



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:06 PM UTC

PDB ID : 7KHK / pdb_00007khk
Title : Crystal structure of KIT kinase domain with a small molecule inhibitor, PLX9486 (bezucastinib) in the DFG-in state
Authors : Zhang, Y.
Deposited on : 2020-10-21
Resolution : 2.34 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

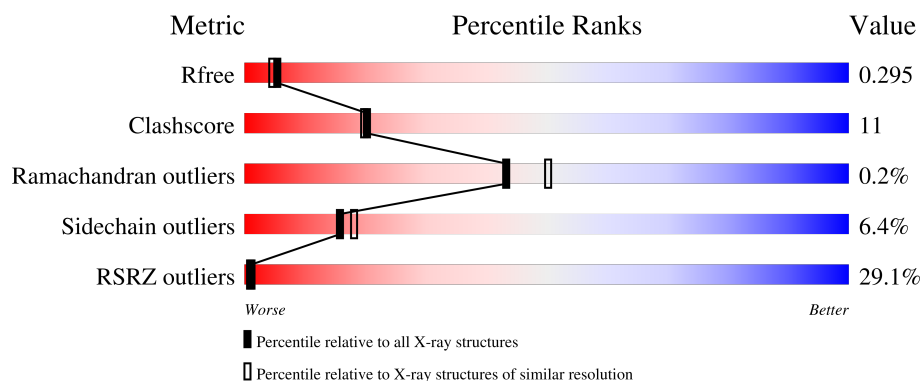
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	335	11% 70% 15% • 13%
1	B	335	37% 57% 20% • 21%

2 Entry composition [i](#)

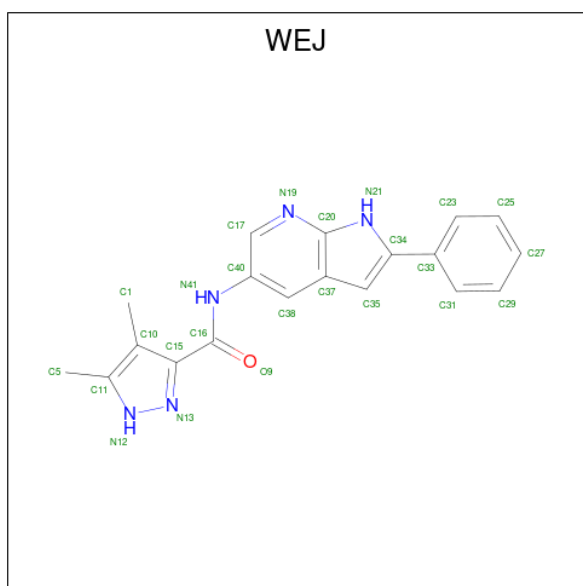
There are 3 unique types of molecules in this entry. The entry contains 4521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mast/stem cell growth factor receptor Kit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2321	1487	389	429	16			
1	B	266	Total	C	N	O	S	0	0	0
			2119	1366	350	388	15			

- Molecule 2 is 4,5-dimethyl-N-(2-phenyl-1H-pyrrolo[2,3-b]pyridin-5-yl)-1H-pyrazole-3-carboxamide (CCD ID: WEJ) (formula: C₁₉H₁₇N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	19	5	1		
2	B	1	Total	C	N	O	0	0
			25	19	5	1		

