



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:47 AM UTC

PDB ID : 7Z5X / pdb_00007z5x
Title : ROS1 with AstraZeneca ligand 2
Authors : Hargreaves, D.
Deposited on : 2022-03-10
Resolution : 2.04 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

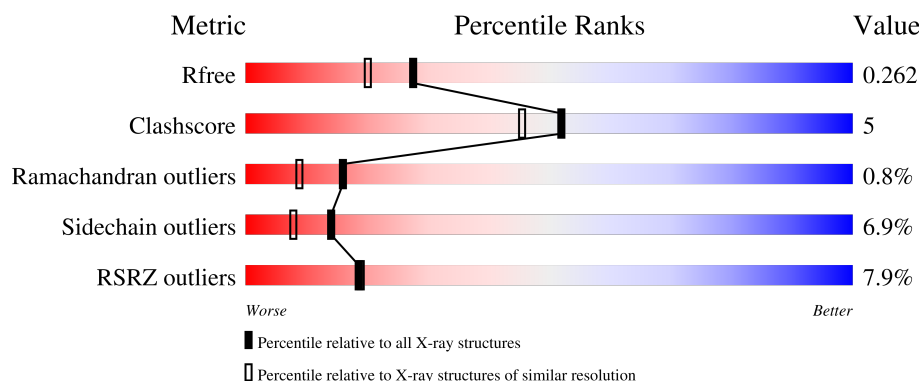
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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	331	5% 68% 13% • 18%
1	B	331	8% 68% 11% • 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4622 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.

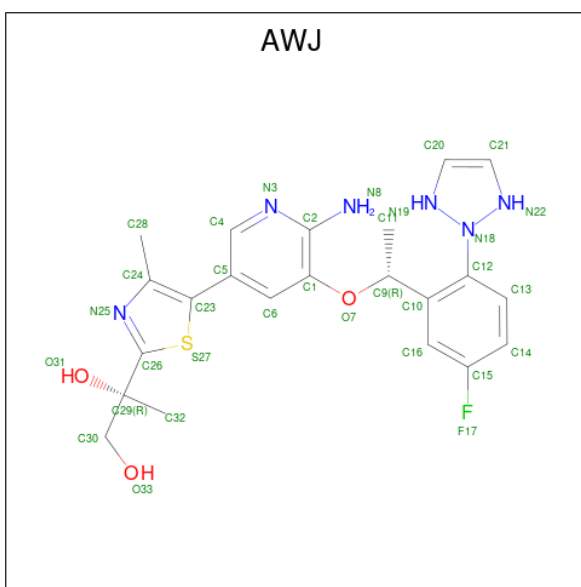
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase ROS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2163	1396	366	388	13			
1	B	271	Total	C	N	O	S	0	0	0
			2171	1402	367	389	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1928	GLY	-	expression tag	UNP P08922
A	1929	SER	-	expression tag	UNP P08922
A	2257	LEU	-	expression tag	UNP P08922
A	2258	GLU	-	expression tag	UNP P08922
B	1928	GLY	-	expression tag	UNP P08922
B	1929	SER	-	expression tag	UNP P08922
B	2257	LEU	-	expression tag	UNP P08922
B	2258	GLU	-	expression tag	UNP P08922

- Molecule 2 is (2R)-2-[5-(6-amino-5-((1R)-1-[2-(1,3-dihydro-2H-1,2,3-triazol-2-yl)-5-fluorophenyl]ethoxy)pyridin-3-yl)-4-methyl-1,3-thiazol-2-yl]propane-1,2-diol (CCD ID: AWJ) (formula: C₂₂H₂₅FN₆O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			33	22	1	6	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			33	22	1	6	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	93	Total	O	0	0
			93	93		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.06Å 41.21Å 85.57Å 90.00° 92.09° 90.00°	Depositor
Resolution (Å)	29.76 – 2.04 29.76 – 2.04	Depositor EDS
% Data completeness (in resolution range)	73.4 (29.76-2.04) 73.3 (29.76-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.227 , 0.266 0.221 , 0.262	Depositor DCC
R_{free} test set	1345 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4622	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.69% 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: AWJ

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	0.74	0/2214	1.04	0/3003
1	B	0.73	0/2222	1.07	3/3014 (0.1%)
All	All	0.74	0/4436	1.05	3/6017 (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	B	2192	ASN	CA-CB-CG	6.84	119.44	112.60
1	B	2187	PRO	CA-C-N	5.60	128.10	120.54
1	B	2187	PRO	C-N-CA	5.60	128.10	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	A	2163	0	2178	24	0
1	B	2171	0	2189	24	0
2	A	33	0	25	0	0
2	B	33	0	25	0	0
3	A	129	0	0	1	0
3	B	93	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4622	0	4417	45	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 5.

