GLU:OE1	1:C:500:ARG:NH2	2.26	0.69
1:D:344:LYS:O	4:D:701:HOH:O	2.11	0.67
1:B:344:LYS:O	4:B:701:HOH:O	2.12	0.66
2:C:601:PL6:O	4:C:701:HOH:O	2.12	0.66
1:A:418:ARG:HH12	1:C:244:LEU:HD21	1.61	0.65
1:B:169:LEU:N	1:B:170:PRO:HD2	2.14	0.62
1:A:169:LEU:N	1:A:170:PRO:HD2	2.15	0.62
1:B:390:GLU:OE2	4:B:702:HOH:O	2.16	0.62
1:C:169:LEU:N	1:C:170:PRO:HD2	2.15	0.61
2:A:601:PL6:OXT	4:A:702:HOH:O	2.16	0.61
1:A:14:VAL:HG21	1:B:365:PRO:HB3	1.84	0.60
1:C:14:VAL:HG21	1:D:365:PRO:HB3	1.84	0.59
1:D:344:LYS:HZ3	2:D:601:PL6:HA	1.67	0.59
2:B:601:PL6:N	2:B:601:PL6:OAH	2.22	0.59
1:C:344:LYS:O	4:C:702:HOH:O	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LYS:NZ	2:D:601:PL6:HA	2.19	0.58
1:A:90:ARG:HD2	4:A:715:HOH:O	2.03	0.58
1:B:180:ASP:OD1	1:B:180:ASP:N	2.32	0.58
1:A:93:GLN:NE2	4:A:706:HOH:O	2.35	0.58
1:B:344:LYS:NZ	2:B:601:PL6:CAJ	2.68	0.57
1:A:397:GLY:HA2	4:A:734:HOH:O	2.05	0.57
1:A:314:VAL:HG11	1:A:330:SER:HB3	1.88	0.55
1:B:66:GLU:HG3	1:B:387:LYS:HE3	1.89	0.54
1:D:496:GLU:OE2	1:D:500:ARG:NH2	2.41	0.54
1:A:481:ARG:HD3	4:A:705:HOH:O	2.09	0.53
1:D:405:GLU:OE2	1:D:406:ARG:HD2	2.09	0.53
1:C:66:GLU:HG2	1:C:387:LYS:HE3	1.91	0.53
1:C:405:GLU:OE2	1:C:406:ARG:HD2	2.09	0.52
1:B:314:VAL:HG11	1:B:330:SER:HB3	1.90	0.52
1:C:314:VAL:HG11	1:C:330:SER:HB3	1.91	0.52
1:B:159:THR:O	1:B:161:THR:N	2.43	0.52
1:C:159:THR:O	1:C:161:THR:N	2.43	0.52
1:C:244:LEU:HD12	1:C:244:LEU:N	2.25	0.52
1:D:314:VAL:HG11	1:D:330:SER:HB3	1.91	0.52
1:B:405:GLU:OE2	1:B:406:ARG:HD2	2.10	0.51
1:D:159:THR:O	1:D:161:THR:N	2.44	0.51
1:C:470:GLU:OE1	4:C:703:HOH:O	2.19	0.51
1:A:159:THR:O	1:A:161:THR:N	2.44	0.50
1:B:138:ARG:NE	4:B:707:HOH:O	2.32	0.50
1:B:66:GLU:HG3	1:B:387:LYS:CE	2.41	0.50
1:C:244:LEU:CD1	1:C:244:LEU:N	2.74	0.50
1:A:225:THR:N	1:A:226:PRO:CD	2.74	0.50
1:D:225:THR:N	1:D:226:PRO:CD	2.75	0.50
1:C:365:PRO:HB3	1:D:14:VAL:HG21	1.93	0.50
1:C:225:THR:N	1:C:226:PRO:CD	2.75	0.49
1:A:344:LYS:HZ3	2:A:601:PL6:HA	1.78	0.49
1:C:402:ARG:HG2	1:C:402:ARG:HH21	1.77	0.49
1:B:56:GLY:O	4:B:703:HOH:O	2.20	0.49
1:A:365:PRO:HB3	1:B:14:VAL:HG21	1.95	0.49
1:A:352:LYS:HD3	1:B:375:PHE:HB3	1.95	0.48
1:B:225:THR:N	1:B:226:PRO:CD	2.75	0.48
1:B:344:LYS:HZ3	2:B:601:PL6:CAJ	2.27	0.48
1:D:138:ARG:NE	4:D:703:HOH:O	2.35	0.48
1:A:405:GLU:OE2	1:A:406:ARG:HD2	2.14	0.47
1:C:344:LYS:NZ	2:C:601:PL6:CAJ	2.77	0.47
1:D:34:ASN:ND2	1:D:490:SER:OG	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:HG2	1:C:387:LYS:CE	2.46	0.46
1:B:165:ASP:C	1:B:165:ASP:OD1	2.54	0.46
1:A:344:LYS:NZ	2:A:601:PL6:HA	2.31	0.46
1:D:344:LYS:NZ	2:D:601:PL6:CA	2.78	0.46
1:A:165:ASP:OD1	1:A:165:ASP:C	2.55	0.46
1:A:221:GLU:N	1:A:222:PRO:HD2	2.30	0.46
1:C:221:GLU:N	1:C:222:PRO:HD2	2.31	0.46
1:C:165:ASP:OD1	1:C:165:ASP:C	2.55	0.45
1:C:235:ARG:NH1	4:C:705:HOH:O	2.29	0.45
1:A:34:ASN:ND2	1:A:490:SER:OG	2.49	0.45
1:B:344:LYS:HZ1	2:B:601:PL6:CAJ	2.30	0.45
1:B:34:ASN:ND2	1:B:490:SER:OG	2.50	0.44
1:B:377:LYS:HE2	4:B:735:HOH:O	2.17	0.44
1:A:262:ASP:O	1:A:264:ASP:N	2.48	0.44
1:B:169:LEU:N	1:B:170:PRO:CD	2.81	0.44
1:B:221:GLU:N	1:B:222:PRO:HD2	2.33	0.44
1:D:165:ASP:OD1	1:D:165:ASP:C	2.55	0.44
1:D:221:GLU:N	1:D:222:PRO:HD2	2.33	0.44
1:D:344:LYS:HZ1	2:D:601:PL6:CA	2.31	0.43
1:C:57:SER:HA	1:C:344:LYS:HB3	2.01	0.43
1:C:34:ASN:ND2	1:C:490:SER:OG	2.50	0.43
1:A:169:LEU:N	1:A:170:PRO:CD	2.82	0.43
1:D:169:LEU:N	1:D:170:PRO:CD	2.82	0.42
1:D:262:ASP:O	1:D:264:ASP:N	2.49	0.42
1:C:405:GLU:OE2	1:C:406:ARG:CD	2.67	0.42
1:B:405:GLU:OE2	1:B:406:ARG:CD	2.68	0.42
1:D:377:LYS:HE2	4:D:761:HOH:O	2.18	0.42
1:B:262:ASP:O	1:B:264:ASP:N	2.50	0.42
1:D:405:GLU:OE2	1:D:406:ARG:CD	2.68	0.42
1:A:93:GLN:HB2	4:A:706:HOH:O	2.20	0.41
1:D:68:ILE:O	1:D:72:LYS:HG3	2.21	0.41
1:A:57:SER:HA	1:A:344:LYS:HB3	2.02	0.41
1:B:168:SER:C	1:B:170:PRO:HD2	2.41	0.41
1:C:169:LEU:N	1:C:170:PRO:CD	2.82	0.41
1:A:405:GLU:OE2	1:A:406:ARG:CD	2.69	0.41
1:C:200:PHE:O	1:C:234:ALA:HA	2.21	0.41
1:C:262:ASP:O	1:C:264:ASP:N	2.48	0.41
1:C:374:THR:OG1	2:D:601:PL6:HBA	2.21	0.41
1:D:289:GLY:HA3	1:D:484:PHE:CD2	2.56	0.41
1:C:204:ASP:HA	1:C:219:GLN:OE1	2.21	0.40
1:D:436:ALA:HA	1:D:485:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:SER:HA	1:D:344:LYS:HB3	2.03	0.40
1:B:376:ALA:O	1:B:377:LYS:HB2	2.21	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	508/523 (97%)	490 (96%)	13 (3%)	5 (1%)	15	13
1	B	508/523 (97%)	488 (96%)	15 (3%)	5 (1%)	15	13
1	C	508/523 (97%)	490 (96%)	13 (3%)	5 (1%)	15	13
1	D	508/523 (97%)	489 (96%)	14 (3%)	5 (1%)	15	13
All	All	2032/2092 (97%)	1957 (96%)	55 (3%)	20 (1%)	15	13

