



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 04:51 PM EDT

PDB ID : 6GL9  
Title : Crystal structure of JAK3 in complex with Compound 10 (FM475)  
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Bountra, C.; Laufer, S.A.; Knapp, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2018-05-23  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

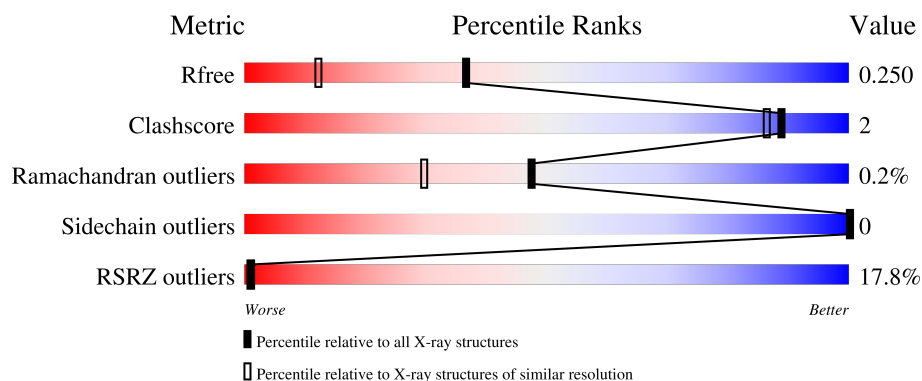
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	294	<div> <div>19%</div> <div>94%</div> <div>6% .</div> </div>
1	B	294	<div> <div>17%</div> <div>94%</div> <div>5% ..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5182 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.

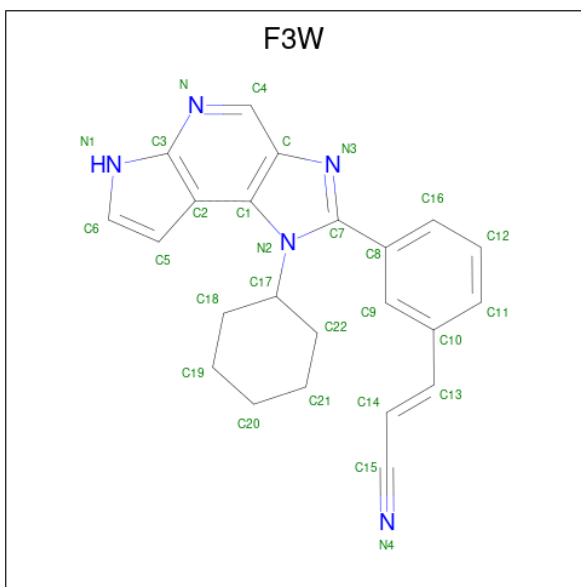
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	9	0
			2382	1518	419	431	14			
1	B	291	Total	C	N	O	S	0	5	0
			2339	1491	410	424	14			

There are 10 discrepancies between the modelled and reference sequences:

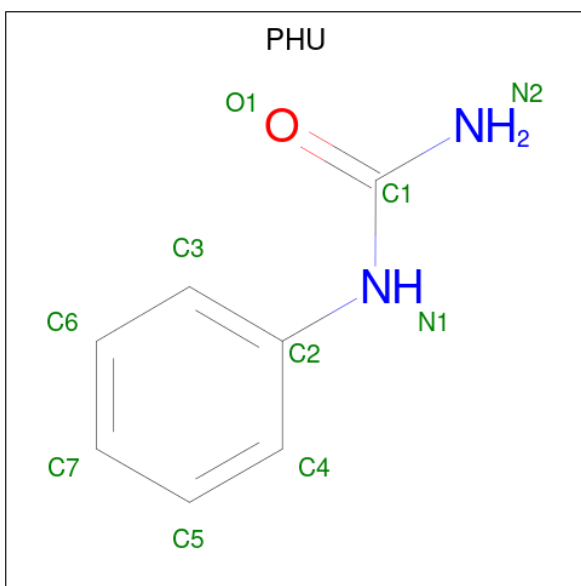
Chain	Residue	Modelled	Actual	Comment	Reference
A	810	SER	-	expression tag	UNP P52333
A	811	MET	-	expression tag	UNP P52333
A	949	ALA	ASP	conflict	UNP P52333
A	1040	SER	CYS	conflict	UNP P52333
A	1048	SER	CYS	conflict	UNP P52333
B	810	SER	-	expression tag	UNP P52333
B	811	MET	-	expression tag	UNP P52333
B	949	ALA	ASP	conflict	UNP P52333
B	1040	SER	CYS	conflict	UNP P52333
B	1048	SER	CYS	conflict	UNP P52333

