Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 07:17 AM EST

PDB ID	:	5EG3
Title	:	Crystal Structure of the Activated FGF Receptor 2 (FGFR2) Kinase Domain in complex with the cSH2 domain of Phospholipase C gamma (PLCgamma)
Authors	:	Huang, Z.; Li, X.; Mohammadi, M.
Deposited on	:	2015-10-26
Resolution	:	2.61 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 (i) 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 (i)) were used in the production of this report:

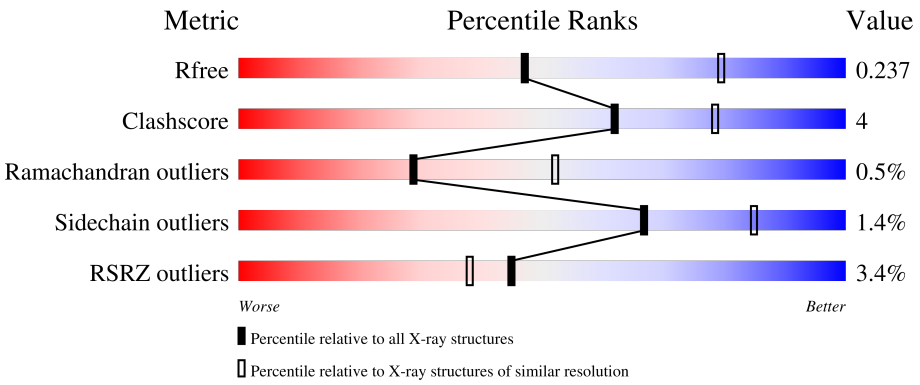
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	334	4% 79% 11% 10%
2	B	114	92% 7% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3414 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
			Total	C	N	O	P	S			
1	A	302	2402	1525	408	448	1	20	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	466	PHE	TYR	engineered mutation	UNP P21802
A	491	ALA	CYS	engineered mutation	UNP P21802
A	565	ALA	GLU	engineered mutation	UNP P21802
A	586	LEU	TYR	engineered mutation	UNP P21802
A	588	PRO	TYR	engineered mutation	UNP P21802
A	656	PHE	TYR	engineered mutation	UNP P21802
A	657	PHE	TYR	engineered mutation	UNP P21802
A	659	GLU	LYS	engineered mutation	UNP P21802

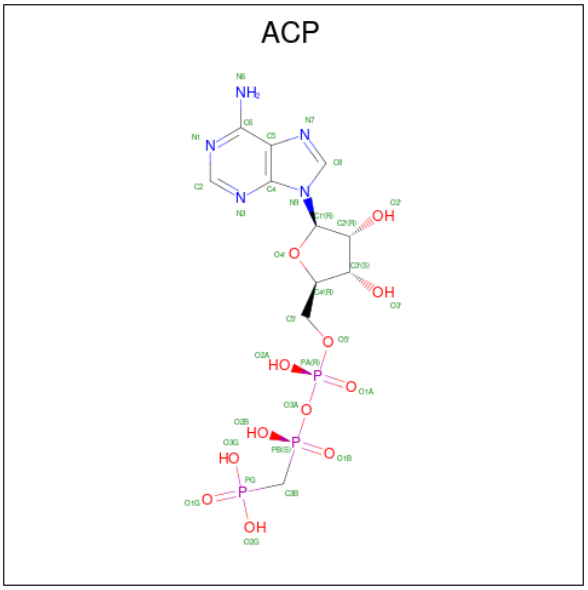
- Molecule 2 is a protein called 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	113	924	580	167	171	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	660	MET	-	initiating methionine	UNP P10686

- Molecule 3 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
			Total	C	N	O	P		
3	A	1	31	11	5	12	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	39	39	39	0	0

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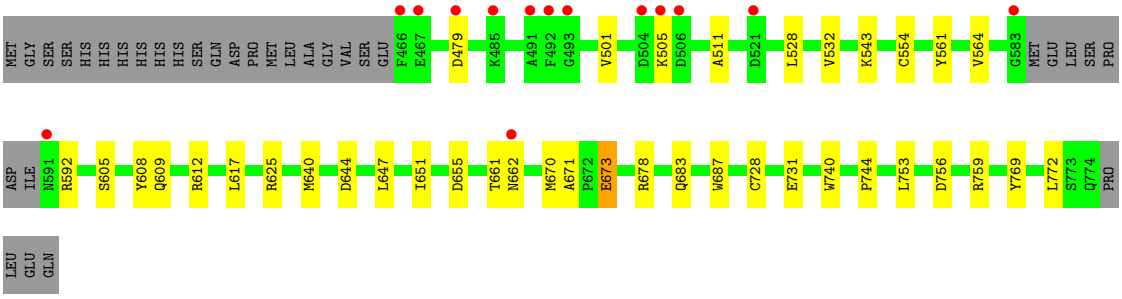
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	16	16	16	0	0