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLY
1	A	263	LYS
1	A	344	LYS
1	B	160	GLY
1	B	263	LYS
1	B	344	LYS
1	C	160	GLY
1	C	263	LYS
1	C	344	LYS
1	D	160	GLY
1	D	263	LYS
1	D	344	LYS
1	A	161	THR

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Mol	Chain	Res	Type
1	B	161	THR
1	C	161	THR
1	D	161	THR
1	B	179	VAL
1	C	179	VAL
1	A	179	VAL
1	D	179	VAL

### 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	416/422 (99%)	400 (96%)	16 (4%)	33	39
1	B	416/422 (99%)	403 (97%)	13 (3%)	40	49
1	C	416/422 (99%)	399 (96%)	17 (4%)	30	36
1	D	416/422 (99%)	397 (95%)	19 (5%)	27	30
All	All	1664/1688 (99%)	1599 (96%)	65 (4%)	32	38

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	197	ARG
1	A	199	LEU
1	A	204	ASP
1	A	235	ARG
1	A	241	GLU
1	A	253	ARG
1	A	260	SER
1	A	272	ASP
1	A	321	ILE
1	A	346	ILE
1	A	365	PRO
1	A	402	ARG
1	A	405	GLU

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Mol	Chain	Res	Type
1	A	426	SER
1	A	448	GLN
1	B	113	ASN
1	B	180	ASP
1	B	197	ARG
1	B	199	LEU
1	B	204	ASP
1	B	244	LEU
1	B	260	SER
1	B	263	LYS
1	B	264	ASP
1	B	321	ILE
1	B	398	ARG
1	B	402	ARG
1	B	448	GLN
1	C	113	ASN
1	C	197	ARG
1	C	199	LEU
1	C	204	ASP
1	C	235	ARG
1	C	241	GLU
1	C	243	GLU
1	C	244	LEU
1	C	253	ARG
1	C	260	SER
1	C	272	ASP
1	C	321	ILE
1	C	398	ARG
1	C	402	ARG
1	C	405	GLU
1	C	444	ASN
1	C	448	GLN
1	D	44	ARG
1	D	113	ASN
1	D	164	LEU
1	D	188	ARG
1	D	192	GLU
1	D	197	ARG
1	D	199	LEU
1	D	204	ASP
1	D	241	GLU
1	D	244	LEU

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Mol	Chain	Res	Type
1	D	260	SER
1	D	263	LYS
1	D	272	ASP
1	D	275	VAL
1	D	321	ILE
1	D	398	ARG
1	D	402	ARG
1	D	448	GLN
1	D	518	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	B	34	ASN
1	B	88	GLN
1	C	34	ASN
1	C	88	GLN
1	C	444	ASN
1	D	34	ASN
1	D	88	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 monosaccharides in this entry.

