



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:21 AM UTC

PDB ID : 4ZHX / pdb_00004zhx
Title : Novel binding site for allosteric activation of AMPK
Authors : Langendorf, C.G.; Ngoei, K.R.; Issa, S.M.A.; Ling, N.; Gorman, M.A.; Parker, M.W.; Sakamoto, K.; Scott, J.W.; Oakhill, J.S.; Kemp, B.E.
Deposited on : 2015-04-27
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

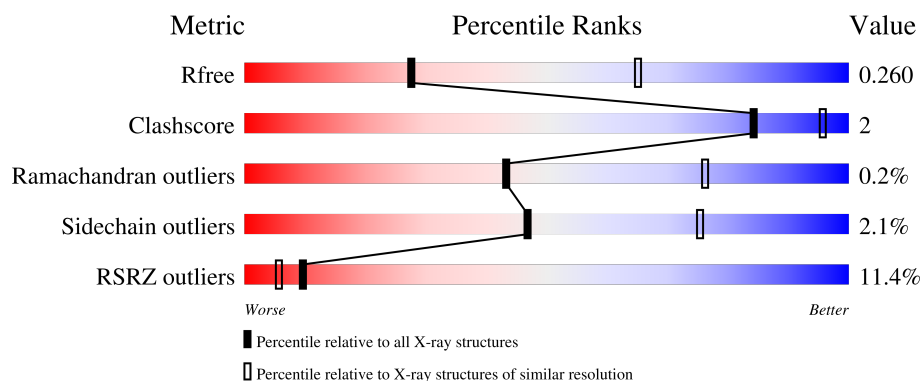
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	565	7% 68% 28%
1	C	565	10% 73% 7% 20%
2	B	270	13% 55% 9% 36%
2	D	270	7% 56% 9% 35%
3	E	336	8% 78% 10% 11%

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Mol	Chain	Length	Quality of chain
3	F	336	8% 82% 7% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14587 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 5'-AMP-activated protein kinase catalytic subunit alpha-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	P	S	0	0	0
			3255	2092	563	577	1	22			
1	C	453	Total	C	N	O	P	S	0	0	0
			3567	2283	617	640	1	26			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP P54646
A	-11	GLY	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	SER	-	expression tag	UNP P54646
A	-8	HIS	-	expression tag	UNP P54646
A	-7	HIS	-	expression tag	UNP P54646
A	-6	HIS	-	expression tag	UNP P54646
A	-5	HIS	-	expression tag	UNP P54646
A	-4	HIS	-	expression tag	UNP P54646
A	-3	HIS	-	expression tag	UNP P54646
A	-2	SER	-	expression tag	UNP P54646
A	-1	GLN	-	expression tag	UNP P54646
A	0	ASP	-	expression tag	UNP P54646
A	1	PRO	-	expression tag	UNP P54646
A	271	GLY	ASP	variant	UNP P54646
C	-12	MET	-	initiating methionine	UNP P54646
C	-11	GLY	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	SER	-	expression tag	UNP P54646
C	-8	HIS	-	expression tag	UNP P54646
C	-7	HIS	-	expression tag	UNP P54646
C	-6	HIS	-	expression tag	UNP P54646
C	-5	HIS	-	expression tag	UNP P54646
C	-4	HIS	-	expression tag	UNP P54646
C	-3	HIS	-	expression tag	UNP P54646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P54646
C	-1	GLN	-	expression tag	UNP P54646
C	0	ASP	-	expression tag	UNP P54646
C	1	PRO	-	expression tag	UNP P54646
C	271	GLY	ASP	variant	UNP P54646

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	P	S	0	0	0
			1310	845	221	240	1	3			
2	D	175	Total	C	N	O	P	S	0	0	0
			1373	884	230	252	1	6			

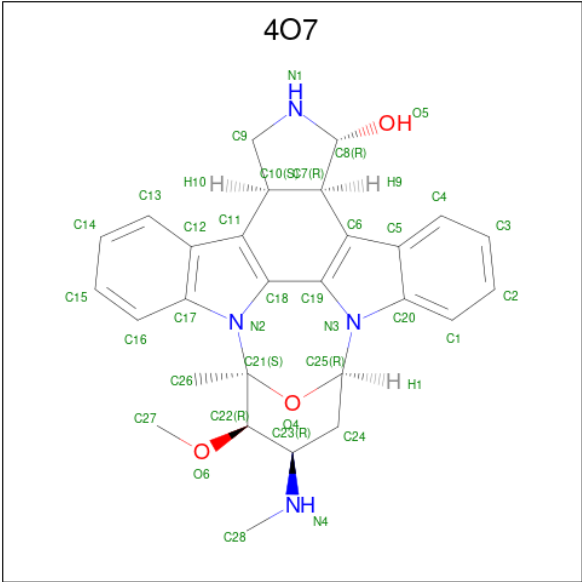
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	298	Total	C	N	O	S		0	2	0
			2381	1553	398	423	7				
3	F	300	Total	C	N	O	S		0	0	0
			2366	1535	396	428	7				

There are 12 discrepancies between the modelled and reference sequences:

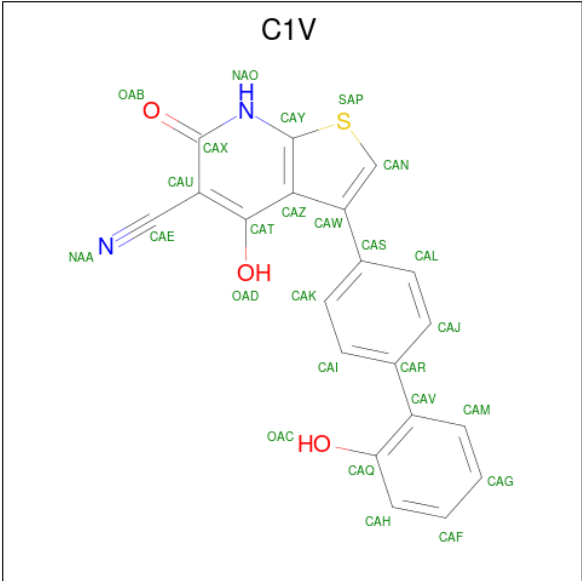
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	UNP P54619
F	-3	ALA	-	expression tag	UNP P54619
F	-2	ASP	-	expression tag	UNP P54619
F	-1	LEU	-	expression tag	UNP P54619
F	0	ASN	-	expression tag	UNP P54619
F	1	TRP	-	expression tag	UNP P54619

- Molecule 4 is (5S,6R,7R,9R,13cR,14R,16aS)-6-methoxy-5-methyl-7-(methylamino)-6,7,8,9,14,15,16,16a-octahydro-5H,13cH-5,9-epoxy-4b,9a,1 5-triazadibenzo[b,h]cyclonona[1,2,3,4-jkl]cyclopenta[e]-as-indacen-14-ol (CCD ID: 4O7) (formula: C₂₈H₃₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 3-[4-(2-hydroxyphenyl)phenyl]-4-oxidanyl-6-oxidanylidene-7H-thieno[2,3-b]pyridine-5-carbonitrile (CCD ID: C1V) (formula: C₂₀H₁₂N₂O₃S).