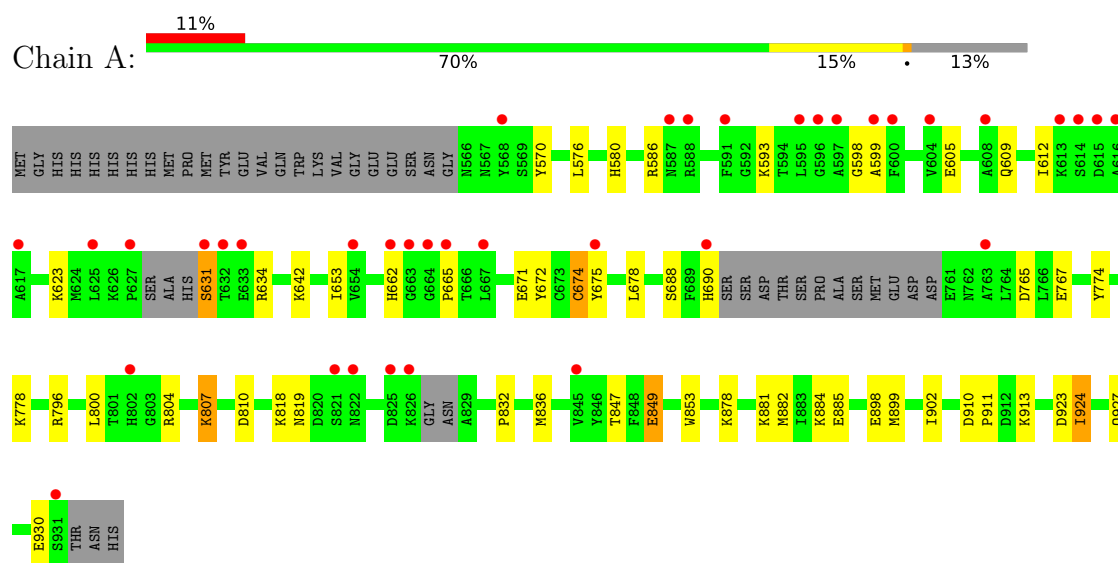
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total 31	O 31	0	0

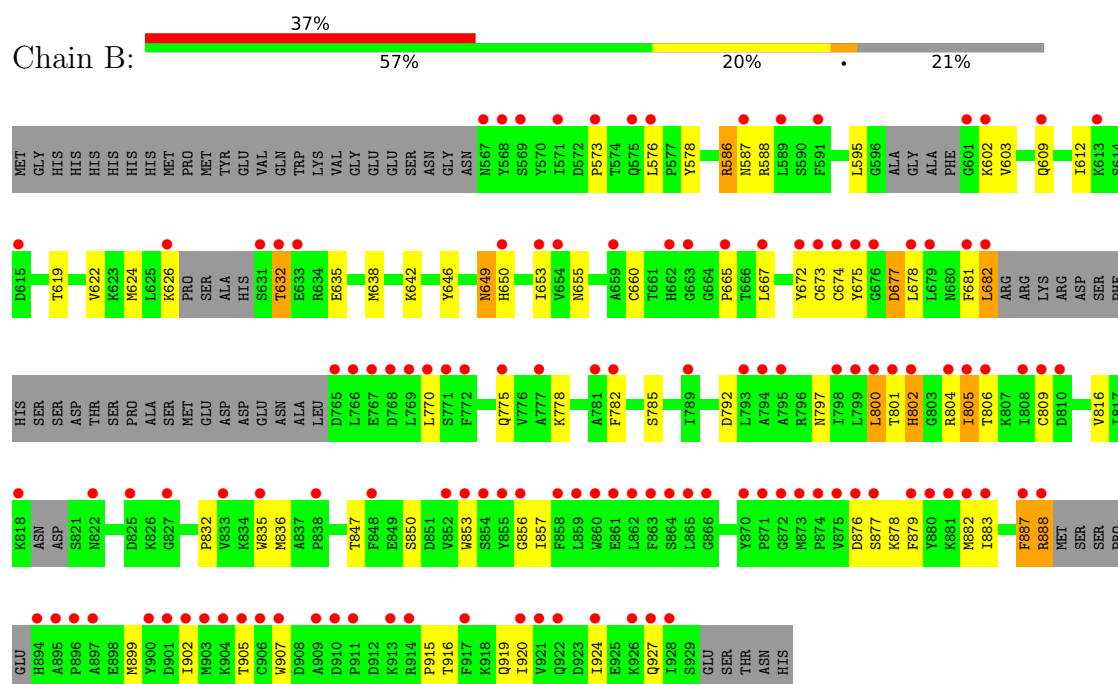
3 Residue-property plots

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: Mast/stem cell growth factor receptor Kit



- Molecule 1: Mast/stem cell growth factor receptor Kit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.98Å 61.91Å 206.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.34 46.06 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.06-2.34) 96.1 (46.06-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.245 , 0.285 0.262 , 0.295	Depositor DCC
R_{free} test set	1534 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4521	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: WEJ

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	0.35	0/2376	0.58	1/3208 (0.0%)
1	B	0.33	0/2167	0.56	0/2924
All	All	0.34	0/4543	0.57	1/6132 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	GLY	N-CA-C	-6.02	98.91	113.18

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	2321	0	2288	37	0
1	B	2119	0	2102	69	0
2	A	25	0	0	1	0
2	B	25	0	0	4	0
3	A	31	0	0	3	0
All	All	4521	0	4390	100	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 11.