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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PL6	D	601	-	19,25,25	1.80	4 (21%)	24,35,35	2.66	6 (25%)
2	PL6	A	601	-	19,25,25	1.50	4 (21%)	24,35,35	2.53	8 (33%)
2	PL6	C	601	-	19,25,25	1.41	3 (15%)	24,35,35	2.43	9 (37%)
2	PL6	B	601	-	19,25,25	1.92	5 (26%)	24,35,35	2.51	7 (29%)
3	GOL	C	602	-	5,5,5	0.14	0	5,5,5	0.41	0
3	GOL	A	602	-	5,5,5	0.15	0	5,5,5	0.30	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
2	PL6	D	601	-	-	2/14/20/20	0/1/1/1
2	PL6	A	601	-	-	4/14/20/20	0/1/1/1
2	PL6	C	601	-	-	2/14/20/20	0/1/1/1
2	PL6	B	601	-	-	3/14/20/20	0/1/1/1
3	GOL	C	602	-	-	4/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	PL6	CAJ-N	4.85	1.36	1.27
2	B	601	PL6	CB-CA	4.70	1.59	1.53
2	B	601	PL6	CAJ-N	3.68	1.34	1.27
2	D	601	PL6	CA-N	3.57	1.50	1.46
2	B	601	PL6	CAV-CAT	-3.56	1.37	1.40
2	A	601	PL6	CA-N	3.53	1.50	1.46
2	C	601	PL6	CAJ-N	3.10	1.33	1.27
2	D	601	PL6	CB-CA	3.04	1.57	1.53
2	A	601	PL6	CAJ-N	2.85	1.32	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PL6	CAW-CAV	-2.53	1.37	1.40
2	C	601	PL6	CAV-CAT	-2.50	1.38	1.40
2	A	601	PL6	CAT-NAO	2.43	1.38	1.33
2	A	601	PL6	CB-CA	2.38	1.56	1.53
2	C	601	PL6	CA-N	2.32	1.49	1.46
2	D	601	PL6	CAV-CAT	-2.22	1.38	1.40
2	B	601	PL6	CA-N	2.18	1.49	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	PL6	CA-N-CAJ	9.07	129.70	117.40
2	B	601	PL6	CA-N-CAJ	8.26	128.60	117.40
2	D	601	PL6	CA-N-CAJ	7.99	128.23	117.40
2	C	601	PL6	CA-N-CAJ	7.02	126.92	117.40
2	D	601	PL6	CG-CB-CA	5.95	126.43	113.28
2	B	601	PL6	CG-CB-CA	4.60	123.44	113.28
2	D	601	PL6	CAV-CAW-CAJ	-4.40	112.22	120.41
2	D	601	PL6	CAU-CAW-CAJ	4.19	128.45	121.56
2	C	601	PL6	CG-CB-CA	3.95	122.01	113.28
2	C	601	PL6	CAV-CAW-CAJ	-3.84	113.26	120.41
2	A	601	PL6	CAW-CAJ-N	-3.82	114.52	123.01
2	B	601	PL6	CAV-CAW-CAJ	-3.69	113.54	120.41
2	B	601	PL6	CAU-CAW-CAJ	3.66	127.57	121.56
2	B	601	PL6	CAA-CAT-CAV	-3.47	116.60	120.89
2	C	601	PL6	CB-CG-CD	-3.20	106.72	113.59
2	D	601	PL6	CAN-CAU-CAK	-3.19	114.12	119.37
2	A	601	PL6	CG-CB-CA	3.14	120.22	113.28
2	C	601	PL6	CAW-CAJ-N	-3.04	116.26	123.01
2	C	601	PL6	CAW-CAV-CAT	-3.00	118.33	120.19
2	A	601	PL6	CAU-CAW-CAJ	2.84	126.23	121.56
2	C	601	PL6	CAN-CAU-CAK	-2.83	114.71	119.37
2	D	601	PL6	CAW-CAJ-N	-2.59	117.26	123.01
2	A	601	PL6	CAV-CAW-CAJ	-2.54	115.68	120.41
2	C	601	PL6	CAU-CAW-CAJ	2.50	125.67	121.56
2	A	601	PL6	OAH-CAV-CAT	2.47	122.87	117.49
2	B	601	PL6	CAW-CAJ-N	-2.24	118.03	123.01
2	C	601	PL6	OAH-CAV-CAT	2.23	122.35	117.49
2	B	601	PL6	CAN-CAU-CAK	-2.19	115.77	119.37
2	A	601	PL6	CAV-CAW-CAU	-2.18	116.59	118.26
2	A	601	PL6	CB-CG-CD	-2.04	109.21	113.59

There are no chirality outliers.

All (17) torsion outliers are listed below:

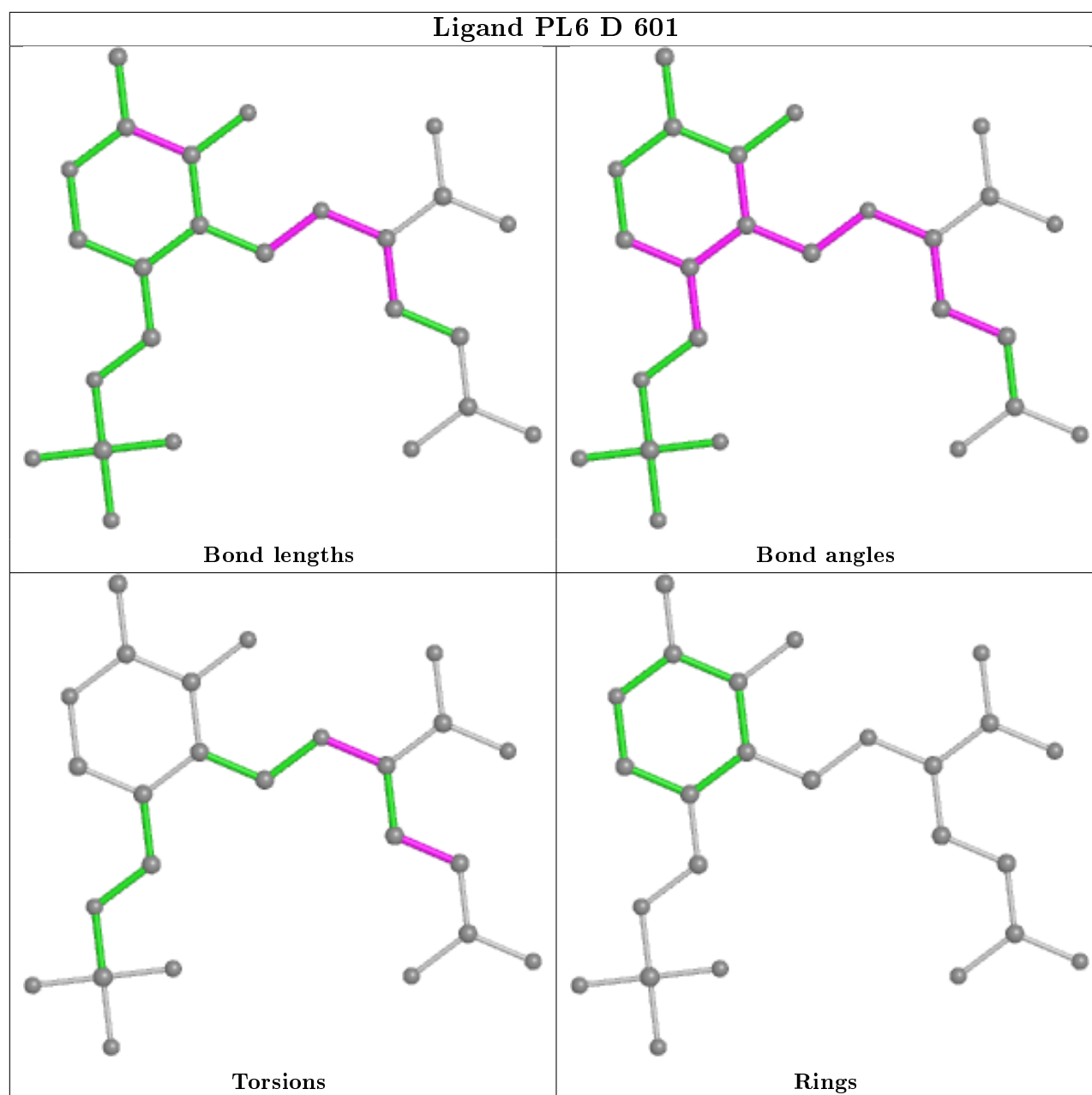
Mol	Chain	Res	Type	Atoms
2	D	601	PL6	CB-CA-N-CAJ
2	D	601	PL6	CA-CB-CG-CD
2	A	601	PL6	CB-CA-N-CAJ
2	A	601	PL6	N-CA-CB-CG
2	A	601	PL6	C-CA-CB-CG
2	C	601	PL6	CB-CA-N-CAJ
2	B	601	PL6	CB-CA-N-CAJ
2	B	601	PL6	N-CA-CB-CG
2	B	601	PL6	C-CA-CB-CG
3	C	602	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-O2
2	C	601	PL6	CA-CB-CG-CD
3	A	602	GOL	O1-C1-C2-O2
3	C	602	GOL	O2-C2-C3-O3
2	A	601	PL6	C-CA-N-CAJ
3	C	602	GOL	C1-C2-C3-O3

There are no ring outliers.

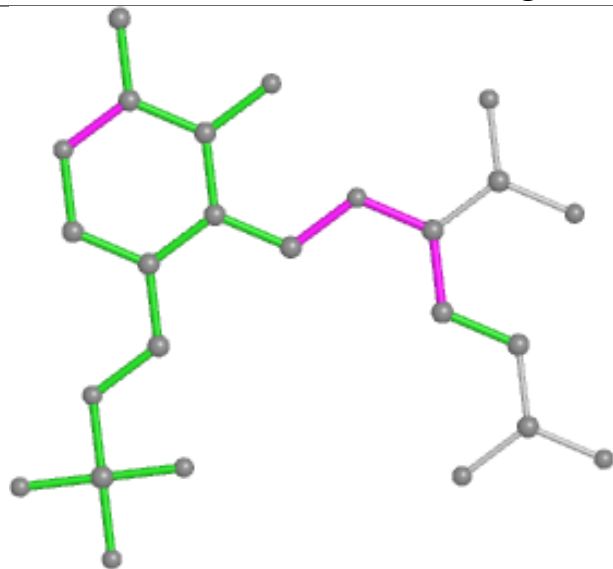
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	PL6	6	0
2	A	601	PL6	4	0
2	C	601	PL6	3	0
2	B	601	PL6	4	0

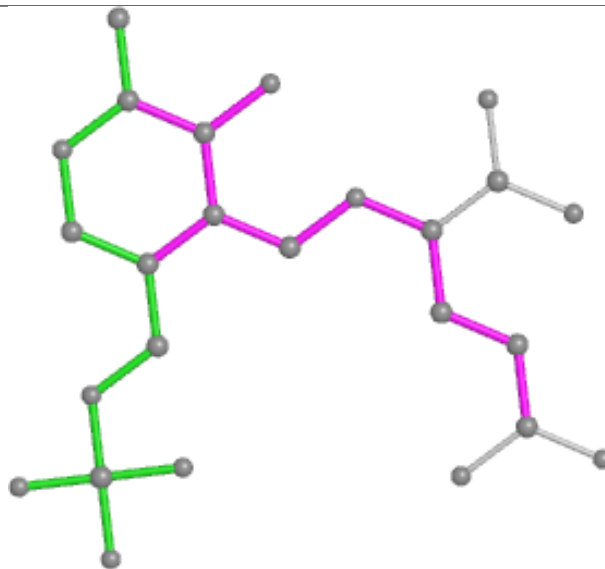
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