All (45) 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:1998:ALA:HA	1:A:2012:GLN:HE22	1.55	0.72
1:B:1998:ALA:HA	1:B:2012:GLN:HE22	1.55	0.71
1:B:1951:LEU:HD11	1:B:1961:GLU:HB2	1.78	0.66
1:A:2201:GLU:H	1:A:2201:GLU:CD	2.05	0.64
1:B:2201:GLU:H	1:B:2201:GLU:CD	2.07	0.63
1:A:2165:HIS:HD2	1:A:2169:ASP:OD2	1.81	0.63
1:B:2063:ILE:HD11	1:B:2098:VAL:HG22	1.82	0.62
1:A:1966:ASP:HA	1:A:1972:SER:HB2	1.83	0.61
1:B:2008:ASN:HD21	1:B:2097:ILE:HD11	1.66	0.60
1:B:1951:LEU:CD1	1:B:1961:GLU:HB2	2.35	0.57
1:A:2140:THR:HG21	3:A:2519:HOH:O	2.05	0.56
1:A:1942:ARG:HG2	1:A:2016:CYS:HB3	1.86	0.56
1:A:2008:ASN:HD21	1:A:2097:ILE:HD11	1.70	0.56
1:B:1969:GLY:O	1:B:1972:SER:HB3	2.06	0.54
1:B:2199:ALA:O	1:B:2205:ARG:HD2	2.10	0.52
1:A:2199:ALA:O	1:A:2205:ARG:HD2	2.10	0.51
1:B:2172:ASN:O	1:B:2176:THR:HB	2.11	0.50
1:A:1965:VAL:HG22	1:A:1974:GLU:HG2	1.94	0.50
1:A:1992:ILE:HD12	1:B:1999:HIS:HB3	1.95	0.49
1:B:2063:ILE:HD11	1:B:2098:VAL:CG2	2.45	0.45
1:A:1953:SER:O	1:A:1957:GLY:O	2.34	0.45
1:A:1942:ARG:H	1:A:1942:ARG:HG3	1.65	0.44
1:B:2057:VAL:HG21	1:B:2218:PHE:HE2	1.82	0.44
1:A:1996:LYS:HG3	1:B:1992:ILE:HG22	2.00	0.44
1:A:2057:VAL:HG21	1:A:2218:PHE:HE2	1.83	0.44
1:A:2174:VAL:O	1:A:2179:ARG:NH2	2.51	0.44
1:A:2201:GLU:CD	1:A:2201:GLU:N	2.73	0.44
1:B:2201:GLU:CD	1:B:2201:GLU:N	2.75	0.43
1:B:2174:VAL:O	1:B:2179:ARG:NH2	2.52	0.43
1:A:2063:ILE:HG21	1:A:2150:LEU:HD21	2.01	0.42
1:B:1966:ASP:HA	1:B:1972:SER:HB3	2.00	0.42
1:A:2000:LEU:HD22	1:A:2075:PHE:HE1	1.83	0.42
1:A:1992:ILE:HG22	1:B:1996:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:ILE:HD11	1:A:2098:VAL:HG22	2.01	0.42
1:A:2012:GLN:HE21	1:A:2024:ILE:HG23	1.85	0.42
1:B:1980:LYS:NZ	3:B:2408:HOH:O	2.52	0.42
1:A:2008:ASN:ND2	1:A:2097:ILE:HD11	2.35	0.41
1:B:2054:VAL:HG13	3:B:2424:HOH:O	2.20	0.41
1:A:2068:VAL:HG21	1:A:2212:GLN:HE21	1.85	0.41
1:B:2134:MET:SD	1:B:2135:ASP:OD2	2.79	0.40
1:B:2226:ILE:HD13	1:B:2226:ILE:HA	1.95	0.40
1:A:2201:GLU:HG2	1:A:2204:GLN:HB2	2.03	0.40
1:B:2012:GLN:HE21	1:B:2024:ILE:HG23	1.86	0.40
1:B:2063:ILE:HG21	1:B:2150:LEU:HD21	2.03	0.40
1:B:2201:GLU:HG2	1:B:2204:GLN:HB2	2.02	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	266/331 (80%)	258 (97%)	6 (2%)	2 (1%)	16	9
1	B	267/331 (81%)	260 (97%)	5 (2%)	2 (1%)	18	10
All	All	533/662 (80%)	518 (97%)	11 (2%)	4 (1%)	16	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2102	ASP
1	A	2102	ASP
1	B	1972	SER
1	A	1972	SER