All (100) 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:674:CYS:HB3	1:B:802:HIS:CD2	2.02	0.94
1:B:675:TYR:HB2	1:B:800:LEU:O	1.71	0.91
1:B:887:PHE:CD1	1:B:888:ARG:HG2	2.10	0.87
1:B:602:LYS:HE3	1:B:624:MET:HG3	1.56	0.87
1:A:586:ARG:NH1	1:A:665:PRO:O	2.08	0.87
1:B:835:TRP:HA	1:B:857:ILE:HD12	1.67	0.76
1:B:809:CYS:HB2	2:B:1001:WEJ:N13	2.00	0.76
1:A:580:HIS:CD2	1:A:662:HIS:HE2	2.04	0.75
1:B:878:LYS:O	1:B:882:MET:HG3	1.88	0.74
1:B:856:GLY:HA3	1:B:907:TRP:HE1	1.51	0.73
1:B:879:PHE:O	1:B:883:ILE:HG12	1.89	0.73
1:B:887:PHE:HD1	1:B:888:ARG:HG2	1.53	0.72
1:B:677:ASP:OD1	1:B:677:ASP:N	2.24	0.70
1:B:586:ARG:NH2	1:B:665:PRO:O	2.23	0.69
1:A:774:TYR:OH	3:A:1101:HOH:O	1.96	0.65
1:A:671:GLU:OE2	1:A:807:LYS:NZ	2.29	0.64
1:A:910:ASP:HB3	1:A:913:LYS:HG3	1.79	0.64
1:B:847:THR:H	1:B:850:SER:HB3	1.62	0.64
1:B:887:PHE:HD1	1:B:888:ARG:CG	2.11	0.64
1:A:672:TYR:HE2	1:B:802:HIS:CD2	2.17	0.63
1:B:887:PHE:CD1	1:B:888:ARG:CG	2.83	0.59
1:B:675:TYR:HB3	1:B:800:LEU:HB3	1.84	0.59
1:B:800:LEU:HD13	1:B:806:THR:HG23	1.85	0.59
1:A:580:HIS:NE2	1:A:662:HIS:NE2	2.50	0.59
1:B:595:LEU:HD13	2:B:1001:WEJ:C35	2.34	0.57
1:A:672:TYR:HE2	1:B:802:HIS:HD2	1.50	0.57
1:A:765:ASP:OD2	1:A:767:GLU:HG2	2.04	0.57
1:A:570:TYR:CD1	1:A:818:LYS:HE2	2.40	0.57
1:A:631:SER:O	1:A:631:SER:OG	2.21	0.57
1:B:832:PRO:O	1:B:836:MET:HG3	2.05	0.56
1:B:660:CYS:HB2	1:B:667:LEU:HB2	1.88	0.56
1:B:802:HIS:ND1	1:B:802:HIS:N	2.53	0.55
1:A:675:TYR:HB2	1:A:800:LEU:O	2.07	0.55
1:A:881:LYS:HE2	1:A:885:GLU:OE2	2.06	0.55
1:A:884:LYS:O	3:A:1102:HOH:O	2.18	0.55
1:B:905:THR:HG23	1:B:915:PRO:HD3	1.89	0.55
1:B:672:TYR:CD1	1:B:672:TYR:C	2.85	0.54
1:B:801:THR:HG22	1:B:805:ILE:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:MET:HE1	1:A:924:ILE:HG12	1.90	0.54
1:B:887:PHE:CE1	1:B:888:ARG:HG2	2.43	0.53
1:B:588:ARG:HD3	1:B:609:GLN:O	2.09	0.53
1:B:673:CYS:O	2:B:1001:WEJ:C31	2.56	0.53
1:A:832:PRO:O	1:A:836:MET:HG3	2.08	0.53
1:B:887:PHE:O	1:B:888:ARG:C	2.51	0.53
1:A:849:GLU:HG3	1:A:911:PRO:HB3	1.91	0.52
1:B:916:THR:OG1	1:B:919:GLN:HG3	2.09	0.52
1:B:650:HIS:HB3	1:B:653:ILE:HG12	1.92	0.52
1:B:775:GLN:OE1	1:B:805:ILE:HA	2.10	0.51
1:A:899:MET:HE2	1:A:902:ILE:HD12	1.93	0.51
