



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 5B7V / pdb_00005b7v
Title : Human FGFR1 kinase in complex with CH5183284
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Deposited on : 2016-06-09
Resolution : 2.15 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

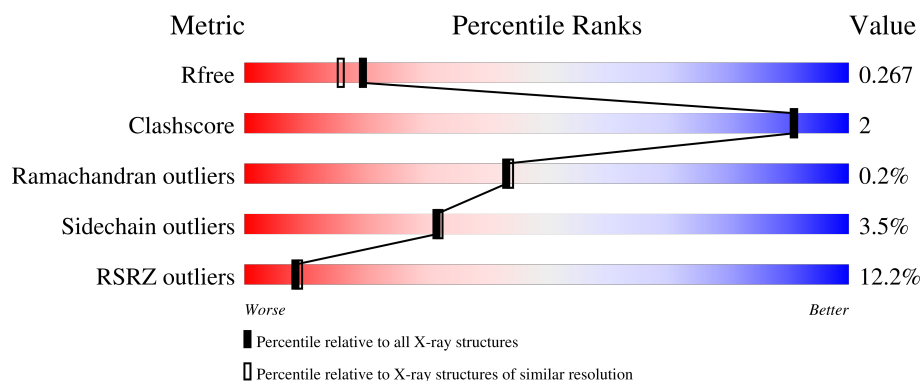
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	310	7% 85% 5% 9%
1	B	310	15% 82% 7% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4580 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.

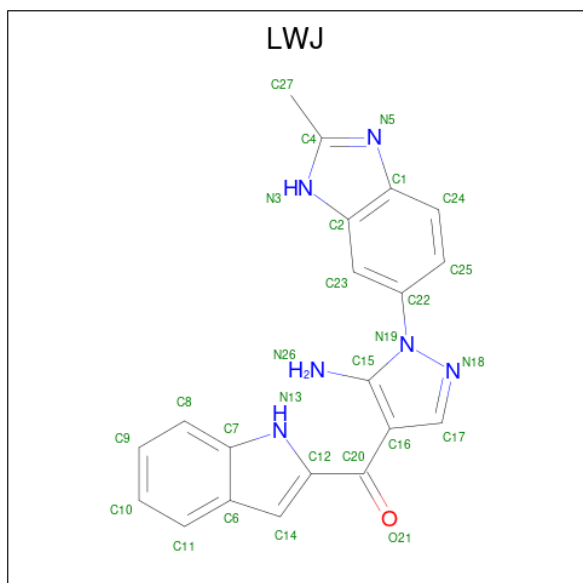
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2246	1429	389	411	17			
1	B	277	Total	C	N	O	S	0	0	0
			2200	1400	376	407	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	VAL	LEU	engineered mutation	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
B	457	VAL	LEU	engineered mutation	UNP P11362
B	488	ALA	CYS	engineered mutation	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362

- Molecule 2 is [5-amino-1-(2-methyl-1H-benzimidazol-6-yl)-1H-pyrazol-4-yl](1H-indol-2-yl)m ethanone (CCD ID: LWJ) (formula: C₂₀H₁₆N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		

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



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

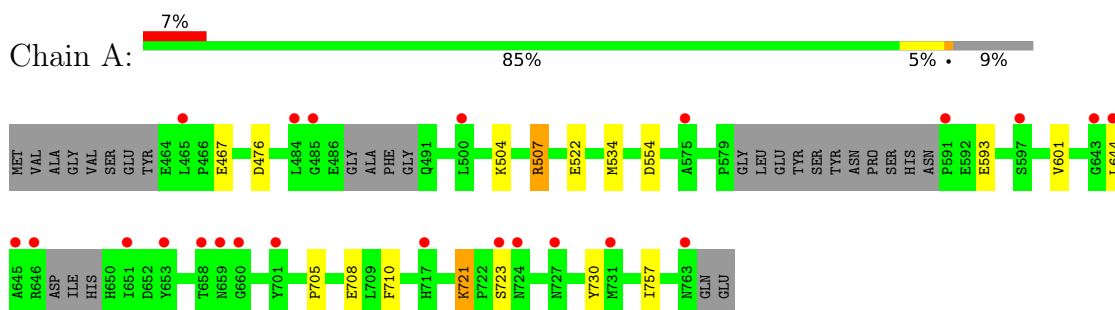
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	23	Total	O	0	0
			23	23		

