



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:16 am BST

PDB ID : 6LVK
Title : Crystal structure of FGFR2 in complex with 1,3,5-triazine derivative
Authors : Echizen, Y.; Amano, Y.; Tateishi, Y.
Deposited on : 2020-02-04
Resolution : 2.29 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

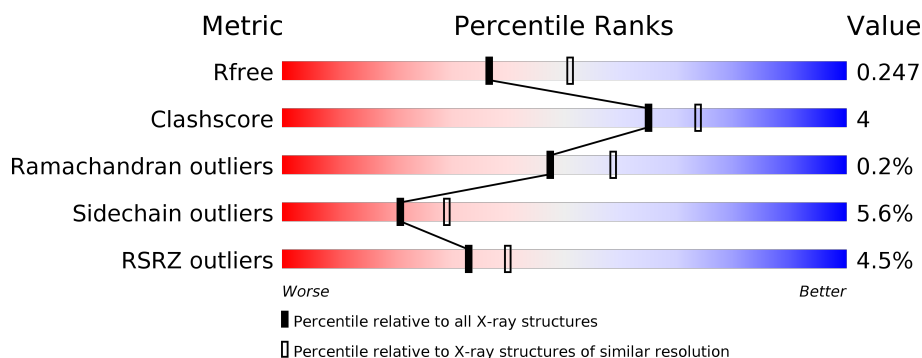
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	313	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	313	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>

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
3	SO4	B	802	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4810 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.

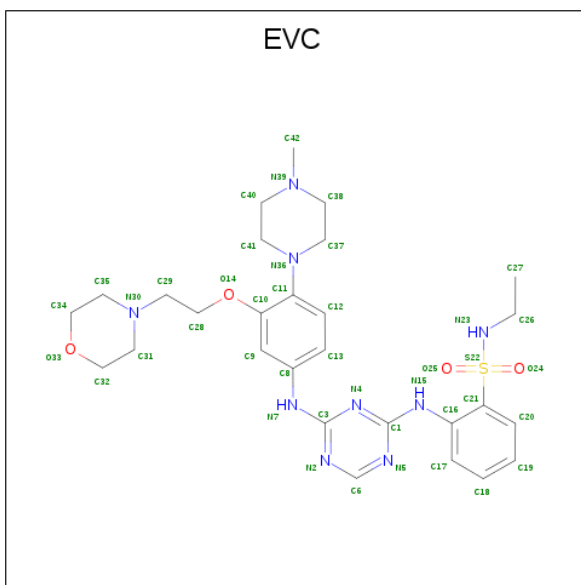
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2296	1457	389	428	1	21			
1	B	286	Total	C	N	O	P	S	0	0	0
			2288	1454	387	425	1	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	GLY	-	expression tag	UNP P21802
A	457	SER	-	expression tag	UNP P21802
A	458	HIS	-	expression tag	UNP P21802
B	456	GLY	-	expression tag	UNP P21802
B	457	SER	-	expression tag	UNP P21802
B	458	HIS	-	expression tag	UNP P21802

- Molecule 2 is N-ethyl-2-[[4-[[4-(4-methylpiperazin-1-yl)-3-(2-morpholin-4-ylethoxy)phenyl]amino]-1,3,5-triazin-2-yl]amino]benzenesulfonamide (three-letter code: EVC) (formula: C₂₈H₃₉N₉O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	28	9	4	1		
2	B	1	Total	C	N	O	S	0	0
			42	28	9	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

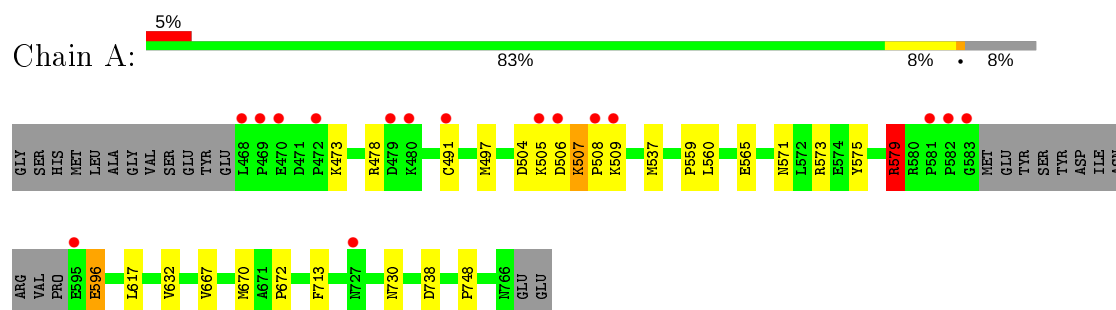
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	67	Total	O	0	0
			67	67		

