



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 09:20 AM EDT

PDB ID : 5UI0  
Title : Crystal Structure of the Tyrosine Kinase Domain of FGF Receptor 2 harboring an E565A/K659M Double Gain-of-Function Mutation  
Authors : Mohammadi, M.; Chen, H.  
Deposited on : 2017-01-12  
Resolution : 2.05 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

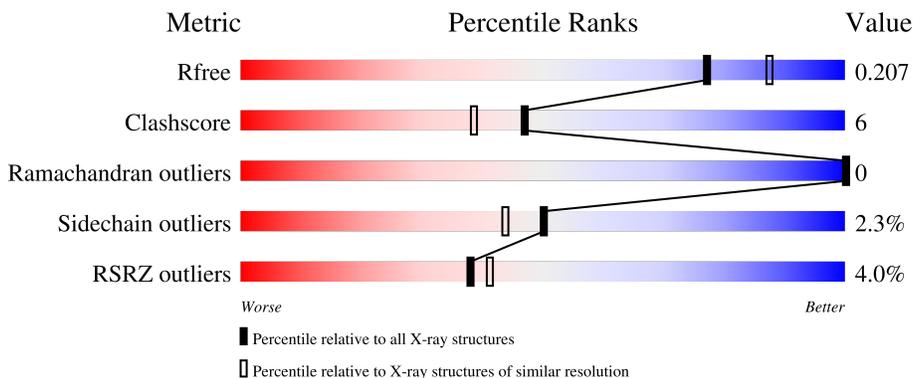
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	324	 4% 81% 12% 7%
1	B	324	 3% 79% 14% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	B	801	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5150 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	S			
1	A	301	2395	1524	402	446	23	0	2	0
1	B	304	2435	1550	409	452	24	0	2	0

There are 32 discrepancies between the modelled and reference sequences:

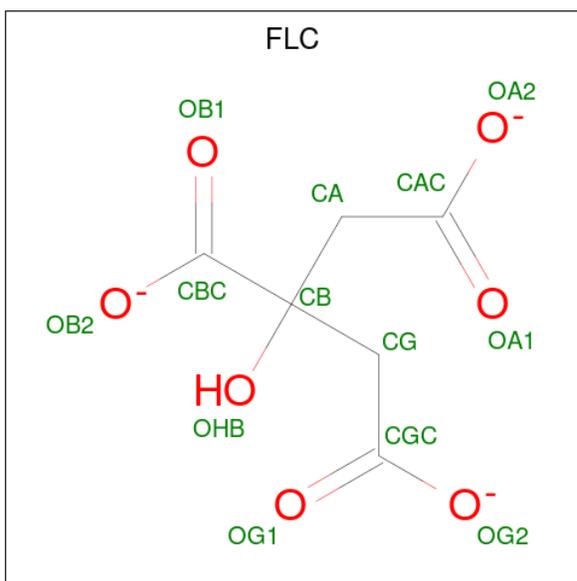
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression 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	491	ALA	CYS	engineered mutation	UNP P21802
A	565	ALA	GLU	engineered mutation	UNP P21802
A	659	MET	LYS	conflict	UNP P21802
B	445	MET	-	initiating methionine	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	491	ALA	CYS	engineered mutation	UNP P21802
B	565	ALA	GLU	engineered mutation	UNP P21802
B	659	MET	LYS	conflict	UNP P21802

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).