1:B:602:LYS:HZ3	1:B:626:LYS:CG	2.24	0.50
1:A:847:THR:OG1	1:A:849:GLU:HG2	2.11	0.50
1:B:632:THR:O	1:B:635:GLU:HG2	2.11	0.50
1:B:882:MET:HE2	1:B:887:PHE:CD2	2.47	0.50
1:B:775:GLN:NE2	1:B:804:ARG:O	2.44	0.50
1:A:623:LYS:NZ	1:A:810:ASP:OD1	2.40	0.50
1:A:923:ASP:OD1	1:A:927:GLN:NE2	2.42	0.50
1:B:782:PHE:O	1:B:785:SER:OG	2.23	0.49
1:B:573:PRO:HB3	1:B:646:TYR:HB2	1.95	0.49
1:B:595:LEU:C	1:B:595:LEU:HD12	2.37	0.49
1:A:899:MET:HE3	1:A:927:GLN:CD	2.38	0.49
1:A:878:LYS:O	1:A:882:MET:HG3	2.14	0.48
1:A:899:MET:HE3	1:A:927:GLN:OE1	2.13	0.48
1:A:593:LYS:HG2	1:A:605:GLU:OE2	2.14	0.48
1:B:675:TYR:CB	1:B:800:LEU:HB3	2.42	0.48
1:B:603:VAL:HA	1:B:622:VAL:O	2.13	0.47
1:A:672:TYR:CE2	1:B:802:HIS:CD2	3.00	0.47
1:B:801:THR:CG2	1:B:805:ILE:HB	2.45	0.47
1:A:765:ASP:CG	1:A:767:GLU:HG2	2.40	0.47
1:B:578:TYR:HB2	1:B:638:MET:HE1	1.96	0.47
1:B:856:GLY:CA	1:B:907:TRP:HE1	2.22	0.47
1:A:674:CYS:HB3	1:B:802:HIS:HD2	1.71	0.47
1:B:675:TYR:HE2	1:B:802:HIS:HA	1.80	0.47
1:B:902:ILE:O	1:B:905:THR:HG22	2.15	0.47
1:B:853:TRP:C	1:B:853:TRP:CD1	2.92	0.46
1:A:609:GLN:NE2	1:B:649:ASN:OD1	2.49	0.46
1:B:602:LYS:HZ1	1:B:626:LYS:HE2	1.81	0.46
1:A:623:LYS:HB2	2:A:1001:WEJ:C1	2.47	0.45
1:B:876:ASP:OD1	1:B:879:PHE:N	2.37	0.45
1:A:631:SER:OG	1:A:634:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:LYS:HE3	1:B:624:MET:CG	2.37	0.45
1:B:899:MET:HA	1:B:899:MET:HE2	1.99	0.44
1:B:576:LEU:O	1:B:642:LYS:HE2	2.18	0.43
1:A:570:TYR:O	1:A:819:ASN:ND2	2.49	0.43
1:A:576:LEU:O	1:A:642:LYS:HE2	2.19	0.43
1:B:887:PHE:CD1	1:B:887:PHE:C	2.96	0.43
1:B:899:MET:HE3	1:B:927:GLN:OE1	2.18	0.43
1:B:682:LEU:H	1:B:682:LEU:HG	1.71	0.42
1:B:778:LYS:HB3	1:B:778:LYS:HE2	1.91	0.42
1:A:853:TRP:CD1	1:A:853:TRP:C	2.98	0.42
1:B:856:GLY:HA3	1:B:907:TRP:NE1	2.26	0.42
1:B:916:THR:O	1:B:920:ILE:HG13	2.20	0.42
1:B:792:ASP:O	1:B:797:ASN:ND2	2.52	0.41
1:B:602:LYS:HZ3	1:B:626:LYS:HG2	1.85	0.41
1:B:673:CYS:O	2:B:1001:WEJ:N21	2.53	0.41
1:A:774:TYR:CE2	1:A:778:LYS:HD2	2.56	0.41
1:A:796:ARG:HG2	3:A:1112:HOH:O	2.20	0.41
1:B:674:CYS:O	1:B:674:CYS:SG	2.79	0.41
1:B:681:PHE:CE2	1:B:800:LEU:HD23	2.56	0.41
1:B:573:PRO:HG2	1:B:816:VAL:HG21	2.03	0.40
1:B:595:LEU:CD1	1:B:603:VAL:HG23	2.51	0.40