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	239/291 (82%)	225 (94%)	14 (6%)	18	10
1	B	240/291 (82%)	221 (92%)	19 (8%)	11	5
All	All	479/582 (82%)	446 (93%)	33 (7%)	14	8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1937	LEU
1	A	1963	THR
1	A	1968	LEU
1	A	1975	ILE
1	A	1983	LYS
1	A	2003	LYS
1	A	2054	VAL
1	A	2131	GLU
1	A	2134	MET
1	A	2171	LEU
1	A	2176	THR
1	A	2179	ARG
1	A	2201	GLU
1	A	2223	LEU
1	B	1937	LEU
1	B	1951	LEU
1	B	1963	THR
1	B	1965	VAL
1	B	1968	LEU
1	B	1975	ILE
1	B	1983	LYS
1	B	2003	LYS
1	B	2054	VAL
1	B	2123	LEU
1	B	2131	GLU
1	B	2134	MET
1	B	2171	LEU

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Mol	Chain	Res	Type
1	B	2176	THR
1	B	2179	ARG
1	B	2188	ASP
1	B	2201	GLU
1	B	2223	LEU
1	B	2226	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2012	GLN
1	A	2022	GLN
1	A	2074	HIS
1	A	2165	HIS
1	A	2167	ASN
1	A	2185	ASN
1	A	2192	ASN
1	A	2212	GLN
1	A	2216	GLN
1	B	2008	ASN
1	B	2012	GLN
1	B	2167	ASN
1	B	2175	GLN
1	B	2185	ASN
1	B	2192	ASN
1	B	2212	GLN
1	B	2216	GLN
1	B	2224	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	AWJ	A	2301	-	34,36,36	0.53	0	37,53,53	0.92	3 (8%)
2	AWJ	B	2301	-	34,36,36	0.58	0	37,53,53	0.93	2 (5%)

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	AWJ	A	2301	-	-	0/18/25/25	0/4/4/4
2	AWJ	B	2301	-	-	1/18/25/25	0/4/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2301	AWJ	O7-C9-C11	3.59	111.73	105.51
2	A	2301	AWJ	C4-C5-C23	2.75	122.80	120.51
2	A	2301	AWJ	C5-C23-C24	2.31	133.95	130.81
2	A	2301	AWJ	O7-C9-C11	2.17	109.28	105.51
2	B	2301	AWJ	C4-C5-C23	2.07	122.24	120.51

There are no chirality outliers.