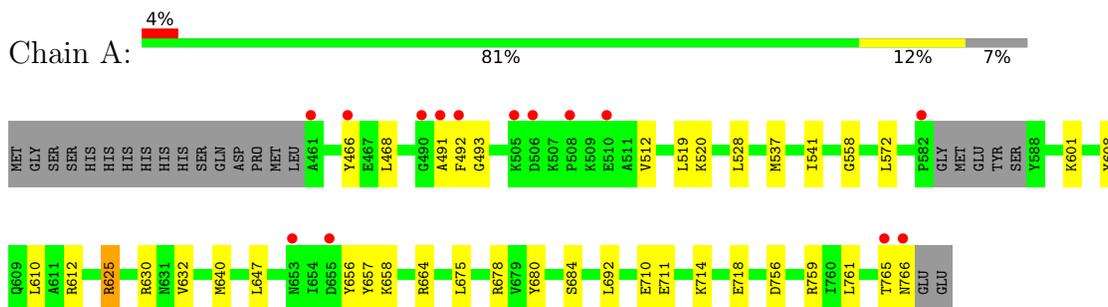


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	110	Total 110	O 110	0	0
5	B	148	Total 148	O 148	0	0

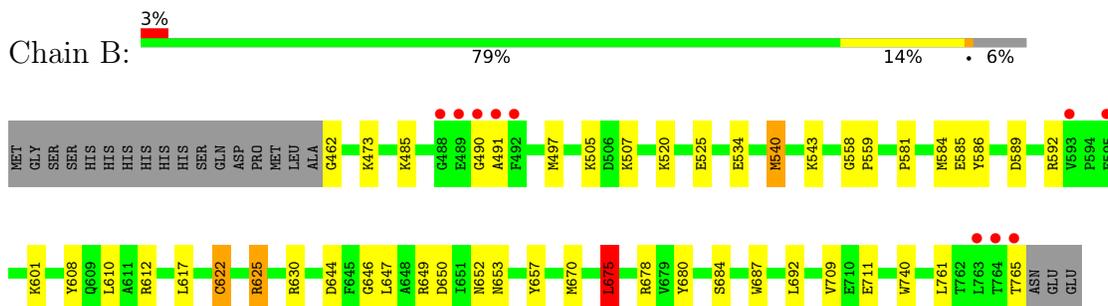
### 3 Residue-property plots [i](#)

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



- Molecule 1: Fibroblast growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.94Å 73.94Å 311.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.14 – 2.05 26.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (26.14-2.05) 98.8 (26.14-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.49 (at 2.04Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.182 , 0.207 0.182 , 0.207	Depositor DCC
$R_{free}$ test set	1998 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ACP, SO4

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	0.41	0/2452	0.59	1/3319 (0.0%)
1	B	0.43	0/2494	0.60	3/3372 (0.1%)
All	All	0.42	0/4946	0.60	4/6691 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	625	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	625	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	625	ARG	NE-CZ-NH1	5.37	122.98	120.30

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	2395	0	2381	25	0
1	B	2435	0	2436	38	0
2	A	13	0	5	3	0
2	B	13	0	5	6	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	14	2	0
5	A	110	0	0	0	0
5	B	148	0	0	6	0
All	All	5150	0	4841	60	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 6.

