Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 09:20 pm BST

PDB ID	:	4F64
Title	:	Crystal structure of Human Fibroblast Growth Factor Receptor 1 Kinase domain in complex with compound 6
Authors	:	Norman, R.A.; Breed, J.; Ogg, D.
Deposited on	:	2012-05-14
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

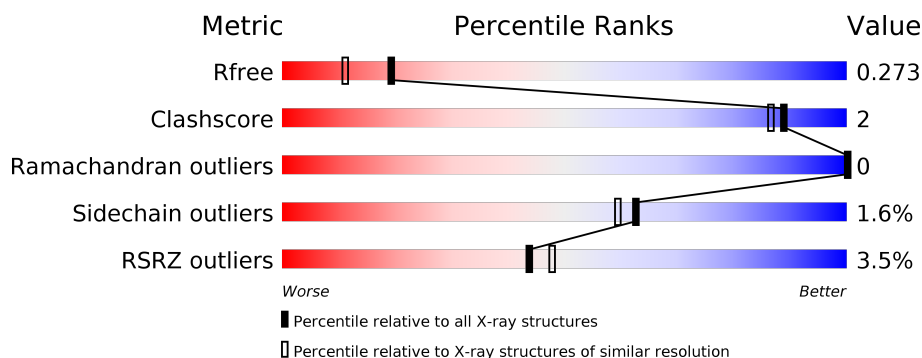|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.273
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		3.5%

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	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 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 <=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	309	3% — 85% — 5% — 10%
1	B	309	3% — 83% — 5% — 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4539 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.
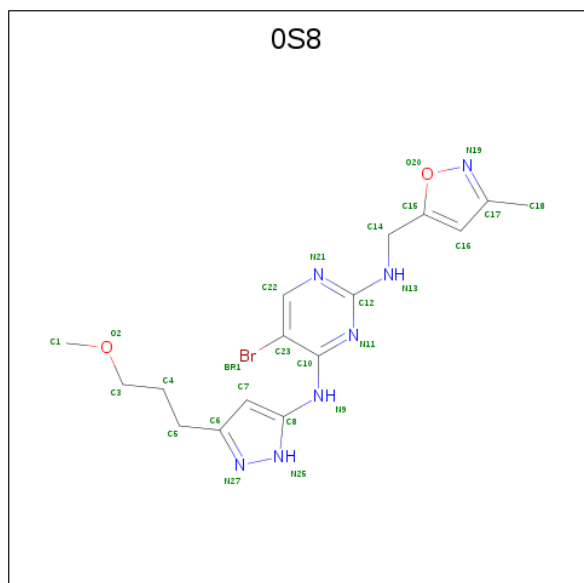
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	1	2	0
			2173	1390	371	395	17			
1	B	272	Total	C	N	O	S	1	1	0
			2077	1329	352	379	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	EXPRESSION TAG	UNP P11362
A	488	ALA	CYS	ENGINEERED MUTATION	UNP P11362
A	584	SER	CYS	ENGINEERED MUTATION	UNP P11362
B	457	GLY	-	EXPRESSION TAG	UNP P11362
B	488	ALA	CYS	ENGINEERED MUTATION	UNP P11362
B	584	SER	CYS	ENGINEERED MUTATION	UNP P11362

- Molecule 2 is 5-bromo-N 4 -[3-(3-methoxypropyl)-1H-pyrazol-5-yl]-N 2 -[(3-methyl-1,2-oxaz ol-5-yl)methyl]pyrimidine-2,4-diamine (three-letter code: 0S8) (formula: $C_{16}H_{20}BrN_7O_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			26	1	16	7	2		
2	B	1	Total	Br	C	N	O	0	0
			26	1	16	7	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 5 is water.

