



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:50 PM UTC

PDB ID : 4GR5 / pdb_00004gr5
Title : Crystal structure of SlgN1deltaAsub in complex with AMPcPP
Authors : Herbst, D.A.; Zocher, G.; Stehle, T.
Deposited on : 2012-08-24
Resolution : 1.92 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

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:

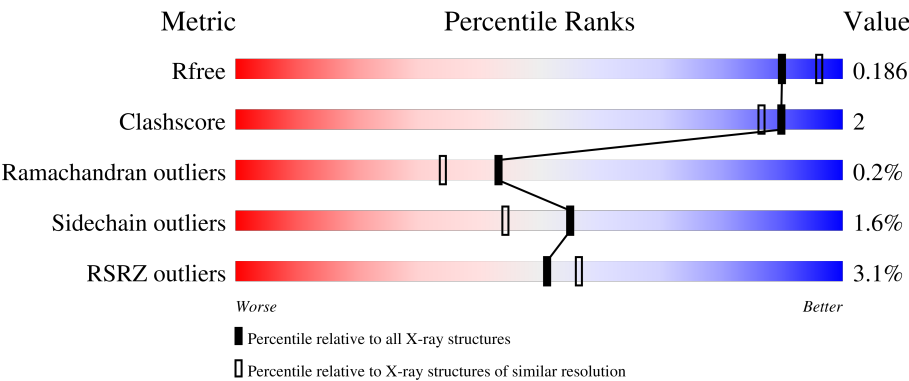
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	570	2% 75% • 21%
1	B	570	2% 75% • 20%
1	C	570	4% 75% 5% 20%
1	D	570	2% 74% • 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14641 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.

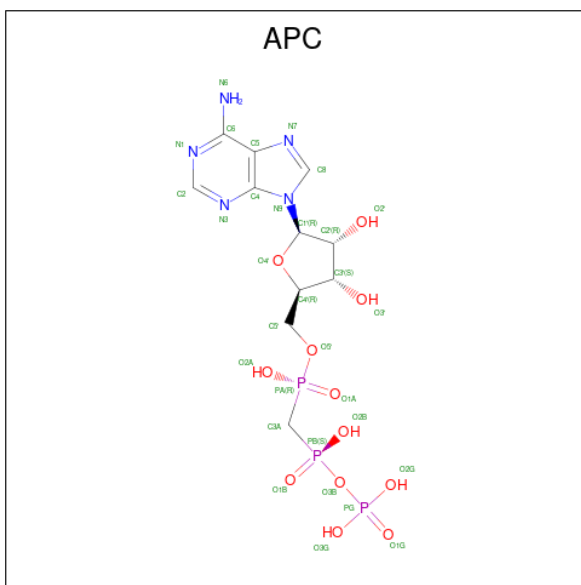
- Molecule 1 is a protein called Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3327	2102	596	617	12			
1	B	455	Total	C	N	O	S	0	2	0
			3375	2129	607	627	12			
1	C	457	Total	C	N	O	S	0	1	0
			3366	2128	602	624	12			
1	D	449	Total	C	N	O	S	0	1	0
			3327	2103	594	618	12			

There are 12 discrepancies between the modelled and reference sequences:

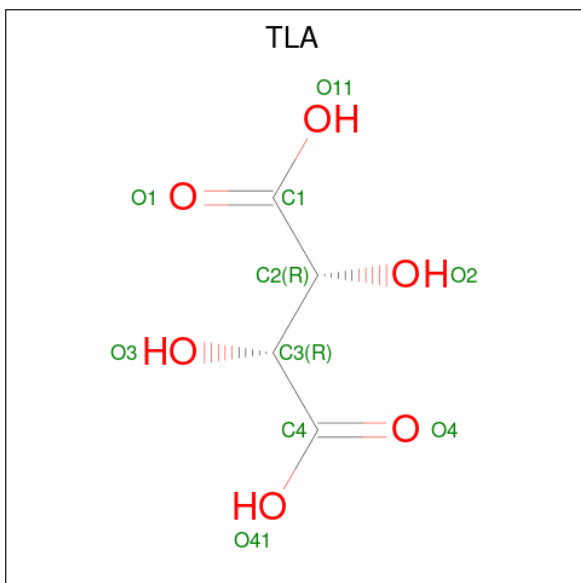
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D1GLU5
A	-1	SER	-	expression tag	UNP D1GLU5
A	0	HIS	-	expression tag	UNP D1GLU5
B	-2	GLY	-	expression tag	UNP D1GLU5
B	-1	SER	-	expression tag	UNP D1GLU5
B	0	HIS	-	expression tag	UNP D1GLU5
C	-2	GLY	-	expression tag	UNP D1GLU5
C	-1	SER	-	expression tag	UNP D1GLU5
C	0	HIS	-	expression tag	UNP D1GLU5
D	-2	GLY	-	expression tag	UNP D1GLU5
D	-1	SER	-	expression tag	UNP D1GLU5
D	0	HIS	-	expression tag	UNP D1GLU5

