



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:40 AM UTC

PDB ID : 7OZY / pdb_00007ozy
Title : FGFR2 kinase domain (residues 461-763) in complex with 38.
Authors : Trinh, C.H.; Turner, L.D.; Fishwick, C.W.G.
Deposited on : 2021-06-29
Resolution : 2.28 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 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

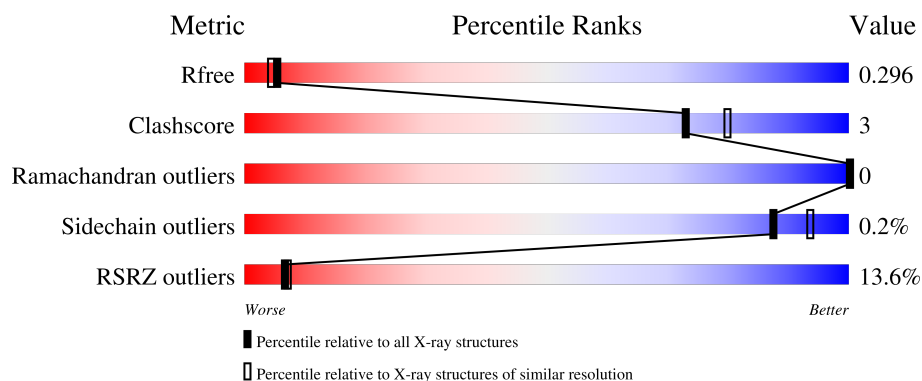
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	303	12% 84% 8% 7%
1	BBB	303	13% 85% 7% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8976 atoms, of which 4435 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.

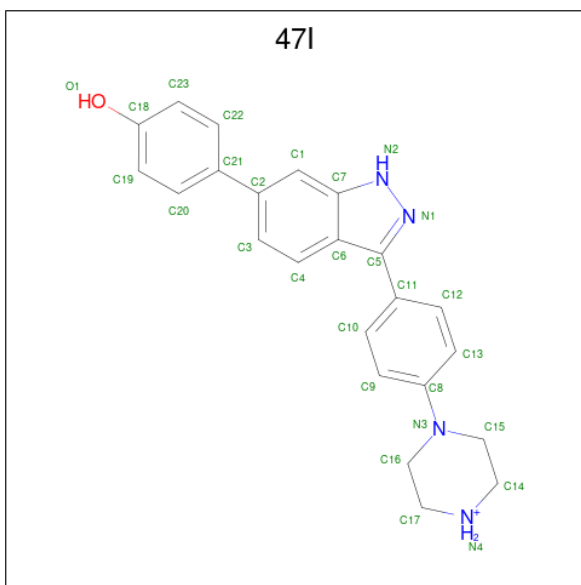
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	281	Total	C	H	N	O	S	97	1	0
			4429	1409	2216	377	405	22			
1	BBB	278	Total	C	H	N	O	S	92	0	0
			4351	1392	2169	366	405	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	461	GLY	-	expression tag	UNP P21802
AAA	462	SER	-	expression tag	UNP P21802
AAA	463	HIS	-	expression tag	UNP P21802
AAA	464	MET	-	expression tag	UNP P21802
BBB	461	GLY	-	expression tag	UNP P21802
BBB	462	SER	-	expression tag	UNP P21802
BBB	463	HIS	-	expression tag	UNP P21802
BBB	464	MET	-	expression tag	UNP P21802

- Molecule 2 is 4-[3-(4-piperazin-4-ium-1-ylphenyl)-1H-indazol-6-yl]phenol (CCD ID: 47I) (formula: C₂₃H₂₃N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			50	23	22	4	1		
2	BBB	1	Total	C	H	N	O	0	0
			50	23	22	4	1		

- 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		
3	BBB	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

