



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 02:50 AM UTC

PDB ID : 7OZF / pdb_00007ozf
Title : FGFR1 kinase domain (residues 458-765) with mutations C488A, C584S in complex with 19.
Authors : Trinh, C.H.; Turner, L.D.; Fishwick, C.W.G.
Deposited on : 2021-06-28
Resolution : 1.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

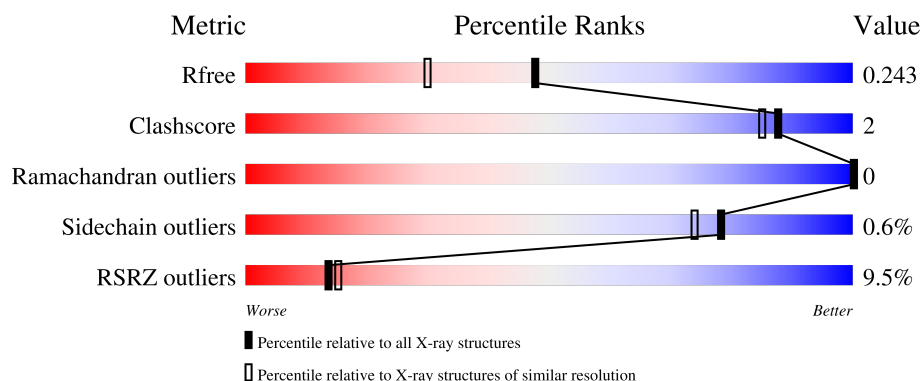
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 $\leq 5\%$. 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	AAA	309	8% 89% 7%
1	BBB	309	9% 85% 6% 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9295 atoms, of which 4548 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.

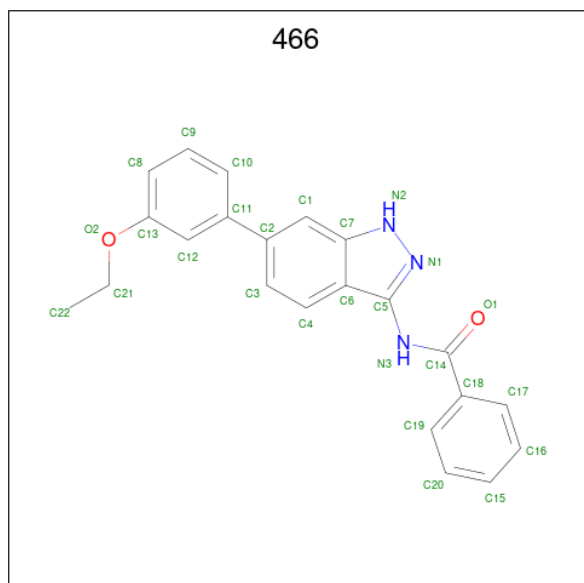
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	288	Total	C	H	N	O	S	109	1	0
			4447	1416	2219	383	411	18			
1	BBB	282	Total	C	H	N	O	S	97	9	0
			4526	1442	2267	385	414	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	457	GLY	-	expression tag	UNP P11362
AAA	488	ALA	CYS	conflict	UNP P11362
AAA	584	SER	CYS	conflict	UNP P11362
BBB	457	GLY	-	expression tag	UNP P11362
BBB	488	ALA	CYS	conflict	UNP P11362
BBB	584	SER	CYS	conflict	UNP P11362

- Molecule 2 is N-[6-(3-ethoxyphenyl)-1H-indazol-3-yl]benzamide (CCD ID: 466) (formula: C₂₂H₁₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