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



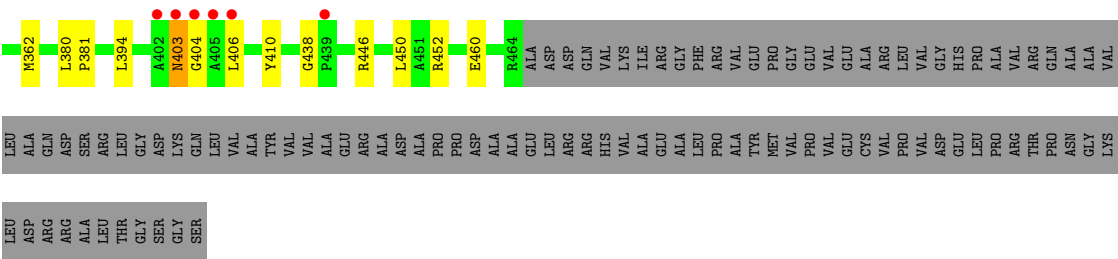
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0
3	B	1	Total C O 10 4 6	0	0
3	B	1	Total C O 10 4 6	0	0
3	C	1	Total C O 10 4 6	0	0
3	D	1	Total C O 10 4 6	0	0
3	D	1	Total C O 10 4 6	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

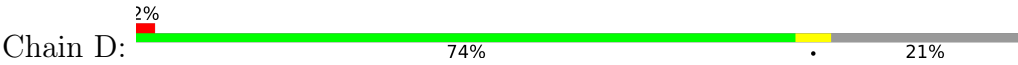
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	313	Total O 313 313	0	0
5	B	246	Total O 246 246	0	0
5	C	211	Total O 211 211	0	0
5	D	291	Total O 291 291	0	0



● Molecule 1: Non-ribosomal peptide synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.90Å 147.79Å 109.92Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	29.83 – 1.92 29.83 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-1.92) 99.7 (29.83-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168, BUSTER 2.10.0	Depositor
R, R_{free}	0.158 , 0.186 0.160 , 0.186	Depositor DCC
R_{free} test set	5872 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14641	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CL, APC, TLA

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	0.45	0/3407	0.76	0/4643
1	B	0.44	0/3456	0.77	5/4709 (0.1%)
1	C	0.42	0/3449	0.76	2/4704 (0.0%)
1	D	0.41	0/3410	0.75	4/4646 (0.1%)
All	All	0.43	0/13722	0.76	11/18702 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	438	GLY	CA-C-N	6.19	126.66	119.47
1	D	438	GLY	C-N-CA	6.19	126.66	119.47
1	B	438	GLY	CA-C-N	5.48	126.69	119.84
1	B	438	GLY	C-N-CA	5.48	126.69	119.84
1	C	438	GLY	CA-C-N	5.43	124.62	118.97
1	C	438	GLY	C-N-CA	5.43	124.62	118.97
1	D	3	ASN	CA-C-N	5.30	124.97	119.56
1	D	3	ASN	C-N-CA	5.30	124.97	119.56
1	B	40	GLY	CA-C-O	-5.20	118.71	122.45
1	B	347	HIS	CA-C-N	5.09	124.88	119.28
1	B	347	HIS	C-N-CA	5.09	124.88	119.28

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	3327	0	3245	13	0
1	B	3375	0	3282	12	0
1	C	3366	0	3276	16	0
1	D	3327	0	3250	8	0
2	A	31	0	14	0	0
2	B	31	0	14	0	0
2	C	31	0	14	0	0
2	D	31	0	14	0	0
3	A	10	0	4	0	0
3	B	20	0	8	0	0
3	C	10	0	4	1	0
3	D	20	0	8	0	0
4	A	1	0	0	0	0
5	A	313	0	0	0	0
5	B	246	0	0	2	0
5	C	211	0	0	2	0
5	D	291	0	0	0	0
All	All	14641	0	13133	49	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 2.