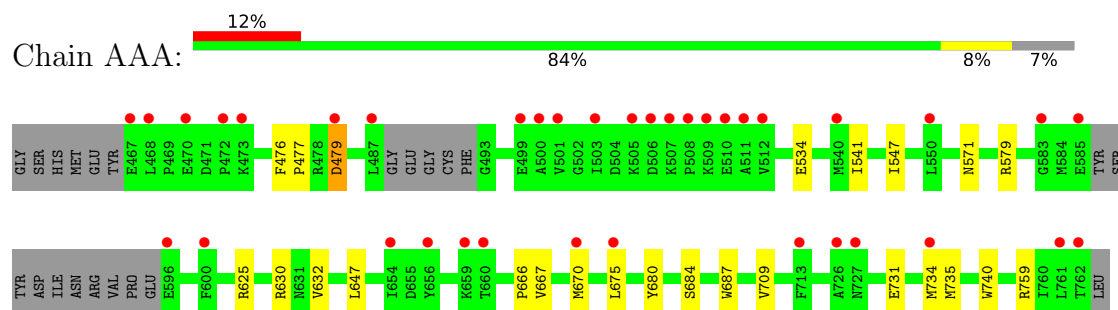
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	49	Total	O	0	0
			49	49		
5	BBB	27	Total	O	0	0
			27	27		

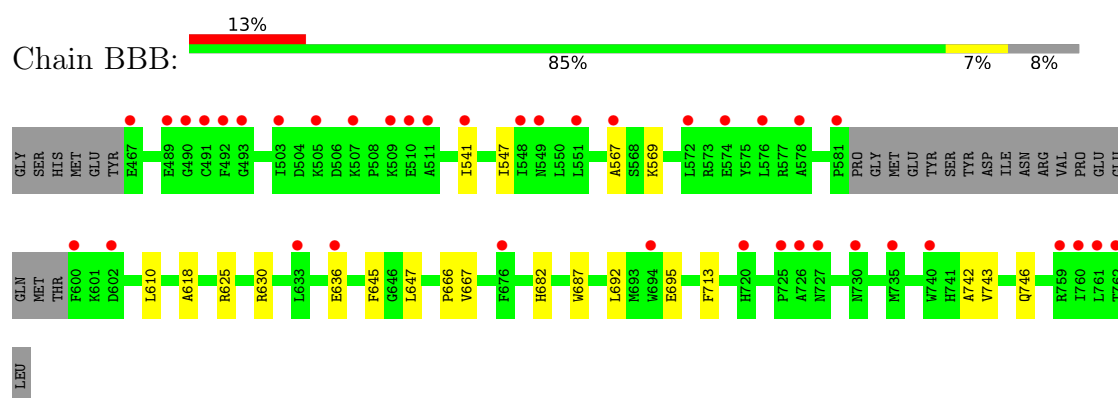
3 Residue-property plots [i](#)

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 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.84Å 113.84Å 117.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.50 – 2.28 80.50 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.3 (80.50-2.28) 98.3 (80.50-2.28)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.240 , 0.296 0.240 , 0.296	Depositor DCC
R_{free} test set	1708 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k 0.002 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: EDO, 47I, 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	AAA	1.02	0/2259	1.41	0/3058
1	BBB	1.02	0/2229	1.44	6/3020 (0.2%)
All	All	1.02	0/4488	1.43	6/6078 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	742	ALA	CA-C-N	5.83	126.56	122.60
1	BBB	742	ALA	C-N-CA	5.83	126.56	122.60
1	BBB	645	PHE	CA-C-N	5.08	125.72	120.03
1	BBB	645	PHE	C-N-CA	5.08	125.72	120.03
1	BBB	567	ALA	CA-C-N	5.01	127.30	120.54
1	BBB	567	ALA	C-N-CA	5.01	127.30	120.54

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	2213	2216	2183	18	0
1	BBB	2182	2169	2140	10	0
2	AAA	28	22	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	28	22	0	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
4	BBB	4	6	6	0	0
5	AAA	49	0	0	0	0
5	BBB	27	0	0	0	0
All	All	4541	4435	4329	28	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 3.