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	283/335 (84%)	278 (98%)	4 (1%)	1 (0%)	30	32
1	B	254/335 (76%)	248 (98%)	6 (2%)	0	100	100
All	All	537/670 (80%)	526 (98%)	10 (2%)	1 (0%)	43	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	599	ALA

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	253/291 (87%)	240 (95%)	13 (5%)	21	26
1	B	231/291 (79%)	213 (92%)	18 (8%)	11	12
All	All	484/582 (83%)	453 (94%)	31 (6%)	16	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	ILE
1	A	631	SER
1	A	653	ILE
1	A	674	CYS
1	A	678	LEU
1	A	688	SER
1	A	690	HIS
1	A	804	ARG
1	A	807	LYS
1	A	849	GLU
1	A	898	GLU
1	A	924	ILE
1	A	930	GLU
1	B	586	ARG
1	B	587	ASN
1	B	612	ILE
1	B	619	THR
1	B	632	THR
1	B	649	ASN
1	B	655	ASN
1	B	677	ASP
1	B	678	LEU

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Mol	Chain	Res	Type
1	B	682	LEU
1	B	770	LEU
1	B	800	LEU
1	B	802	HIS
1	B	805	ILE
1	B	877	SER
1	B	887	PHE
1	B	888	ARG
1	B	924	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	690	HIS
1	A	822	ASN

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](#)

2 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	WEJ	A	1001	-	28,28,28	1.16	4 (14%)	38,40,40	1.65	7 (18%)
2	WEJ	B	1001	-	28,28,28	1.15	4 (14%)	38,40,40	1.66	8 (21%)

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	WEJ	A	1001	-	-	4/12/12/12	0/4/4/4
2	WEJ	B	1001	-	-	4/12/12/12	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	WEJ	C15-N13	2.77	1.37	1.34
2	B	1001	WEJ	C15-N13	2.72	1.37	1.34
2	A	1001	WEJ	C37-C20	-2.34	1.38	1.42
2	B	1001	WEJ	C37-C20	-2.28	1.38	1.42
2	B	1001	WEJ	C11-C10	2.22	1.43	1.37
2	A	1001	WEJ	C11-C10	2.19	1.43	1.37
2	A	1001	WEJ	C15-C10	-2.18	1.39	1.45
2	B	1001	WEJ	C15-C10	-2.14	1.39	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	WEJ	C15-N13-N12	5.97	115.06	104.90
2	A	1001	WEJ	C15-N13-N12	5.95	115.03	104.90
2	A	1001	WEJ	C11-N12-N13	-3.69	103.47	111.93
2	B	1001	WEJ	C11-N12-N13	-3.68	103.49	111.93
2	B	1001	WEJ	C16-C15-C10	2.98	133.84	127.72
2	A	1001	WEJ	C10-C11-N12	2.88	112.24	107.35
2	B	1001	WEJ	C10-C11-N12	2.87	112.22	107.35
2	A	1001	WEJ	C16-C15-C10	2.84	133.55	127.72
2	A	1001	WEJ	C40-C17-N19	2.44	126.10	124.07
2	B	1001	WEJ	C40-C17-N19	2.44	126.09	124.07
2	A	1001	WEJ	C10-C15-N13	-2.31	104.60	110.64
2	B	1001	WEJ	C10-C15-N13	-2.30	104.62	110.64
2	B	1001	WEJ	C35-C34-N21	-2.07	105.98	108.65
2	A	1001	WEJ	C35-C34-N21	-2.05	106.01	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	WEJ	C20-N21-C34	2.00	110.68	108.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