All (49) 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:42:ASP:OD1	1:D:43:SER:N	2.30	0.64
1:C:452:ARG:NH2	1:C:460:GLU:OE1	2.32	0.63
1:A:308:ALA:HB3	1:A:333:GLU:HG3	1.82	0.61
1:B:38:ARG:HD3	1:B:50:HIS:NE2	2.16	0.59
1:A:52:GLU:HG3	1:A:425:ALA:HB2	1.84	0.58
1:C:344:ARG:NH1	5:C:906:HOH:O	2.31	0.58
1:D:308:ALA:HB3	1:D:333:GLU:HG3	1.86	0.58
1:B:406:LEU:HD11	1:B:450:LEU:HB3	1.87	0.57
1:C:42:ASP:OD1	1:C:43:SER:N	2.37	0.57
1:C:406:LEU:HB3	1:C:450:LEU:HD11	1.87	0.56
1:D:44:ARG:NH2	1:D:429:GLU:OE2	2.36	0.56
1:B:52:GLU:HG3	1:B:425:ALA:HB2	1.89	0.55
1:A:121:PRO:HA	1:A:146:GLY:O	2.08	0.53
1:C:160:ARG:NH1	1:C:219:THR:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:HG2	1:A:29:ILE:HD12	1.92	0.51
1:C:156:PHE:CZ	1:C:220:SER:HA	2.46	0.51
1:D:13:VAL:HG12	1:D:41:THR:HA	1.93	0.49
1:A:117:LEU:HD22	1:C:117:LEU:HD22	1.96	0.48
1:D:52:GLU:HG2	1:D:425:ALA:HB2	1.95	0.47
1:D:270:PHE:HB3	1:D:274:LEU:HD22	1.95	0.47
1:A:3:ASN:ND2	1:A:446:ARG:HD2	2.30	0.47
1:C:410:TYR:CE2	1:C:446:ARG:HB3	2.50	0.47
1:A:461:TYR:CE2	1:A:463:GLY:HA2	2.51	0.46
1:B:109:ARG:NH1	5:B:901:HOH:O	2.48	0.46
1:C:153:ASP:CG	1:C:155:GLN:HG2	2.42	0.45
1:C:406:LEU:HD13	1:C:450:LEU:HD21	1.97	0.45
1:A:454:ARG:HG3	1:A:456:ASP:OD1	2.16	0.44
1:A:44:ARG:NH2	1:A:429:GLU:OE1	2.47	0.44
1:C:403:ASN:OD1	1:C:403:ASN:N	2.31	0.43
1:A:74:VAL:HG13	1:A:274:LEU:HD11	1.99	0.43
1:B:112:HIS:CE1	1:B:200:PRO:HG2	2.54	0.43
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.90	0.43
1:B:406:LEU:HD21	1:B:450:LEU:HD13	2.00	0.42
1:C:340:VAL:HG13	1:C:352:LEU:HD13	2.01	0.42
1:B:199:ALA:HA	1:B:200:PRO:HD3	1.95	0.42
1:B:454:ARG:HB3	1:B:456:ASP:OD1	2.20	0.42
1:B:160:ARG:NH2	1:B:219:THR:O	2.53	0.42
1:B:249:GLY:O	1:B:277:ALA:HB2	2.20	0.42
1:B:443:ARG:NH1	5:B:940:HOH:O	2.34	0.41
1:D:365:THR:HG21	1:D:411:VAL:HB	2.02	0.41
3:C:602:TLA:O41	5:C:836:HOH:O	2.22	0.41
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.82	0.41
1:C:380:LEU:HA	1:C:381:PRO:HD3	1.96	0.41
1:A:156:PHE:CZ	1:A:220:SER:HA	2.56	0.41
1:A:160:ARG:NH2	1:A:222:SER:O	2.54	0.41
1:D:179:LEU:O	1:D:182:ARG:HG3	2.21	0.41
1:C:394:LEU:HD12	1:C:410:TYR:CD1	2.57	0.40
1:C:404:GLY:HA2	1:C:452:ARG:HE	1.87	0.40
1:B:163:LEU:HA	1:B:163:LEU:HD12	1.83	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	445/570 (78%)	439 (99%)	5 (1%)	1 (0%)	43	34
1	B	451/570 (79%)	443 (98%)	7 (2%)	1 (0%)	43	34
1	C	454/570 (80%)	445 (98%)	8 (2%)	1 (0%)	43	34
1	D	444/570 (78%)	438 (99%)	5 (1%)	1 (0%)	43	34
All	All	1794/2280 (79%)	1765 (98%)	25 (1%)	4 (0%)	43	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	MET
1	A	362	MET
1	C	362	MET
1	D	362	MET

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	330/425 (78%)	328 (99%)	2 (1%)	78	75
1	B	334/425 (79%)	329 (98%)	5 (2%)	57	47
1	C	332/425 (78%)	326 (98%)	6 (2%)	51	39
1	D	331/425 (78%)	323 (98%)	8 (2%)	43	28
All	All	1327/1700 (78%)	1306 (98%)	21 (2%)	55	44

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	274	LEU
1	B	6	GLU
1	B	163	LEU
1	B	167	ASP
1	B	198	ASP
1	B	204	LEU
1	C	37	VAL
1	C	223	THR
1	C	241	LEU
1	C	256	GLN
1	C	344	ARG
1	C	403	ASN
1	D	6	GLU
1	D	29	ILE
1	D	61	THR
1	D	274	LEU
1	D	294	GLU
1	D	423	ARG
1	D	443	ARG
1	D	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	B	22	HIS
1	B	53	HIS
1	B	54	HIS
1	B	112	HIS
1	B	155	GLN
1	B	286	ASN
1	C	22	HIS
1	C	305	GLN
1	D	50	HIS
1	D	54	HIS
1	D	155	GLN
1	D	286	ASN
1	D	305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	APC	A	601	-	29,33,33	1.66	5 (17%)	44,52,52	1.68	11 (25%)
3	TLA	B	602	-	9,9,9	1.18	0	12,12,12	1.19	1 (8%)
2	APC	B	601	-	29,33,33	1.57	5 (17%)	44,52,52	1.74	10 (22%)
3	TLA	B	603	-	9,9,9	1.24	1 (11%)	12,12,12	1.17	1 (8%)
2	APC	C	601	-	29,33,33	1.57	5 (17%)	44,52,52	1.80	12 (27%)
3	TLA	C	602	-	9,9,9	1.24	0	12,12,12	0.99	0
3	TLA	A	602	-	9,9,9	1.12	0	12,12,12	1.20	1 (8%)
3	TLA	D	602	-	9,9,9	1.32	0	12,12,12	1.25	2 (16%)
3	TLA	D	603	-	9,9,9	1.19	0	12,12,12	0.97	0
2	APC	D	601	-	29,33,33	1.53	5 (17%)	44,52,52	1.78	10 (22%)