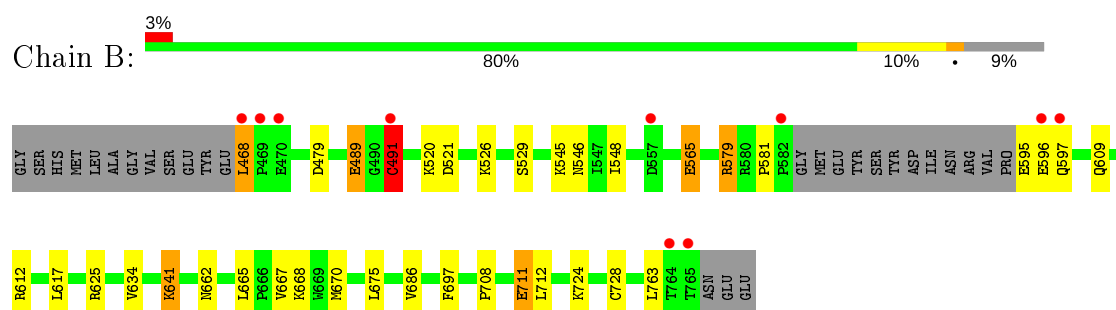
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	64.27Å 105.57Å 116.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.29 48.06 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.06-2.29) 99.6 (48.06-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.203 , 0.247 0.203 , 0.247	Depositor DCC
R_{free} test set	1775 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4810	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: EVC, SO4, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	1/2326 (0.0%)	0.72	3/3142 (0.1%)
1	B	0.31	0/2318	0.71	1/3130 (0.0%)
All	All	0.34	1/4644 (0.0%)	0.71	4/6272 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	560	LEU	C-O	-6.02	1.11	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	ARG	CG-CD-NE	9.61	131.97	111.80
1	A	579	ARG	CB-CA-C	7.18	124.76	110.40
1	B	579	ARG	CB-CA-C	5.79	121.98	110.40
1	A	560	LEU	CA-C-O	5.10	130.81	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	504	ASP	Peptide
1	B	491	CYS	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	2296	0	2286	13	0
1	B	2288	0	2288	21	0
2	A	42	0	0	2	0
2	B	42	0	0	2	0
3	A	5	0	0	0	0
3	B	15	0	0	3	0
4	A	55	0	0	1	0
4	B	67	0	0	2	0
All	All	4810	0	4574	38	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 (38) 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:506:ASP:O	1:A:508:PRO:HD3	1.66	0.94
1:A:667:VAL:HG13	1:A:713:PHE:HE2	1.56	0.70
1:A:667:VAL:HG13	1:A:713:PHE:CE2	2.28	0.68
1:B:708:PRO:HG2	1:B:711:GLU:HG2	1.77	0.67
1:A:506:ASP:C	1:A:508:PRO:HD3	2.18	0.63
1:A:478:ARG:NH1	1:A:559:PRO:O	2.31	0.63
1:B:662:ASN:HB3	1:B:670:MET:CE	2.33	0.58
2:A:801:EVC:C41	2:A:801:EVC:O14	2.52	0.58
2:B:801:EVC:O14	2:B:801:EVC:C37	2.56	0.54
1:B:625:ARG:NH1	3:B:802:SO4:O3	2.39	0.54
1:B:708:PRO:HG2	1:B:711:GLU:CG	2.41	0.50
1:B:697:PHE:CD1	1:B:728:CYS:HB3	2.47	0.50
1:B:548:ILE:CD1	1:B:565:GLU:HG2	2.42	0.50
3:B:802:SO4:O4	4:B:901:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:VAL:HA	1:A:670:MET:HE2	1.94	0.49
1:A:672:PRO:HA	1:A:713:PHE:HE1	1.77	0.48
3:B:802:SO4:O2	4:B:902:HOH:O	2.20	0.48
1:B:545:LYS:O	1:B:641:LYS:HE2	2.14	0.48
1:B:724:LYS:NZ	1:B:728:CYS:O	2.47	0.47
1:B:546:ASN:ND2	1:B:609:GLN:HB3	2.31	0.46
1:A:575:TYR:O	1:A:579:ARG:HD2	2.15	0.45
1:B:489:GLU:HG2	1:B:520:LYS:HD3	1.98	0.45
1:A:491:CYS:SG	1:B:491:CYS:HB2	2.56	0.45
1:A:559:PRO:HB3	1:B:708:PRO:HB3	1.99	0.45
1:B:595:GLU:HB3	1:B:596:GLU:H	1.67	0.45
2:A:801:EVC:C41	4:A:912:HOH:O	2.65	0.44
1:B:665:LEU:HD12	1:B:670:MET:HE3	1.99	0.44
1:B:662:ASN:O	1:B:670:MET:HE1	2.18	0.44
1:B:668:LYS:HG2	1:B:712:LEU:HD22	2.00	0.44
1:B:548:ILE:HD11	1:B:565:GLU:HG2	1.99	0.43
2:B:801:EVC:N4	2:B:801:EVC:C17	2.81	0.43
1:B:581:PRO:HA	1:B:597:GLN:NE2	2.33	0.43
1:B:675:LEU:HA	1:B:675:LEU:HD12	1.89	0.43
1:B:468:LEU:HA	1:B:468:LEU:HD12	1.86	0.42
1:A:596:GLU:H	1:A:596:GLU:HG3	1.59	0.41
1:A:571:ASN:HA	1:A:632:VAL:O	2.21	0.40
1:A:738:ASP:HB3	1:A:748:PRO:HD3	2.03	0.40
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.92	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	283/313 (90%)	275 (97%)	7 (2%)	1 (0%)	34 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/313 (90%)	278 (99%)	3 (1%)	0	100	100
All	All	564/626 (90%)	553 (98%)	10 (2%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	LYS