All (28) 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:670:MET:SD	1:AAA:675:LEU:HD23	2.27	0.75
1:BBB:692:LEU:O	1:BBB:695:GLU:HB2	2.04	0.57
1:BBB:687:TRP:C	1:BBB:687:TRP:CD1	2.84	0.55
1:AAA:579:ARG:HH11	1:AAA:579:ARG:HG3	1.74	0.52
1:BBB:630:ARG:HH22	1:BBB:666:PRO:HG2	1.75	0.52
1:BBB:667:VAL:HG13	1:BBB:713:PHE:CE2	2.47	0.49
1:BBB:625:ARG:HD3	1:BBB:647:LEU:O	2.12	0.49
1:AAA:670:MET:SD	1:AAA:675:LEU:CD2	2.99	0.49
1:AAA:731:GLU:OE2	1:AAA:759:ARG:NH2	2.41	0.49
1:BBB:618:ALA:HA	1:BBB:682:HIS:CD2	2.48	0.48
1:AAA:630:ARG:NH2	1:AAA:666:PRO:HG2	2.30	0.47
1:AAA:630:ARG:HH22	1:AAA:666:PRO:HG2	1.80	0.47
1:AAA:667:VAL:HG21	1:AAA:709:VAL:HB	1.96	0.46
1:AAA:534:GLU:OE2	2:AAA:801:47I:O1	2.32	0.46
1:BBB:610:LEU:HD13	1:BBB:692:LEU:HD21	1.97	0.45
1:AAA:687:TRP:CE3	1:AAA:740:TRP:HA	2.52	0.45
1:BBB:541:ILE:HD12	1:BBB:547:ILE:HD12	2.00	0.44
1:AAA:735:MET:HE3	1:AAA:735:MET:HB2	1.75	0.43
1:AAA:579:ARG:HG3	1:AAA:579:ARG:NH1	2.33	0.43
1:AAA:680:TYR:CE1	1:AAA:684:SER:HB2	2.54	0.42
1:AAA:571:ASN:HA	1:AAA:632:VAL:O	2.20	0.42
1:AAA:734:MET:HA	1:AAA:734:MET:HE2	2.01	0.42
1:BBB:569:LYS:NZ	1:BBB:636:GLU:O	2.53	0.42
1:AAA:541:ILE:HD12	1:AAA:547:ILE:HD12	2.02	0.41
1:AAA:479:ASP:OD1	1:AAA:479:ASP:N	2.48	0.41
1:BBB:743:VAL:HB	1:BBB:746:GLN:HG3	2.03	0.41
1:AAA:476:PHE:HA	1:AAA:477:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:625:ARG:HD3	1:AAA:647:LEU:O	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	AAA	276/303 (91%)	269 (98%)	7 (2%)	0	100	100
1	BBB	274/303 (90%)	265 (97%)	9 (3%)	0	100	100
All	All	550/606 (91%)	534 (97%)	16 (3%)	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	236/266 (89%)	235 (100%)	1 (0%)	84	91
1	BBB	232/266 (87%)	232 (100%)	0	100	100
All	All	468/532 (88%)	467 (100%)	1 (0%)	87	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	479	ASP

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](#)

5 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	AAA	802	-	4,4,4	0.37	0	6,6,6	0.15	0
4	EDO	BBB	803	-	3,3,3	0.18	0	2,2,2	0.11	0
2	47I	BBB	801	-	32,32,32	1.65	5 (15%)	44,45,45	1.70	5 (11%)
2	47I	AAA	801	-	32,32,32	1.59	4 (12%)	44,45,45	1.69	5 (11%)
3	SO4	BBB	802	-	4,4,4	0.39	0	6,6,6	0.09	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	BBB	803	-	-	0/1/1/1	-
2	47I	BBB	801	-	-	3/12/20/20	0/5/5/5
2	47I	AAA	801	-	-	3/12/20/20	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	801	47I	C11-C5	-5.43	1.41	1.49
2	BBB	801	47I	C11-C5	-5.39	1.41	1.49
2	BBB	801	47I	O1-C18	-5.35	1.25	1.37
2	AAA	801	47I	O1-C18	-5.20	1.25	1.37
2	AAA	801	47I	C6-C5	-2.57	1.41	1.47
2	BBB	801	47I	C5-N1	2.50	1.35	1.33
2	BBB	801	47I	C6-C5	-2.36	1.41	1.47
2	AAA	801	47I	C5-N1	2.08	1.35	1.33
2	BBB	801	47I	C6-C7	-2.00	1.38	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	801	47I	C6-C5-N1	-8.42	105.55	110.36
2	AAA	801	47I	C6-C5-N1	-7.63	106.00	110.36
2	AAA	801	47I	C16-N3-C15	4.09	120.78	111.57
2	AAA	801	47I	C12-C11-C5	3.49	124.95	120.64
2	BBB	801	47I	C12-C11-C5	3.12	124.50	120.64
2	AAA	801	47I	C10-C11-C5	-2.95	116.99	120.64
2	BBB	801	47I	C16-N3-C15	2.88	118.04	111.57
2	BBB	801	47I	C1-C7-C6	-2.39	120.61	122.52
2	AAA	801	47I	C17-C16-N3	-2.26	105.47	110.38
2	BBB	801	47I	C11-C5-N1	2.09	123.94	119.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

