WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 01:58 PM EST

PDB ID	:	6V6Q
Title	:	Crystal Structure of Monophosphorylated FGF Receptor 2 isoform IIIb with PTR657
Authors	:	Lin, C.-C.; Wieteska, L.; Poncet-Montange, G.; Suen, K.M.; Arold, S.T.; Ahmed, Z.; Ladbury, J.E.
Deposited on	:	2019-12-05
Resolution	:	2.46 Å(reported)

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

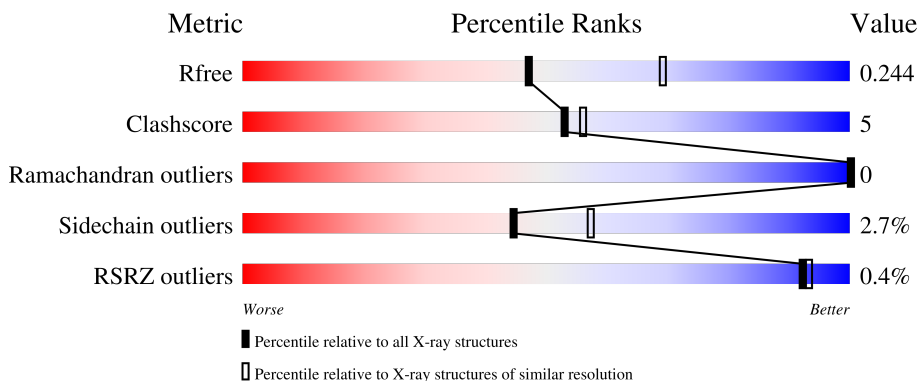|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.46 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		0.4%

Worse ◼ *Better*

◼ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	411	61% 9% 30%
1	B	411	61% 9% • 29%
1	C	411	59% 9% 32%
1	D	411	.% 57% 10% 33%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9267 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total 2287	C 1461	N 388	O 416	P 1	S 21	0	0	0
1	B	291	Total 2323	C 1478	N 394	O 428	P 1	S 22	0	0	0
1	C	279	Total 2215	C 1413	N 377	O 403	S 22		0	0	0
1	D	276	Total 2193	C 1400	N 375	O 397	S 21		0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	GLY	-	expression tag	UNP P21802
A	412	SER	-	expression tag	UNP P21802
A	466	PHE	TYR	engineered mutation	UNP P21802
A	561	PHE	TYR	engineered mutation	UNP P21802
A	566	PHE	TYR	engineered mutation	UNP P21802
A	575	PHE	TYR	engineered mutation	UNP P21802
A	586	PHE	TYR	engineered mutation	UNP P21802
A	588	PHE	TYR	engineered mutation	UNP P21802
A	608	PHE	TYR	engineered mutation	UNP P21802
A	616	PHE	TYR	engineered mutation	UNP P21802
A	657	PHE	TYR	engineered mutation	UNP P21802
A	733	PHE	TYR	engineered mutation	UNP P21802
B	411	GLY	-	expression tag	UNP P21802
B	412	SER	-	expression tag	UNP P21802
B	466	PHE	TYR	engineered mutation	UNP P21802
B	561	PHE	TYR	engineered mutation	UNP P21802
B	566	PHE	TYR	engineered mutation	UNP P21802
B	575	PHE	TYR	engineered mutation	UNP P21802
B	586	PHE	TYR	engineered mutation	UNP P21802
B	588	PHE	TYR	engineered mutation	UNP P21802
B	608	PHE	TYR	engineered mutation	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	616	PHE	TYR	engineered mutation	UNP P21802
B	657	PHE	TYR	engineered mutation	UNP P21802
B	733	PHE	TYR	engineered mutation	UNP P21802
C	411	GLY	-	expression tag	UNP P21802
C	412	SER	-	expression tag	UNP P21802
C	466	PHE	TYR	engineered mutation	UNP P21802
C	561	PHE	TYR	engineered mutation	UNP P21802
C	566	PHE	TYR	engineered mutation	UNP P21802
C	575	PHE	TYR	engineered mutation	UNP P21802
C	586	PHE	TYR	engineered mutation	UNP P21802
C	588	PHE	TYR	engineered mutation	UNP P21802
C	608	PHE	TYR	engineered mutation	UNP P21802
C	616	PHE	TYR	engineered mutation	UNP P21802
C	657	PHE	TYR	engineered mutation	UNP P21802
C	733	PHE	TYR	engineered mutation	UNP P21802
D	411	GLY	-	expression tag	UNP P21802
D	412	SER	-	expression tag	UNP P21802
D	466	PHE	TYR	engineered mutation	UNP P21802
D	561	PHE	TYR	engineered mutation	UNP P21802
D	566	PHE	TYR	engineered mutation	UNP P21802
D	575	PHE	TYR	engineered mutation	UNP P21802
D	586	PHE	TYR	engineered mutation	UNP P21802
D	588	PHE	TYR	engineered mutation	UNP P21802
D	608	PHE	TYR	engineered mutation	UNP P21802
D	616	PHE	TYR	engineered mutation	UNP P21802
D	657	PHE	TYR	engineered mutation	UNP P21802
D	733	PHE	TYR	engineered mutation	UNP P21802