All (60) 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:B:649:ARG:HH21	2:B:801:FLC:HG1	1.26	0.98
1:A:632:VAL:HG11	1:A:640:MET:HE3	1.74	0.69
1:A:678:ARG:NH2	1:B:525:GLU:OE2	2.27	0.68
1:A:664:ARG:NH2	2:A:801:FLC:OA1	2.30	0.62
1:A:756:ASP:OD1	1:A:759:ARG:NH2	2.35	0.60
1:A:657:TYR:OH	2:A:801:FLC:OB1	2.13	0.60
1:A:625:ARG:HD3	1:A:647:LEU:O	2.03	0.59
1:B:625:ARG:HD3	1:B:647:LEU:O	2.04	0.57
1:B:657:TYR:OH	2:B:801:FLC:HG2	2.05	0.57
1:B:581:PRO:HG2	1:B:584:MET:HE2	1.88	0.56
2:B:801:FLC:OG1	2:B:801:FLC:OHB	2.18	0.56
1:B:601:LYS:HE3	1:B:765:THR:HG22	1.87	0.56
1:B:491:ALA:O	5:B:901:HOH:O	2.18	0.55
1:A:710:GLU:CG	1:B:559:PRO:HA	2.37	0.55
1:B:490:GLY:O	1:B:520:LYS:NZ	2.32	0.54
1:B:761:LEU:O	1:B:765:THR:HG23	2.07	0.54
1:A:710:GLU:HG3	1:B:559:PRO:HA	1.90	0.54
1:A:537:MET:O	1:A:541:ILE:HG12	2.10	0.52
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.91	0.52
1:B:649:ARG:NH2	2:B:801:FLC:HG1	2.10	0.52
1:B:540:MET:HE1	1:B:650:ASP:HB2	1.92	0.52
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.45	0.51
1:B:608:TYR:CZ	1:B:612:ARG:HD2	2.46	0.51
1:A:608:TYR:CZ	1:A:612:ARG:HD2	2.46	0.51
4:B:802:ACP:O5'	4:B:802:ACP:H8	2.11	0.50
1:B:657:TYR:HH	2:B:801:FLC:HG2	1.76	0.50
1:B:680:TYR:CE1	1:B:684:SER:HB2	2.47	0.49
1:B:485:LYS:HE2	1:B:497:MET:HE3	1.93	0.49
1:A:761:LEU:O	1:A:765:THR:HG23	2.13	0.49
1:A:765:THR:O	1:A:766:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:GLY:N	5:B:907:HOH:O	2.45	0.48
2:A:801:FLC:OA1	2:A:801:FLC:OHB	2.29	0.48
1:A:632:VAL:CG1	1:A:640:MET:HE3	2.43	0.47
1:B:670:MET:SD	1:B:675:LEU:HD13	2.54	0.47
1:B:505:LYS:HE3	5:B:974:HOH:O	2.15	0.47
1:B:709:VAL:HG13	5:B:1019:HOH:O	2.15	0.47
1:B:585:GLU:OE2	1:B:585:GLU:N	2.33	0.46
1:A:656:TYR:HE1	1:A:658:LYS:HE2	1.78	0.46
1:A:714:LYS:HE2	1:A:718:GLU:OE2	2.16	0.46
1:B:585:GLU:HG2	1:B:586:TYR:CD1	2.52	0.45
1:B:678:ARG:HD3	5:B:952:HOH:O	2.17	0.45
1:B:644:ASP:OD2	4:B:802:ACP:H3B1	2.16	0.45
1:B:617:LEU:HD11	1:B:622[A]:CYS:SG	2.57	0.45
1:A:572:LEU:HD13	1:A:640:MET:HE1	1.99	0.44
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.99	0.44
1:B:485:LYS:HE2	1:B:497:MET:CE	2.48	0.44
1:A:493:GLY:O	1:A:520:LYS:HE3	2.18	0.43
1:B:589:ASP:O	5:B:902:HOH:O	2.21	0.43
1:A:601:LYS:HE3	1:A:765:THR:HG22	2.01	0.42
1:A:466:TYR:HE2	1:A:468:LEU:HD23	1.84	0.42
1:B:534:GLU:HB2	1:B:646:GLY:HA2	2.01	0.42
1:B:652:ASN:O	1:B:653:ASN:HB2	2.20	0.42
1:B:581:PRO:HD2	1:B:584:MET:HE3	2.02	0.41
1:B:608:TYR:CE2	1:B:612:ARG:HD2	2.55	0.41
1:A:519:LEU:HD11	1:A:528:LEU:HD13	2.03	0.41
1:A:711:GLU:OE2	1:B:558:GLY:HA2	2.20	0.41
1:B:625:ARG:HH12	2:B:801:FLC:HA2	1.86	0.41
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.56	0.41
1:A:558:GLY:HA2	1:B:711:GLU:OE2	2.21	0.40
1:A:491:ALA:HB2	1:B:491:ALA:CB	2.51	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	299/324 (92%)	296 (99%)	3 (1%)	0	100	100
1	B	304/324 (94%)	301 (99%)	3 (1%)	0	100	100
All	All	603/648 (93%)	597 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	261/283 (92%)	257 (98%)	4 (2%)	65	62
1	B	267/283 (94%)	258 (97%)	9 (3%)	37	30
All	All	528/566 (93%)	515 (98%)	13 (2%)	50	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	PHE
1	A	512	VAL
1	A	630	ARG
1	A	675	LEU
1	B	473	LYS
1	B	507	LYS
1	B	540	MET
1	B	543	LYS
1	B	592	ARG
1	B	622[A]	CYS
1	B	622[B]	CYS
1	B	630	ARG
1	B	675	LEU