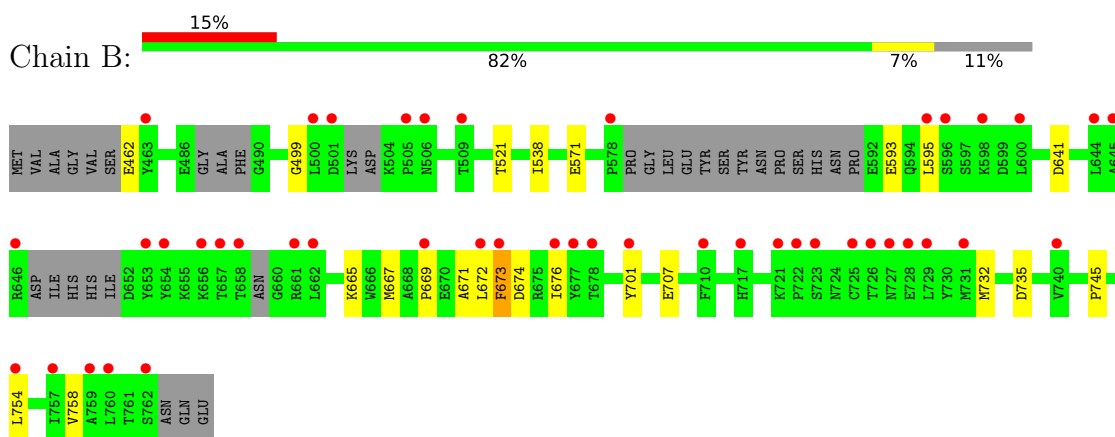
3 Residue-property plots [i](#)

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 1



• 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	211.21Å 56.75Å 65.45Å 90.00° 107.43° 90.00°	Depositor
Resolution (Å)	31.24 – 2.15 31.24 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.24-2.15) 96.9 (31.24-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.223 , 0.256 0.229 , 0.267	Depositor DCC
R_{free} test set	1983 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4580	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.85	0/2291	1.27	2/3094 (0.1%)
1	B	0.83	0/2241	1.29	7/3025 (0.2%)
All	All	0.84	0/4532	1.28	9/6119 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	673	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	476	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	710	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	521	THR	CA-C-N	5.32	128.14	120.38
1	B	521	THR	C-N-CA	5.32	128.14	120.38
1	B	571	GLU	CA-C-N	5.09	127.06	120.44
1	B	571	GLU	C-N-CA	5.09	127.06	120.44
1	B	671	ALA	CA-C-N	5.08	127.53	120.63
1	B	671	ALA	C-N-CA	5.08	127.53	120.63

There are no chirality outliers.

There are no planarity outliers.

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	2246	0	2267	4	0
1	B	2200	0	2196	9	0
2	A	27	0	16	1	0
2	B	27	0	16	2	0
3	A	5	0	0	0	0
4	A	52	0	0	0	0
4	B	23	0	0	0	0
All	All	4580	0	4495	15	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 (15) 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)
2:B:801:LWJ:H8	2:B:801:LWJ:H9	1.74	0.69
1:B:669:PRO:O	1:B:672:LEU:HB2	2.02	0.59
1:A:705:PRO:HD2	1:A:708:GLU:HB2	1.90	0.53
2:A:801:LWJ:H8	2:A:801:LWJ:H9	1.92	0.51
1:B:754:LEU:O	1:B:758:VAL:HG23	2.12	0.50
1:A:504:LYS:HB3	1:A:507:ARG:HG2	1.95	0.48
1:B:667:MET:HB3	1:B:672:LEU:CD1	2.43	0.48
1:B:669:PRO:HA	1:B:672:LEU:HD22	1.94	0.47
1:B:665:LYS:HE2	1:B:701:TYR:HB2	1.97	0.46
1:B:732:MET:HE1	1:B:754:LEU:HG	1.99	0.45
1:B:641:ASP:H	2:B:801:LWJ:H1	1.65	0.45
1:B:735:ASP:HB3	1:B:745:PRO:HD3	2.00	0.43
1:A:601:VAL:HG11	1:A:757:ILE:HG22	2.02	0.41
1:A:721:LYS:HD3	1:A:730:TYR:HB2	2.03	0.41
1:B:667:MET:SD	1:B:672:LEU:HD12	2.61	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	274/310 (88%)	270 (98%)	4 (2%)	0	100	100
1	B	265/310 (86%)	257 (97%)	7 (3%)	1 (0%)	30	26
All	All	539/620 (87%)	527 (98%)	11 (2%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	GLY