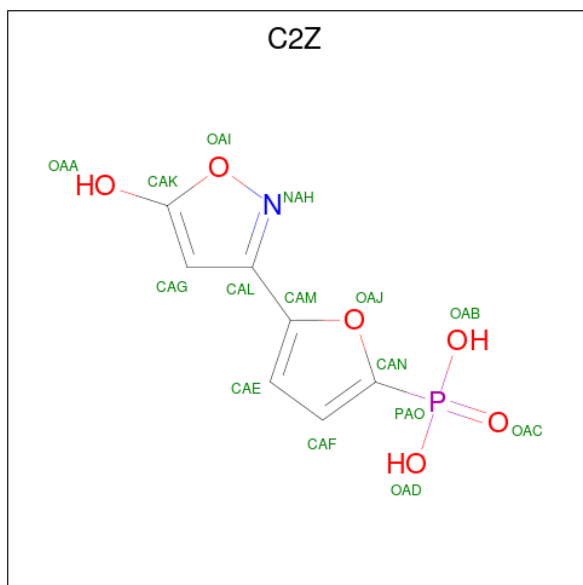
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

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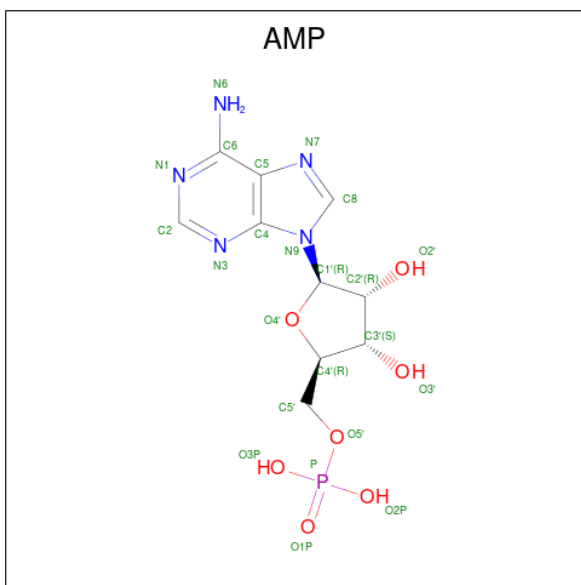
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

- Molecule 6 is 5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid (CCD ID: C2Z) (formula: $C_7H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

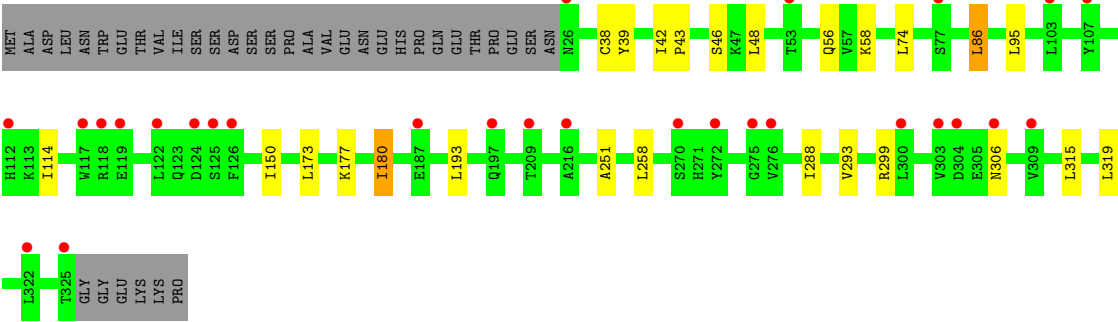
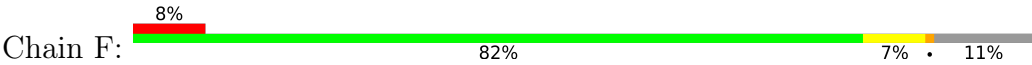
- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total	O	0	0
			28	28		
8	B	13	Total	O	0	0
			13	13		
8	C	33	Total	O	0	0
			33	33		
8	D	16	Total	O	0	0
			16	16		
8	E	26	Total	O	0	0
			26	26		
8	F	21	Total	O	0	0
			21	21		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.95Å 134.24Å 141.48Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	43.78 – 2.99 43.78 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.78-2.99) 98.5 (43.78-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.225 , 0.243 0.241 , 0.260	Depositor DCC
R_{free} test set	2868 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14587	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, AMP, C1V, 4O7, C2Z

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	0.72	0/3316	1.26	2/4477 (0.0%)
1	C	0.72	0/3637	1.28	6/4918 (0.1%)
2	B	0.73	0/1335	1.16	0/1825
2	D	0.70	0/1400	1.13	0/1908
3	E	0.73	0/2437	1.26	0/3309
3	F	0.74	0/2414	1.29	2/3284 (0.1%)
All	All	0.72	0/14539	1.25	10/19721 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	HIS	CA-C-N	6.20	125.29	120.33
1	C	218	HIS	C-N-CA	6.20	125.29	120.33
1	C	428	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	428	PHE	CA-CB-CG	5.97	119.77	113.80
1	C	174	CYS	N-CA-C	5.74	117.79	108.26

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	3255	0	3224	9	0
1	C	3567	0	3505	16	1
2	B	1310	0	1240	12	0
2	D	1373	0	1342	12	1
3	E	2381	0	2443	17	0
3	F	2366	0	2400	11	0
4	A	35	0	0	0	0
4	C	35	0	0	0	0
5	B	26	0	12	0	0
5	C	26	0	12	0	0
6	E	30	0	0	0	0
7	F	46	0	24	0	0
8	A	28	0	0	0	0
8	B	13	0	0	0	0
8	C	33	0	0	1	0
8	D	16	0	0	0	0
8	E	26	0	0	0	0
8	F	21	0	0	0	0
All	All	14587	0	14202	67	1

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 2.