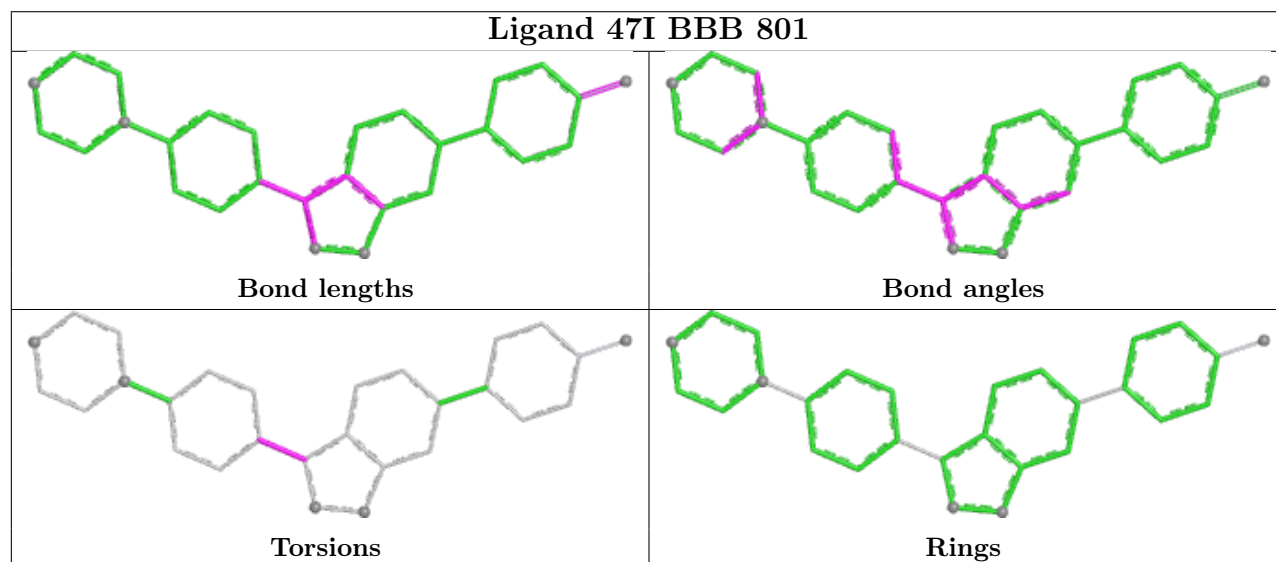
Mol	Chain	Res	Type	Atoms
2	BBB	801	47I	C12-C11-C5-C6
2	AAA	801	47I	C12-C11-C5-C6
2	BBB	801	47I	C10-C11-C5-C6
2	AAA	801	47I	C10-C11-C5-C6
2	AAA	801	47I	C12-C11-C5-N1
2	BBB	801	47I	C12-C11-C5-N1