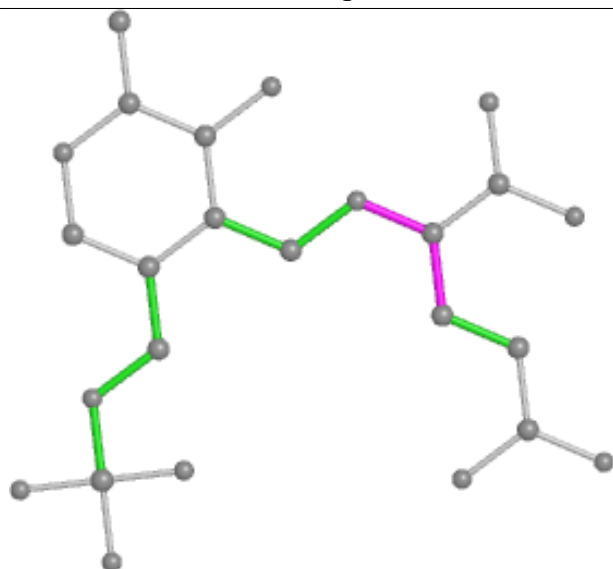
## Ligand PL6 A 601



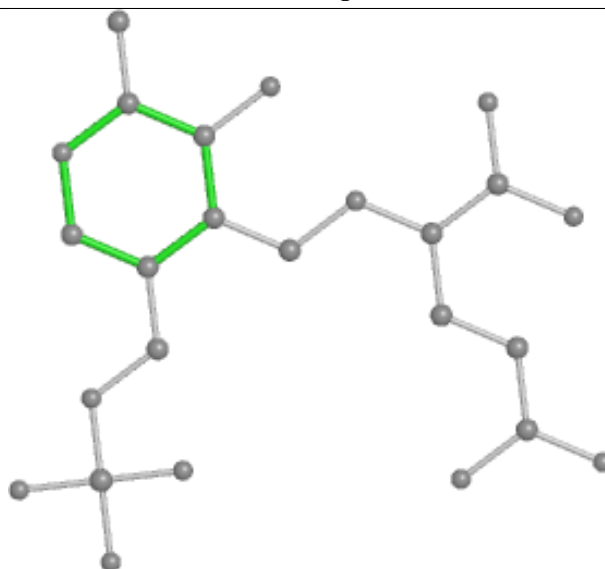
Bond lengths



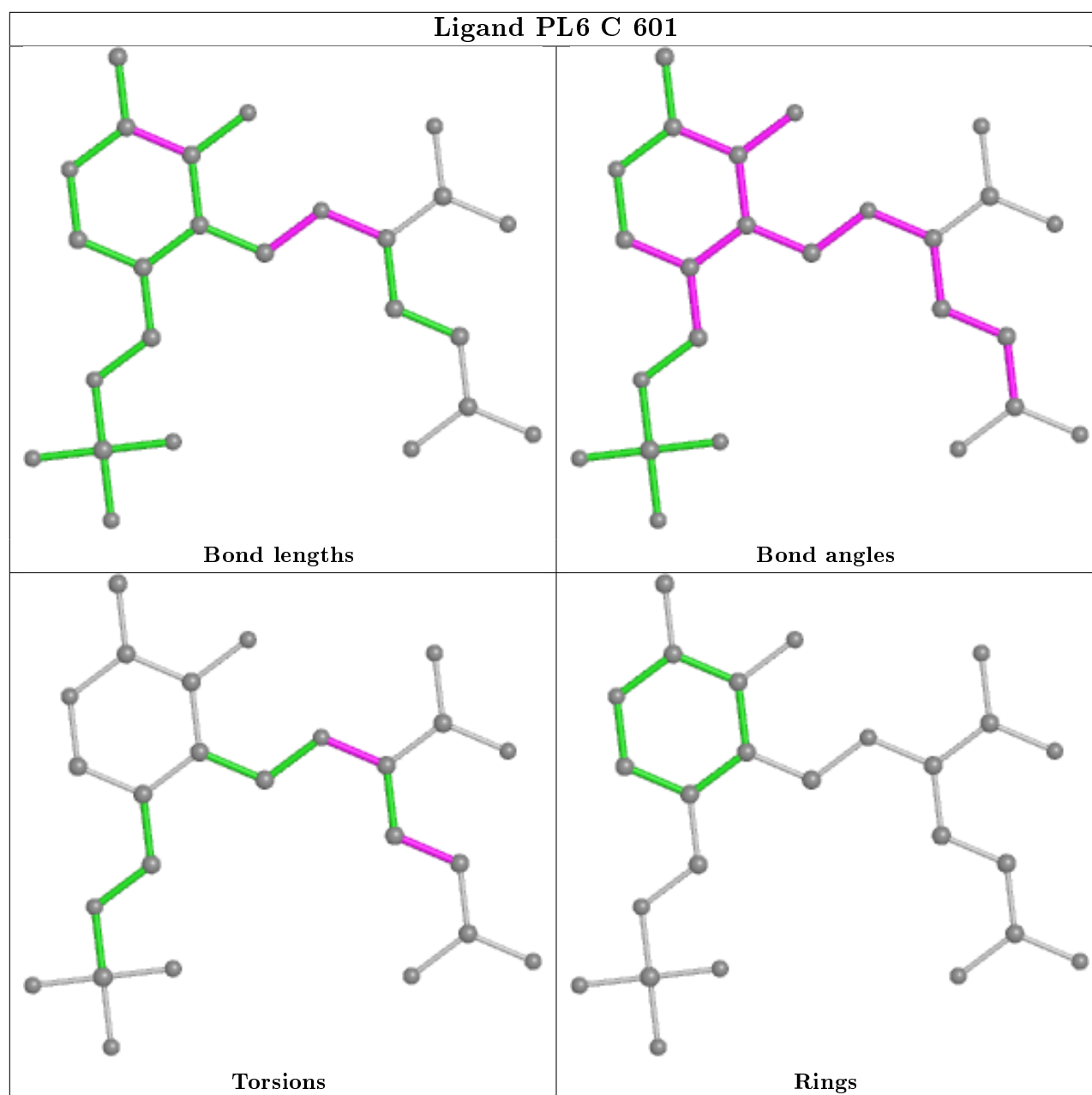
Bond angles

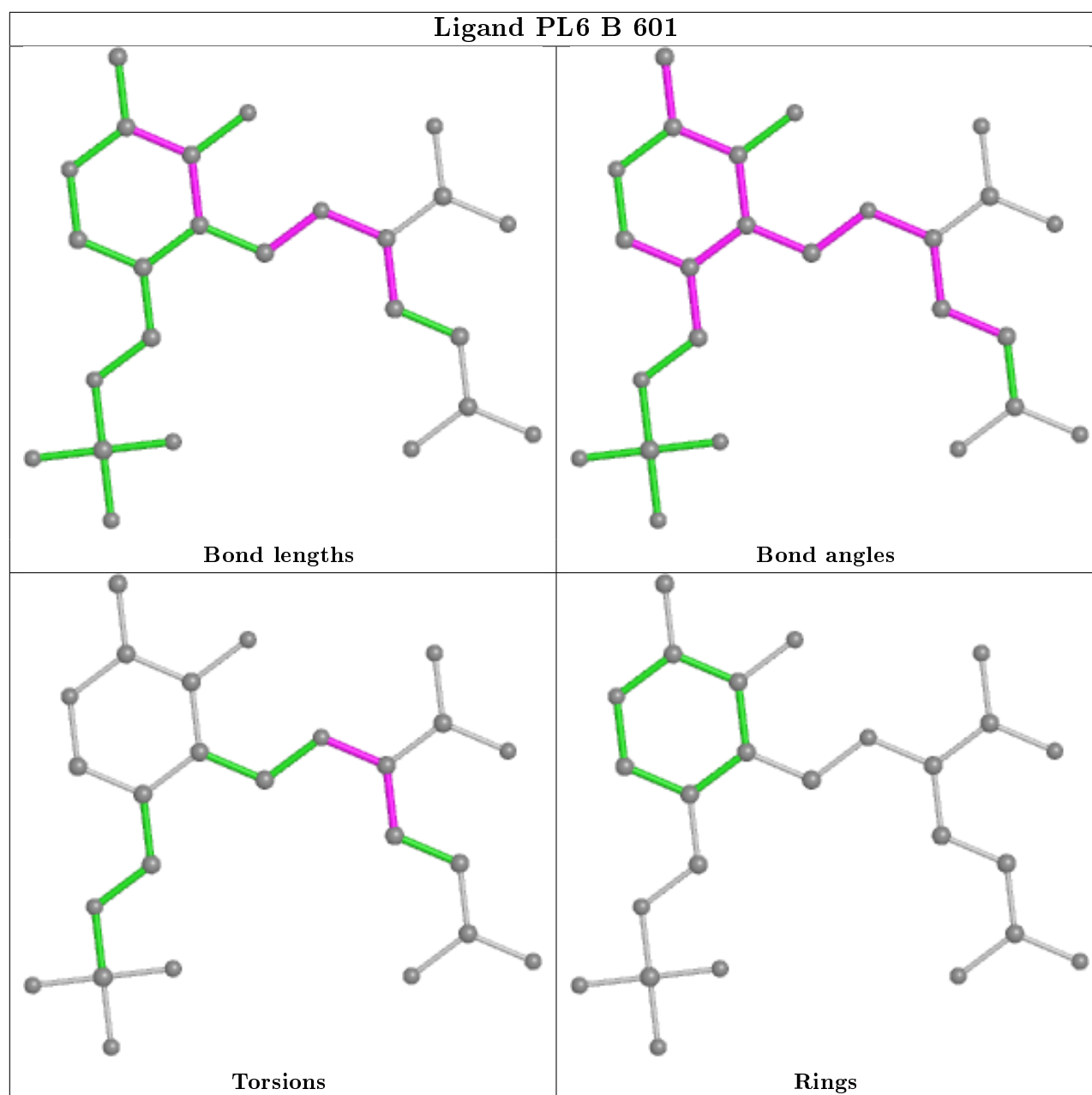


Torsions



Rings





## 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, 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	512/523 (97%)	-0.03	30 (5%)	22	24	16, 28, 61, 96	0
1	B	512/523 (97%)	-0.07	22 (4%)	35	37	15, 27, 62, 87	0
1	C	512/523 (97%)	0.02	33 (6%)	19	21	14, 27, 69, 96	0
1	D	512/523 (97%)	-0.05	22 (4%)	35	37	15, 27, 59, 90	0
All	All	2048/2092 (97%)	-0.03	107 (5%)	27	30	14, 27, 62, 96	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	5.8
1	A	263	LYS	5.4
1	A	161	THR	5.0
1	D	179	VAL	4.8
1	A	164	LEU	4.8
1	B	179	VAL	4.6
1	A	159	THR	4.5
1	D	158	THR	4.4
1	C	161	THR	4.3
1	D	160	GLY	4.2
1	C	166	THR	4.1
1	C	164	LEU	4.1
1	A	179	VAL	4.1
1	C	179	VAL	4.0
1	D	159	THR	4.0
1	C	170	PRO	3.9
1	C	158	THR	3.8
1	B	160	GLY	3.7
1	A	158	THR	3.7
1	B	155	GLU	3.6
1	D	166	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	161	THR	3.5
1	C	155	GLU	3.5
1	D	155	GLU	3.4
1	C	156	ALA	3.4
1	A	155	GLU	3.4
1	C	181	GLY	3.2
1	C	153	ALA	3.2
1	C	154	ARG	3.2
1	D	154	ARG	3.2
1	C	171	LEU	3.1
1	C	169	LEU	3.1
1	C	172	VAL	3.0
1	B	159	THR	3.0
1	A	172	VAL	3.0