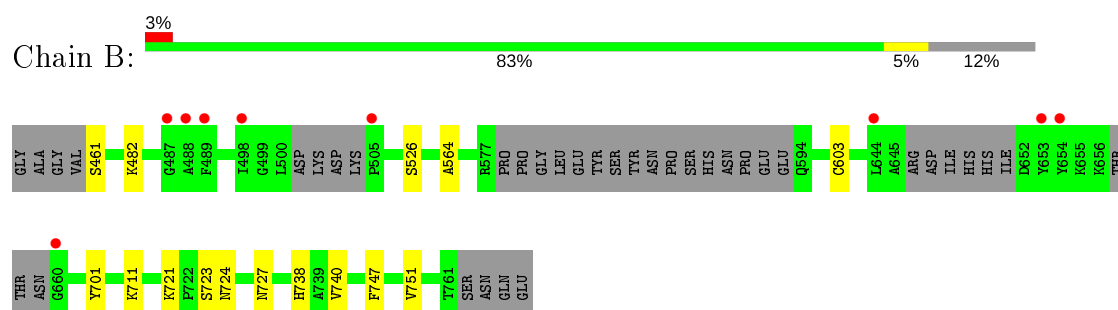| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total 148	O 148	0	0
5	B	68	Total 68	O 68	0	0

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 1

Chain A:

- Molecule 1: Fibroblast growth factor receptor 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	208.81Å 57.28Å 65.43Å 90.00° 107.55° 90.00°	Depositor
Resolution (Å)	61.90 – 2.05 43.36 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.4 (61.90-2.05) 95.4 (43.36-2.05)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.13	Depositor
$<I/\sigma(I)>$ [1]	1.97 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.269 0.227 , 0.273	Depositor DCC
R_{free} test set	2264 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.5	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0S8, SO4, EDO

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	1.05	2/2217 (0.1%)	0.75	1/3004 (0.0%)
1	B	0.72	2/2117 (0.1%)	0.73	0/2871
All	All	0.91	4/4334 (0.1%)	0.74	1/5875 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603[A]	CYS	CB-SG	-26.49	1.37	1.82
1	A	603[B]	CYS	CB-SG	-26.49	1.37	1.82
1	B	603[A]	CYS	CB-SG	-11.97	1.61	1.82
1	B	603[B]	CYS	CB-SG	-11.97	1.61	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	NE-CZ-NH2	-6.93	116.83	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	2173	0	2151	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2077	0	2014	7	0
2	A	26	0	20	2	0
2	B	26	0	20	1	0
3	A	8	0	12	2	0
3	B	8	0	12	1	0
4	A	5	0	0	0	0
5	A	148	0	0	1	0
5	B	68	0	0	0	0
All	All	4539	0	4229	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (16) 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:564:ALA:H	2:B:801:0S8:H20	1.34	0.74
1:A:564:ALA:H	2:A:801:0S8:H20	1.37	0.73
1:A:530:SER:OG	5:A:1029:HOH:O	2.13	0.64
1:B:738:HIS:HD2	1:B:740:VAL:H	1.54	0.54
1:A:737:TRP:CE3	3:A:803:EDO:H22	2.46	0.51
1:B:721:LYS:CE	1:B:727:ASN:ND2	2.75	0.50
1:A:737:TRP:CD2	3:A:803:EDO:H22	2.47	0.49
1:B:723:SER:O	1:B:724:ASN:HB2	2.15	0.47
1:B:721:LYS:CE	1:B:727:ASN:HD21	2.27	0.47
1:B:701:TYR:OH	3:B:803:EDO:H12	2.16	0.45
1:A:598:LYS:NZ	1:A:761:THR:O	2.38	0.45
1:A:667:MET:HE3	1:A:677:TYR:OH	2.20	0.42
2:A:801:0S8:H10	2:A:801:0S8:N11	2.34	0.42
1:B:747:PHE:O	1:B:751:VAL:HG23	2.20	0.42
1:A:610:GLY:HA3	1:A:639:ILE:HD12	2.02	0.42
1:A:684:TRP:CD1	1:A:684:TRP:C	2.94	0.41