The worst 5 of 67 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)
3:F:43:PRO:HG2	3:F:46:SER:HB3	1.76	0.66
1:A:35:HIS:HB3	1:A:39:GLY:H	1.70	0.56
1:C:138:ARG:HH12	1:C:172:TPO:HB	1.73	0.54
3:F:177:LYS:HA	3:F:180:ILE:HD12	1.90	0.54
3:E:61:PHE:HA	3:E:64:LEU:HD12	1.90	0.53

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ALA:O	2:D:144:SER:OG[2_946]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/565 (71%)	388 (97%)	11 (3%)	1 (0%)	36	70
1	C	442/565 (78%)	423 (96%)	18 (4%)	1 (0%)	43	76
2	B	165/270 (61%)	156 (94%)	9 (6%)	0	100	100
2	D	168/270 (62%)	161 (96%)	5 (3%)	2 (1%)	10	40
3	E	298/336 (89%)	291 (98%)	7 (2%)	0	100	100
3	F	298/336 (89%)	290 (97%)	8 (3%)	0	100	100
All	All	1771/2342 (76%)	1709 (96%)	58 (3%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ASP
1	C	316	PRO
2	D	258	LYS
2	D	194	PRO

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	344/497 (69%)	339 (98%)	5 (2%)	57	80
1	C	378/497 (76%)	368 (97%)	10 (3%)	40	72
2	B	135/239 (56%)	132 (98%)	3 (2%)	45	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	152/239 (64%)	150 (99%)	2 (1%)	61	81
3	E	265/308 (86%)	260 (98%)	5 (2%)	50	76
3	F	262/308 (85%)	255 (97%)	7 (3%)	39	71
All	All	1536/2088 (74%)	1504 (98%)	32 (2%)	47	75

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	180	ILE
3	F	299	ARG
1	C	237	LEU
1	C	176	SER
3	F	306	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	150	ASN
3	E	80	GLN
3	F	93	ASN
3	E	67	ASN
3	E	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPO	C	172	1	8,10,11	1.32	1 (12%)	10,14,16	1.65	1 (10%)
1	TPO	A	172	1	8,10,11	1.37	1 (12%)	10,14,16	1.84	1 (10%)
2	SEP	B	108	2	8,9,10	1.01	1 (12%)	7,12,14	2.26	1 (14%)
2	SEP	D	108	2	8,9,10	1.00	0	7,12,14	1.72	1 (14%)

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
1	TPO	C	172	1	-	2/9/11/13	-
1	TPO	A	172	1	-	0/9/11/13	-
2	SEP	B	108	2	-	2/6/8/10	-
2	SEP	D	108	2	-	2/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-3.34	1.53	1.59
1	C	172	TPO	P-OG1	-3.11	1.54	1.59
2	B	108	SEP	P-OG	-2.23	1.53	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	OG-CB-CA	5.39	113.39	108.14
1	A	172	TPO	P-OG1-CB	-4.96	109.84	123.33
1	C	172	TPO	P-OG1-CB	-4.20	111.91	123.33
2	D	108	SEP	OG-CB-CA	3.53	111.58	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	108	SEP	N-CA-CB-OG
2	B	108	SEP	C-CA-CB-OG
2	D	108	SEP	C-CA-CB-OG
2	D	108	SEP	N-CA-CB-OG
1	C	172	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	172	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
7	AMP	F	401	-	25,25,25	0.38	0	37,38,38	0.43	0
5	C1V	C	602	-	28,29,29	3.23	8 (28%)	32,42,42	5.28	6 (18%)
4	4O7	A	601	-	38,42,42	3.31	9 (23%)	33,68,68	3.23	14 (42%)
5	C1V	B	301	-	28,29,29	3.24	8 (28%)	32,42,42	5.22	6 (18%)
6	C2Z	E	401	-	14,16,16	3.54	7 (50%)	13,24,24	2.08	5 (38%)
6	C2Z	E	402	-	14,16,16	3.50	7 (50%)	13,24,24	2.12	5 (38%)
7	AMP	F	402	-	25,25,25	0.14	0	37,38,38	0.34	0
4	4O7	C	601	-	38,42,42	3.29	9 (23%)	33,68,68	3.21	14 (42%)

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
7	AMP	F	401	-	-	3/10/26/26	0/3/3/3
5	C1V	C	602	-	-	0/8/10/10	0/4/4/4
4	4O7	A	601	-	-	2/4/58/58	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	C1V	B	301	-	-	0/8/10/10	0/4/4/4
6	C2Z	E	401	-	-	0/4/10/10	0/2/2/2
6	C2Z	E	402	-	-	0/4/10/10	0/2/2/2
7	AMP	F	402	-	-	2/10/26/26	0/3/3/3
4	4O7	C	601	-	-	2/4/58/58	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	4O7	C18-C11	11.18	1.49	1.37
4	C	601	4O7	C18-C11	11.13	1.49	1.37
4	A	601	4O7	C19-C6	10.18	1.48	1.37
4	C	601	4O7	C19-C6	10.14	1.48	1.37
5	C	602	C1V	CAE-NAA	9.86	1.32	1.14

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	C1V	CAU-CAE-NAA	-25.23	120.02	177.39
5	C	602	C1V	CAU-CAE-NAA	-25.13	120.24	177.39
5	C	602	C1V	CAN-SAP-CAY	12.89	99.53	90.33
5	B	301	C1V	CAN-SAP-CAY	12.23	99.06	90.33
4	C	601	4O7	C18-C19-C6	-9.03	115.58	122.87

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

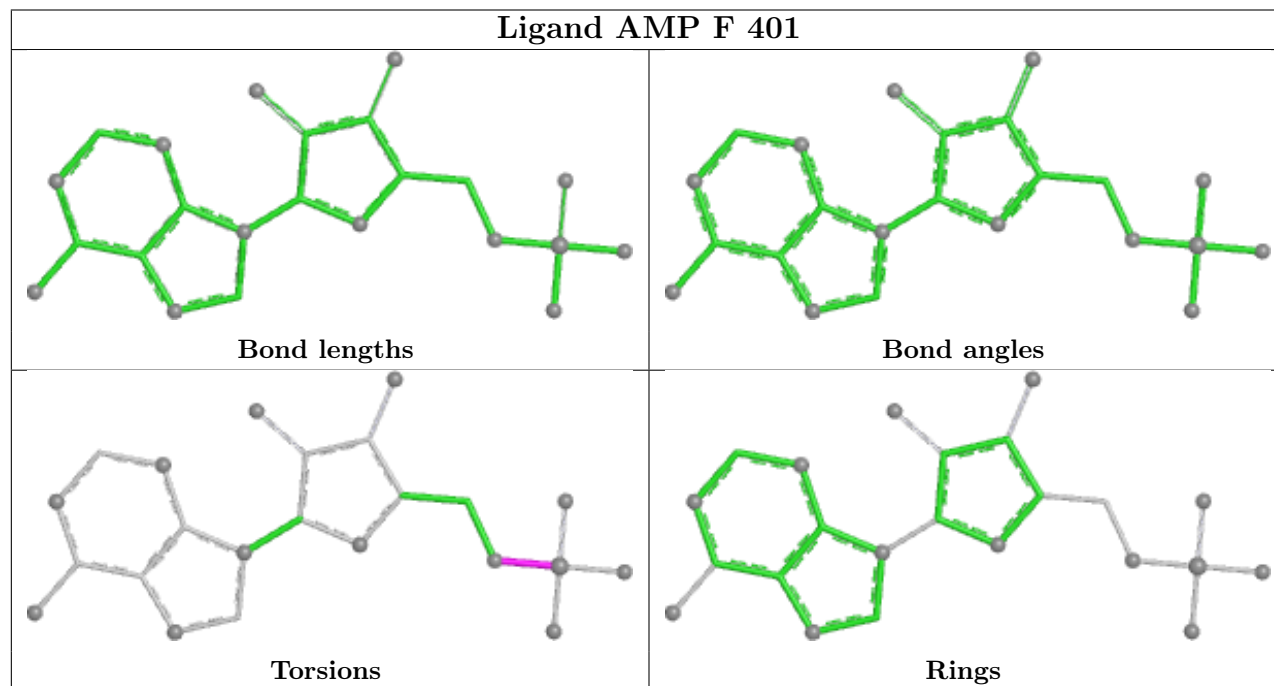
Mol	Chain	Res	Type	Atoms
4	A	601	4O7	C22-C23-N4-C28
4	C	601	4O7	C22-C23-N4-C28
7	F	401	AMP	C5'-O5'-P-O3P
7	F	402	AMP	C5'-O5'-P-O1P
7	F	402	AMP	C5'-O5'-P-O3P