- Molecule 2 is ( {E} )-3-[3-(3-cyclohexyl-3,5,8,10-tetrazatricyclo[7.3.0.0<sup>2,6</sup> ]dodeca-1(9),2(6),4,7,11-pentaen-4-yl)phenyl]prop-2-enenitrile (three-letter code: F3W) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			28	23	5		
2	B	1	Total	C	N	0	0
			28	23	5		

- Molecule 3 is 1-phenylurea (three-letter code: PHU) (formula:  $C_7H_8N_2O$ ).



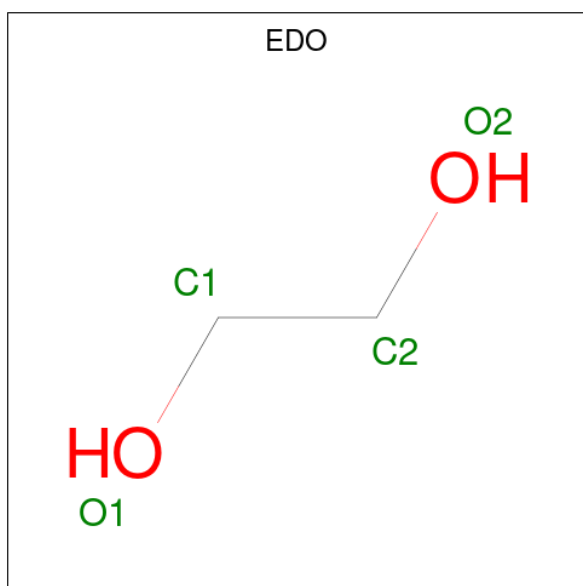
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	2	1		
3	B	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

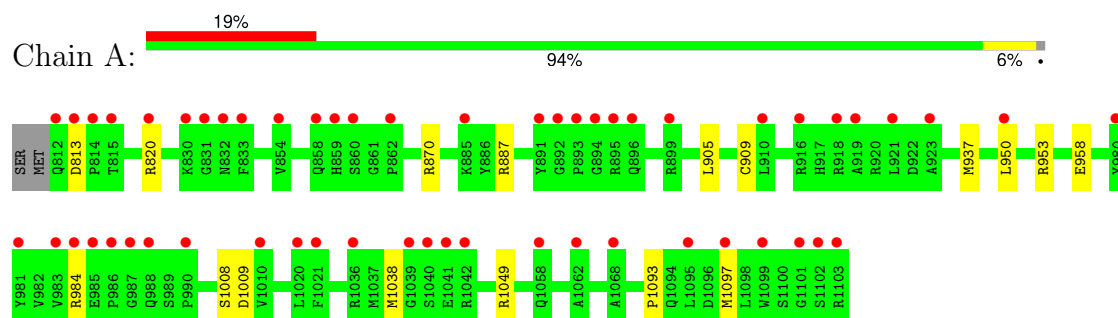
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	155	Total O 155 155	0	0
6	B	166	Total O 166 166	0	0