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

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 27	C 11	N 5	O 9	P 2	0	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total 29	O 29	0	0

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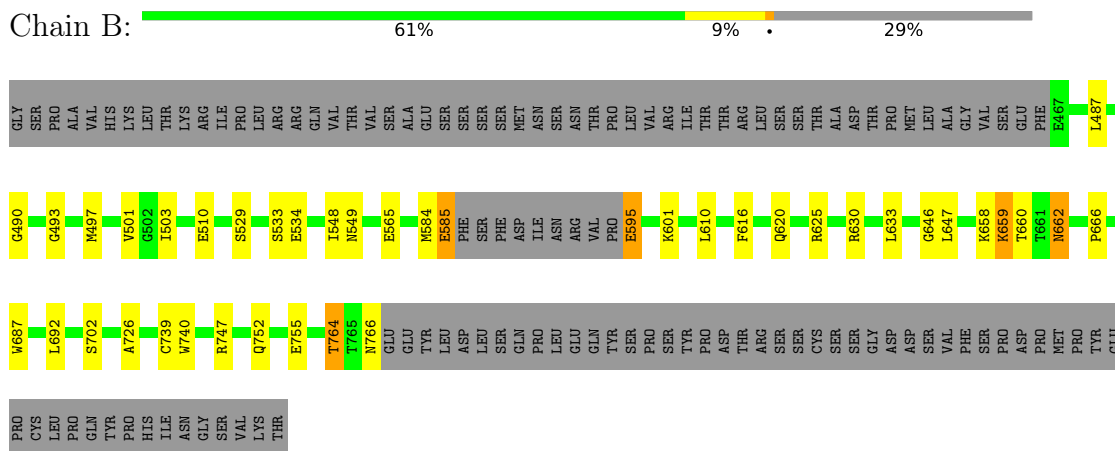| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	63	Total 63	O 63	0	0
4	C	23	Total 23	O 23	0	0
4	D	10	Total 10	O 10	0	0

3 Residue-property plots ⓘ

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.
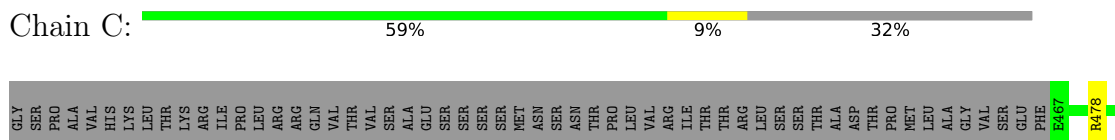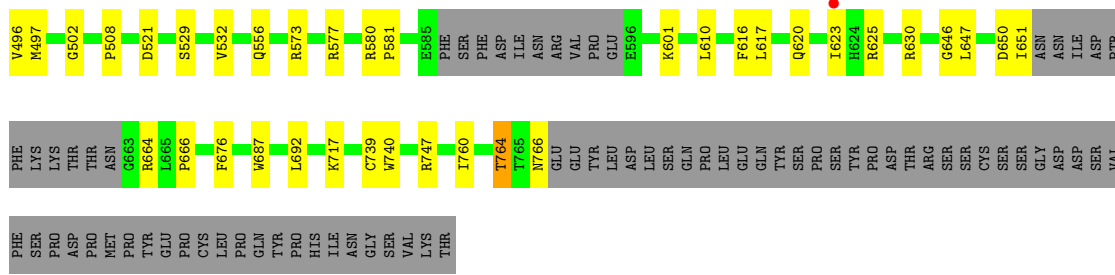
• Molecule 1: Fibroblast growth factor receptor 2