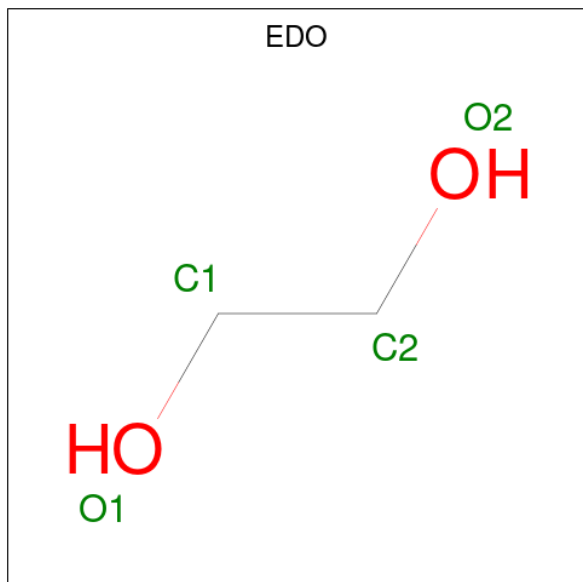
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			46	22	19	3	2		
2	BBB	1	Total	C	H	N	O	0	0
			46	22	19	3	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C H O 10 2 6 2	1	0
4	AAA	1	Total C H O 10 2 6 2	1	0
4	BBB	1	Total C H O 10 2 6 2	1	0
4	BBB	1	Total C H O 10 2 6 2	1	0

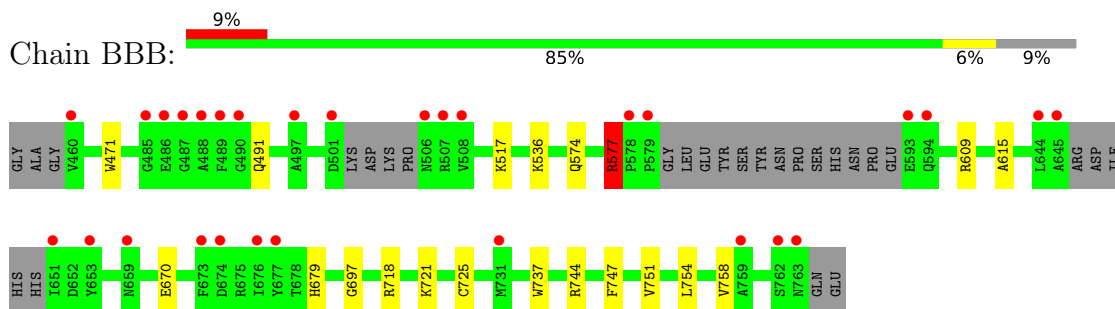
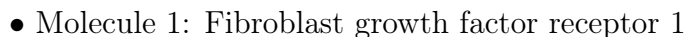
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Cl 1 1	0	0
5	BBB	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	100	Total O 100 100	0	0
6	BBB	83	Total O 83 83	0	0

- Molecule 1: Fibroblast growth factor receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.32Å 57.77Å 65.94Å 90.00° 107.17° 90.00°	Depositor
Resolution (Å)	63.00 – 1.82 63.00 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.7 (63.00-1.82) 98.7 (63.00-1.82)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.242 0.204 , 0.243	Depositor DCC
R_{free} test set	3411 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9295	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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: 466, SO4, CL, 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	AAA	1.03	0/2275	1.32	0/3084
1	BBB	1.01	0/2304	1.33	3/3116 (0.1%)
All	All	1.02	0/4579	1.32	3/6200 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	577	ARG	CB-CA-C	6.41	118.68	109.26
1	BBB	697	GLY	CA-C-N	5.61	125.42	120.10
1	BBB	697	GLY	C-N-CA	5.61	125.42	120.10

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	AAA	2228	2219	2172	8	0
1	BBB	2259	2267	2230	9	0
2	AAA	27	19	0	0	0
2	BBB	27	19	0	1	0
3	AAA	5	0	0	0	0
4	AAA	8	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	8	12	12	0	0
5	AAA	1	0	0	1	0
5	BBB	1	0	0	0	0
6	AAA	100	0	0	0	0
6	BBB	83	0	0	0	0
All	All	4747	4548	4426	18	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.