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: Fibroblast growth factor receptor 2

Chain A:



• Molecule 2: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-1

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.61Å 53.23Å 127.66Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	37.86 – 2.61 37.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.86-2.61) 95.3 (37.86-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.78 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.185 , 0.237 0.188 , 0.237	Depositor DCC
R_{free} test set	1598 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3414	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, ACP, MG

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	1/2434 (0.0%)	0.57	0/3289
2	B	0.49	0/945	0.57	0/1271
All	All	0.46	1/3379 (0.0%)	0.57	0/4560

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	CYS	CB-SG	-5.89	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2402	0	2386	24	0
2	B	924	0	897	5	0
3	A	31	0	14	1	0
4	A	2	0	0	0	0
5	A	39	0	0	4	0
5	B	16	0	0	1	0
All	All	3414	0	3297	29	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 4.

All (29) 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:505:LYS:H	1:A:505:LYS:HD2	1.50	0.76
3:A:801:ACP:O3G	5:A:901:HOH:O	2.12	0.67
1:A:592:ARG:NH2	5:A:904:HOH:O	2.35	0.58
1:A:505:LYS:HD2	1:A:505:LYS:N	2.17	0.57
1:A:608:TYR:CZ	1:A:612:ARG:HD2	2.42	0.54
1:A:651:ILE:HD12	1:A:655:ASP:HA	1.92	0.52
1:A:501:VAL:HA	1:A:511:ALA:HA	1.91	0.52
1:A:554:CYS:HB2	1:A:561:TYR:HB2	1.93	0.50
1:A:671:ALA:HB1	1:A:673:GLU:OE2	2.11	0.50
2:B:695:LYS:HE3	5:B:805:HOH:O	2.14	0.47
1:A:501:VAL:HG12	1:A:511:ALA:HB2	1.95	0.47
2:B:708:ALA:HB2	2:B:750:MET:HE2	1.97	0.46
1:A:772:LEU:HD12	2:B:726:LEU:HD11	1.96	0.46
2:B:696:ARG:HD3	2:B:703:ALA:HB2	1.96	0.46
1:A:543:LYS:HB3	1:A:543:LYS:HE3	1.62	0.45
1:A:731:GLU:OE2	1:A:759:ARG:NH1	2.46	0.45
1:A:608:TYR:OH	1:A:612:ARG:HD2	2.18	0.43
1:A:605:SER:O	1:A:609:GLN:HG3	2.19	0.42
1:A:625:ARG:HD3	1:A:647:LEU:O	2.19	0.42
1:A:756:ASP:OD1	1:A:759:ARG:NH2	2.52	0.42
1:A:753:LEU:HD23	1:A:753:LEU:HA	1.91	0.42
1:A:683:GLN:HG2	1:A:744:PRO:O	2.20	0.41
1:A:640:MET:HE2	1:A:640:MET:HB3	1.84	0.41
1:A:678:ARG:HA	1:A:678:ARG:HD3	1.86	0.41
1:A:687:TRP:CE3	1:A:740:TRP:HA	2.55	0.41
1:A:670:MET:HA	5:A:926:HOH:O	2.21	0.41
1:A:756:ASP:OD2	5:A:902:HOH:O	2.22	0.41
2:B:684:ARG:HA	2:B:766:THR:HG22	2.02	0.41
1:A:528:LEU:O	1:A:532:VAL:HG23	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	297/334 (89%)	290 (98%)	5 (2%)	2 (1%)	22	43
2	B	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
All	All	408/448 (91%)	397 (97%)	9 (2%)	2 (0%)	29	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	662	ASN
1	A	644	ASP

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	259/292 (89%)	254 (98%)	5 (2%)	57	79
2	B	97/98 (99%)	97 (100%)	0	100	100
All	All	356/390 (91%)	351 (99%)	5 (1%)	67	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	564	VAL
1	A	617	LEU
1	A	661	THR