Chain A:
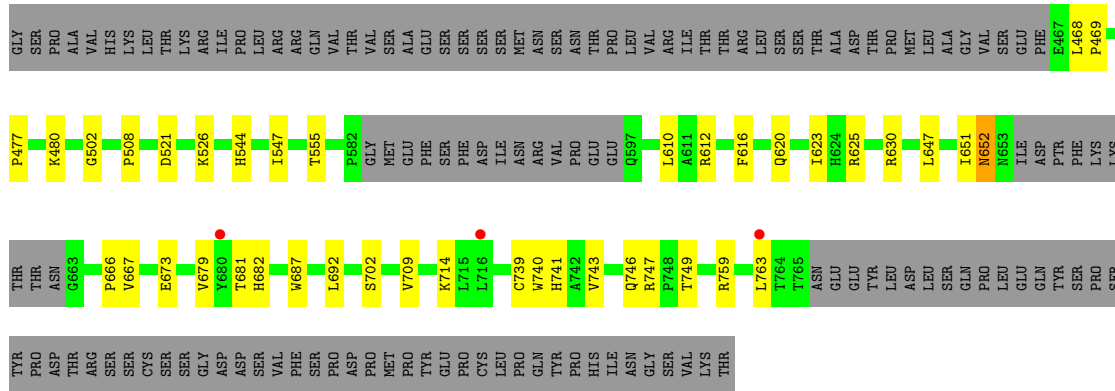

• Molecule 1: Fibroblast growth factor receptor 2

Chain B:

• Molecule 1: Fibroblast growth factor receptor 2

Chain C:

V496 M497 G502 P508 D521 S529 V532 Q556 R573 R577 R580 P581 E585 PHE SER PHE ASP ILE ASN ARG VAL PRO GLU E596 K601 L610 F616 L617 Q620 I623 H624 R625 R630 G646 L647 D650 I651 ASN ASN ILE ASP PTR

PHE LYS LYS THR THR ASN G663 R664 L665 P666 F676 W687 L692 K717 C739 W740 R747 I760 T764 T765 N766 GLU GLU TYR LEU ASP LEU SER GLN PRO LEU GLU GLN TYR SER PRO SER TYR PRO ASP THR ARG SER SER CYS SER SER GLY ASP ASP SER VAL

PHE SER PRO ASP PRO MET PRO TYR GLU CYS LEU PRO GLN TYR PRO HIS ILE ASN GLY SER VAL LYS THR

• Molecule 1: Fibroblast growth factor receptor 2

Chain D:

%

57%   10%   33%

GLY SER PRO ALA VAL HIS LYS LYS LEU THR LYS ARG ILE PRO LEU ARG ARG GLN VAL THR VAL SER ALA GLU SER SER SER SER MET ASN SER ASN THR PRO LEU VAL ARG ILE THR THR ARG LEU SER SER THR ALA ASP THR PRO MET LEU ALA GLY VAL SER GLU PHE E467 L468 P469

P477 K480 G502 P508 D521 K526 H544 I547 T555 P582 GLY MET GLU PHE SER PHE ASP ILE ASN ARG VAL PRO GLU GLU Q597 L610 A611 R612 F616 Q620 I623 H624 R625 R630 L647 I651 N652 N653 ILE ASP PTR PHE LYS LYS

THR THR ASN G663 P666 V667 E673 V679 Y680 T681 H682 W687 L692 S702 V709 K714 L715 L716 C739 W740 H741 A742 V743 Q746 R747 P748 T749 R759 L763 T764 T765 ASN GLU GLU TYR LEU ASP LEU SER GLN PRO LEU GLU GLN TYR SER PRO SER

TYR PRO ASP THR ARG SER SER CYS SER SER GLY ASP ASP SER VAL PHE SER PRO ASP PRO MET PRO TYR GLU CYS LEU PRO GLN TYR PRO HIS ILE ASN GLY SER VAL LYS THR

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.97Å 86.54Å 254.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.06 – 2.46 81.92 – 2.46	Depositor EDS
% Data completeness (in resolution range)	95.9 (82.06-2.46) 95.9 (81.92-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.211 , 0.239 0.219 , 0.244	Depositor DCC
R_{free} test set	2574 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9267	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ACP, MG, PTR

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	#$\lvert Z \rvert$ >5	RMSZ	#$\lvert Z \rvert$ >5
1	A	0.66	0/2318	0.77	0/3124
1	B	0.67	0/2353	0.81	0/3170
1	C	0.65	0/2260	0.78	0/3045
1	D	0.62	0/2238	0.77	0/3017
All	All	0.65	0/9169	0.79	0/12356

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	646	GLY	Peptide

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	2287	0	2301	25	0
1	B	2323	0	2328	25	0
1	C	2215	0	2232	25	0
1	D	2193	0	2214	31	0
2	A	31	0	14	2	0
2	B	31	0	14	1	0
2	C	27	0	12	0	0
2	D	31	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	29	0	0	1	0
4	B	63	0	0	1	0
4	C	23	0	0	0	0
4	D	10	0	0	0	0
All	All	9267	0	9129	99	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 5.