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	249/273 (91%)	237 (95%)	12 (5%)	25	36
1	B	249/273 (91%)	233 (94%)	16 (6%)	17	23
All	All	498/546 (91%)	470 (94%)	28 (6%)	21	29

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	LYS
1	A	497	MET
1	A	505	LYS
1	A	507	LYS
1	A	509	LYS
1	A	537	MET
1	A	565	GLU
1	A	573	ARG
1	A	579	ARG
1	A	596	GLU
1	A	617	LEU
1	A	730	ASN
1	B	468	LEU
1	B	479	ASP
1	B	489	GLU

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Mol	Chain	Res	Type
1	B	491	CYS
1	B	521	ASP
1	B	526	LYS
1	B	529	SER
1	B	565	GLU
1	B	579	ARG
1	B	612	ARG
1	B	634	VAL
1	B	641	LYS
1	B	667	VAL
1	B	686	VAL
1	B	711	GLU
1	B	763	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	A	631	ASN
1	A	766	ASN
1	B	631	ASN
1	B	637	ASN
1	B	653	ASN
1	B	683	GLN

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	A	561	1	15,16,17	1.17	1 (6%)	19,22,24	1.52	1 (5%)
1	PTR	B	561	1	15,16,17	1.13	1 (6%)	19,22,24	1.31	3 (15%)