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	246/271 (91%)	237 (96%)	9 (4%)	30	30
1	B	238/271 (88%)	230 (97%)	8 (3%)	32	33
All	All	484/542 (89%)	467 (96%)	17 (4%)	32	32

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	GLU
1	A	507	ARG
1	A	522	GLU
1	A	534	MET
1	A	554	ASP
1	A	593	GLU
1	A	644	LEU
1	A	721	LYS
1	A	723	SER
1	B	462	GLU
1	B	538	ILE
1	B	593	GLU

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Mol	Chain	Res	Type
1	B	595	LEU
1	B	673	PHE
1	B	674	ASP
1	B	676	ILE
1	B	707	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	553	GLN
1	A	594	GLN
1	A	679	HIS
1	A	717	HIS
1	A	743	GLN
1	B	491	GLN
1	B	506	ASN
1	B	635	ASN
1	B	680	GLN
1	B	717	HIS

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](#)

3 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	LWJ	A	801	-	31,31,31	2.09	11 (35%)	43,46,46	1.09	4 (9%)
2	LWJ	B	801	-	31,31,31	1.72	7 (22%)	43,46,46	1.02	3 (6%)
3	SO4	A	802	-	4,4,4	0.27	0	6,6,6	0.11	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	LWJ	A	801	-	-	2/12/12/12	0/5/5/5
2	LWJ	B	801	-	-	2/12/12/12	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LWJ	C15-N19	4.89	1.41	1.36
2	B	801	LWJ	C15-N19	4.87	1.41	1.36
2	A	801	LWJ	C16-C15	4.82	1.43	1.39
2	A	801	LWJ	C17-C16	4.17	1.46	1.41
2	A	801	LWJ	N19-N18	2.84	1.41	1.38
2	A	801	LWJ	C24-C1	2.73	1.44	1.40
2	B	801	LWJ	C2-C1	2.70	1.43	1.40
2	A	801	LWJ	C25-C22	2.61	1.44	1.39
2	B	801	LWJ	C6-C7	2.61	1.45	1.41
2	A	801	LWJ	C2-C1	2.59	1.43	1.40
2	A	801	LWJ	C4-N3	2.58	1.40	1.35
2	B	801	LWJ	C10-C9	2.58	1.43	1.38
2	B	801	LWJ	C4-N3	2.57	1.40	1.35
2	B	801	LWJ	C16-C15	2.52	1.41	1.39
2	B	801	LWJ	C25-C22	2.39	1.43	1.39
2	A	801	LWJ	C10-C9	2.38	1.43	1.38
2	A	801	LWJ	C4-N5	2.29	1.36	1.33
2	A	801	LWJ	C8-C7	2.14	1.43	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	LWJ	C22-N19-N18	2.70	122.13	118.85
2	B	801	LWJ	C23-C22-N19	-2.64	115.43	119.27
2	B	801	LWJ	C25-C22-C23	2.43	123.95	119.12
2	A	801	LWJ	C22-N19-C15	-2.26	126.17	129.40
2	A	801	LWJ	C23-C22-N19	-2.14	116.16	119.27
2	B	801	LWJ	C10-C11-C6	-2.13	117.73	120.95
2	A	801	LWJ	C25-C22-C23	2.09	123.28	119.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