The worst 5 of 99 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:760:ILE:O	1:A:764:THR:HG23	1.51	1.08
1:D:667:VAL:HG21	1:D:709:VAL:HG13	1.36	1.08
1:C:760:ILE:O	1:C:764:THR:HG23	1.50	1.08
1:D:468:LEU:HD11	1:D:555:THR:HB	1.41	0.98
1:A:724:LYS:HE3	1:A:728:CYS:O	1.63	0.97

There are no symmetry-related clashes.

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	281/411 (68%)	275 (98%)	6 (2%)	0	100	100
1	B	286/411 (70%)	279 (98%)	7 (2%)	0	100	100
1	C	273/411 (66%)	269 (98%)	4 (2%)	0	100	100
1	D	270/411 (66%)	266 (98%)	4 (2%)	0	100	100
All	All	1110/1644 (68%)	1089 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	250/366 (68%)	246 (98%)	4 (2%)	62	74
1	B	254/366 (69%)	242 (95%)	12 (5%)	26	34
1	C	243/366 (66%)	240 (99%)	3 (1%)	71	81
1	D	241/366 (66%)	233 (97%)	8 (3%)	38	49
All	All	988/1464 (68%)	961 (97%)	27 (3%)	44	57

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	764	THR
1	C	764	THR
1	D	681	THR
1	C	623	ILE
1	C	766	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	727	ASN
1	D	653	ASN
1	D	544	HIS

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Mol	Chain	Res	Type
1	C	720	HIS
1	D	652	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	PTR	B	656	1	15,16,17	0.52	0	19,22,24	0.71	0
1	PTR	A	656	1	15,16,17	0.66	0	19,22,24	0.67	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
1	PTR	B	656	1	-	<mark>2/10/11/13</mark>	0/1/1/1
1	PTR	A	656	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	656	PTR	CE2-CZ-OH-P

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Mol	Chain	Res	Type	Atoms
1	B	656	PTR	CE1-CZ-OH-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ACP	D	901	3	27,33,33	0.91	1 (3%)	32,52,52	0.96	2 (6%)
2	ACP	A	901	3	27,33,33	0.88	1 (3%)	32,52,52	0.84	1 (3%)
2	ACP	C	901	3	25,29,33	0.91	1 (4%)	26,45,52	0.86	1 (3%)
2	ACP	B	901	3	27,33,33	0.82	1 (3%)	32,52,52	0.88	2 (6%)

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	ACP	D	901	3	-	6/15/38/38	0/3/3/3
2	ACP	A	901	3	-	6/15/38/38	0/3/3/3
2	ACP	C	901	3	-	7/9/32/38	0/3/3/3
2	ACP	B	901	3	-	4/15/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	ACP	PB-C3B	2.40	1.83	1.77
2	A	901	ACP	PB-O2B	-2.31	1.50	1.56
2	D	901	ACP	PB-O2B	-2.31	1.51	1.56
2	B	901	ACP	PB-O2B	-2.24	1.51	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	ACP	O1G-PG-C3B	-2.54	105.76	111.24
2	B	901	ACP	C5-C6-N6	2.47	124.10	120.35
2	A	901	ACP	C5-C6-N6	2.45	124.07	120.35
2	D	901	ACP	C5-C6-N6	2.31	123.86	120.35
2	C	901	ACP	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ACP	PG-C3B-PB-O1B
2	B	901	ACP	PB-C3B-PG-O1G
2	B	901	ACP	PB-C3B-PG-O2G
2	B	901	ACP	PB-C3B-PG-O3G
2	C	901	ACP	C5'-O5'-PA-O2A