The worst 5 of 18 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:AAA:516:LEU:HD11	1:AAA:525:LEU:HD13	1.77	0.67
1:BBB:721:LYS:NZ	1:BBB:725:CYS:O	2.29	0.64
1:AAA:489:PHE:O	1:AAA:514:LYS:HE3	2.05	0.57
1:AAA:661:ARG:HD2	5:AAA:805:CL:CL	2.52	0.47
1:BBB:471:TRP:CD1	1:BBB:536:LYS:HE2	2.52	0.45

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	AAA	283/309 (92%)	277 (98%)	6 (2%)	0	100	100
1	BBB	283/309 (92%)	278 (98%)	5 (2%)	0	100	100
All	All	566/618 (92%)	555 (98%)	11 (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	AAA	233/269 (87%)	232 (100%)	1 (0%)	84	81
1	BBB	237/269 (88%)	235 (99%)	2 (1%)	73	67
All	All	470/538 (87%)	467 (99%)	3 (1%)	78	74

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	609	ARG
1	BBB	577	ARG
1	BBB	609	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	EDO	AAA	803	-	3,3,3	0.22	0	2,2,2	0.60	0
4	EDO	BBB	802	-	3,3,3	0.20	0	2,2,2	0.44	0
2	466	AAA	801	-	30,30,30	1.37	5 (16%)	38,41,41	1.16	5 (13%)
2	466	BBB	801	-	30,30,30	1.17	2 (6%)	38,41,41	1.19	5 (13%)
3	SO4	AAA	802	-	4,4,4	0.30	0	6,6,6	0.06	0
4	EDO	AAA	804	-	3,3,3	0.17	0	2,2,2	0.07	0
4	EDO	BBB	803	-	3,3,3	0.16	0	2,2,2	0.42	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
4	EDO	AAA	803	-	-	1/1/1/1	-
4	EDO	BBB	802	-	-	1/1/1/1	-
2	466	AAA	801	-	-	0/15/15/15	0/4/4/4
2	466	BBB	801	-	-	0/15/15/15	0/4/4/4
4	EDO	AAA	804	-	-	1/1/1/1	-
4	EDO	BBB	803	-	-	1/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	801	466	C6-C5	-5.14	1.39	1.47
2	BBB	801	466	C6-C5	-4.37	1.41	1.47
2	AAA	801	466	C5-N1	2.55	1.34	1.32
2	AAA	801	466	C14-N3	-2.40	1.33	1.37
2	AAA	801	466	C7-N2	-2.22	1.32	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	801	466	C18-C14-N3	4.20	122.31	116.25
2	AAA	801	466	C18-C14-N3	3.04	120.63	116.25
2	BBB	801	466	N3-C5-N1	-2.80	115.59	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	801	466	N3-C5-N1	-2.78	115.66	123.09
2	BBB	801	466	C6-C5-N3	2.43	133.63	123.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