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	561	1	-	2/10/11/13	0/1/1/1
1	PTR	B	561	1	-	3/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	561	PTR	P-OH	3.84	1.65	1.59
1	A	561	PTR	P-OH	3.44	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	PTR	CB-CA-C	-4.86	102.36	111.47
1	B	561	PTR	CB-CA-C	-3.08	105.70	111.47
1	B	561	PTR	O2P-P-OH	-2.15	98.51	105.24
1	B	561	PTR	O2P-P-O1P	2.10	118.91	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	561	PTR	CA-CB-CG-CD2
1	A	561	PTR	CA-CB-CG-CD1
1	B	561	PTR	CA-CB-CG-CD2
1	B	561	PTR	CA-CB-CG-CD1
1	B	561	PTR	CZ-OH-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.27	0
2	EVC	B	801	-	46,46,46	1.34	2 (4%)	61,63,63	1.90	17 (27%)
3	SO4	B	802	-	4,4,4	0.30	0	6,6,6	0.45	0
2	EVC	A	801	-	46,46,46	1.12	2 (4%)	61,63,63	1.97	21 (34%)
3	SO4	B	803	-	4,4,4	0.23	0	6,6,6	0.34	0
3	SO4	A	802	-	4,4,4	0.17	0	6,6,6	0.80	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
2	EVC	B	801	-	-	6/28/46/46	0/5/5/5
2	EVC	A	801	-	-	5/28/46/46	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	EVC	S22-N23	6.83	1.72	1.61
2	A	801	EVC	S22-N23	5.16	1.69	1.61
2	B	801	EVC	C3-N7	2.53	1.41	1.36
2	A	801	EVC	C40-N39	2.05	1.50	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	EVC	C21-S22-N23	-5.20	101.07	107.82
2	A	801	EVC	C21-S22-N23	-4.89	101.47	107.82
2	A	801	EVC	N2-C3-N4	-4.86	121.94	126.55
2	B	801	EVC	N2-C3-N4	-4.79	122.01	126.55
2	A	801	EVC	C28-O14-C10	-4.59	106.45	117.69
2	B	801	EVC	C40-N39-C38	4.04	115.17	109.52
2	B	801	EVC	C41-C40-N39	-4.02	106.27	110.80
2	B	801	EVC	C42-N39-C40	4.00	116.65	110.66
2	A	801	EVC	C42-N39-C40	3.52	115.93	110.66
2	A	801	EVC	C26-N23-S22	-3.49	112.98	119.69
2	B	801	EVC	C21-C16-N15	-3.18	118.44	121.45
2	A	801	EVC	N5-C1-N4	-3.17	123.54	126.55
2	B	801	EVC	N5-C1-N4	-3.10	123.61	126.55
2	A	801	EVC	C21-C16-N15	-3.01	118.60	121.45
2	A	801	EVC	C40-N39-C38	2.86	113.52	109.52
2	B	801	EVC	C41-N36-C11	2.84	123.01	116.27
2	B	801	EVC	C28-O14-C10	-2.82	110.79	117.69
2	A	801	EVC	C37-N36-C11	2.74	122.75	116.27
2	A	801	EVC	C41-N36-C11	2.69	122.66	116.27
2	A	801	EVC	C42-N39-C38	2.61	114.56	110.66
2	B	801	EVC	O24-S22-C21	2.60	111.94	107.66
2	A	801	EVC	C37-C38-N39	-2.56	107.91	110.80
2	A	801	EVC	C1-N4-C3	2.56	118.22	113.89
2	B	801	EVC	C1-N4-C3	2.52	118.16	113.89
2	B	801	EVC	C20-C21-C16	2.45	122.30	120.28
2	A	801	EVC	C28-C29-N30	-2.38	106.85	113.31
2	A	801	EVC	O24-S22-C21	2.32	111.48	107.66
2	A	801	EVC	O25-S22-O24	2.32	122.40	119.55
2	B	801	EVC	C42-N39-C38	2.21	113.97	110.66
2	A	801	EVC	O25-S22-C21	-2.21	104.03	107.66
2	A	801	EVC	C41-C40-N39	-2.19	108.33	110.80
2	B	801	EVC	C38-C37-N36	2.18	114.94	110.70
2	A	801	EVC	O24-S22-N23	2.12	110.35	107.04
2	B	801	EVC	C37-N36-C11	2.11	121.27	116.27
2	B	801	EVC	O14-C10-C11	2.05	119.42	116.28
2	B	801	EVC	O25-S22-O24	2.03	122.04	119.55
2	A	801	EVC	C34-O33-C32	2.02	116.64	109.89
2	A	801	EVC	O14-C10-C9	-2.01	118.95	123.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