There are no ring outliers.
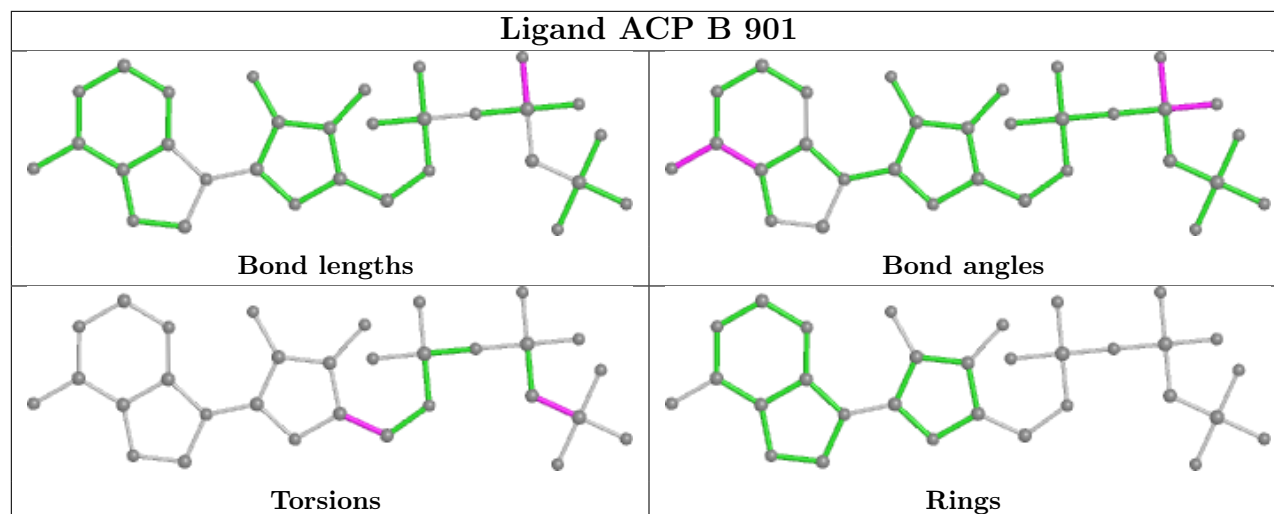
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ACP	2	0
2	B	901	ACP	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 then 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 ACP D 901

Bond lengths — Bond angles — Torsions — Rings

Ligand ACP A 901

Bond lengths — Bond angles — Torsions — Rings

Ligand ACP C 901

Bond lengths — Bond angles — Torsions — Rings

Ligand ACP B 901	
Bond lengths	Bond angles
Torsions	Rings
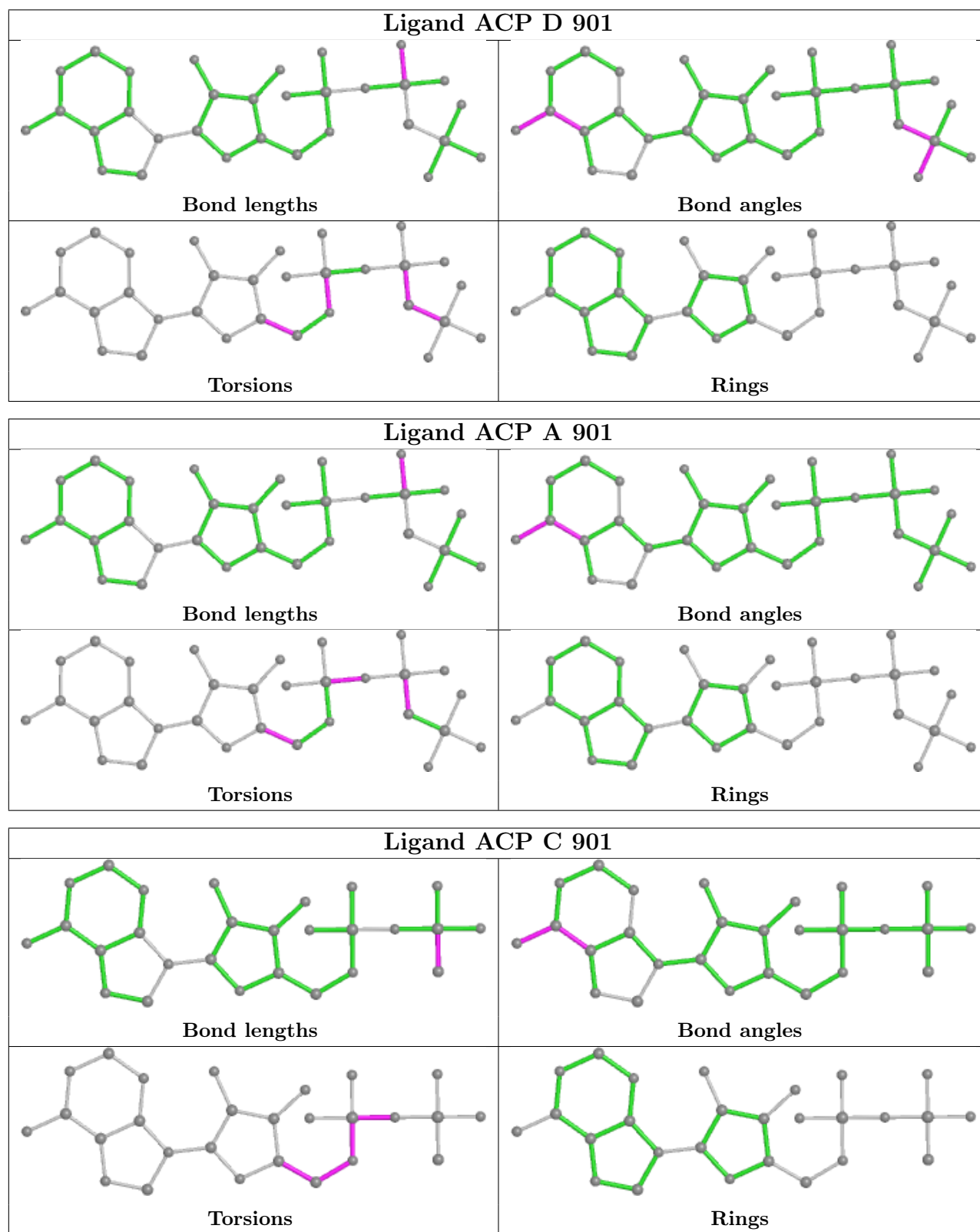
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	285/411 (69%)	-0.19	1 (0%) 92	93	39, 71, 111, 128	0
1	B	290/411 (70%)	-0.30	0 100	100	30, 48, 81, 128	0
1	C	279/411 (67%)	-0.16	1 (0%) 92	93	38, 73, 117, 149	0
1	D	276/411 (67%)	-0.03	3 (1%) 80	80	60, 87, 123, 143	0
All	All	1130/1644 (68%)	-0.17	5 (0%) 92	93	30, 71, 114, 149	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	727	ASN	3.7
1	D	716	LEU	2.8
1	D	680	TYR	2.4
1	C	623	ILE	2.3
1	D	763	LEU	2.1