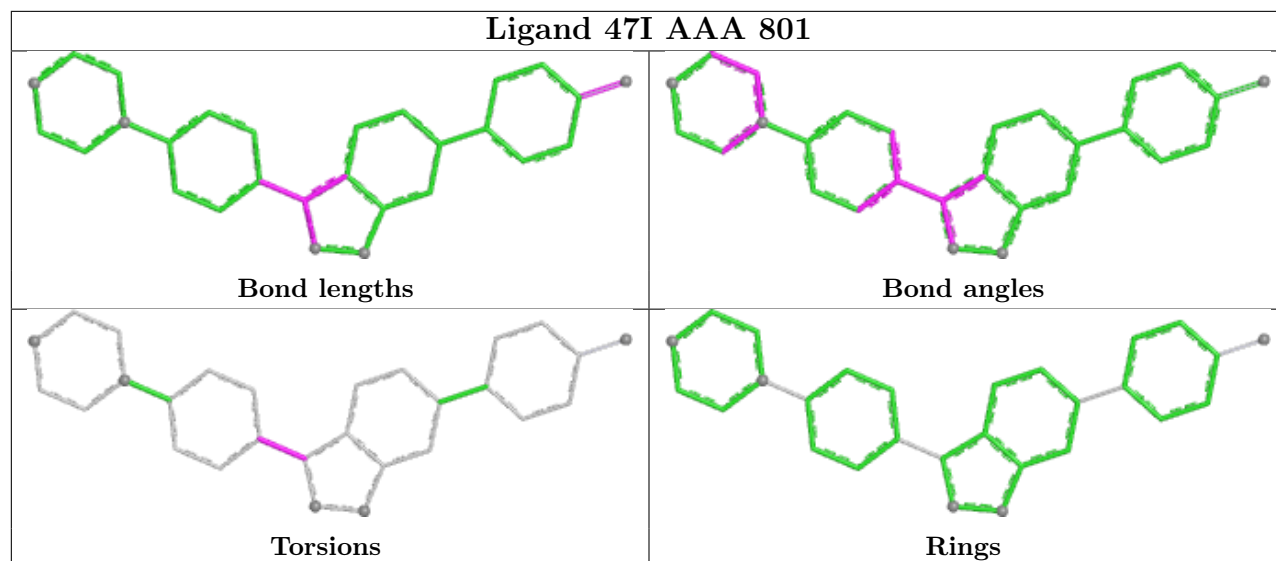
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	801	47I	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 ⓘ

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	AAA	281/303 (92%)	0.74	37 (13%) 7 7	18, 47, 81, 98	1 (0%)
1	BBB	278/303 (91%)	0.97	39 (14%) 6 7	32, 56, 91, 130	0
All	All	559/606 (92%)	0.86	76 (13%) 7 7	18, 52, 86, 130	1 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	492	PHE	8.2
1	BBB	491	CYS	7.6
1	BBB	727	ASN	6.2
1	AAA	675	LEU	5.4
1	BBB	581	PRO	5.3
1	AAA	467	GLU	4.5
1	AAA	727	ASN	4.2
1	BBB	490	GLY	4.0
1	AAA	510	GLU	4.0
1	AAA	487	LEU	4.0
1	AAA	585	GLU	3.8
1	AAA	473	LYS	3.6
1	AAA	470	GLU	3.6
1	AAA	500	ALA	3.6
1	AAA	505	LYS	3.4
1	BBB	505	LYS	3.4
1	AAA	762	THR	3.3
1	BBB	600	PHE	3.3
1	BBB	578	ALA	3.2
1	AAA	506	ASP	3.2
1	AAA	512	VAL	3.1
1	BBB	509	LYS	3.1
1	AAA	508	PRO	3.0
1	BBB	759	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	BBB	762	THR	2.9
1	AAA	656	TYR	2.8
1	BBB	493	GLY	2.8
1	AAA	596	GLU	2.8
1	BBB	510	GLU	2.8
1	BBB	761	LEU	2.8
1	AAA	654	ILE	2.7
1	AAA	511	ALA	2.7
1	BBB	726	ALA	2.7
1	BBB	503	ILE	2.7
1	AAA	726	ALA	2.7
1	BBB	507	LYS	2.6
1	BBB	676	PHE	2.6
1	BBB	730	ASN	2.6
1	AAA	660	THR	2.6
1	BBB	567	ALA	2.6
1	BBB	740	TRP	2.6
1	AAA	713	PHE	2.6
1	BBB	541	ILE	2.6
1	BBB	760	ILE	2.6
1	AAA	468	LEU	2.5
1	BBB	694	TRP	2.5
1	BBB	720	HIS	2.5
1	BBB	574	GLU	2.4
1	AAA	550	LEU	2.4
1	BBB	633	LEU	2.4
1	BBB	636	GLU	2.4
1	AAA	583	GLY	2.4
1	BBB	467	GLU	2.4
1	AAA	659	LYS	2.3
1	AAA	501	VAL	2.3
1	AAA	479	ASP	2.3
1	AAA	734	MET	2.3
1	BBB	549	ASN	2.3
1	BBB	725	PRO	2.3
1	AAA	499	GLU	2.3
1	AAA	509	LYS	2.3
1	BBB	548	ILE	2.3
1	BBB	551	LEU	2.2
1	AAA	472	PRO	2.2
1	AAA	540	MET	2.2
1	AAA	670	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	507	LYS	2.2
1	AAA	761	LEU	2.1
1	BBB	735	MET	2.1
1	BBB	511	ALA	2.1
1	AAA	600	PHE	2.1
1	BBB	572	LEU	2.1
1	BBB	576	LEU	2.1
1	AAA	503	ILE	2.1
1	BBB	489	GLU	2.0
1	BBB	602	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