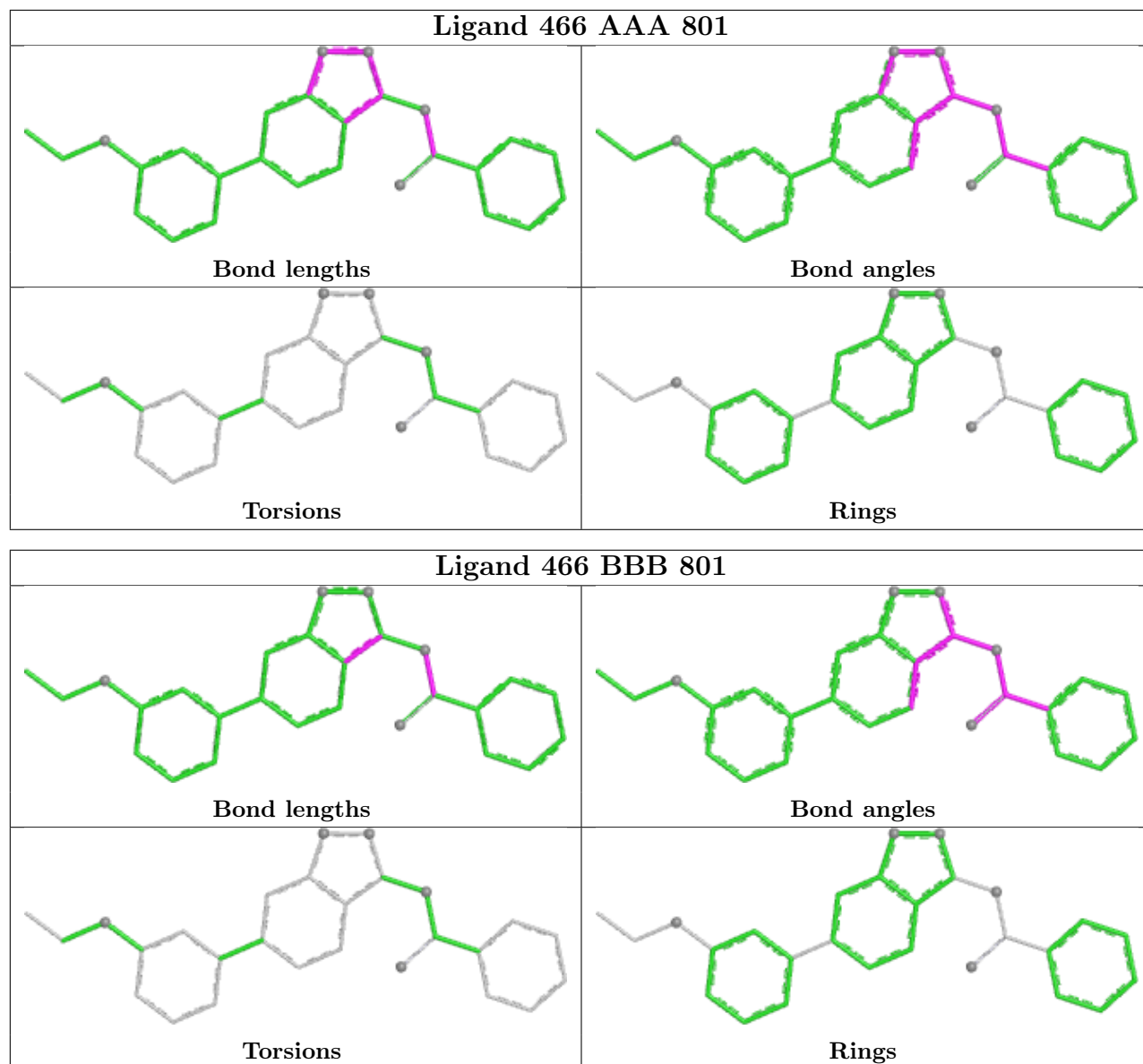
Mol	Chain	Res	Type	Atoms
4	AAA	803	EDO	O1-C1-C2-O2
4	BBB	802	EDO	O1-C1-C2-O2
4	AAA	804	EDO	O1-C1-C2-O2
4	BBB	803	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	801	466	1	0
4	AAA	804	EDO	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 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 [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	AAA	288/309 (93%)	0.61	25 (8%) 16 18	18, 46, 76, 103	1 (0%)
1	BBB	282/309 (91%)	0.86	29 (10%) 12 13	20, 46, 72, 91	9 (3%)
All	All	570/618 (92%)	0.73	54 (9%) 14 15	18, 46, 73, 103	10 (1%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	488[A]	ALA	15.6
1	BBB	489[A]	PHE	14.5
1	BBB	487[A]	GLY	10.9
1	BBB	651	ILE	6.8
1	BBB	763	ASN	6.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

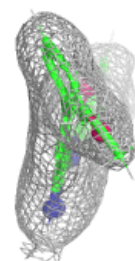
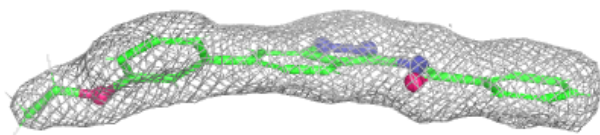
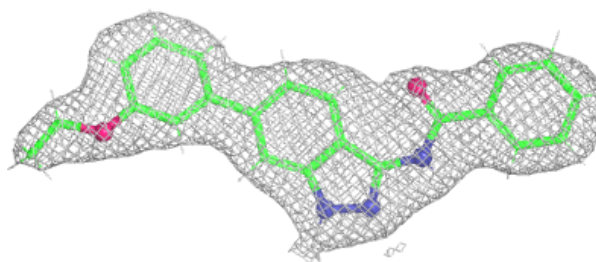
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