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	272/309 (88%)	264 (97%)	8 (3%)	0	100	100
1	B	263/309 (85%)	259 (98%)	4 (2%)	0	100	100
All	All	535/618 (87%)	523 (98%)	12 (2%)	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	230/269 (86%)	227 (99%)	3 (1%)	69	67
1	B	211/269 (78%)	207 (98%)	4 (2%)	57	53
All	All	441/538 (82%)	434 (98%)	7 (2%)	62	59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	SER
1	A	609	ARG
1	A	618	LYS
1	B	461	SER
1	B	482	LYS
1	B	526	SER
1	B	711	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	738	HIS
1	B	680	GLN
1	B	727	ASN
1	B	738	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	0S8	B	801	-	25,28,28	1.32	3 (12%)	23,37,37	2.39	12 (52%)
2	0S8	A	801	-	25,28,28	1.27	2 (8%)	23,37,37	2.24	10 (43%)
3	EDO	A	802	-	3,3,3	0.47	0	2,2,2	0.22	0
4	SO4	A	804	-	4,4,4	0.32	0	6,6,6	0.29	0
3	EDO	B	803	-	3,3,3	0.38	0	2,2,2	0.36	0
3	EDO	A	803	-	3,3,3	0.35	0	2,2,2	0.52	0
3	EDO	B	802	-	3,3,3	0.45	0	2,2,2	0.05	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	0S8	B	801	-	-	1/10/14/14	0/3/3/3
2	0S8	A	801	-	-	3/10/14/14	0/3/3/3
3	EDO	A	802	-	-	0/1/1/1	-
3	EDO	B	803	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	0S8	C6-N27	-3.68	1.29	1.34
2	A	801	0S8	C12-N13	3.60	1.39	1.34
2	A	801	0S8	C6-N27	-2.94	1.30	1.34
2	B	801	0S8	C12-N13	2.55	1.38	1.34
2	B	801	0S8	C16-C17	2.13	1.44	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	0S8	N21-C12-N11	-5.54	121.30	126.55
2	B	801	0S8	N21-C12-N11	-5.31	121.52	126.55
2	B	801	0S8	C7-C8-N25	-4.08	104.63	110.47
2	A	801	0S8	C22-N21-C12	3.57	121.26	115.88
2	B	801	0S8	C22-N21-C12	3.45	121.08	115.88
2	B	801	0S8	C23-C22-N21	-3.37	118.95	123.09
2	A	801	0S8	C23-C22-N21	-3.31	119.02	123.09
2	B	801	0S8	C8-C7-C6	3.12	109.01	105.95
2	A	801	0S8	C18-C17-N19	2.97	125.95	120.06
2	B	801	0S8	BR1-C23-C10	2.86	123.01	120.15
2	A	801	0S8	C16-C17-N19	-2.77	105.70	110.85
2	B	801	0S8	C15-C14-N13	-2.69	106.88	112.71
2	B	801	0S8	C18-C17-N19	2.61	125.23	120.06
2	A	801	0S8	N13-C12-N11	2.59	121.68	117.19
2	B	801	0S8	C14-N13-C12	-2.59	119.66	123.28
2	A	801	0S8	C7-C8-N25	-2.57	106.78	110.47
2	B	801	0S8	C16-C17-N19	-2.48	106.24	110.85
2	B	801	0S8	C7-C6-N27	-2.43	108.01	111.44
2	A	801	0S8	N9-C10-N11	2.38	122.66	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	0S8	C12-N11-C10	2.31	121.69	116.39
2	A	801	0S8	C5-C4-C3	-2.31	105.57	113.34
2	A	801	0S8	C7-C6-N27	-2.26	108.25	111.44