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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FLC	B	801	-	12,12,12	1.87	3 (25%)	17,17,17	1.51	3 (17%)
3	SO4	A	802	-	4,4,4	0.13	0	6,6,6	0.13	0
2	FLC	A	801	-	12,12,12	1.85	4 (33%)	17,17,17	2.09	3 (17%)
4	ACP	B	802	-	27,33,33	2.43	10 (37%)	32,52,52	1.30	3 (9%)

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	FLC	B	801	-	-	9/16/16/16	-
2	FLC	A	801	-	-	7/16/16/16	-
4	ACP	B	802	-	-	4/15/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	ACP	O4'-C1'	6.16	1.49	1.41
4	B	802	ACP	C2'-C1'	-5.82	1.44	1.53
4	B	802	ACP	C2'-C3'	-4.12	1.42	1.53
2	B	801	FLC	CG-CB	-3.72	1.49	1.53
4	B	802	ACP	C2-N3	3.31	1.37	1.32
4	B	802	ACP	PG-O1G	3.21	1.56	1.50
4	B	802	ACP	C6-N6	3.03	1.45	1.34
2	A	801	FLC	CG-CB	-3.00	1.50	1.53
2	B	801	FLC	CA-CB	-2.97	1.50	1.53
2	A	801	FLC	CB-CBC	-2.96	1.50	1.53
2	A	801	FLC	CA-CB	-2.77	1.50	1.53
2	A	801	FLC	OHB-CB	-2.70	1.38	1.43
4	B	802	ACP	PB-O1B	2.59	1.57	1.51
4	B	802	ACP	C3'-C4'	-2.43	1.46	1.53
2	B	801	FLC	OHB-CB	-2.36	1.38	1.43
4	B	802	ACP	PB-O2B	-2.28	1.51	1.56
4	B	802	ACP	PB-O3A	2.19	1.60	1.58

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FLC	OB2-CBC-CB	5.81	123.13	113.05
4	B	802	ACP	N3-C2-N1	-5.08	120.74	128.68
2	A	801	FLC	OB1-CBC-CB	-3.94	116.67	122.25
2	B	801	FLC	OB2-CBC-CB	2.58	117.54	113.05
2	B	801	FLC	CB-CA-CAC	-2.49	107.79	113.81
4	B	802	ACP	C4-C5-N7	-2.25	107.05	109.40
2	A	801	FLC	OA2-CAC-CA	2.17	121.31	114.35
4	B	802	ACP	PB-O3A-PA	-2.10	125.92	132.56
2	B	801	FLC	CG-CB-CBC	-2.04	105.73	110.11

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FLC	CAC-CA-CB-CBC
2	A	801	FLC	CAC-CA-CB-CG
2	A	801	FLC	CAC-CA-CB-OHB
2	A	801	FLC	CG-CB-CBC-OB1
2	A	801	FLC	CG-CB-CBC-OB2
2	A	801	FLC	OHB-CB-CBC-OB1
2	A	801	FLC	OHB-CB-CBC-OB2