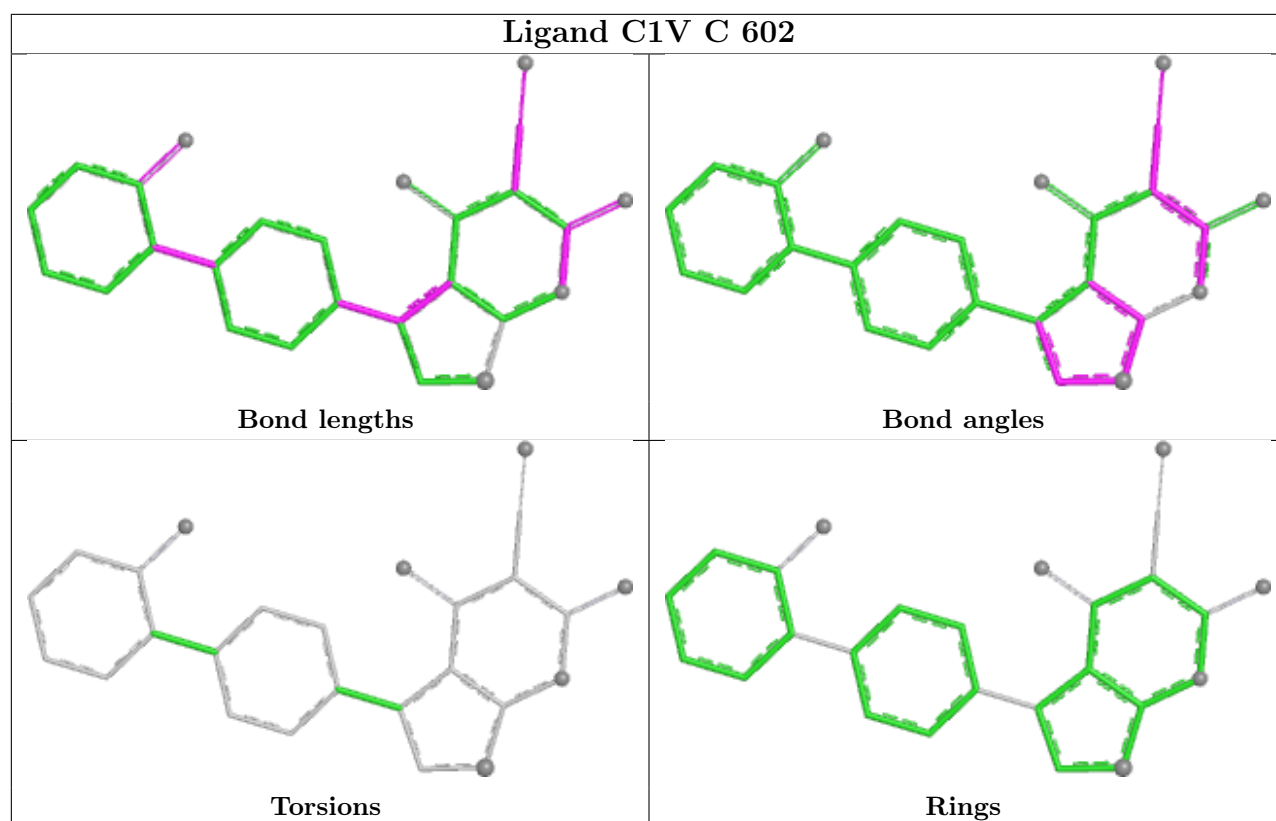
There are no ring outliers.

No monomer is involved in short contacts.

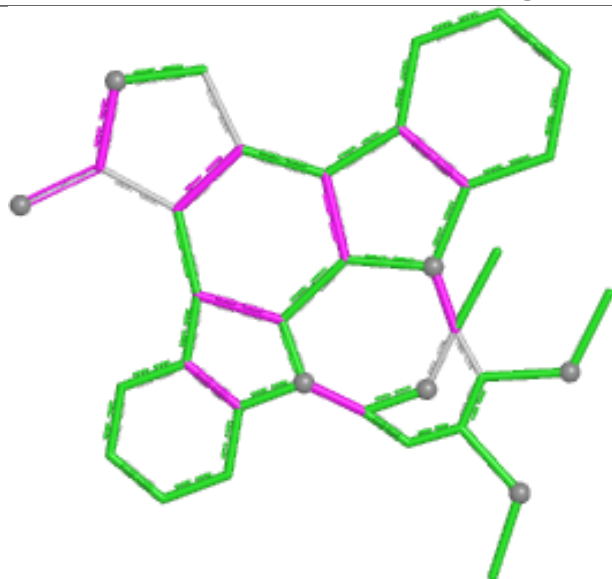
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