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	APC	A	601	-	-	3/19/38/38	0/3/3/3
3	TLA	B	602	-	-	10/12/12/12	-
2	APC	B	601	-	-	1/19/38/38	0/3/3/3
3	TLA	B	603	-	-	7/12/12/12	-
2	APC	C	601	-	-	5/19/38/38	0/3/3/3
3	TLA	C	602	-	-	3/12/12/12	-
3	TLA	A	602	-	-	0/12/12/12	-
3	TLA	D	602	-	-	8/12/12/12	-
3	TLA	D	603	-	-	3/12/12/12	-
2	APC	D	601	-	-	5/19/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	APC	C5-C4	4.69	1.47	1.39
2	A	601	APC	PB-O3B	4.68	1.63	1.58
2	A	601	APC	C5-C4	4.60	1.47	1.39
2	D	601	APC	C5-C4	4.52	1.47	1.39
2	B	601	APC	C5-C4	4.32	1.46	1.39
2	B	601	APC	PB-O3B	4.24	1.63	1.58
2	C	601	APC	PB-O3B	3.65	1.62	1.58
2	D	601	APC	PB-O3B	3.47	1.62	1.58
2	C	601	APC	C5-C6	2.76	1.48	1.41
2	A	601	APC	C8-N7	2.64	1.36	1.31
2	D	601	APC	C5-C6	2.55	1.48	1.41
2	B	601	APC	C5-C6	2.53	1.48	1.41
2	D	601	APC	C8-N7	2.49	1.36	1.31
2	A	601	APC	C5-C6	2.45	1.47	1.41
2	C	601	APC	C8-N7	2.41	1.36	1.31
2	B	601	APC	C8-N7	2.33	1.36	1.31
3	B	603	TLA	O41-C4	-2.26	1.23	1.30
2	A	601	APC	C4-N9	-2.22	1.33	1.37
2	C	601	APC	C4-N9	-2.18	1.33	1.37
2	D	601	APC	C5-N7	-2.06	1.35	1.39
2	B	601	APC	PB-O2B	-2.02	1.51	1.56

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	APC	C5-C4-N3	-5.35	119.35	126.72
2	D	601	APC	C5-C4-N3	-5.22	119.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	APC	C5-C4-N3	-4.84	120.05	126.72
2	A	601	APC	C5-C4-N3	-4.76	120.16	126.72
2	B	601	APC	N3-C4-N9	4.39	134.63	127.17
2	D	601	APC	N3-C4-N9	4.05	134.06	127.17
2	C	601	APC	N3-C4-N9	3.96	133.90	127.17
2	A	601	APC	N3-C4-N9	3.75	133.54	127.17
2	C	601	APC	N3-C2-N1	-3.62	123.10	128.58
2	D	601	APC	C2-N3-C4	3.58	120.57	111.83
2	B	601	APC	C2-N3-C4	3.47	120.30	111.83
2	C	601	APC	C2-N3-C4	3.45	120.26	111.83
2	D	601	APC	N3-C2-N1	-3.44	123.37	128.58
2	D	601	APC	C4-C5-N7	-3.42	106.67	110.58
2	A	601	APC	N3-C2-N1	-3.38	123.46	128.58
2	B	601	APC	N3-C2-N1	-3.32	123.56	128.58
2	A	601	APC	C2-N3-C4	3.30	119.88	111.83
2	A	601	APC	C4-C5-N7	-3.21	106.92	110.58
2	C	601	APC	C4-N9-C8	3.14	109.03	105.74
2	A	601	APC	C4-N9-C8	3.09	108.98	105.74
2	C	601	APC	C4-C5-N7	-3.07	107.07	110.58
2	B	601	APC	C4-N9-C8	3.05	108.94	105.74
2	B	601	APC	C4-C5-N7	-3.04	107.10	110.58
2	D	601	APC	O2A-PA-O1A	2.90	119.38	109.95
2	C	601	APC	O2A-PA-O1A	2.89	119.36	109.95
2	D	601	APC	C4-N9-C8	2.78	108.65	105.74
3	B	602	TLA	O41-C4-C3	2.60	120.55	113.31
2	D	601	APC	C5-N7-C8	2.48	107.35	103.45
2	B	601	APC	O2A-PA-O1A	2.47	118.00	109.95
2	A	601	APC	O2A-PA-O1A	2.40	117.78	109.95
3	A	602	TLA	O11-C1-C2	2.39	119.96	113.31
2	B	601	APC	O2B-PB-O1B	2.35	117.61	109.95
2	C	601	APC	C2-N1-C6	2.34	122.57	118.73
2	C	601	APC	O2B-PB-O1B	2.34	117.56	109.95
2	C	601	APC	C5-N7-C8	2.30	107.06	103.45
2	B	601	APC	C5-N7-C8	2.28	107.03	103.45
2	C	601	APC	C6-C5-N7	2.26	136.46	132.09
2	D	601	APC	C6-C5-N7	2.25	136.44	132.09
2	A	601	APC	C6-C5-N7	2.24	136.41	132.09
2	C	601	APC	N9-C8-N7	-2.22	110.78	113.94
3	B	603	TLA	O41-C4-C3	2.13	119.24	113.31
2	B	601	APC	N9-C8-N7	-2.13	110.91	113.94
2	D	601	APC	N9-C8-N7	-2.13	110.92	113.94
2	A	601	APC	C2-N1-C6	2.11	122.19	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	TLA	O11-C1-C2	2.10	119.14	113.31
2	A	601	APC	O1B-PB-C3A	2.03	114.41	109.05
2	A	601	APC	C5-N7-C8	2.02	106.63	103.45
3	D	602	TLA	O2-C2-C3	-2.02	106.05	110.17