1	C	263	LYS	3.0
1	D	263	LYS	3.0
1	C	268	VAL	3.0
1	A	157	LEU	3.0
1	D	243	GLU	3.0
1	C	267	ARG	3.0
1	B	263	LYS	3.0
1	A	166	THR	3.0
1	D	161	THR	2.9
1	C	168	SER	2.9
1	A	168	SER	2.8
1	A	171	LEU	2.8
1	B	265	THR	2.8
1	A	154	ARG	2.8
1	A	268	VAL	2.8
1	B	166	THR	2.8
1	D	170	PRO	2.7
1	A	182	VAL	2.7
1	B	169	LEU	2.7
1	D	6	GLY	2.7
1	C	157	LEU	2.7
1	C	163	THR	2.7
1	B	151	ASP	2.6
1	D	264	ASP	2.6
1	A	163	THR	2.5
1	A	169	LEU	2.5
1	A	6	GLY	2.5
1	B	168	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	243	GLU	2.5
1	A	265	THR	2.5
1	B	154	ARG	2.5
1	D	169	LEU	2.5
1	C	160	GLY	2.4
1	A	41	ASP	2.4
1	D	157	LEU	2.4
1	D	163	THR	2.4
1	D	180	ASP	2.4
1	A	264	ASP	2.4
1	C	44	ARG	2.4
1	C	151	ASP	2.4
1	B	164	LEU	2.4
1	A	162	ALA	2.4
1	B	180	ASP	2.4
1	C	159	THR	2.4
1	B	41	ASP	2.4
1	D	188	ARG	2.3
1	C	6	GLY	2.3
1	B	6	GLY	2.3
1	B	156	ALA	2.3
1	A	152	THR	2.3
1	C	182	VAL	2.3
1	C	180	ASP	2.3
1	D	178	ASP	2.3
1	C	260	SER	2.3
1	C	265	THR	2.3
1	B	44	ARG	2.2
1	D	164	LEU	2.2
1	B	243	GLU	2.2
1	B	158	THR	2.2
1	A	188	ARG	2.2
1	C	41	ASP	2.2
1	D	183	ILE	2.2
1	A	170	PRO	2.2
1	A	180	ASP	2.2
1	C	184	ALA	2.1
1	B	152	THR	2.1
1	D	395	ASP	2.1
1	B	184	ALA	2.1
1	A	184	ALA	2.1
1	A	185	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	188	ARG	2.0
1	A	267	ARG	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](#)