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Mol	Chain	Res	Type
1	A	673	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	A	769	1	15,16,17	1.35	1 (6%)	19,22,24	0.86	1 (5%)

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	A	769	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	769	PTR	OH-CZ	-4.38	1.30	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	769	PTR	O3P-P-OH	2.60	113.37	105.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	ACP	A	801	4	27,33,33	2.33	10 (37%)	32,52,52	1.81	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	801	4	-	3/15/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ACP	O4'-C1'	5.97	1.49	1.41
3	A	801	ACP	C2'-C1'	-4.41	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ACP	C2'-C3'	-4.05	1.42	1.53
3	A	801	ACP	PG-O1G	3.50	1.57	1.50
3	A	801	ACP	C3'-C4'	-3.19	1.44	1.53
3	A	801	ACP	C6-N6	3.16	1.45	1.34
3	A	801	ACP	PB-O2B	-3.04	1.49	1.56
3	A	801	ACP	PB-O3A	2.59	1.61	1.58
3	A	801	ACP	C2-N3	2.53	1.36	1.32
3	A	801	ACP	PG-O3G	-2.24	1.49	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	ACP	N3-C2-N1	-5.07	120.76	128.68
3	A	801	ACP	C3'-C2'-C1'	3.42	106.12	100.98
3	A	801	ACP	C4-C5-N7	-3.07	106.20	109.40
3	A	801	ACP	C5'-C4'-C3'	-3.01	103.91	115.18
3	A	801	ACP	O2G-PG-C3B	2.75	113.07	106.40
3	A	801	ACP	PB-O3A-PA	-2.54	124.52	132.56
3	A	801	ACP	C2'-C3'-C4'	2.42	107.34	102.64
3	A	801	ACP	O5'-C5'-C4'	2.22	116.64	108.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ACP	C5'-O5'-PA-O3A
3	A	801	ACP	PB-O3A-PA-O5'
3	A	801	ACP	C5'-O5'-PA-O2A

There are no ring outliers.

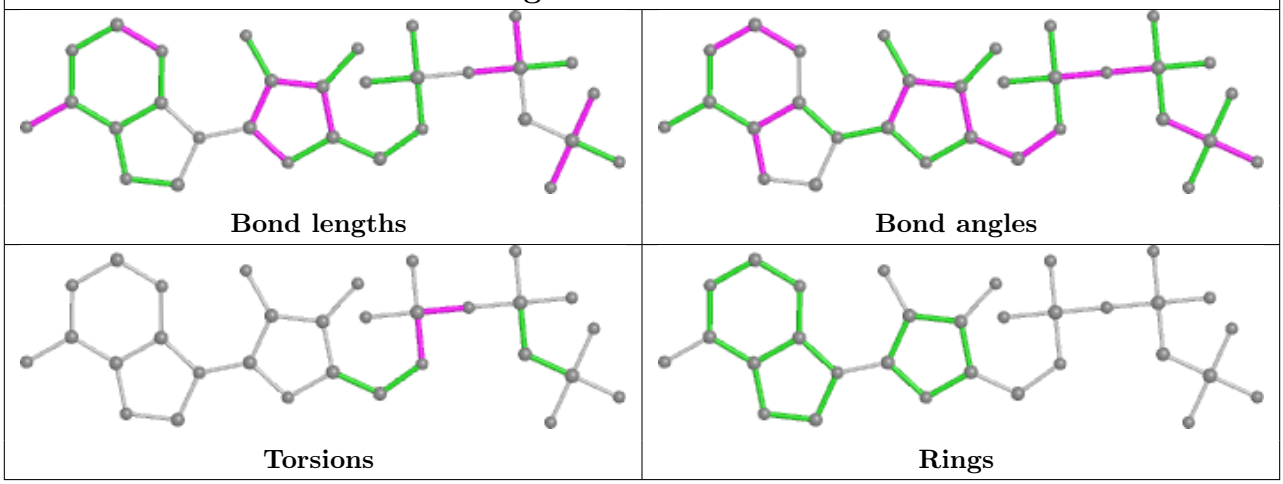
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	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 A 801