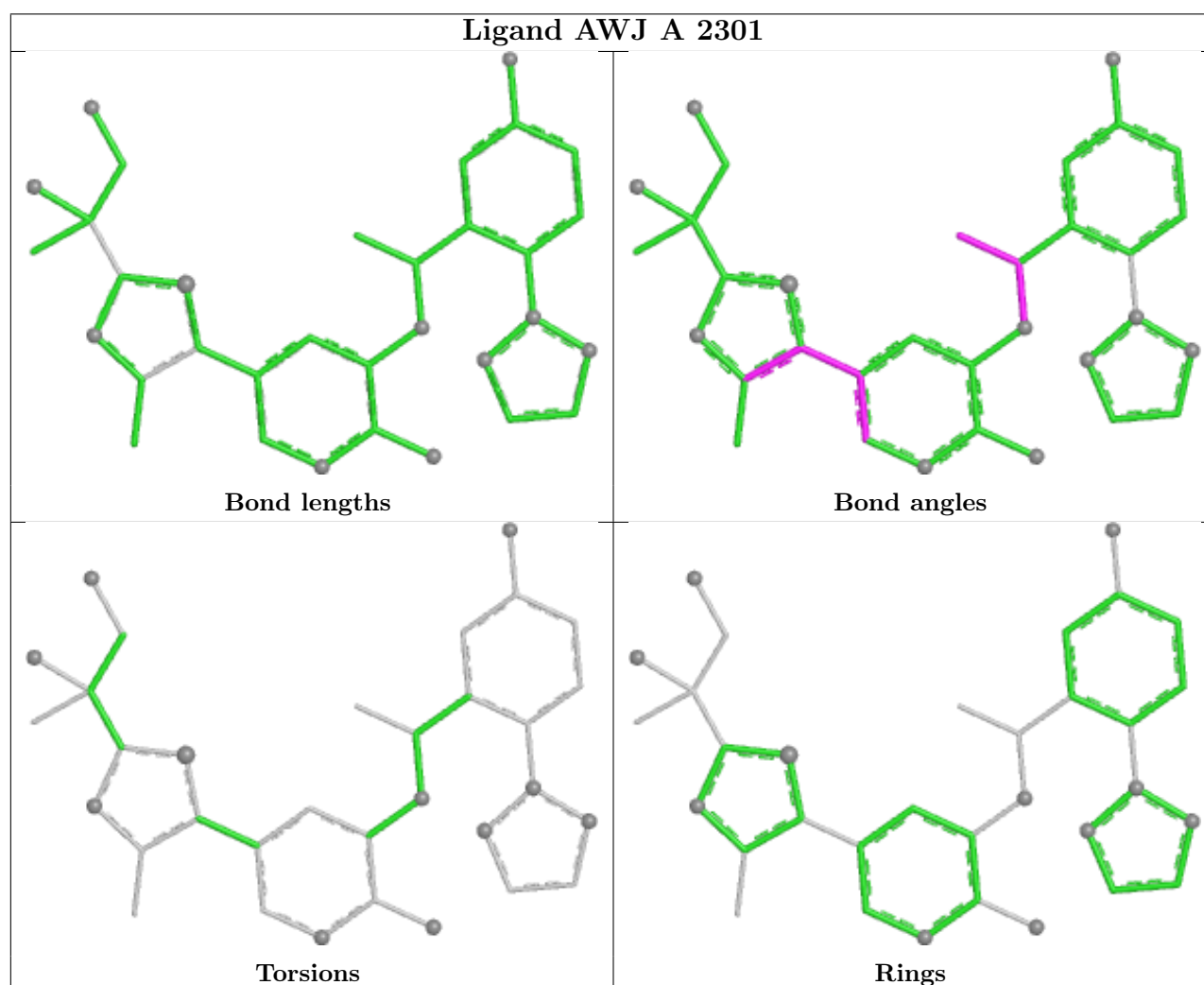
All (1) torsion outliers are listed below:

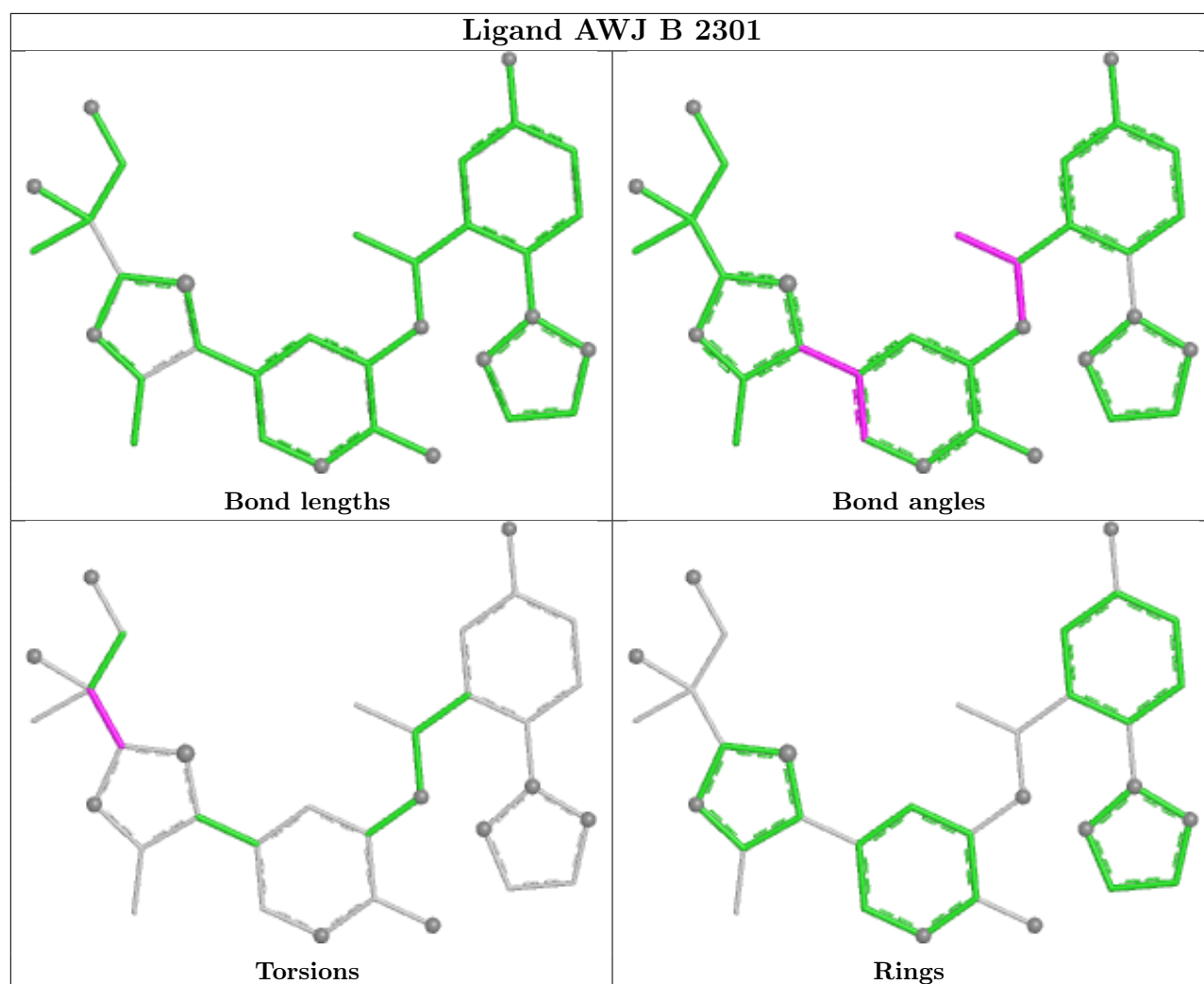
Mol	Chain	Res	Type	Atoms
2	B	2301	AWJ	S27-C26-C29-C32