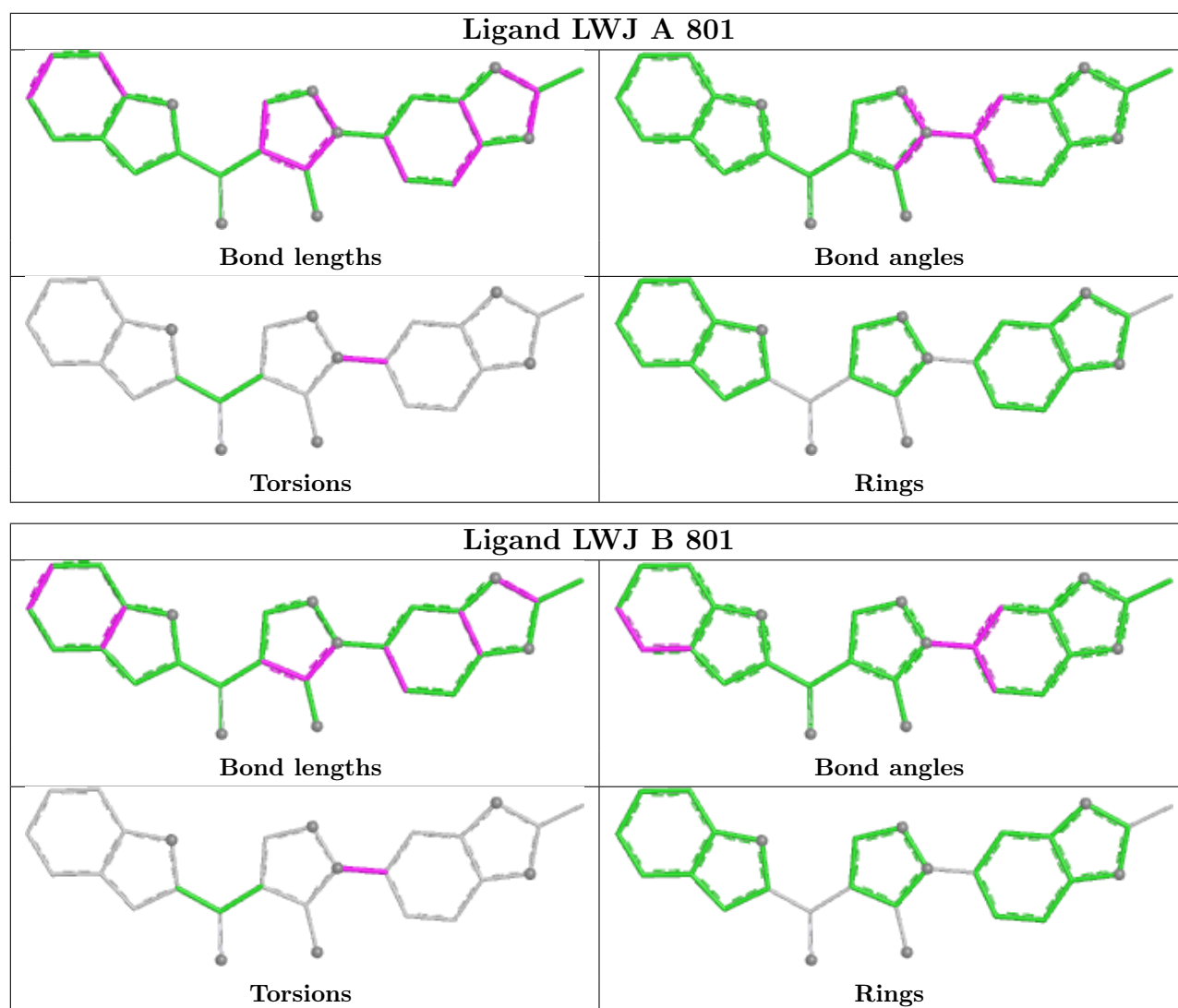
Mol	Chain	Res	Type	Atoms
2	B	801	LWJ	C23-C22-N19-N18
2	A	801	LWJ	C23-C22-N19-N18
2	B	801	LWJ	C25-C22-N19-N18
2	A	801	LWJ	C25-C22-N19-N18