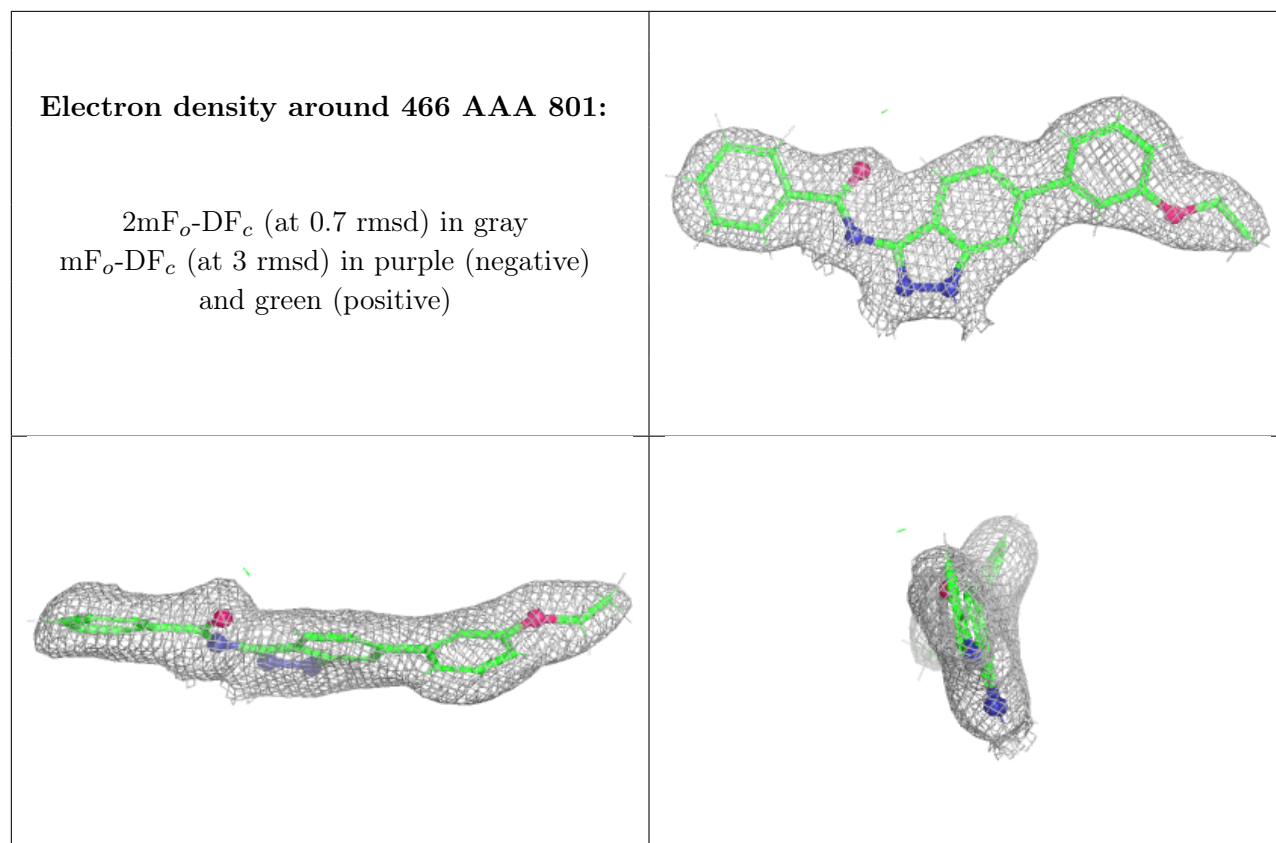
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	AAA	802	5/5	0.65	0.13	102,103,106,110	0
4	EDO	BBB	802	4/4	0.92	0.12	51,55,56,57	1
5	CL	AAA	805	1/1	0.92	0.23	61,61,61,61	0
2	466	BBB	801	27/27	0.93	0.11	40,46,66,67	0
5	CL	BBB	804	1/1	0.93	0.22	58,58,58,58	0
4	EDO	BBB	803	4/4	0.95	0.11	53,54,58,58	1
4	EDO	AAA	804	4/4	0.95	0.14	42,46,47,47	1
2	466	AAA	801	27/27	0.95	0.08	37,47,55,56	0
4	EDO	AAA	803	4/4	0.96	0.07	47,50,52,54	1

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 466 BBB 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.