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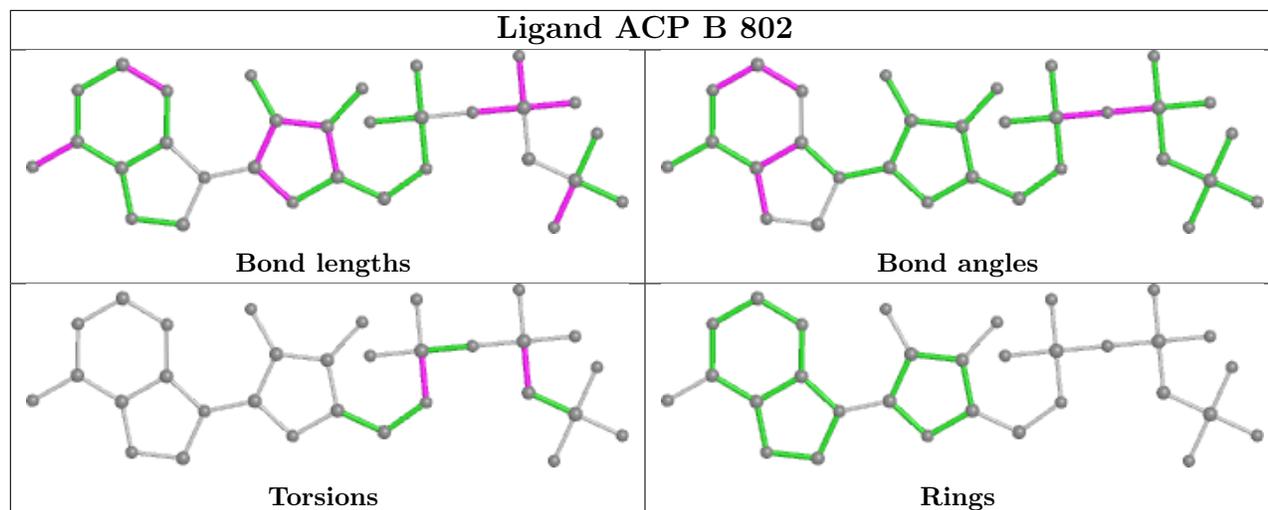
Mol	Chain	Res	Type	Atoms
2	B	801	FLC	CG-CB-CBC-OB1
2	B	801	FLC	CG-CB-CBC-OB2
2	B	801	FLC	OHB-CB-CBC-OB1
2	B	801	FLC	OHB-CB-CBC-OB2
2	B	801	FLC	CA-CB-CG-CGC
2	B	801	FLC	CBC-CB-CG-CGC
2	B	801	FLC	OHB-CB-CG-CGC
4	B	802	ACP	PG-C3B-PB-O1B
4	B	802	ACP	PG-C3B-PB-O2B
4	B	802	ACP	PG-C3B-PB-O3A
2	B	801	FLC	CA-CB-CBC-OB1
2	B	801	FLC	CA-CB-CBC-OB2
4	B	802	ACP	C5'-O5'-PA-O1A

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	FLC	6	0
2	A	801	FLC	3	0
4	B	802	ACP	2	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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	301/324 (92%)	-0.20	14 (4%) 31 33	14, 25, 51, 79	0
1	B	304/324 (93%)	-0.22	10 (3%) 46 50	12, 22, 49, 104	0
All	All	605/648 (93%)	-0.21	24 (3%) 38 41	12, 24, 51, 104	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	ALA	7.2
1	A	490	GLY	6.6
1	B	489	GLU	6.1
1	B	492	PHE	5.2
1	B	490	GLY	4.6
1	A	582	PRO	4.0
1	A	766	ASN	3.7
1	A	491	ALA	3.7
1	B	593	VAL	3.5
1	A	653	ASN	3.5
1	A	461	ALA	3.3
1	B	764	THR	3.3
1	B	763	LEU	3.2
1	B	765	THR	3.1
1	A	655	ASP	3.0
1	B	488	GLY	2.9
1	A	508	PRO	2.7
1	A	765	THR	2.7
1	A	505	LYS	2.6
1	A	510	GLU	2.6
1	A	506	ASP	2.5
1	B	595	GLU	2.5
1	A	492	PHE	2.2
1	A	466	TYR	2.1