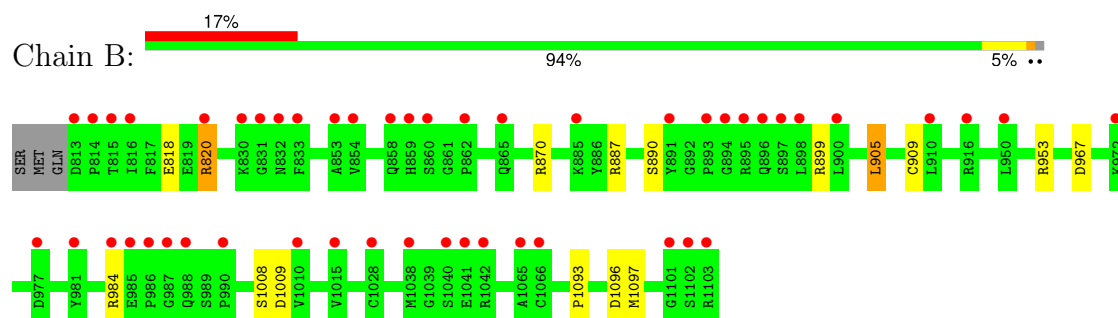
### 3 Residue-property plots [i](#)

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: Tyrosine-protein kinase JAK3



#### • Molecule 1: Tyrosine-protein kinase JAK3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.02Å 50.42Å 61.59Å 91.93° 90.03° 92.80°	Depositor
Resolution (Å)	19.81 – 1.70 19.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.81-1.70) 97.5 (19.71-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.207 , 0.244 0.216 , 0.250	Depositor DCC
$R_{free}$ test set	2503 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, PHU, F3W, 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	A	0.77	0/2463	0.87	5/3328 (0.2%)
1	B	0.82	0/2408	0.95	10/3257 (0.3%)
All	All	0.80	0/4871	0.91	15/6585 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	905[A]	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	B	905[B]	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	B	820	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	B	870	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	953	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	953	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	B	984	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	1009	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	1009	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	870	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	820	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	887	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	887	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	887	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	887	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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	2382	0	2386	11	0
1	B	2339	0	2330	8	0
2	A	28	0	0	2	0
2	B	28	0	0	2	0
3	A	10	0	8	0	0
3	B	10	0	8	0	0
4	A	6	0	8	1	0
4	B	6	0	8	1	0
5	A	28	0	42	0	0
5	B	24	0	36	0	0
6	A	155	0	0	1	0
6	B	166	0	0	0	0
All	All	5182	0	4826	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.

All (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:B:909:CYS:SG	2:B:1201:F3W:C13	2.79	0.71
1:A:984:ARG:NH2	1:B:1096:ASP:OD2	2.26	0.68
1:A:909:CYS:SG	2:A:1201:F3W:C13	2.85	0.65
1:A:1038:MET:SD	1:A:1049:ARG:HG2	2.41	0.61
1:A:905[A]:LEU:HD21	1:A:958:GLU:OE1	2.03	0.57
1:B:818:GLU:HG3	1:B:820:ARG:HG2	1.90	0.54
1:B:890[B]:SER:OG	1:B:899:ARG:HB2	2.07	0.54
1:B:909:CYS:SG	2:B:1201:F3W:C14	2.98	0.52
1:A:1008:SER:C	4:A:1203:GOL:H32	2.31	0.52
1:B:1008:SER:C	4:B:1203:GOL:H32	2.33	0.49
1:A:909:CYS:SG	2:A:1201:F3W:C14	3.02	0.48
1:A:1093:PRO:O	1:A:1097:MET:HG2	2.17	0.45
1:B:1093:PRO:O	1:B:1097:MET:HG2	2.18	0.43
1:A:870[B]:ARG:HD3	6:A:1351:HOH:O	2.19	0.42
1:B:905[A]:LEU:HD23	1:B:905[A]:LEU:HA	1.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:MET:CE	1:A:950[B]:LEU:HD11	2.49	0.41
1:A:813:ASP:OD1	1:A:813:ASP:N	2.54	0.41

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	A	299/294 (102%)	290 (97%)	9 (3%)	0	100	100
1	B	294/294 (100%)	285 (97%)	8 (3%)	1 (0%)	41	24
All	All	593/588 (101%)	575 (97%)	17 (3%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	967	ASP

### 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	A	261/256 (102%)	261 (100%)	0	100	100
1	B	255/256 (100%)	255 (100%)	0	100	100
All	All	516/512 (101%)	516 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