There are no chirality outliers.
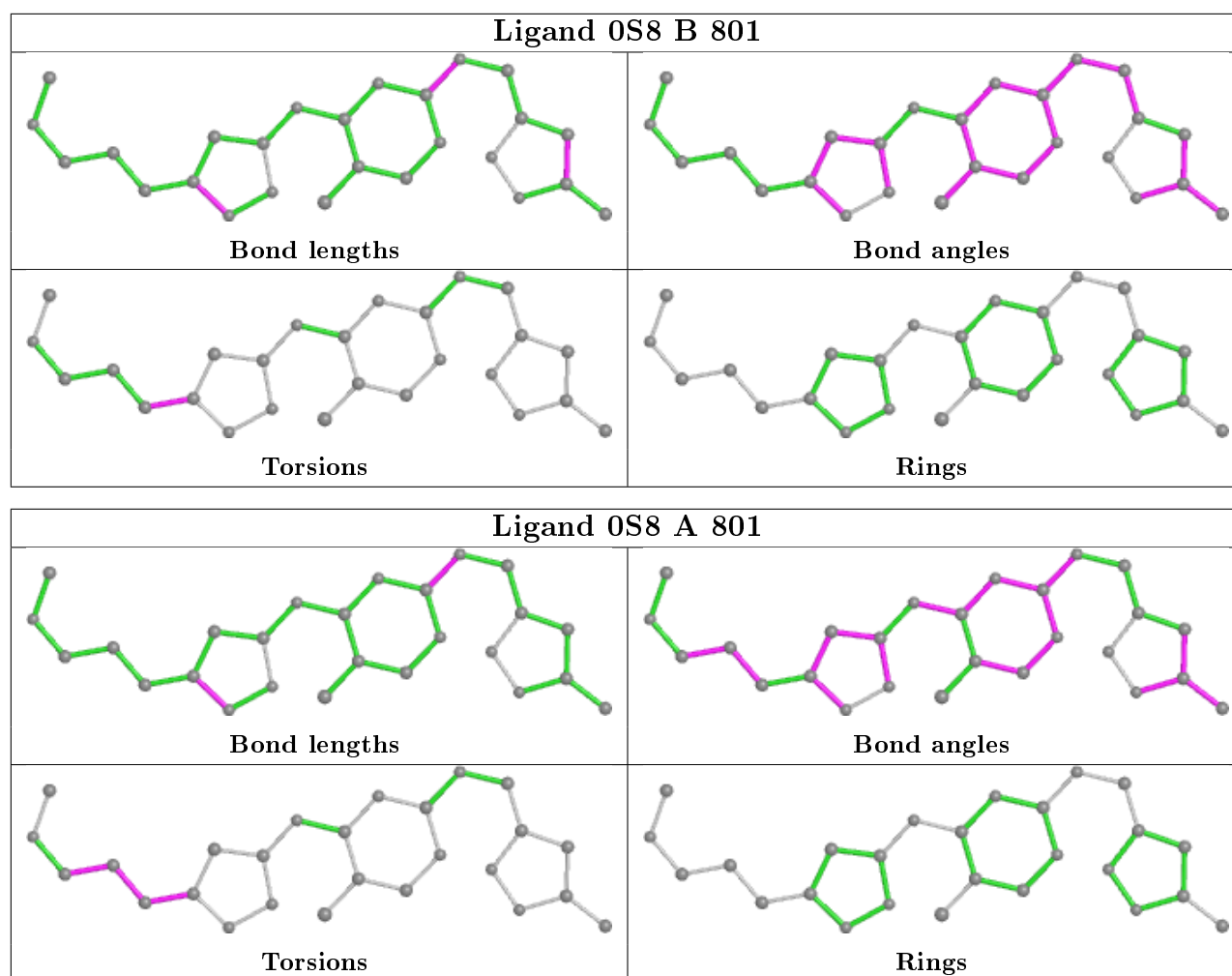
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	0S8	C4-C5-C6-N27
2	A	801	0S8	C4-C5-C6-N27
3	B	803	EDO	O1-C1-C2-O2
2	A	801	0S8	O2-C3-C4-C5
2	A	801	0S8	C3-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	0S8	1	0
2	A	801	0S8	2	0
3	B	803	EDO	1	0
3	A	803	EDO	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 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 0S8 B 801