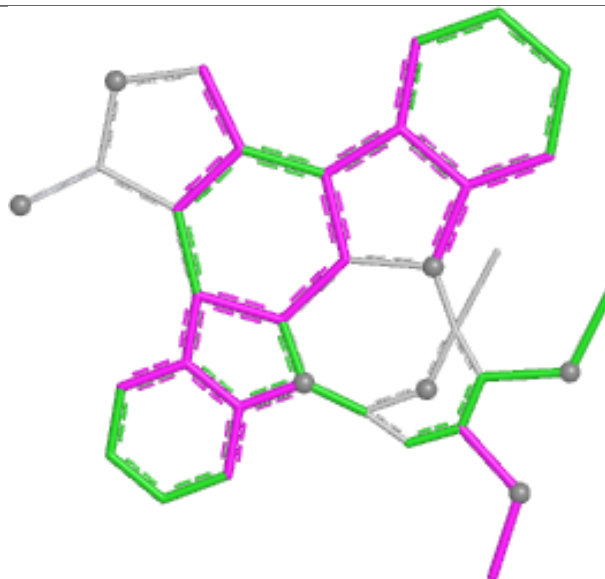




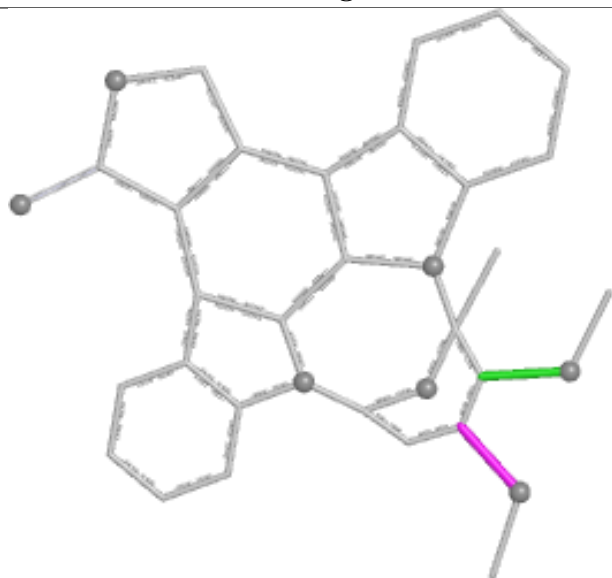
Ligand 4O7 A 601



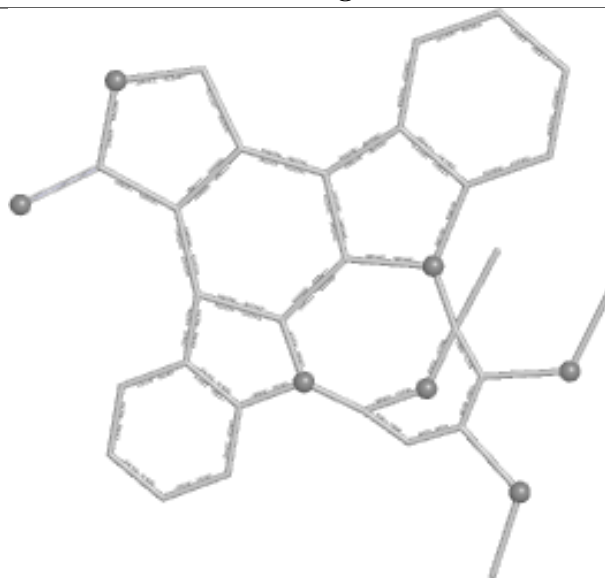
Bond lengths



Bond angles

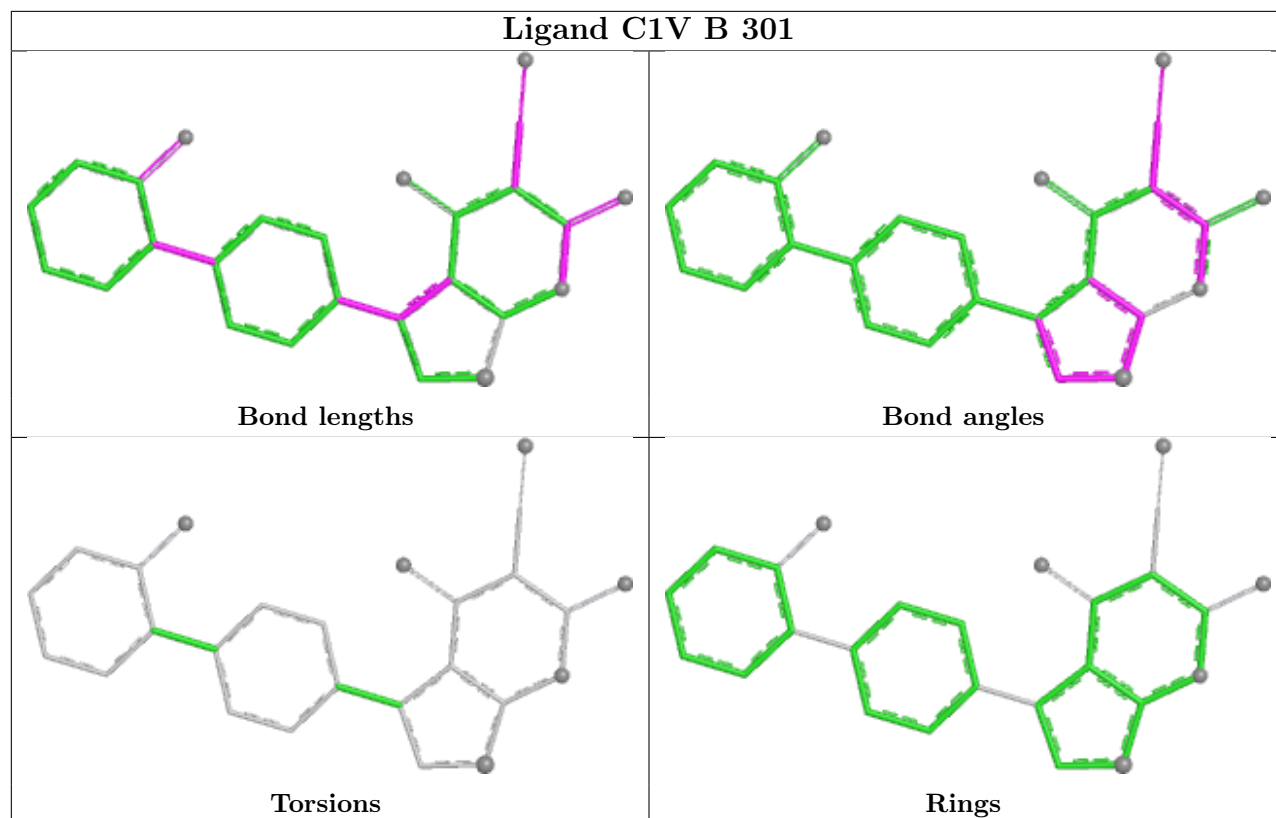


Torsions

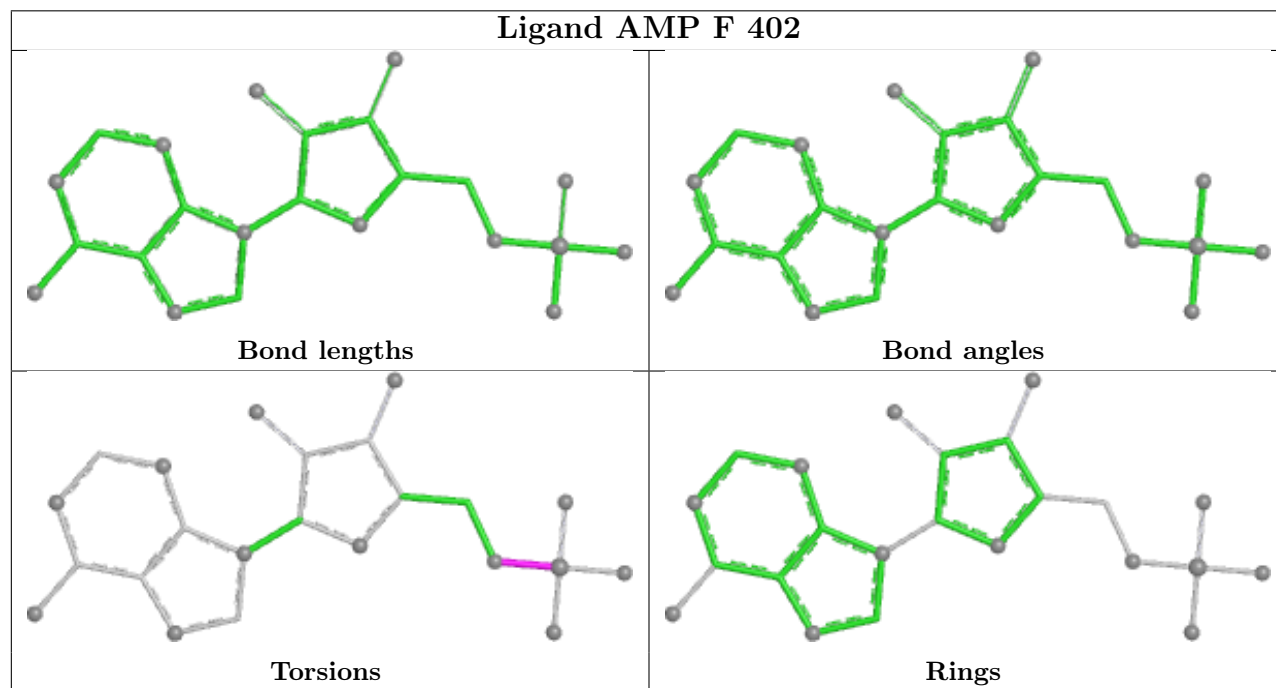


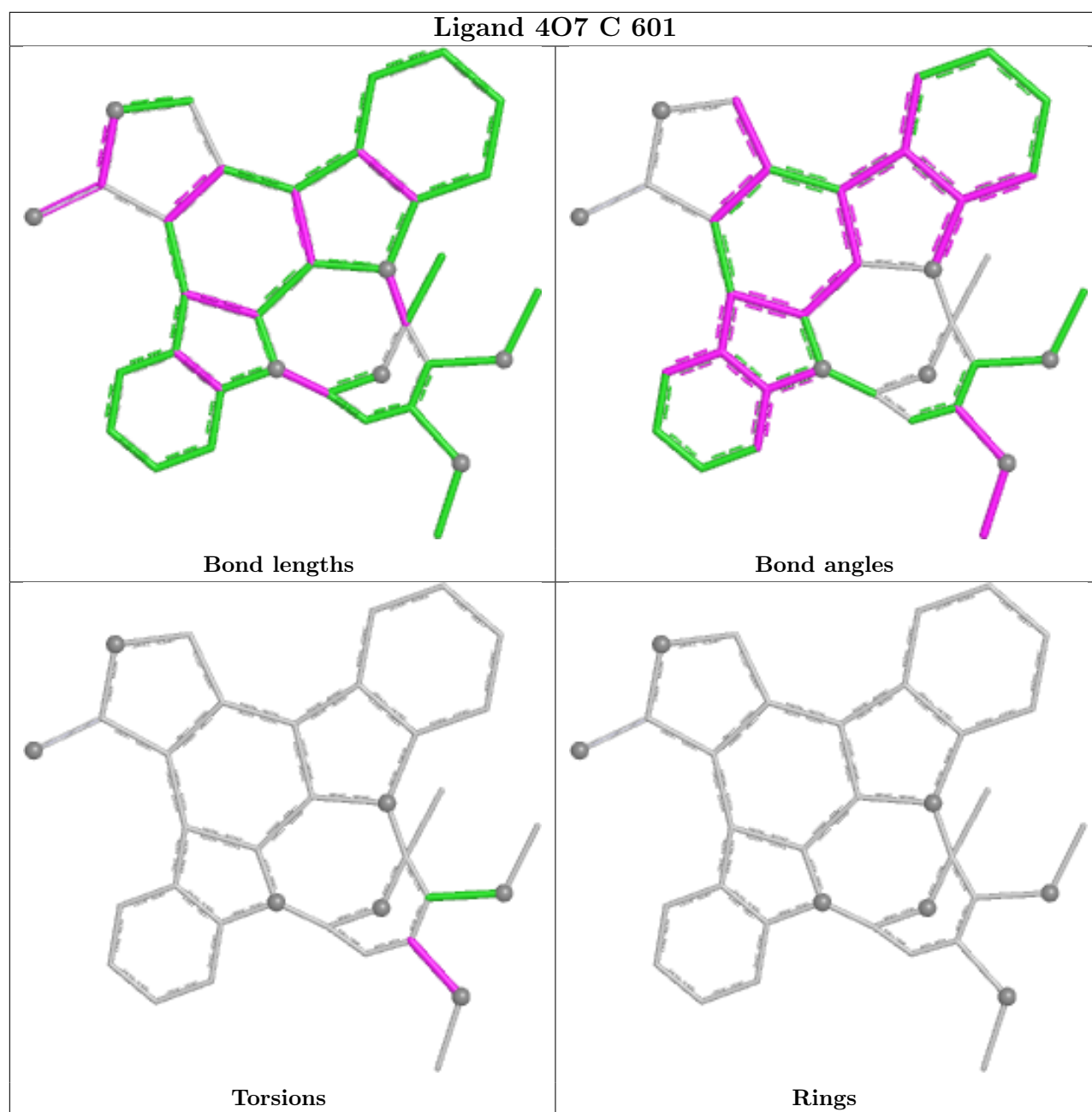
Rings

Ligand C1V B 301



Ligand AMP F 402





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	408/565 (72%)	0.99	40 (9%) 13 7	42, 69, 110, 163	0
1	C	452/565 (80%)	1.01	56 (12%) 8 5	33, 65, 108, 167	0
2	B	171/270 (63%)	1.40	35 (20%) 2 2	41, 85, 113, 142	0
2	D	174/270 (64%)	0.94	19 (10%) 10 6	43, 62, 103, 156	0
3	E	298/336 (88%)	0.86	27 (9%) 15 8	37, 62, 94, 113	2 (0%)
3	F	300/336 (89%)	0.87	28 (9%) 14 7	36, 61, 93, 108	0
All	All	1803/2342 (76%)	0.99	205 (11%) 10 6	33, 66, 106, 167	2 (0%)