19 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
5	EDO	B	1207	-	3,3,3	0.39	0	2,2,2	0.38	0
5	EDO	A	1207	-	3,3,3	0.35	0	2,2,2	0.53	0
4	GOL	B	1203	-	5,5,5	0.63	0	5,5,5	0.89	0
5	EDO	A	1209	-	3,3,3	0.60	0	2,2,2	0.31	0
5	EDO	A	1208	-	3,3,3	0.27	0	2,2,2	0.65	0
5	EDO	B	1204	-	3,3,3	0.51	0	2,2,2	0.31	0
2	F3W	B	1201	-	25,32,32	0.81	1 (4%)	30,45,45	1.68	4 (13%)
5	EDO	A	1204	-	3,3,3	0.42	0	2,2,2	0.57	0
5	EDO	B	1206	-	3,3,3	0.34	0	2,2,2	0.44	0
2	F3W	A	1201	-	25,32,32	0.72	1 (4%)	30,45,45	1.69	4 (13%)
5	EDO	A	1210	-	3,3,3	0.50	0	2,2,2	0.43	0
5	EDO	B	1208	-	3,3,3	0.40	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	1209	-	3,3,3	0.42	0	2,2,2	0.24	0
5	EDO	B	1205	-	3,3,3	0.41	0	2,2,2	0.12	0
4	GOL	A	1203	-	5,5,5	0.54	0	5,5,5	1.19	1 (20%)
3	PHU	A	1202	-	10,10,10	0.61	0	12,12,12	0.46	0
5	EDO	A	1205	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	A	1206	-	3,3,3	0.26	0	2,2,2	0.74	0
3	PHU	B	1202	-	10,10,10	0.36	0	12,12,12	0.24	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
5	EDO	B	1207	-	-	1/1/1/1	-
5	EDO	A	1207	-	-	0/1/1/1	-
4	GOL	B	1203	-	-	2/4/4/4	-
5	EDO	A	1209	-	-	0/1/1/1	-
5	EDO	A	1208	-	-	0/1/1/1	-
5	EDO	B	1204	-	-	0/1/1/1	-
2	F3W	B	1201	-	-	0/7/20/20	0/5/5/5
5	EDO	A	1204	-	-	1/1/1/1	-
5	EDO	B	1206	-	-	0/1/1/1	-
2	F3W	A	1201	-	-	0/7/20/20	0/5/5/5
5	EDO	A	1210	-	-	0/1/1/1	-
5	EDO	B	1208	-	-	1/1/1/1	-
5	EDO	B	1209	-	-	1/1/1/1	-
5	EDO	B	1205	-	-	0/1/1/1	-
4	GOL	A	1203	-	-	3/4/4/4	-
3	PHU	A	1202	-	-	0/4/4/4	0/1/1/1
5	EDO	A	1205	-	-	1/1/1/1	-
5	EDO	A	1206	-	-	0/1/1/1	-
3	PHU	B	1202	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	F3W	C4-N	3.10	1.34	1.30
2	A	1201	F3W	C4-N	2.78	1.33	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	F3W	C2-C1-C	-5.19	117.25	120.03
2	A	1201	F3W	C2-C1-C	-4.92	117.40	120.03
2	B	1201	F3W	C2-C1-N2	4.72	139.42	130.91
2	A	1201	F3W	C2-C1-N2	4.41	138.87	130.91
2	A	1201	F3W	C4-N-C3	-4.28	114.80	117.40
2	B	1201	F3W	C4-N-C3	-3.52	115.26	117.40
2	B	1201	F3W	C16-C8-C7	-2.21	115.61	120.60
2	A	1201	F3W	C18-C17-C22	2.11	114.21	110.19
4	A	1203	GOL	O2-C2-C3	-2.02	100.83	109.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	GOL	C1-C2-C3-O3
4	B	1203	GOL	C1-C2-C3-O3
4	A	1203	GOL	O2-C2-C3-O3
4	B	1203	GOL	O2-C2-C3-O3
5	B	1207	EDO	O1-C1-C2-O2
5	A	1204	EDO	O1-C1-C2-O2
5	B	1209	EDO	O1-C1-C2-O2
5	B	1208	EDO	O1-C1-C2-O2
5	A	1205	EDO	O1-C1-C2-O2
4	A	1203	GOL	O1-C1-C2-O2