Ligand 0S8 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	278/309 (89%)	-0.01	10 (3%)	42	46	9, 22, 43, 56	1 (0%)
1	B	272/309 (88%)	0.02	9 (3%)	46	50	15, 29, 46, 60	1 (0%)
All	All	550/618 (88%)	0.00	19 (3%)	44	48	9, 25, 45, 60	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	PHE	3.3
1	B	653	TYR	3.0
1	A	647	ASP	2.8
1	A	519	ASP	2.7
1	B	505	PRO	2.7
1	A	520	ALA	2.6
1	A	650	HIS	2.5
1	A	658	THR	2.5
1	B	660	GLY	2.5
1	B	654	TYR	2.4
1	A	649	HIS	2.3
1	A	521	THR	2.3
1	A	648	ILE	2.3
1	B	487	GLY	2.2
1	B	498	ILE	2.1
1	A	518	SER	2.1
1	B	488	ALA	2.1
1	A	756	ARG	2.1
1	B	644	LEU	2.0

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)

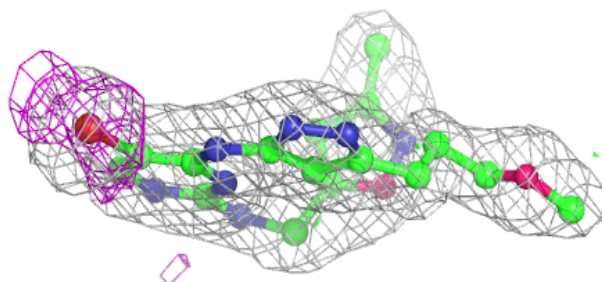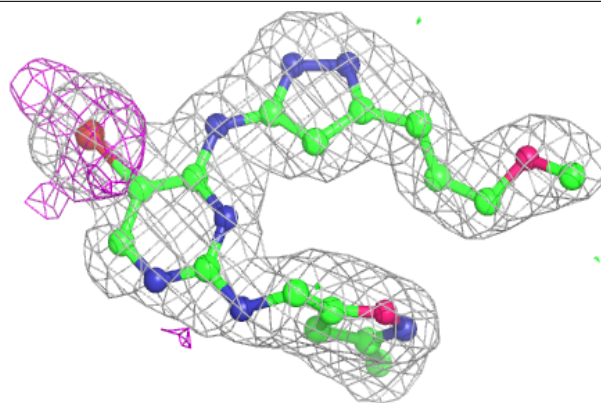There are no carbohydrates in this entry.

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.

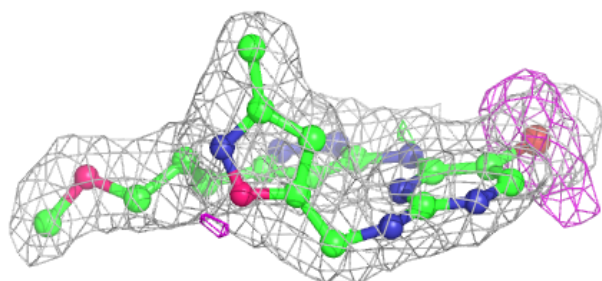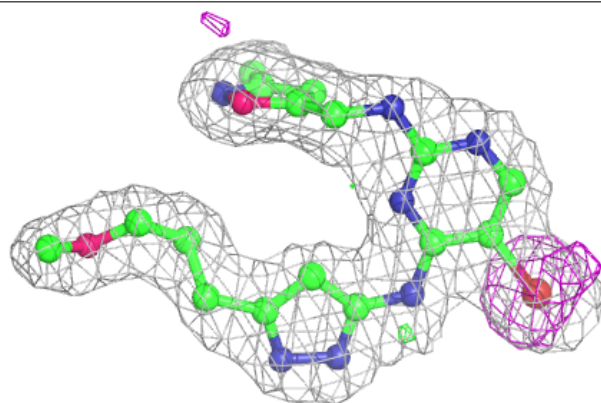| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0S8	B	801	26/26	0.90	0.12	21,30,34,51	0
3	EDO	B	803	4/4	0.90	0.16	37,38,38,38	0
3	EDO	A	802	4/4	0.93	0.11	25,28,29,31	0
2	0S8	A	801	26/26	0.93	0.11	17,26,30,44	0
3	EDO	B	802	4/4	0.93	0.15	34,36,36,36	0
3	EDO	A	803	4/4	0.96	0.18	31,32,32,32	0
4	SO4	A	804	5/5	0.98	0.11	37,37,38,38	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 0S8 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 0S8 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.