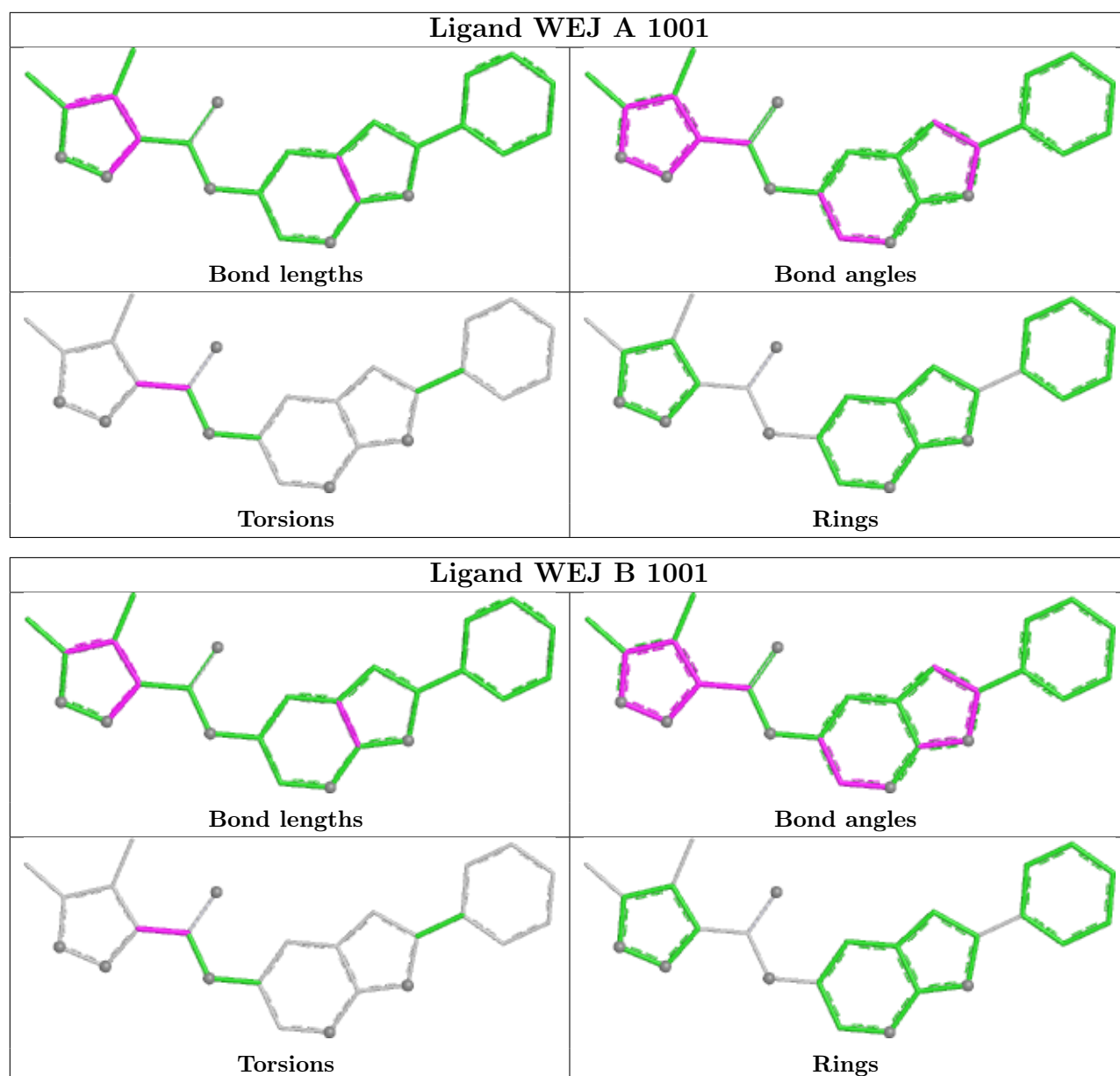
Mol	Chain	Res	Type	Atoms
2	A	1001	WEJ	C10-C15-C16-N41
2	A	1001	WEJ	C10-C15-C16-O9
2	A	1001	WEJ	N13-C15-C16-N41
2	A	1001	WEJ	N13-C15-C16-O9
2	B	1001	WEJ	N13-C15-C16-N41
2	B	1001	WEJ	N13-C15-C16-O9
2	B	1001	WEJ	C10-C15-C16-N41
2	B	1001	WEJ	C10-C15-C16-O9