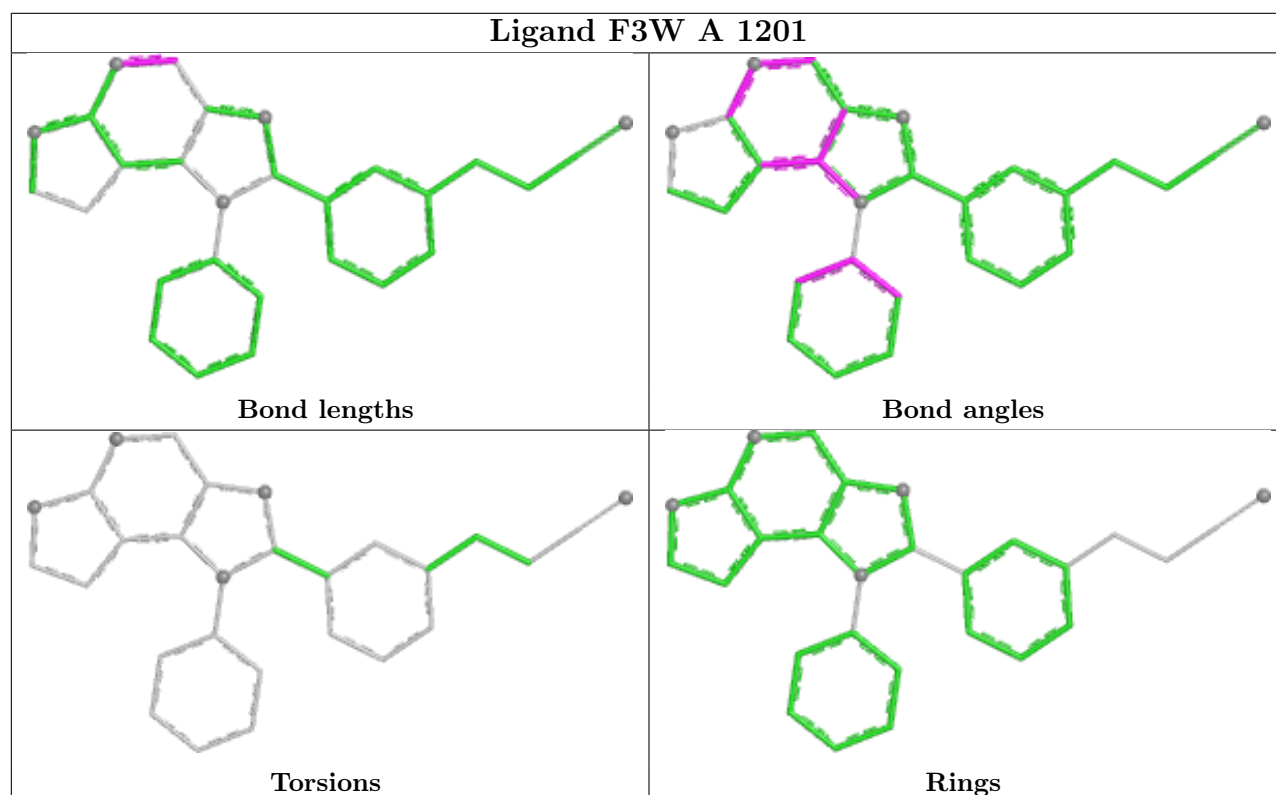
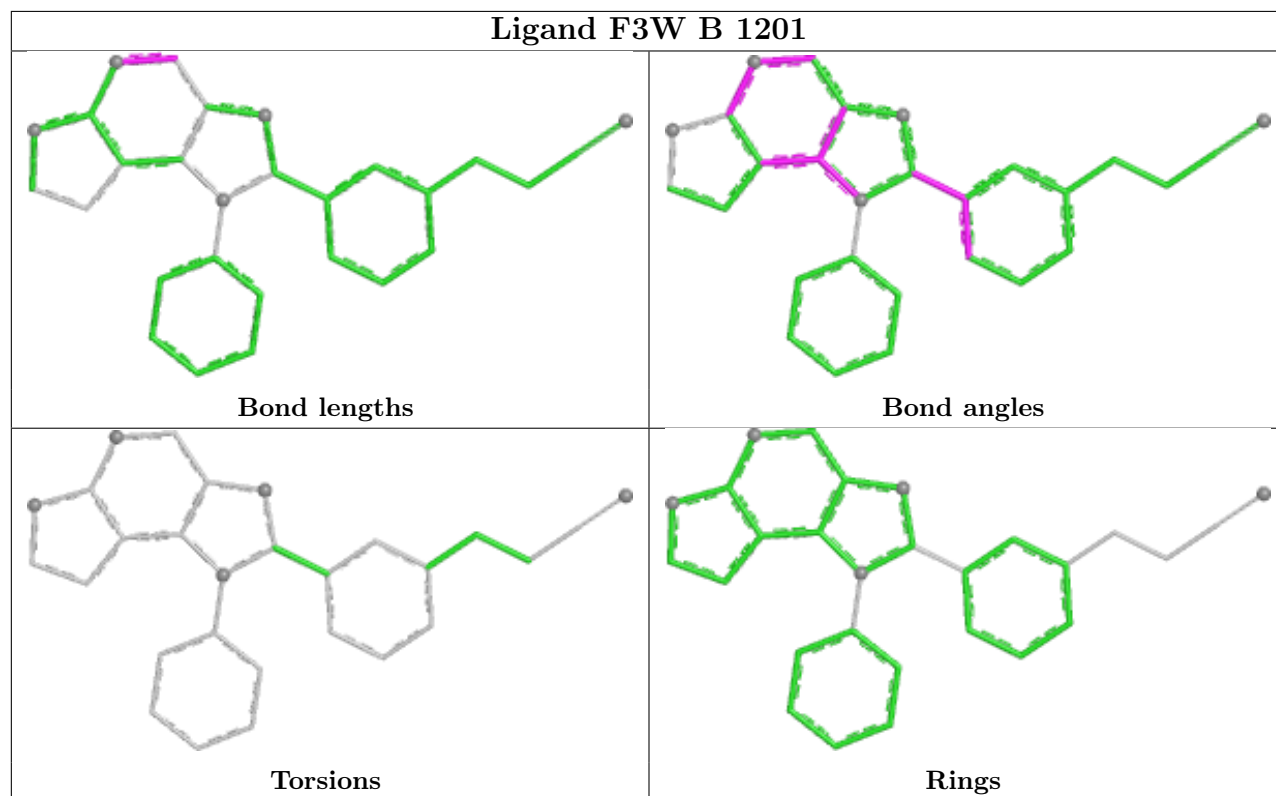
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1203	GOL	1	0
2	B	1201	F3W	2	0
2	A	1201	F3W	2	0
4	A	1203	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/294 (99%)	1.39	55 (18%)  	11, 22, 51, 79	0
1	B	291/294 (98%)	1.22	49 (16%)  	12, 22, 45, 73	0
All	All	583/588 (99%)	1.30	104 (17%)  	11, 22, 46, 79	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	986	PRO	13.2
1	B	986	PRO	11.8
1	B	987	GLY	10.7
1	A	812	GLN	10.1
1	A	1039	GLY	9.0
1	A	987	GLY	8.9
1	A	833	PHE	8.0
1	B	814	PRO	7.9
1	B	833	PHE	7.8
1	A	814	PRO	7.6
1	A	894	GLY	7.5
1	B	832	ASN	7.4
1	A	919	ALA	6.4
1	B	859	HIS	6.1
1	A	1040	SER	6.1
1	A	813	ASP	6.0
1	B	896	GLN	5.8
1	A	984	ARG	5.4
1	A	893	PRO	5.4
1	B	985	GLU	5.4