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	301/334 (90%)	0.05	14 (4%) 31 25	14, 31, 75, 106	0
2	B	113/114 (99%)	-0.21	0 100 100	17, 31, 54, 68	0
All	All	414/448 (92%)	-0.02	14 (3%) 45 38	14, 31, 68, 106	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	LYS	4.5
1	A	662	ASN	3.6
1	A	479	ASP	3.2
1	A	466	PHE	3.2
1	A	492	PHE	3.1
1	A	504	ASP	2.8
1	A	583	GLY	2.7
1	A	506	ASP	2.7
1	A	485	LYS	2.7
1	A	491	ALA	2.6
1	A	521	ASP	2.6
1	A	493	GLY	2.5
1	A	467	GLU	2.4
1	A	591	ASN	2.2

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	PTR	A	769	16/17	0.98	0.11	21,23,25,26	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

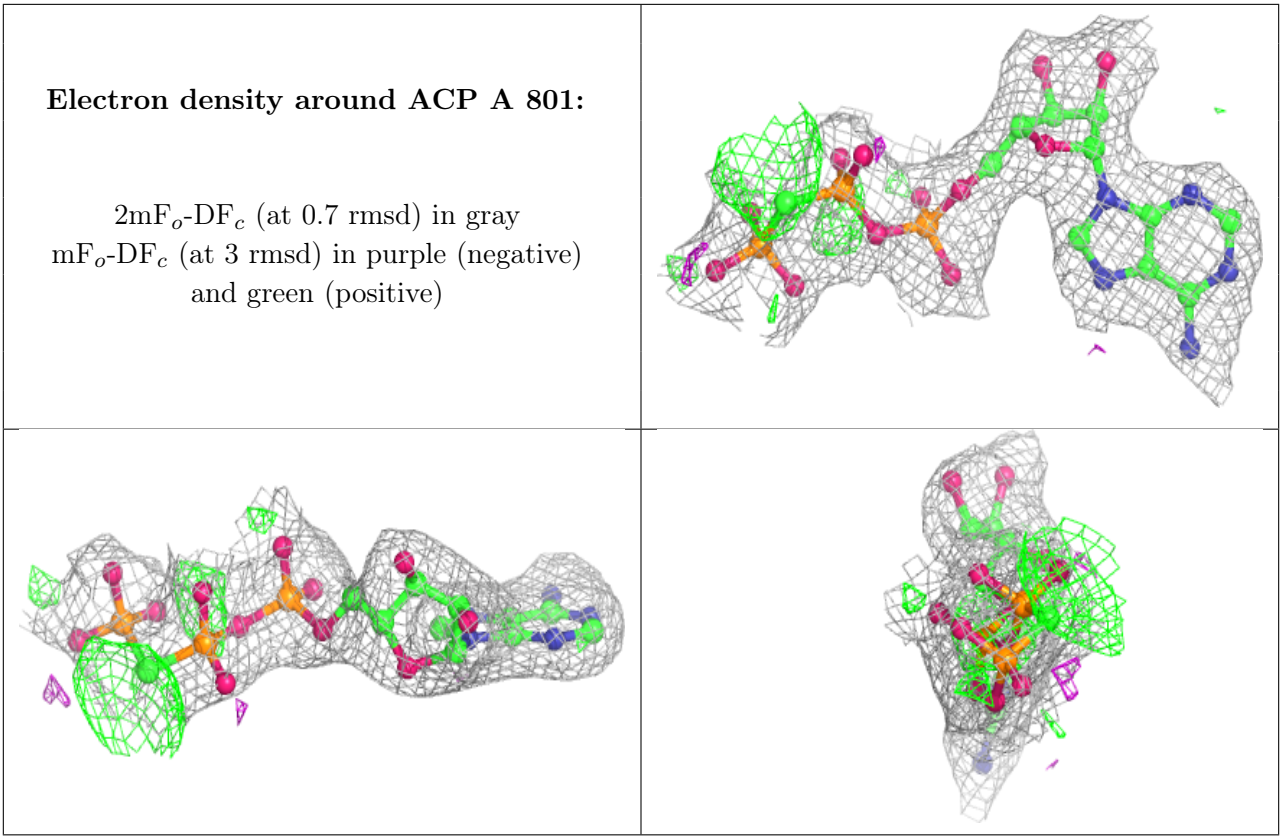
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACP	A	801	31/31	0.94	0.15	21,27,65,74	0
4	MG	A	802	1/1	0.95	0.17	37,37,37,37	0
4	MG	A	803	1/1	0.96	0.15	28,28,28,28	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 A 801:

$2mF_o$-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.