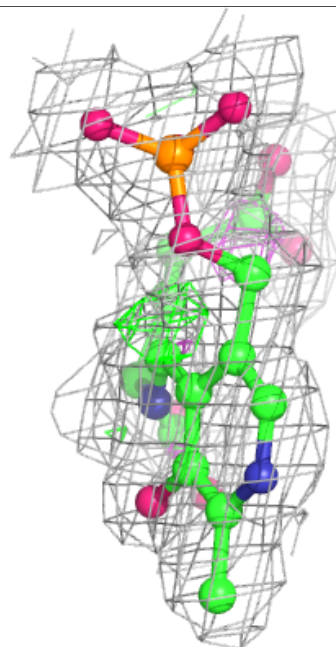
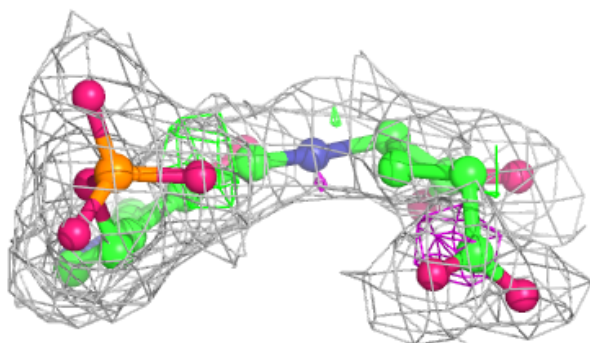
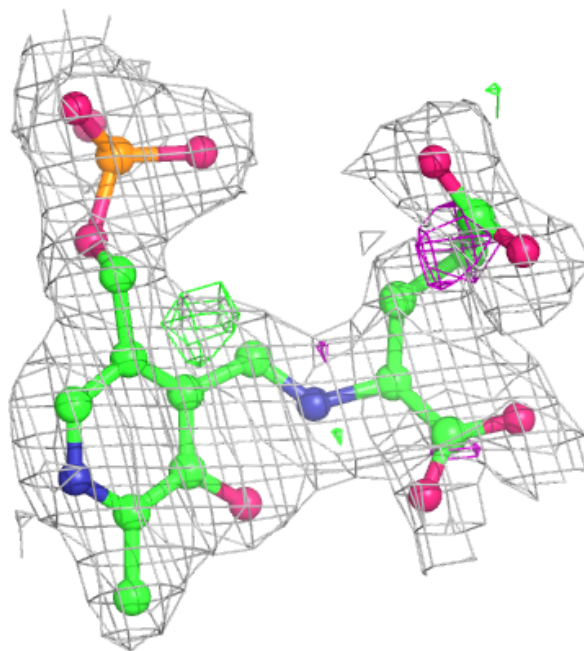
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GOL	A	602	6/6	0.90	0.17	41,43,46,47	0
3	GOL	C	602	6/6	0.94	0.17	45,48,50,55	0
2	PL6	D	601	25/25	0.95	0.18	18,25,51,58	0
2	PL6	B	601	25/25	0.96	0.17	19,24,58,62	0
2	PL6	C	601	25/25	0.97	0.14	19,26,56,66	0
2	PL6	A	601	25/25	0.97	0.17	20,25,65,69	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.

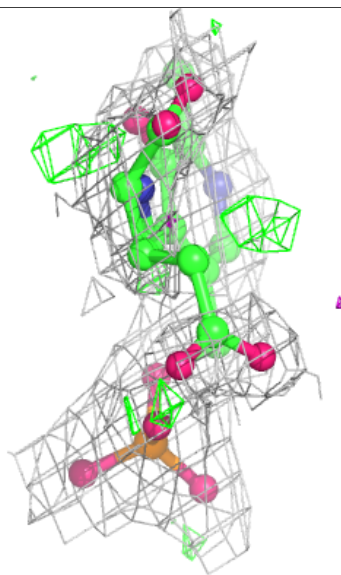
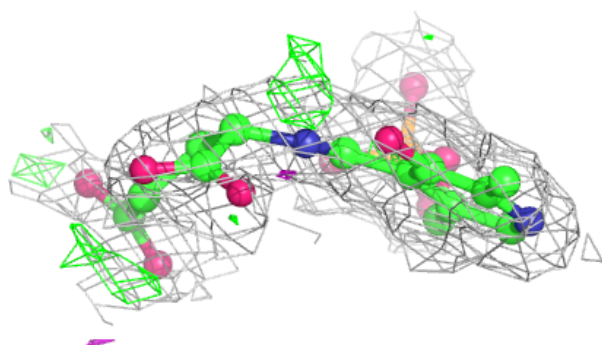
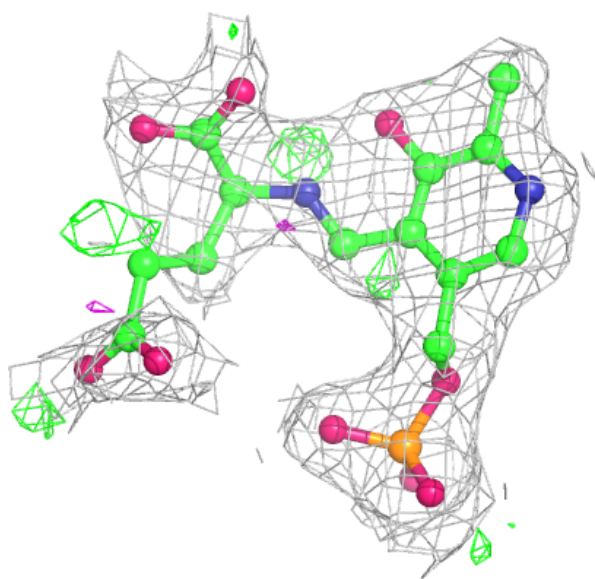
**Electron density around PL6 D 601:**