1	A	950[A]	LEU	5.4
1	A	895	ARG	5.3
1	B	950[A]	LEU	5.3
1	A	859	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	813	ASP	4.8
1	B	895	ARG	4.5
1	B	1103	ARG	4.5
1	A	985	GLU	4.4
1	B	860	SER	4.4
1	A	896	GLN	4.3
1	A	832	ASN	4.2
1	A	815	THR	4.2
1	A	981	TYR	4.1
1	B	862	PRO	4.1
1	B	1065	ALA	3.9
1	A	1042	ARG	3.8
1	A	860	SER	3.8
1	B	815	THR	3.7
1	B	897	SER	3.7
1	B	891	TYR	3.5
1	A	990	PRO	3.5
1	A	892	GLY	3.4
1	A	1103	ARG	3.4
1	A	988	GLN	3.4
1	B	1042	ARG	3.3
1	B	831	GLY	3.2
1	B	981	TYR	3.1
1	A	862	PRO	3.0
1	B	893	PRO	3.0
1	B	853	ALA	2.9
1	A	1036	ARG	2.9
1	B	1041	GLU	2.9
1	B	900	LEU	2.8
1	A	983	VAL	2.8
1	B	1038	MET	2.8
1	B	854	VAL	2.8
1	A	885	LYS	2.8
1	B	1102	SER	2.7
1	B	830	LYS	2.7
1	B	984	ARG	2.7
1	A	916	ARG	2.7
1	B	820	ARG	2.7
1	A	910	LEU	2.7
1	B	1040	SER	2.7