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	WEJ	1	0
2	B	1001	WEJ	4	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	291/335 (86%)	0.85	37 (12%) 8 9	38, 58, 96, 134	0
1	B	266/335 (79%)	2.10	125 (46%) 0 0	54, 100, 126, 158	0
All	All	557/670 (83%)	1.45	162 (29%) 1 1	38, 80, 123, 158	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	862	LEU	7.3
1	B	768	ASP	5.8
1	B	863	PHE	5.2
1	B	924	ILE	5.2
1	B	765	ASP	5.1
1	A	600	PHE	4.9
1	B	673	CYS	4.9
1	A	822	ASN	4.9
1	B	679	LEU	4.7
1	B	866	GLY	4.7
1	B	860	TRP	4.4
1	B	897	ALA	4.4
1	B	928	ILE	4.4
1	A	662	HIS	4.3
1	A	599	ALA	4.3
1	A	625	LEU	4.3
1	B	682	LEU	4.3
1	B	766	LEU	4.3
1	A	615	ASP	4.2
1	B	865	LEU	4.2
1	B	793	LEU	4.2
1	B	907	TRP	4.0
1	B	800	LEU	4.0
1	B	894	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	665	PRO	3.9
1	B	772	PHE	3.9
1	B	900	TYR	3.9
1	A	613	LYS	3.9
1	B	875	VAL	3.8
1	B	901	ASP	3.8
1	B	856	GLY	3.8
1	B	662	HIS	3.8
1	B	769	LEU	3.7
1	B	879	PHE	3.6
1	B	613	LYS	3.6
1	B	770	LEU	3.6
1	B	576	LEU	3.6
1	B	859	LEU	3.6
1	A	627	PRO	3.5
1	B	609	GLN	3.5
1	B	883	ILE	3.5
1	B	882	MET	3.4
1	B	663	GLY	3.4
1	B	858	PHE	3.4
1	B	801	THR	3.4
1	B	896	PRO	3.4
1	B	575	GLN	3.4
1	B	887	PHE	3.3
1	B	567	ASN	3.3
1	A	663	GLY	3.3
1	B	808	ILE	3.3
1	B	674	CYS	3.2
1	B	681	PHE	3.2
1	B	781	ALA	3.2
1	B	626	LYS	3.2
1	B	825	ASP	3.2
1	B	864	SER	3.2
1	B	602	LYS	3.2
1	B	799	LEU	3.2
1	A	826	LYS	3.1
1	B	802	HIS	3.1
1	B	920	ILE	3.1
1	B	615	ASP	3.1
1	B	911	PRO	3.1
1	B	921	VAL	3.1
1	B	822	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	802	HIS	3.0
1	B	659	ALA	3.0
1	B	855	TYR	3.0
1	B	927	GLN	3.0
1	B	926	LYS	3.0
1	B	880	TYR	3.0
1	B	827	GLY	3.0
1	B	917	PHE	2.9
1	B	895	ALA	2.9
1	B	852	VAL	2.9
1	B	874	PRO	2.9
1	B	650	HIS	2.9
1	B	667	LEU	2.9
1	B	569	SER	2.9
1	B	601	GLY	2.9
1	B	853	TRP	2.9
1	B	888	ARG	2.9
1	B	775	GLN	2.9
1	B	877	SER	2.9
1	B	678	LEU	2.9
1	B	906	CYS	2.9
1	B	913	LYS	2.8
1	A	664	GLY	2.8
1	A	763	ALA	2.8
1	B	794	ALA	2.8
1	A	568	TYR	2.7
1	A	597	ALA	2.7
1	A	825	ASP	2.7
1	B	805	ILE	2.7
1	A	931	SER	2.7
1	B	903	MET	2.7
1	B	795	ALA	2.7
1	B	571	ILE	2.7
1	B	861	GLU	2.6
1	B	902	ILE	2.6
1	B	809	CYS	2.6
1	B	914	ARG	2.6
1	B	589	LEU	2.6
1	A	608	ALA	2.6
1	A	616	ALA	2.6
1	B	587	ASN	2.6
1	B	806	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	573	PRO	2.5
1	B	676	GLY	2.5
1	B	905	THR	2.5
1	A	596	GLY	2.5
1	A	690	HIS	2.5
1	B	871	PRO	2.4
1	B	675	TYR	2.4
1	A	587	ASN	2.4
1	A	617	ALA	2.4
1	B	854	SER	2.4
1	B	872	GLY	2.4
1	B	909	ALA	2.4
1	A	845	VAL	2.4
1	B	653	ILE	2.4
1	B	804	ARG	2.4
1	A	633	GLU	2.4
1	B	910	ASP	2.3
1	B	838	PRO	2.3
1	B	591	PHE	2.3
1	B	870	TYR	2.3
1	A	631	SER	2.3
1	B	665	PRO	2.3
1	A	821	SER	2.3
1	A	591	PHE	2.3
1	B	818	LYS	2.3
1	A	588	ARG	2.3
1	B	922	GLN	2.3
1	B	672	TYR	2.2
1	A	654	VAL	2.2
1	B	848	PHE	2.2
1	B	568	TYR	2.2
1	B	835	TRP	2.2
1	B	782	PHE	2.2
1	B	873	MET	2.2
1	B	881	LYS	2.2
1	B	904	LYS	2.2
1	A	675	TYR	2.1
1	B	767	GLU	2.1
1	A	614	SER	2.1
1	B	798	ILE	2.1
1	B	777	ALA	2.1
1	B	633	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	789	ILE	2.1
1	B	810	ASP	2.1
1	B	654	VAL	2.1
1	A	632	THR	2.1
1	B	631	SER	2.1
1	A	667	LEU	2.1
1	A	604	VAL	2.1
1	B	833	VAL	2.1
1	A	595	LEU	2.0
1	B	876	ASP	2.0
1	B	632	THR	2.0
1	B	771	SER	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](#)