There are no ring outliers.

No monomer is involved in short contacts.

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	270/331 (81%)	0.50	17 (6%) 26 26	22, 36, 55, 71	0
1	B	271/331 (81%)	0.70	26 (9%) 13 13	24, 40, 62, 83	0
All	All	541/662 (81%)	0.60	43 (7%) 18 19	22, 38, 60, 83	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2221	PHE	4.4
1	B	2226	ILE	4.3
1	A	2222	PHE	4.2
1	A	1956	PHE	4.1
1	B	2222	PHE	3.9
1	A	2123	LEU	3.9
1	B	1956	PHE	3.8
1	A	2046	PHE	3.8
1	B	2174	VAL	3.6
1	B	2134	MET	3.6
1	A	2223	LEU	3.3
1	B	2223	LEU	3.1
1	A	2102	ASP	2.9
1	B	1953	SER	2.9
1	A	1953	SER	2.7
1	B	2171	LEU	2.7
1	A	2221	PHE	2.6
1	B	2176	THR	2.6
1	B	2047	TYR	2.5
1	A	2134	MET	2.5
1	B	2191	TRP	2.5
1	A	1968	LEU	2.5
1	B	2140	THR	2.5
1	A	1955	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1955	ALA	2.5
1	B	2044	ALA	2.4
1	B	2164	ALA	2.4
1	B	2204	GLN	2.4
1	B	1949	LEU	2.3
1	B	2046	PHE	2.3
1	B	2177	GLY	2.3
1	B	2224	ASN	2.3
1	A	2164	ALA	2.3
1	A	2124	PRO	2.3
1	B	1968	LEU	2.3
1	A	2103	PHE	2.2
1	B	2133	LEU	2.2
1	A	2225	SER	2.2
1	B	2209	HIS	2.1
1	B	2168	LEU	2.1
1	A	2101	GLY	2.1
1	B	2175	GLN	2.0
1	A	1954	GLY	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.