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	LWJ	1	0
2	B	801	LWJ	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	282/310 (90%)	0.56	23 (8%) 17 19	34, 52, 92, 120	0
1	B	277/310 (89%)	0.95	45 (16%) 4 5	39, 58, 104, 122	0
All	All	559/620 (90%)	0.75	68 (12%) 8 9	34, 55, 96, 122	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	645	ALA	5.8
1	B	653	TYR	5.3
1	B	501	ASP	4.8
1	B	657	THR	4.8
1	B	673	PHE	4.7
1	A	591	PRO	4.6
1	A	644	LEU	4.1
1	A	651	ILE	4.1
1	B	727	ASN	3.9
1	B	676	ILE	3.9
1	B	644	LEU	3.9
1	B	710	PHE	3.7
1	A	643	GLY	3.6
1	B	760	LEU	3.4
1	A	658	THR	3.4
1	B	463	TYR	3.3
1	B	740	VAL	3.3
1	A	763	ASN	3.3
1	A	646	ARG	3.3
1	B	726	THR	3.2
1	B	672	LEU	3.2
1	A	731	MET	3.1
1	A	701	TYR	3.0
1	B	725	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	658	THR	3.0
1	B	717	HIS	3.0
1	B	654	TYR	3.0
1	B	578	PRO	2.9
1	A	723	SER	2.8
1	A	653	TYR	2.8
1	B	661	ARG	2.8
1	B	728	GLU	2.8
1	B	731	MET	2.7
1	A	485	GLY	2.7
1	B	721	LYS	2.7
1	B	678	THR	2.7
1	B	505	PRO	2.7
1	B	759	ALA	2.7
1	B	646	ARG	2.7
1	B	595	LEU	2.6
1	A	465	LEU	2.6
1	B	669	PRO	2.5
1	B	662	LEU	2.5
1	B	596	SER	2.5
1	B	677	TYR	2.5
1	A	575	ALA	2.5
1	B	645	ALA	2.5
1	B	701	TYR	2.4
1	B	656	LYS	2.4
1	B	600	LEU	2.3
1	A	500	LEU	2.3
1	B	757	ILE	2.3
1	A	717	HIS	2.2
1	A	724	ASN	2.2
1	A	660	GLY	2.2
1	B	722	PRO	2.2
1	A	597	SER	2.2
1	B	500	LEU	2.2
1	B	762	SER	2.2
1	B	598	LYS	2.2
1	B	506	ASN	2.2
1	A	659	ASN	2.1
1	B	509	THR	2.1
1	A	484	LEU	2.1
1	B	723	SER	2.1
1	B	729	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	727	ASN	2.0
1	B	754	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

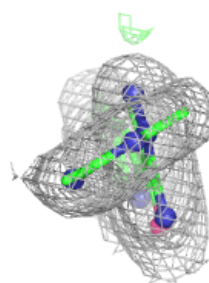
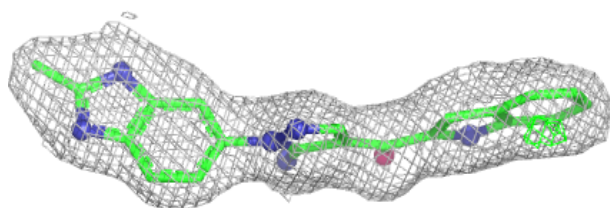
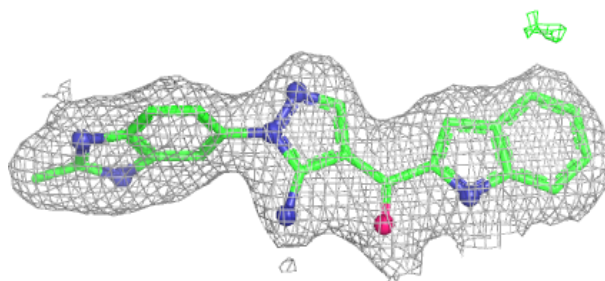
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	802	5/5	0.73	0.15	88,91,92,93	0
2	LWJ	A	801	27/27	0.95	0.07	41,46,53,54	0
2	LWJ	B	801	27/27	0.96	0.07	39,45,50,52	0

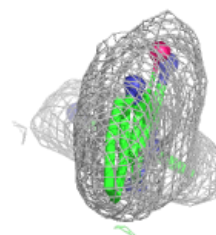
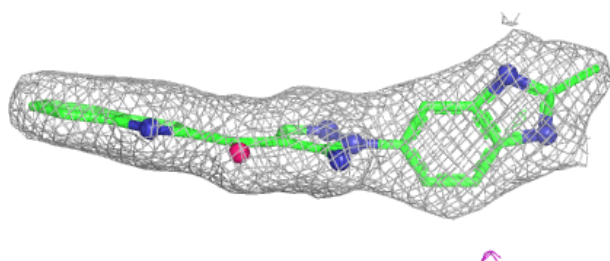
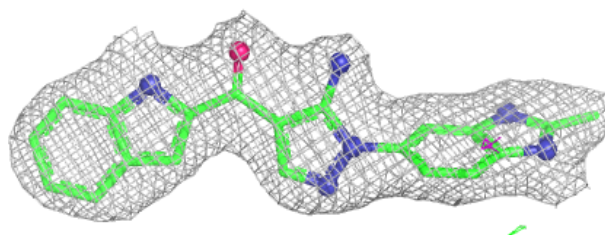
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LWJ 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)

**Electron density around LWJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.