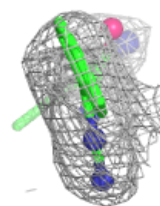
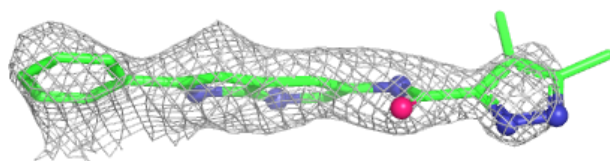
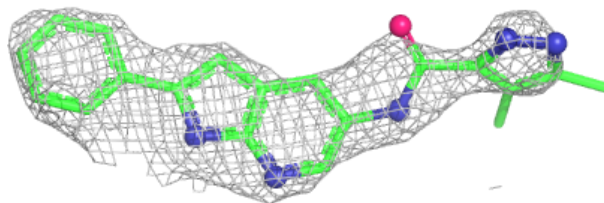
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	WEJ	B	1001	25/25	0.81	0.17	105,106,112,113	0
2	WEJ	A	1001	25/25	0.87	0.21	105,105,106,106	0

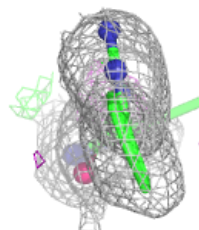
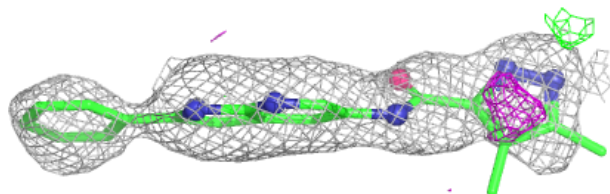
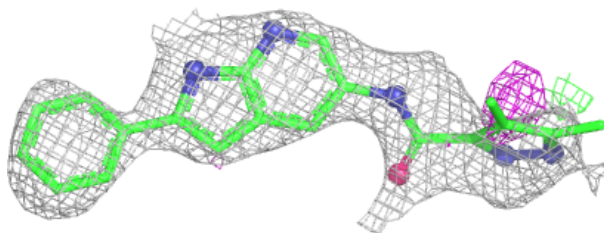
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WEJ B 1001:

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

**Electron density around WEJ A 1001:**

$2mF_o-DF_c$ (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.