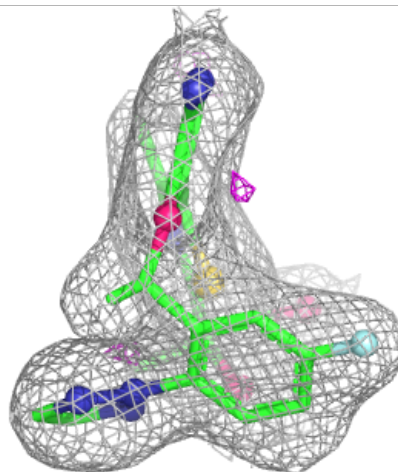
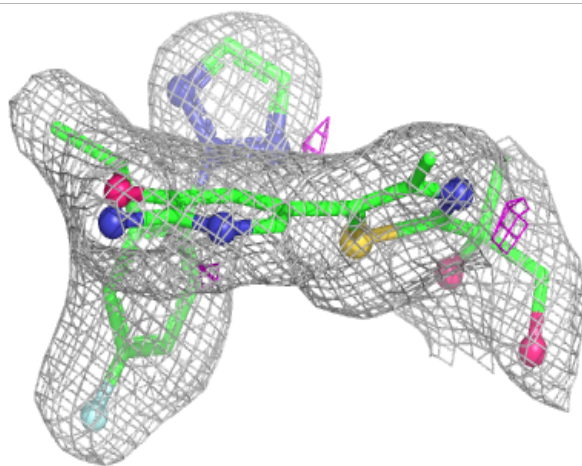
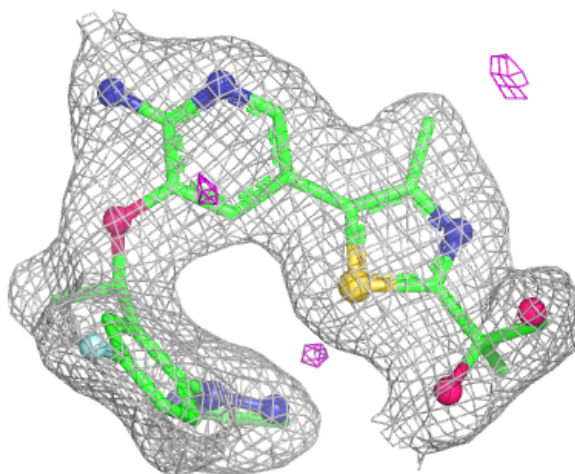
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AWJ	A	2301	33/33	0.94	0.07	25,29,31,31	0
2	AWJ	B	2301	33/33	0.94	0.07	26,29,31,32	0

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.

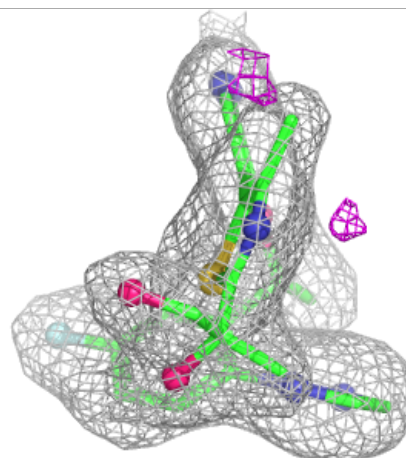
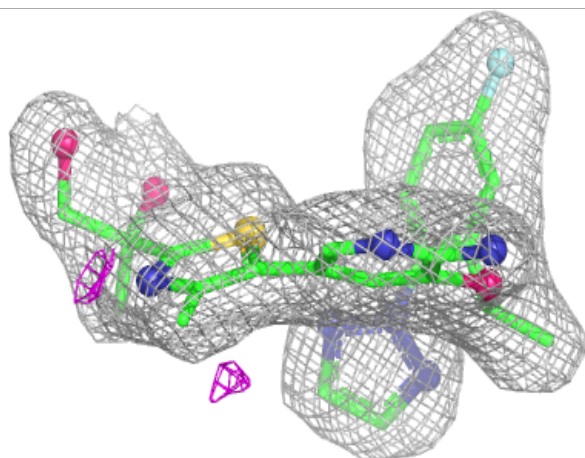
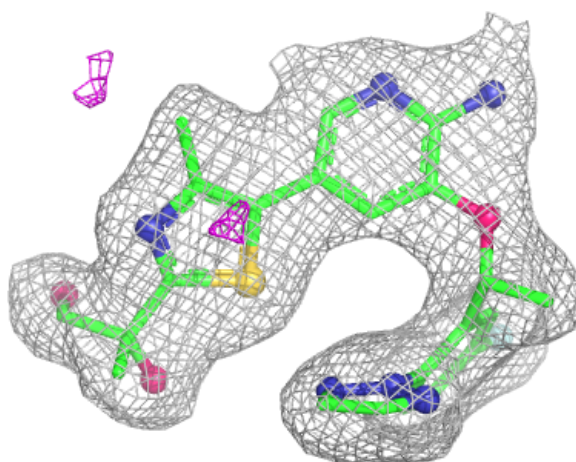
Electron density around AWJ A 2301:

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



Electron density around AWJ B 2301:

$2mF_o-DF_c$ (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.