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



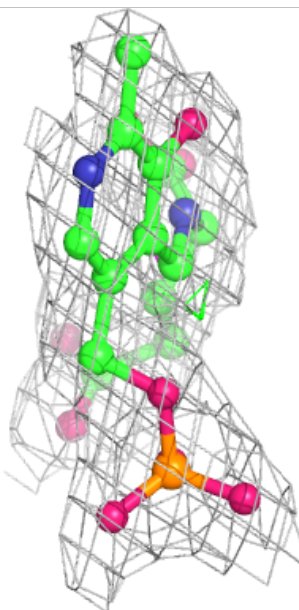
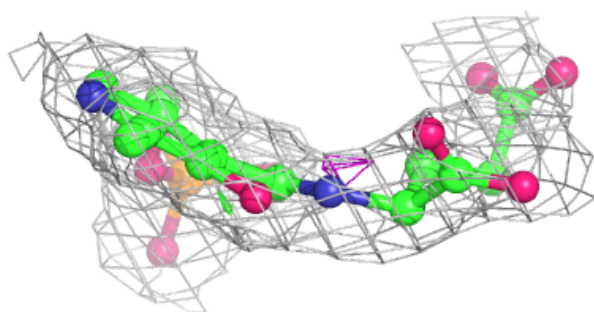
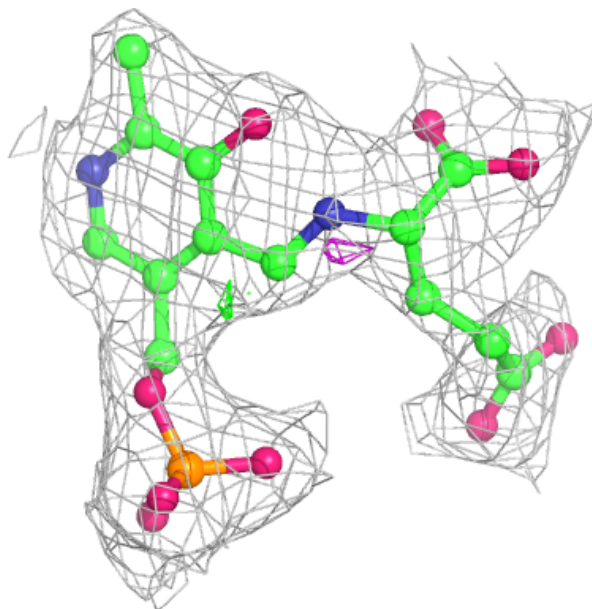
**Electron density around PL6 B 601:**

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



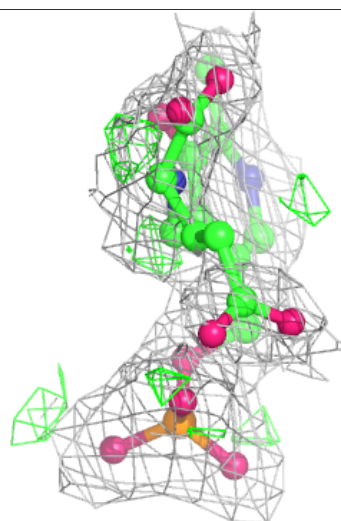
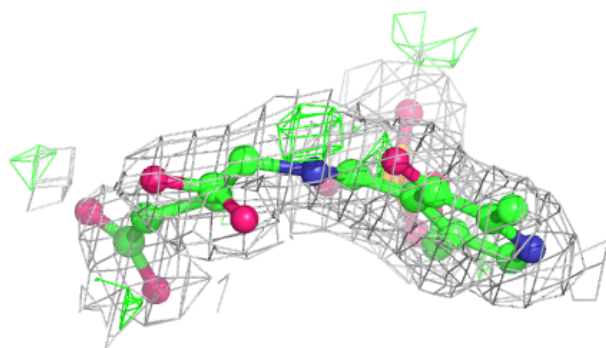
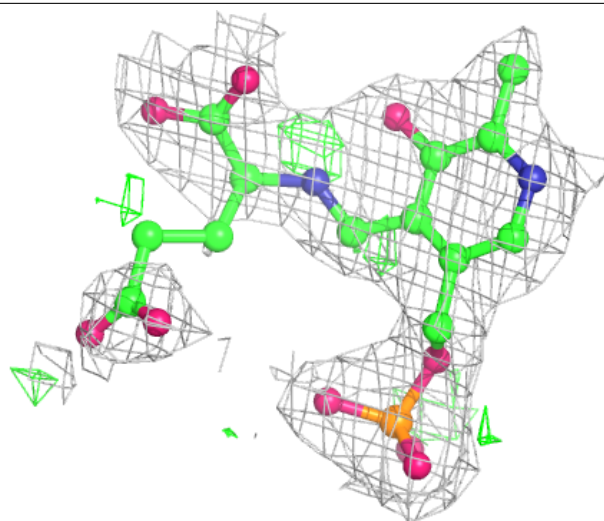
**Electron density around PL6 C 601:**

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



**Electron density around PL6 A 601:**

$2mF_o-DF_c$  (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.