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

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

## 6.3 Carbohydrates [i](#)

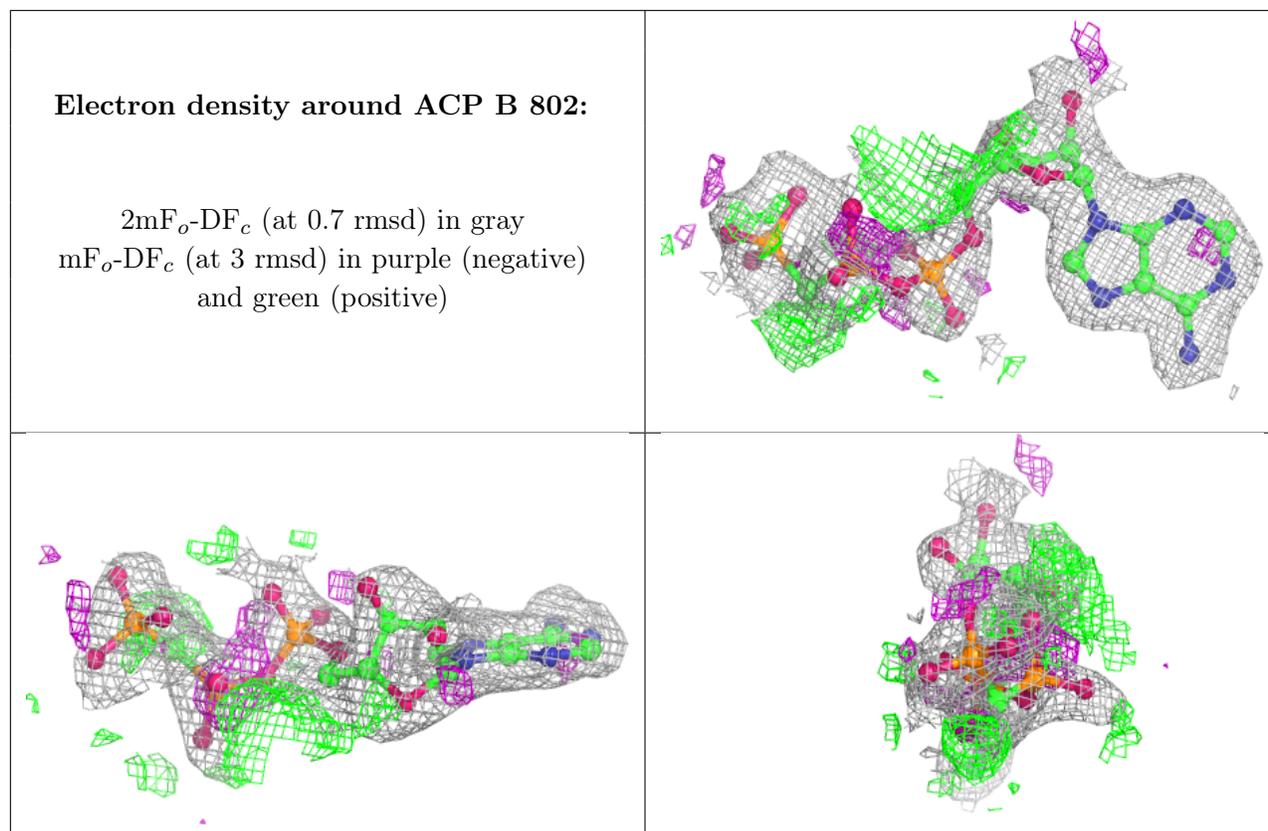
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FLC	B	801	13/13	0.63	0.25	39,61,64,65	0
2	FLC	A	801	13/13	0.73	0.25	45,60,66,66	0
4	ACP	B	802	31/31	0.84	0.16	23,50,95,95	0
3	SO4	A	802	5/5	0.94	0.20	66,66,69,70	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.