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	APC	PB-O3B-PG-O3G
3	D	602	TLA	C1-C2-C3-O3
3	D	602	TLA	O2-C2-C3-O3
3	D	602	TLA	O2-C2-C3-C4
3	D	602	TLA	C1-C2-C3-C4
3	B	602	TLA	O1-C1-C2-O2
3	B	602	TLA	O11-C1-C2-O2
3	B	602	TLA	O3-C3-C4-O4
3	B	602	TLA	O3-C3-C4-O41
3	B	602	TLA	C2-C3-C4-O4
3	B	602	TLA	C2-C3-C4-O41
3	D	603	TLA	O11-C1-C2-O2
3	D	603	TLA	O1-C1-C2-O2
3	B	602	TLA	O2-C2-C3-C4
3	B	602	TLA	C1-C2-C3-O3
3	D	602	TLA	O1-C1-C2-O2
3	D	602	TLA	O1-C1-C2-C3
3	B	602	TLA	C1-C2-C3-C4
3	D	602	TLA	O11-C1-C2-C3
3	D	602	TLA	O11-C1-C2-O2
2	C	601	APC	O4'-C4'-C5'-O5'
3	B	602	TLA	O2-C2-C3-O3
3	B	603	TLA	O2-C2-C3-C4
2	C	601	APC	C3'-C4'-C5'-O5'
3	C	602	TLA	C1-C2-C3-O3
3	B	603	TLA	O1-C1-C2-C3
3	B	603	TLA	O11-C1-C2-O2
3	B	603	TLA	C1-C2-C3-O3
3	C	602	TLA	O2-C2-C3-C4
3	B	603	TLA	O11-C1-C2-C3
3	B	603	TLA	C1-C2-C3-C4
3	C	602	TLA	C1-C2-C3-C4
3	D	603	TLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	601	APC	PB-O3B-PG-O1G
3	B	603	TLA	O1-C1-C2-O2
2	A	601	APC	PB-C3A-PA-O1A
2	C	601	APC	PB-C3A-PA-O1A
2	D	601	APC	PB-C3A-PA-O1A
2	A	601	APC	PB-O3B-PG-O3G
2	C	601	APC	PB-O3B-PG-O2G
2	D	601	APC	PB-O3B-PG-O2G
2	D	601	APC	PB-O3B-PG-O3G
2	A	601	APC	PB-O3B-PG-O1G
2	C	601	APC	C4'-C5'-O5'-PA
2	D	601	APC	C4'-C5'-O5'-PA

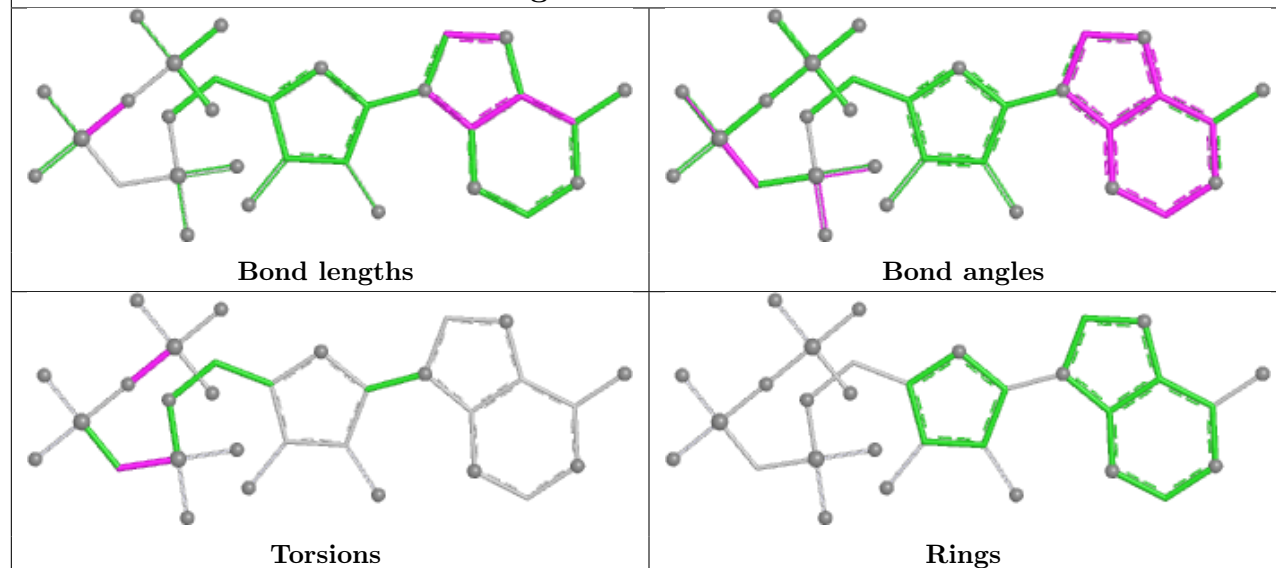
There are no ring outliers.