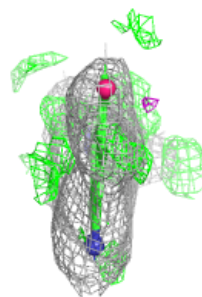
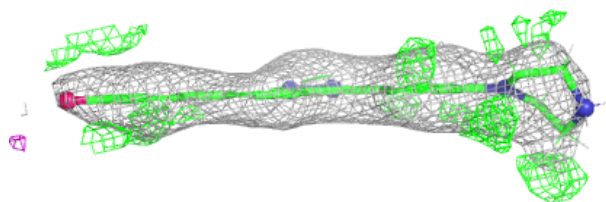
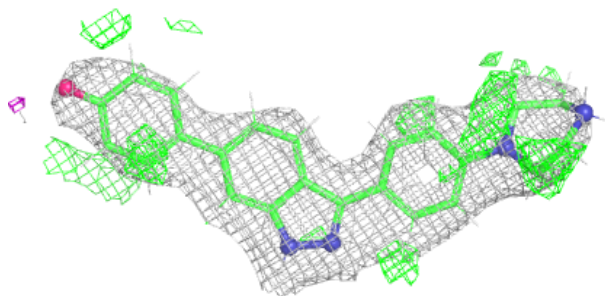
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.82	0.14	73,81,85,85	0
2	47I	BBB	801	28/28	0.87	0.21	41,47,64,64	50
2	47I	AAA	801	28/28	0.88	0.14	43,53,67,72	3
3	SO4	BBB	802	5/5	0.91	0.10	50,51,58,59	0
4	EDO	BBB	803	4/4	0.92	0.12	43,52,57,58	1

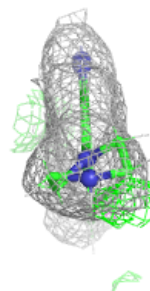
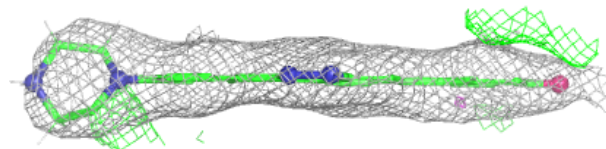
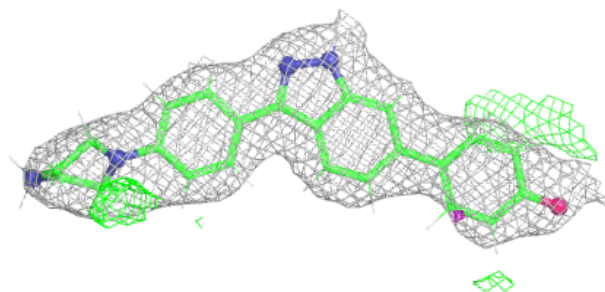
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 47I 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)

**Electron density around 47I AAA 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 ⓘ

There are no such residues in this entry.