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	LYS	5.0
1	C	319	GLN	4.9
3	E	306	ASN	4.9
1	A	293	VAL	4.6
1	A	110	ARG	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	172	11/12	0.75	0.16	70,71,74,76	4
1	TPO	A	172	11/12	0.78	0.17	60,62,65,66	4
2	SEP	B	108	10/11	0.91	0.10	76,78,85,86	0
2	SEP	D	108	10/11	0.92	0.11	60,63,67,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

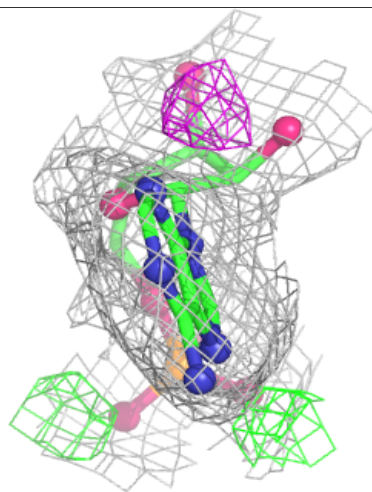
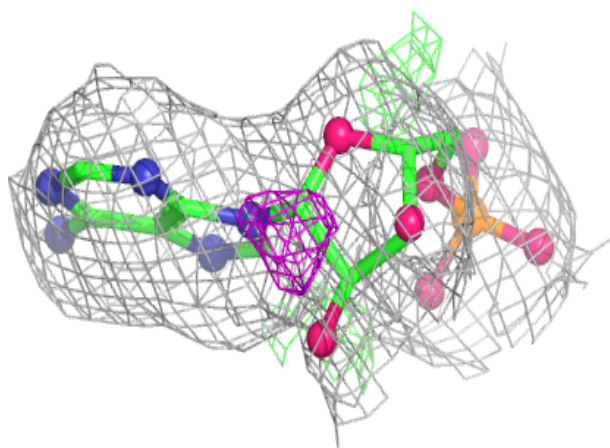
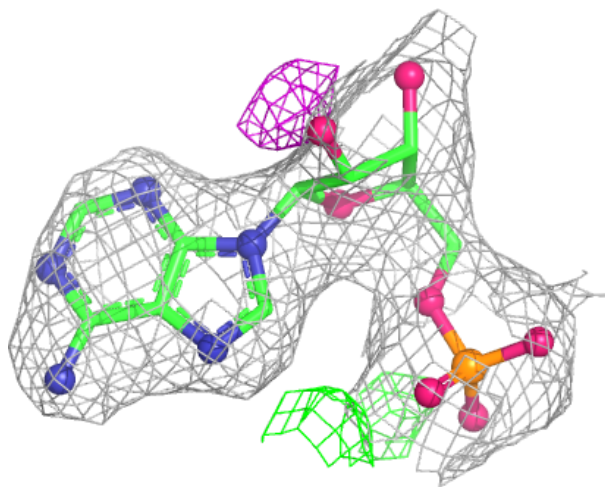
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	C2Z	E	402	15/15	0.79	0.19	95,95,95,95	0
6	C2Z	E	401	15/15	0.84	0.15	88,88,89,89	0
7	AMP	F	402	23/23	0.92	0.11	60,64,68,69	0
7	AMP	F	401	23/23	0.93	0.11	63,68,71,72	0
5	C1V	B	301	26/26	0.93	0.12	58,61,67,69	0
4	4O7	A	601	35/35	0.94	0.10	37,39,41,41	0
4	4O7	C	601	35/35	0.96	0.09	33,35,36,37	0
5	C1V	C	602	26/26	0.96	0.08	39,42,43,45	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.

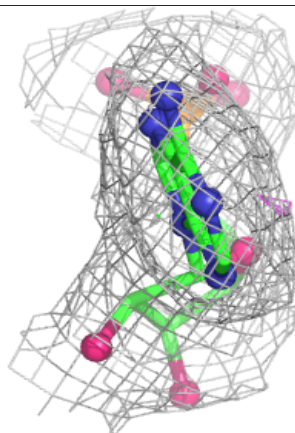
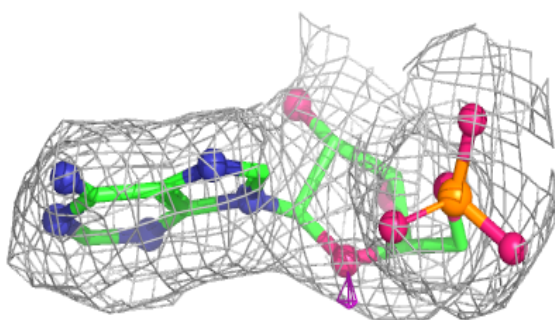
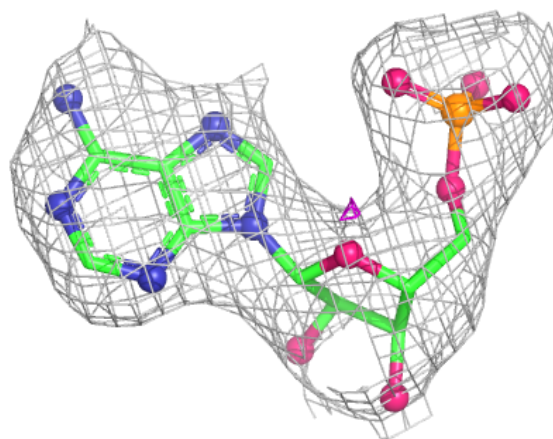
Electron density around AMP F 402:

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

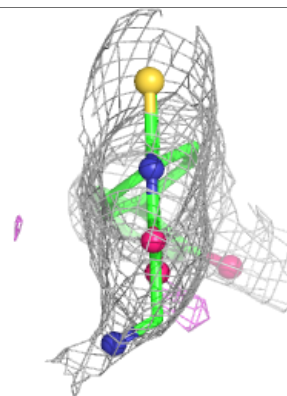
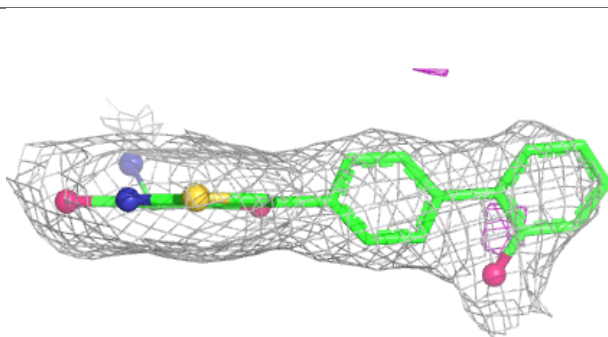
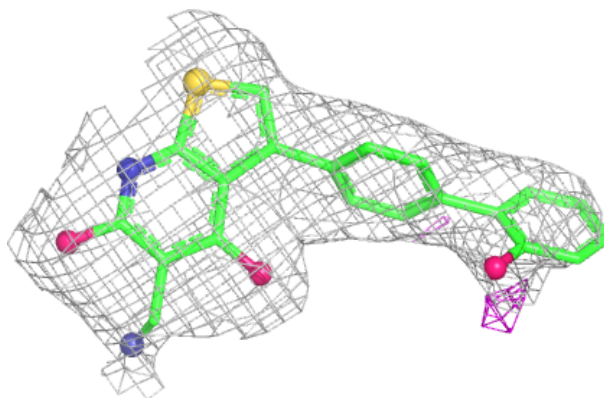