1	A	899	ARG	2.6
1	A	858	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	918	ARG	2.6
1	A	891	TYR	2.6
1	B	885	LYS	2.6
1	A	921	LEU	2.6
1	A	923	ALA	2.6
1	B	865	GLN	2.5
1	B	988	GLN	2.5
1	B	1101	GLY	2.5
1	A	1010	VAL	2.5
1	B	990	PRO	2.4
1	B	1010	VAL	2.4
1	A	1021	PHE	2.4
1	B	910	LEU	2.4
1	A	980	TYR	2.4
1	A	1058	GLN	2.4
1	A	1097	MET	2.4
1	A	1062	ALA	2.4
1	B	816	ILE	2.3
1	A	1102	SER	2.3
1	B	1015	VAL	2.3
1	A	1020	LEU	2.3
1	A	1095	LEU	2.3
1	A	1068	ALA	2.2
1	A	1101	GLY	2.2
1	B	894	GLY	2.2
1	A	830	LYS	2.2
1	B	898	LEU	2.2
1	A	1099	TRP	2.2
1	B	1028	CYS	2.2
1	A	854	VAL	2.2
1	A	831	GLY	2.2
1	B	977	ASP	2.2
1	B	916	ARG	2.1
1	B	1066	CYS	2.1
1	B	972[A]	LYS	2.1
1	A	820	ARG	2.1
1	B	858	GLN	2.1
1	A	1041	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates

There are no monosaccharides in this entry.

## 6.4 Ligands

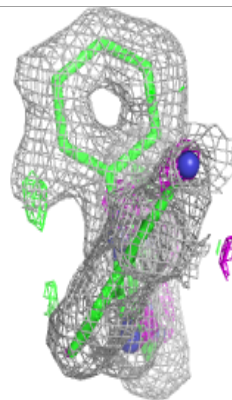
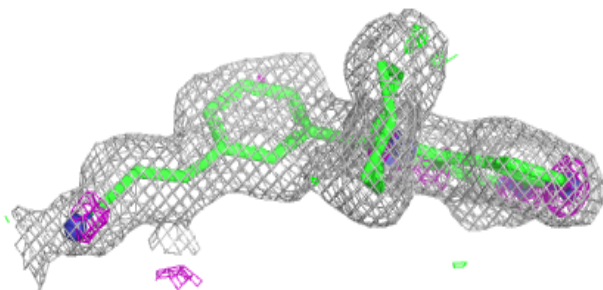
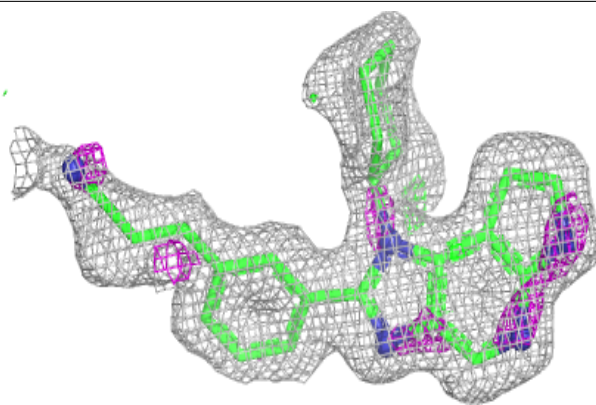
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	EDO	B	1204	4/4	0.55	0.22	37,39,40,41	0
5	EDO	A	1207	4/4	0.61	0.21	40,41,43,43	0
5	EDO	B	1207	4/4	0.61	0.22	45,46,46,51	0
5	EDO	A	1204	4/4	0.62	0.19	33,36,37,43	0
5	EDO	A	1205	4/4	0.66	0.20	40,41,42,43	0
5	EDO	A	1209	4/4	0.67	0.18	27,28,28,29	0
5	EDO	B	1206	4/4	0.71	0.17	41,41,43,43	0
4	GOL	A	1203	6/6	0.74	0.26	21,23,25,27	0
5	EDO	A	1208	4/4	0.74	0.25	39,39,39,41	0
5	EDO	A	1210	4/4	0.77	0.17	29,30,30,31	0
5	EDO	A	1206	4/4	0.78	0.18	29,30,30,33	0
5	EDO	B	1208	4/4	0.78	0.14	28,29,29,30	0
4	GOL	B	1203	6/6	0.79	0.21	21,21,25,26	0
5	EDO	B	1205	4/4	0.84	0.13	33,33,34,38	0
2	F3W	A	1201	28/28	0.89	0.12	12,14,27,29	0
2	F3W	B	1201	28/28	0.90	0.13	12,13,26,30	0
3	PHU	A	1202	10/10	0.90	0.16	14,17,19,19	0
5	EDO	B	1209	4/4	0.90	0.14	42,43,43,44	0
3	PHU	B	1202	10/10	0.91	0.18	12,14,16,16	0

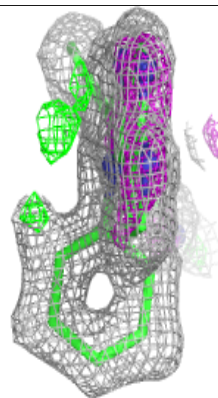
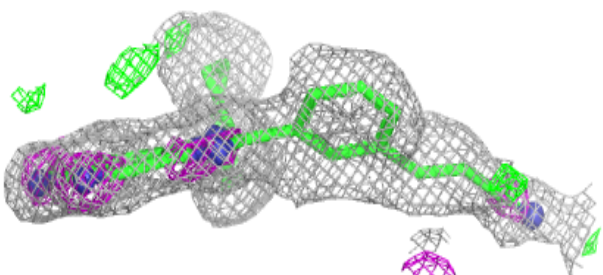
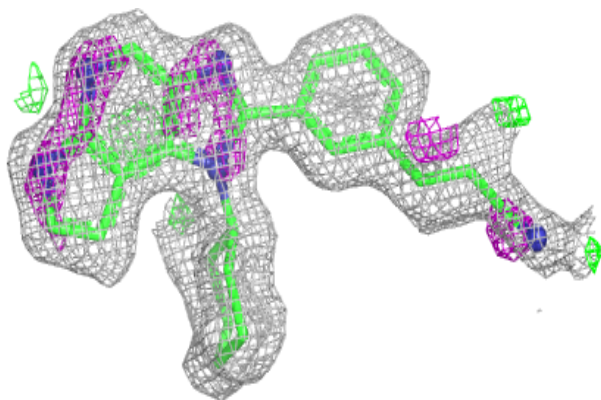
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around F3W A 1201:**

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

**Electron density around F3W B 1201:**

$2mF_o-DF_c$  (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.