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

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(Å²)	Q<0.9
1	PTR	A	656	16/17	0.96	0.12	65,69,72,75	0
1	PTR	B	656	16/17	0.98	0.10	42,48,55,56	0

6.3 Carbohydrates ⓘ
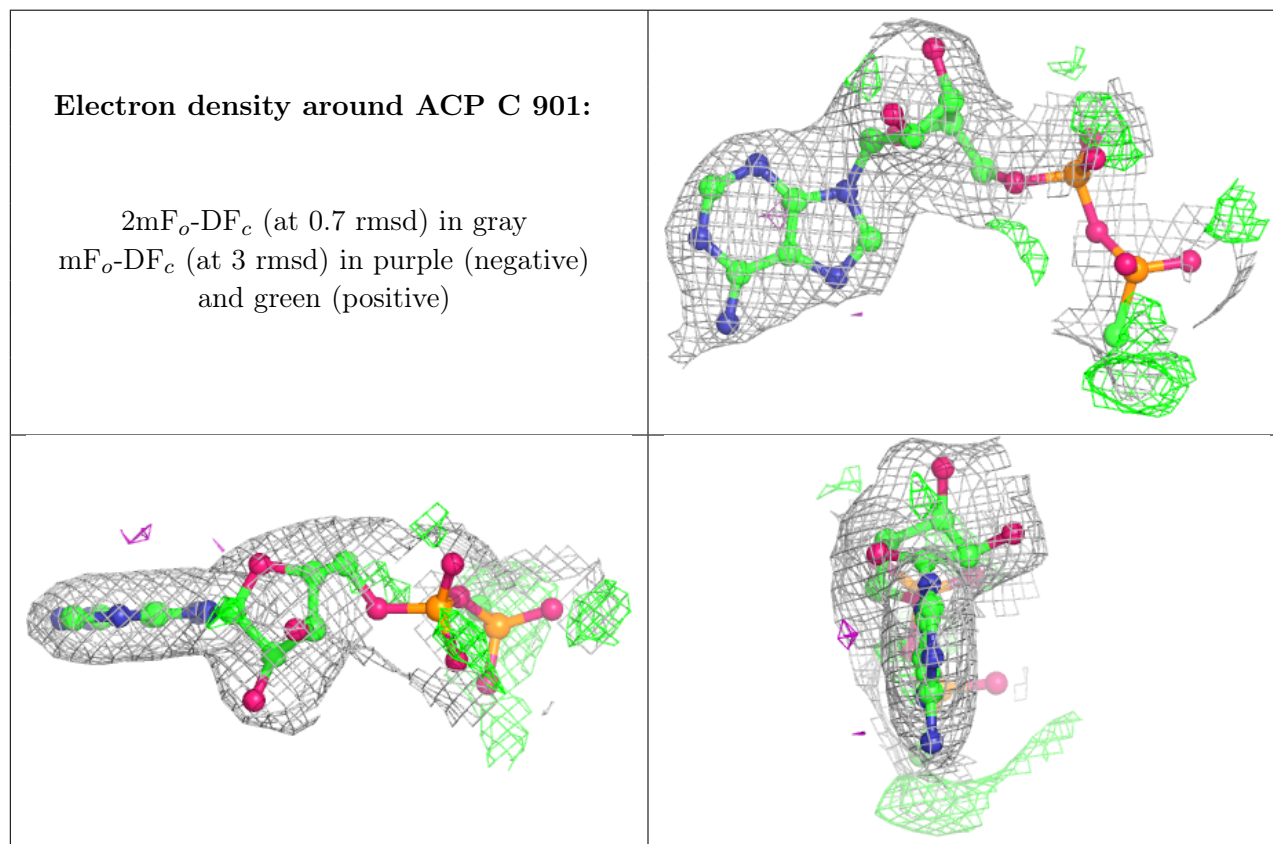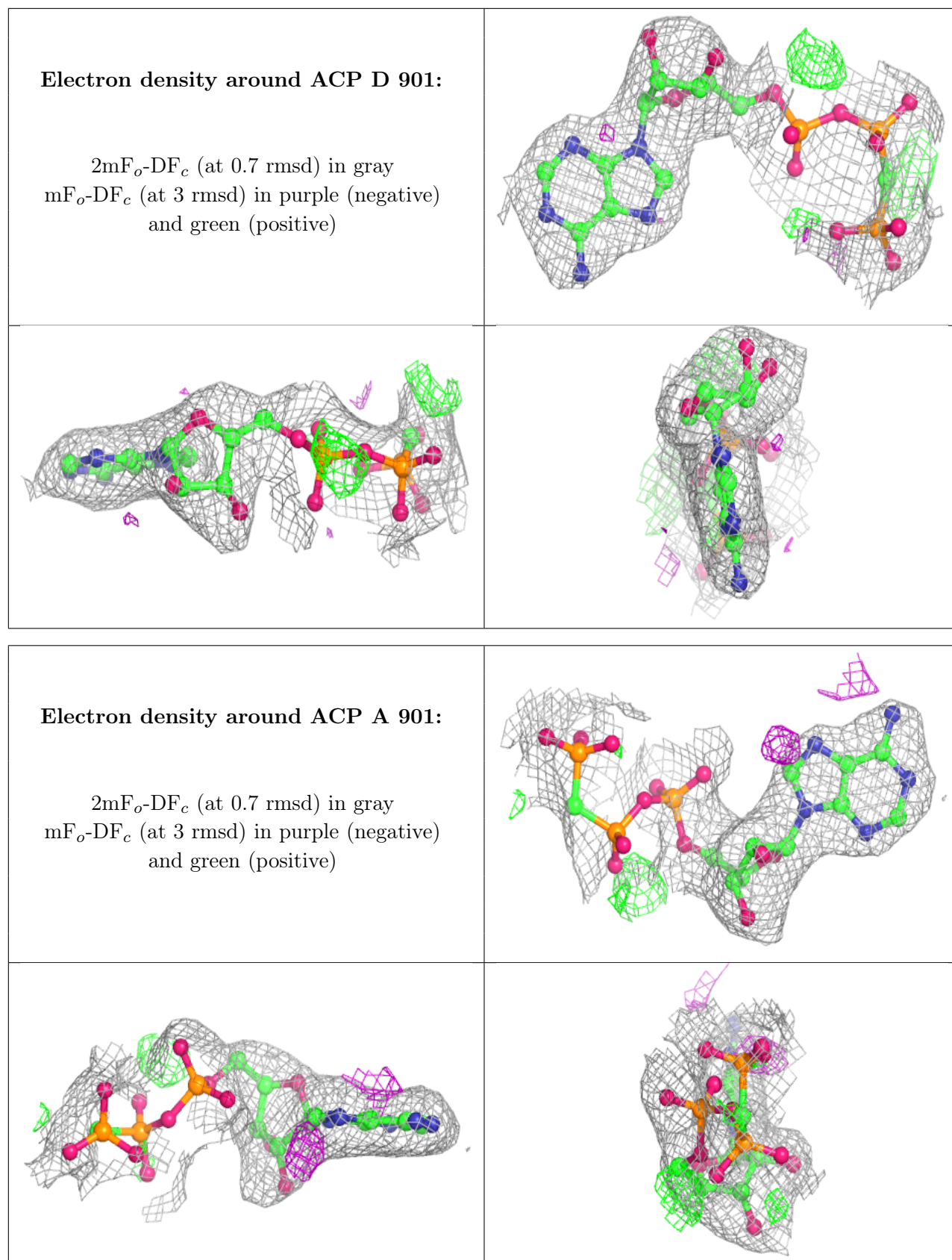
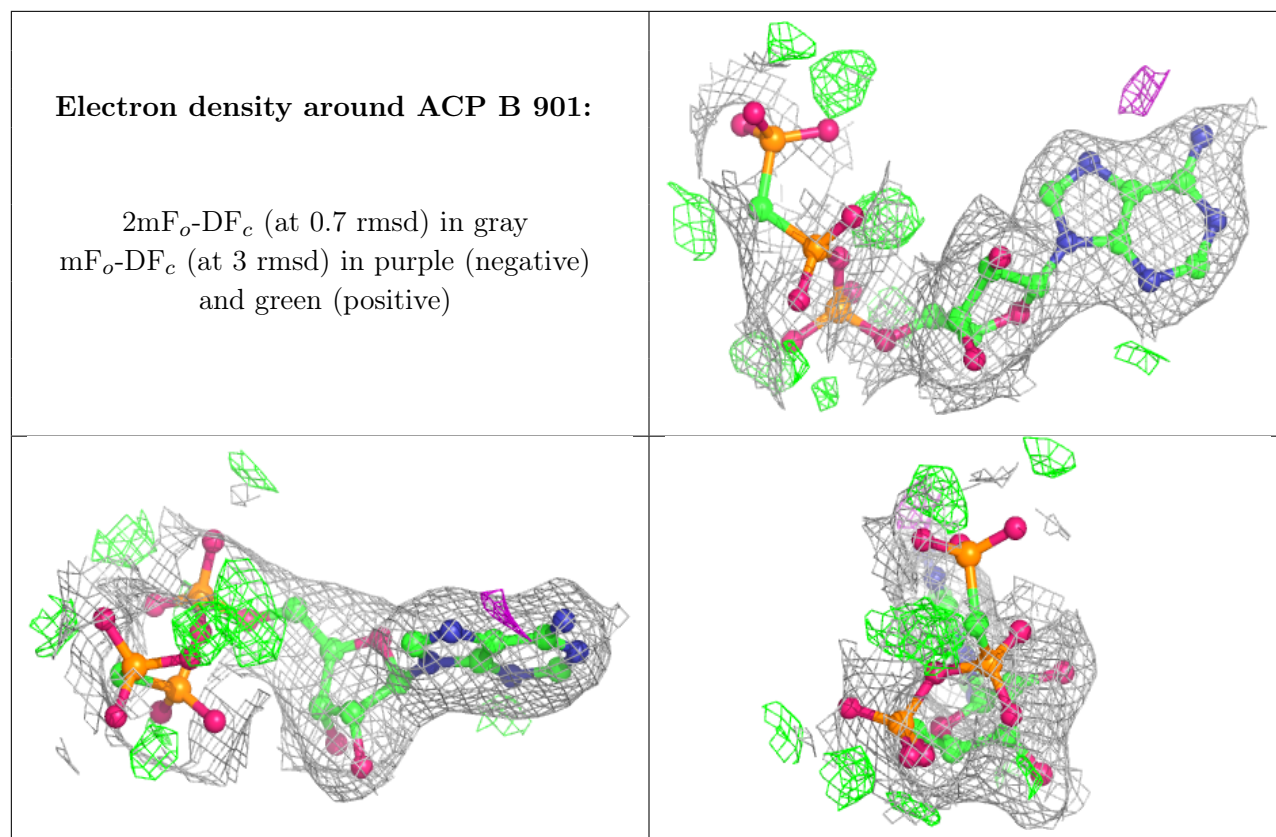There are no monosaccharides in this entry.

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, 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
3	MG	D	902	1/1	0.83	0.12	139,139,139,139	0
2	ACP	C	901	27/31	0.87	0.13	56,79,123,125	0
2	ACP	D	901	31/31	0.90	0.13	59,87,140,146	0
2	ACP	A	901	31/31	0.90	0.12	48,73,117,123	0
3	MG	B	902	1/1	0.92	0.11	50,50,50,50	0
3	MG	C	902	1/1	0.92	0.12	72,72,72,72	0
3	MG	A	902	1/1	0.92	0.06	53,53,53,53	0
2	ACP	B	901	31/31	0.94	0.13	34,55,94,105	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 ACP C 901:

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

Electron density around ACP D 901:

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

Electron density around ACP A 901:

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

Electron density around ACP B 901:

$2mF_o$-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 ⓘ

There are no such residues in this entry.