Electron density around AMP F 401:

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

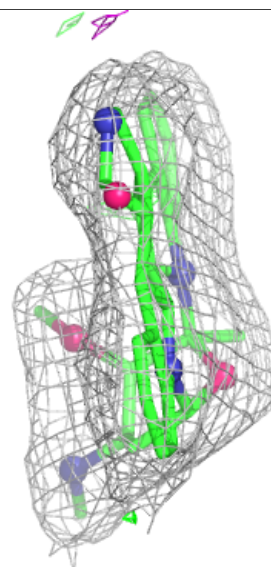
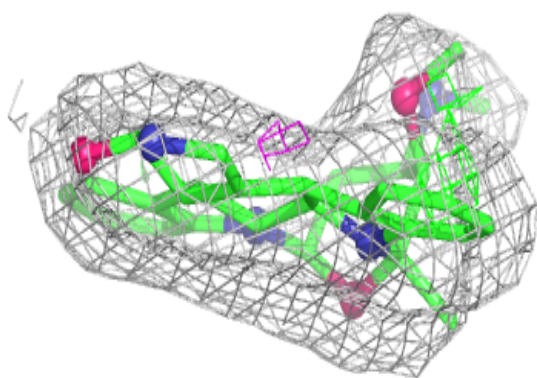
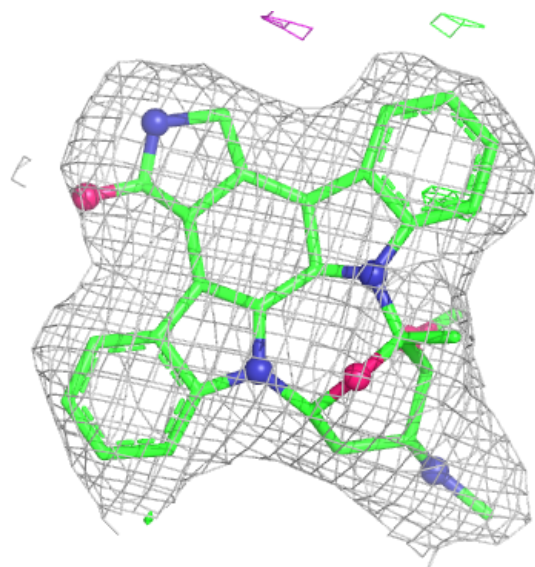
**Electron density around C1V B 301:**

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



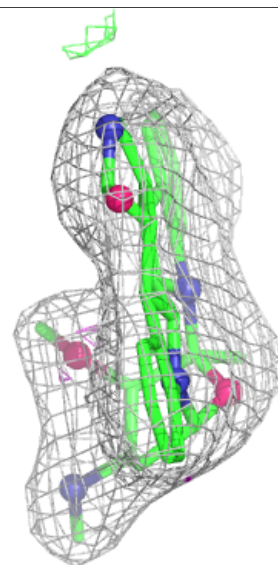
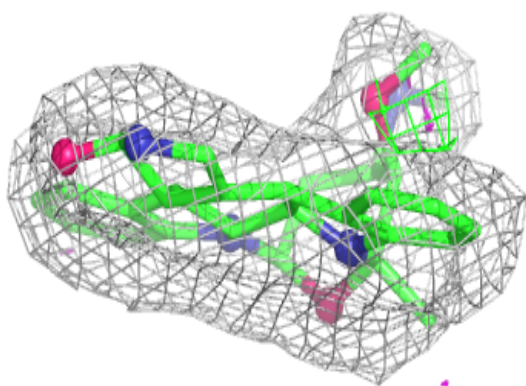
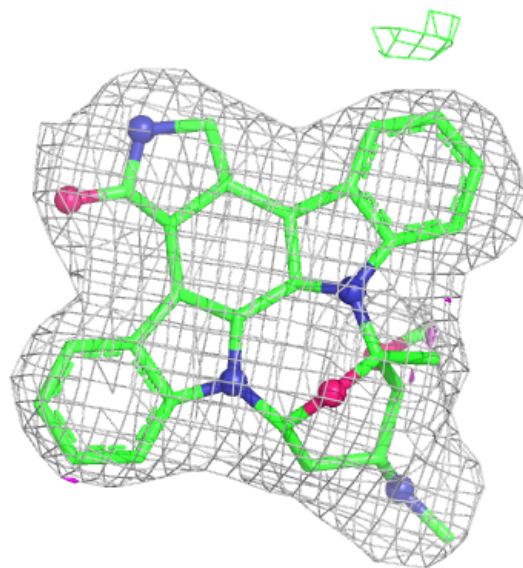
Electron density around 4O7 A 601:

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



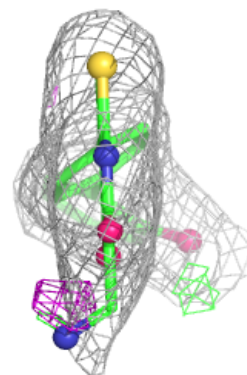
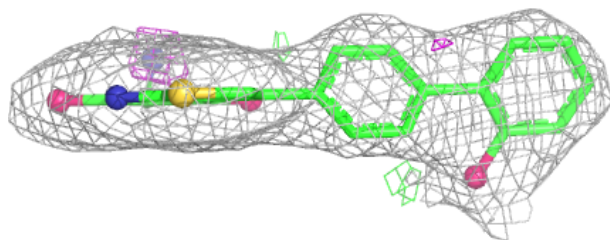
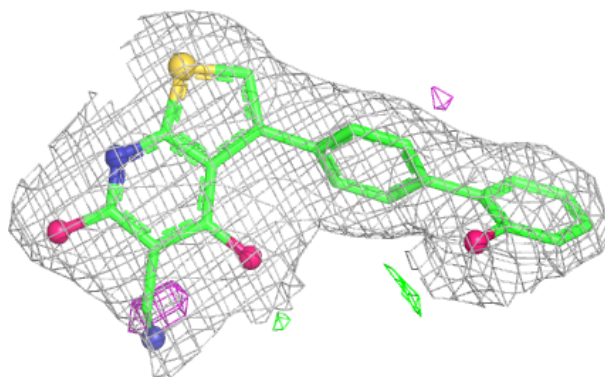
Electron density around 4O7 C 601:

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 C1V C 602:

$2mF_o - DF_c$ (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.