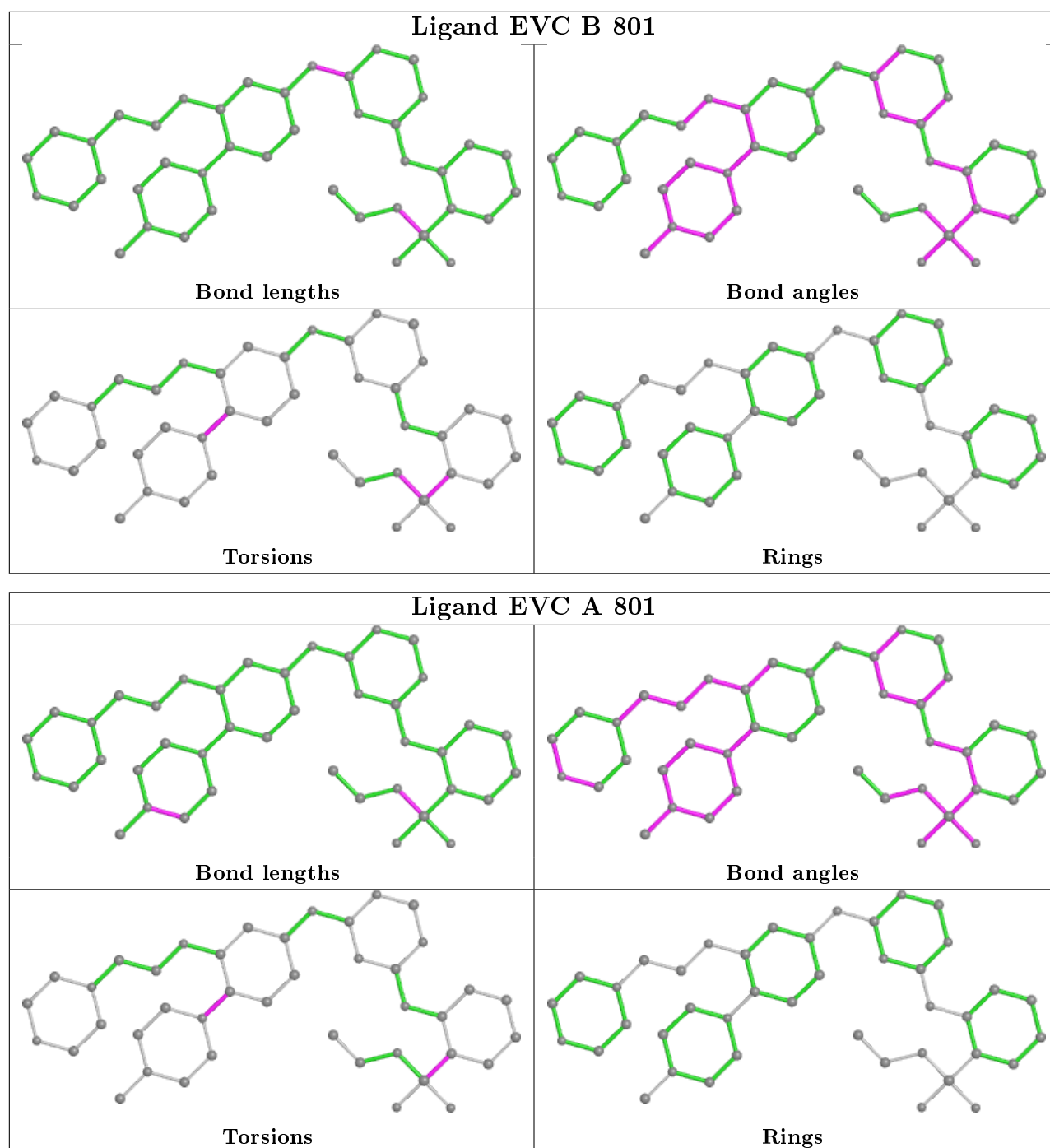
Mol	Chain	Res	Type	Atoms
2	B	801	EVC	C10-C11-N36-C37
2	A	801	EVC	C10-C11-N36-C41
2	B	801	EVC	C12-C11-N36-C37
2	A	801	EVC	C12-C11-N36-C41
2	B	801	EVC	C20-C21-S22-O24
2	A	801	EVC	C20-C21-S22-O24
2	A	801	EVC	C20-C21-S22-N23
2	A	801	EVC	C20-C21-S22-O25
2	B	801	EVC	C20-C21-S22-N23
2	B	801	EVC	C26-N23-S22-O24
2	B	801	EVC	C20-C21-S22-O25

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	EVC	2	0
3	B	802	SO4	3	0
2	A	801	EVC	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, 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	287/313 (91%)	0.04	16 (5%) 24 30	16, 28, 67, 100	0
1	B	285/313 (91%)	0.03	10 (3%) 44 51	18, 29, 55, 83	0
All	All	572/626 (91%)	0.04	26 (4%) 33 40	16, 29, 63, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	7.0
1	A	727	ASN	4.4
1	B	582	PRO	4.2
1	A	506	ASP	4.1
1	A	469	PRO	4.1
1	B	596	GLU	3.8
1	A	582	PRO	3.7
1	A	480	LYS	3.6
1	A	505	LYS	3.5
1	B	557	ASP	3.3
1	B	765	THR	3.2
1	A	470	GLU	3.2
1	A	508	PRO	3.1
1	A	509	LYS	3.0
1	B	468	LEU	2.8
1	A	479	ASP	2.8
1	B	470	GLU	2.8
1	B	469	PRO	2.6
1	B	491	CYS	2.5
1	A	468	LEU	2.5
1	A	491	CYS	2.4
1	A	472	PRO	2.4
1	B	597	GLN	2.3
1	B	764	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	581	PRO	2.1
1	A	595	GLU	2.1