1 monomer is involved in 1 short contact:

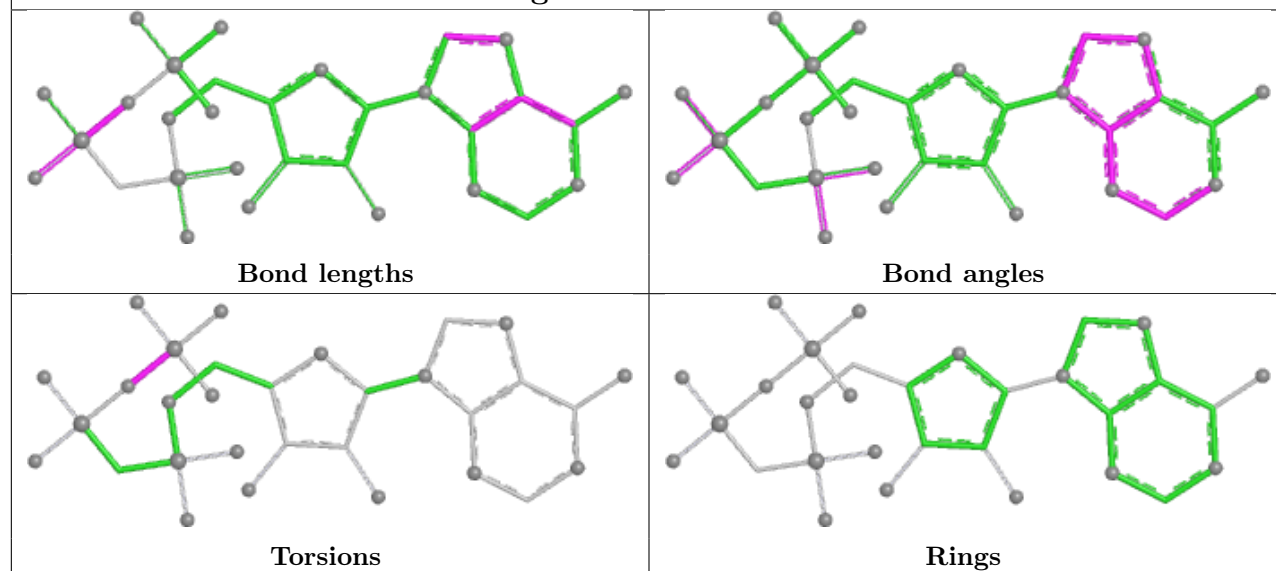
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	TLA	1	0

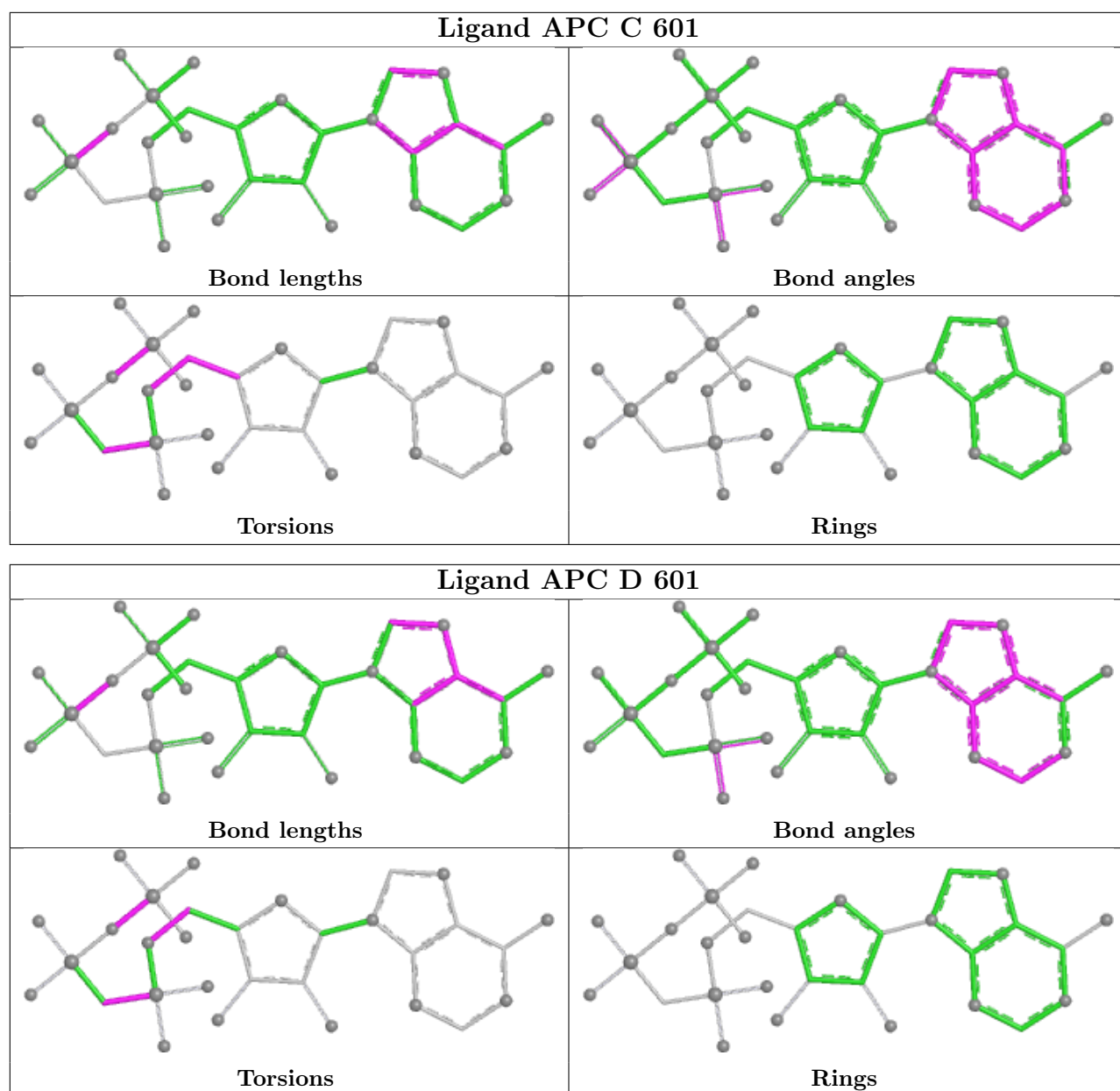
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand APC A 601