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	561	16/17	0.95	0.12	29,37,46,47	0
1	PTR	B	561	16/17	0.97	0.14	27,35,45,46	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

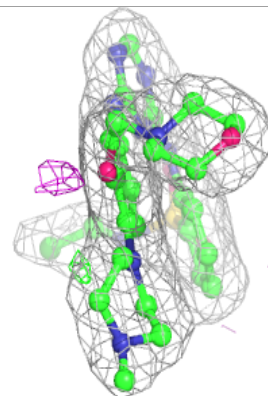
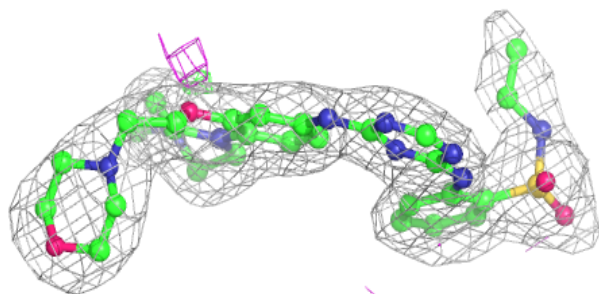
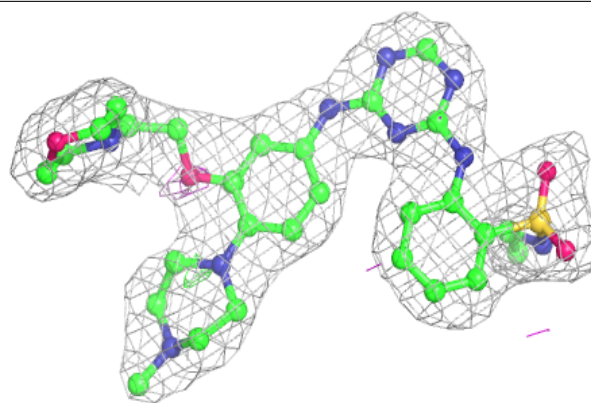
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	802	5/5	0.83	0.19	43,54,64,64	0
3	SO4	B	804	5/5	0.91	0.24	79,79,83,85	0
2	EVC	B	801	42/42	0.95	0.12	20,25,33,33	0
2	EVC	A	801	42/42	0.96	0.13	21,28,41,43	0
3	SO4	B	803	5/5	0.97	0.12	44,46,49,50	0
3	SO4	B	802	5/5	0.98	0.17	47,51,56,56	0

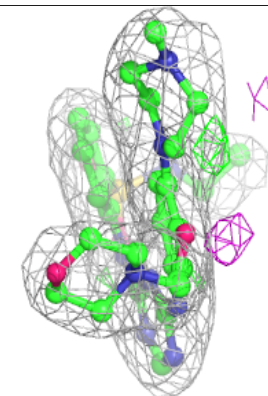
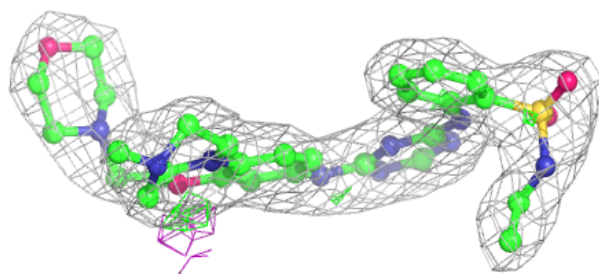
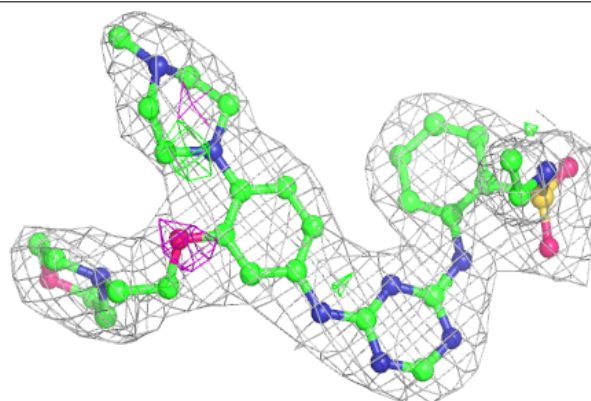
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EVC B 801:

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

**Electron density around EVC 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.