Ligand APC B 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/570 (79%)	-0.26	10 (2%) 62 69	22, 33, 62, 104	0
1	B	455/570 (79%)	-0.18	12 (2%) 57 63	21, 35, 67, 112	2 (0%)
1	C	457/570 (80%)	0.07	21 (4%) 37 42	21, 39, 83, 109	1 (0%)
1	D	449/570 (78%)	-0.02	14 (3%) 51 56	23, 38, 82, 109	1 (0%)
All	All	1812/2280 (79%)	-0.10	57 (3%) 51 56	21, 36, 77, 112	4 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	5.2
1	D	201	ALA	4.8
1	D	439	PRO	4.2
1	B	40	GLY	4.0
1	A	201	ALA	4.0
1	C	406	LEU	3.9
1	C	200	PRO	3.9
1	B	63	PRO	3.9
1	B	197	SER	3.7
1	C	404	GLY	3.7
1	A	69	PRO	3.6
1	A	68	ALA	3.6
1	C	68	ALA	3.6
1	D	61	THR	3.5
1	B	62	GLY	3.4
1	C	402	ALA	3.4
1	D	438	GLY	3.3
1	D	68	ALA	3.2
1	C	9	ASP	3.2
1	C	222	SER	3.1
1	C	439	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASP	3.0
1	C	221	GLY	3.0
1	B	220	SER	3.0
1	C	220	SER	2.9
1	C	10	GLY	2.9
1	C	223	THR	2.9
1	C	69	PRO	2.8
1	B	61	THR	2.8
1	B	439	PRO	2.7
1	C	65	VAL	2.7
1	C	405	ALA	2.7
1	C	40	GLY	2.6
1	D	193	ASP	2.6
1	D	8	TYR	2.6
1	A	70	ALA	2.6
1	B	28	GLY	2.5
1	D	440	GLY	2.5
1	D	221	GLY	2.5
1	C	63	PRO	2.5
1	C	64	ALA	2.4
1	B	402	ALA	2.4
1	C	403	ASN	2.3
1	B	1	MET	2.3
1	A	2	SER	2.3
1	D	223	THR	2.2
1	A	221	GLY	2.2
1	A	9	ASP	2.2
1	D	3	ASN	2.2
1	C	2	SER	2.2
1	D	9	ASP	2.1
1	B	222	SER	2.1
1	A	224	GLY	2.1
1	D	38	ARG	2.1
1	A	455	ALA	2.1
1	D	7	GLU	2.0
1	C	61	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

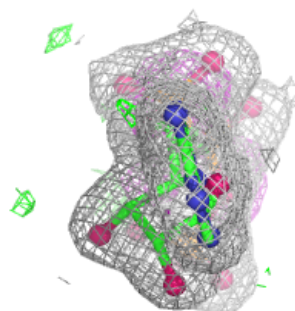
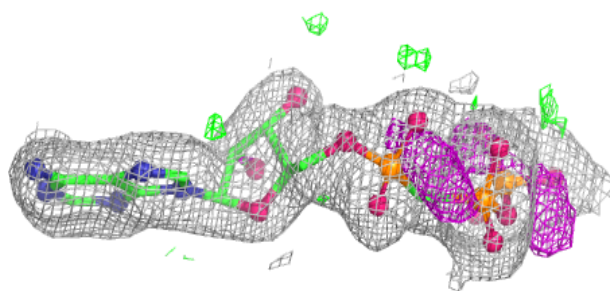
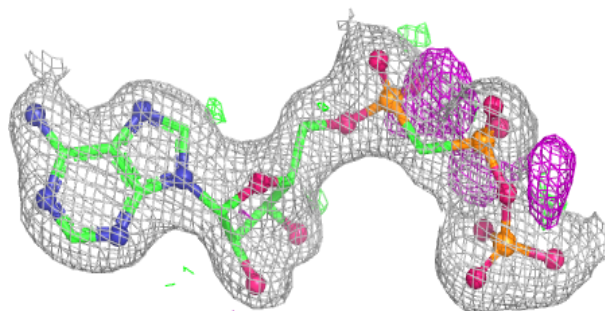
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	TLA	D	602	10/10	0.71	0.20	45,54,58,62	10
3	TLA	B	602	10/10	0.83	0.11	53,81,86,87	0
3	TLA	A	602	10/10	0.88	0.15	22,36,38,41	10
3	TLA	C	602	10/10	0.89	0.15	32,42,52,56	10
3	TLA	B	603	10/10	0.89	0.15	19,38,43,44	10
3	TLA	D	603	10/10	0.90	0.16	30,45,50,51	10
2	APC	C	601	31/31	0.94	0.08	38,44,67,88	0
2	APC	B	601	31/31	0.97	0.06	27,34,47,53	0
2	APC	A	601	31/31	0.98	0.05	25,28,40,46	0
2	APC	D	601	31/31	0.98	0.05	26,34,43,49	0
4	CL	A	603	1/1	0.98	0.12	51,51,51,51	0

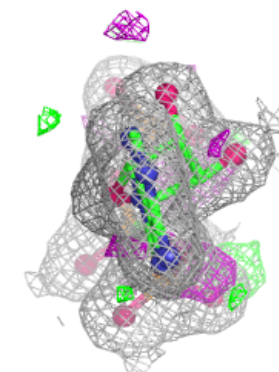
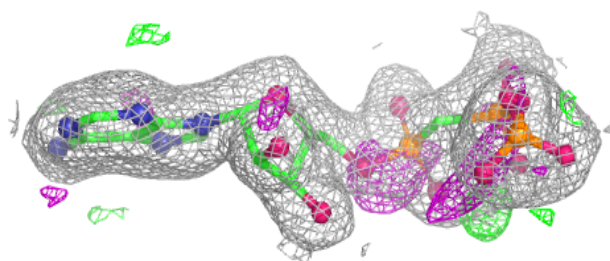
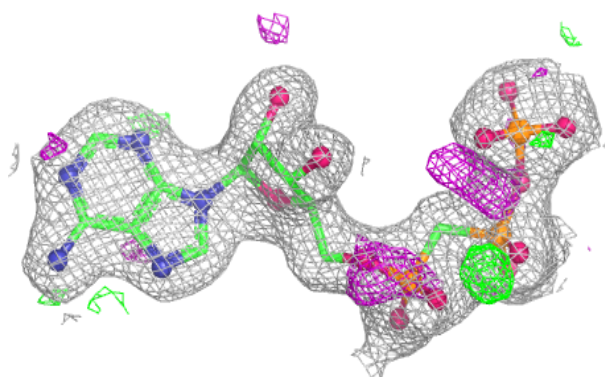
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC 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)

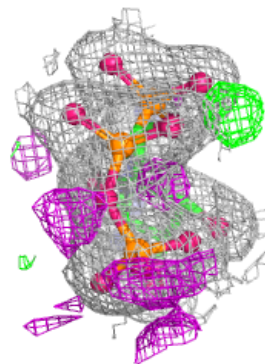
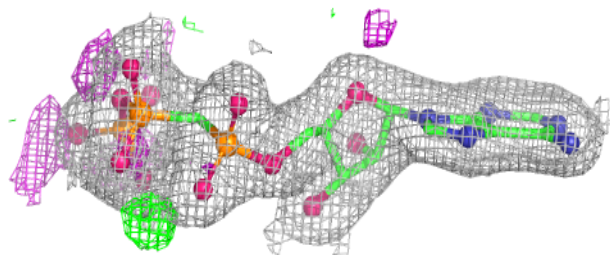
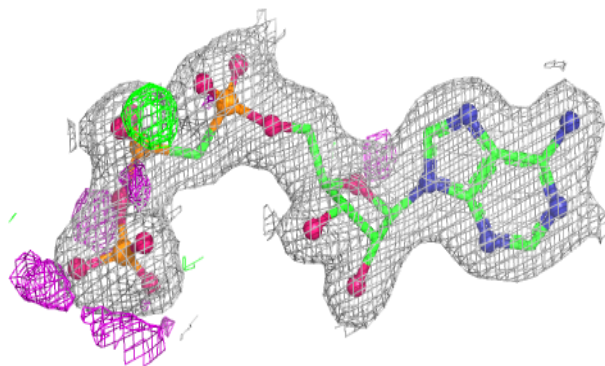
**Electron density around APC B 601:**

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

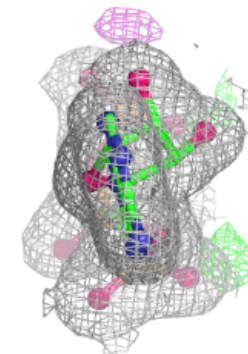
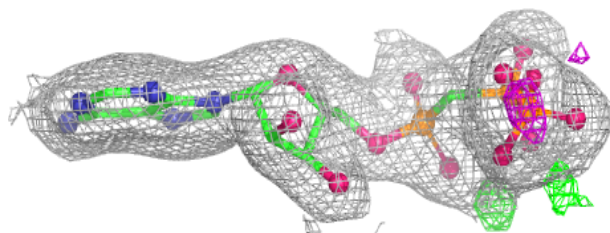
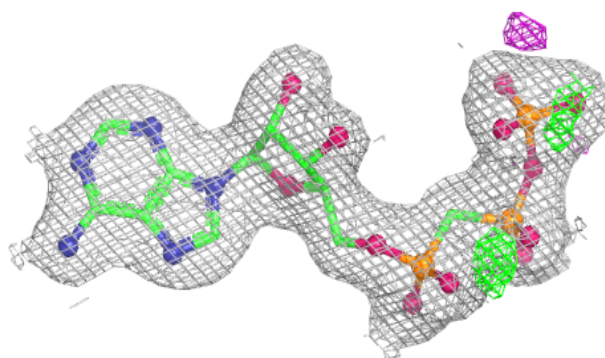


Electron density around APC A 601:

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

**Electron density around APC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.