Full wwPDB X-ray Structure Validation Report (i)

Oct 28, 2024 – 11:19 am GMT

PDB ID	:	6SM8
Title	:	Human jak1 kinase domain in complex with inhibitor
Authors	:	Read, J.A.; Steuber, H.
Deposited on	:	2019-08-21
Resolution	:	1.85 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 (i) 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 (i)) were used in the production of this report:

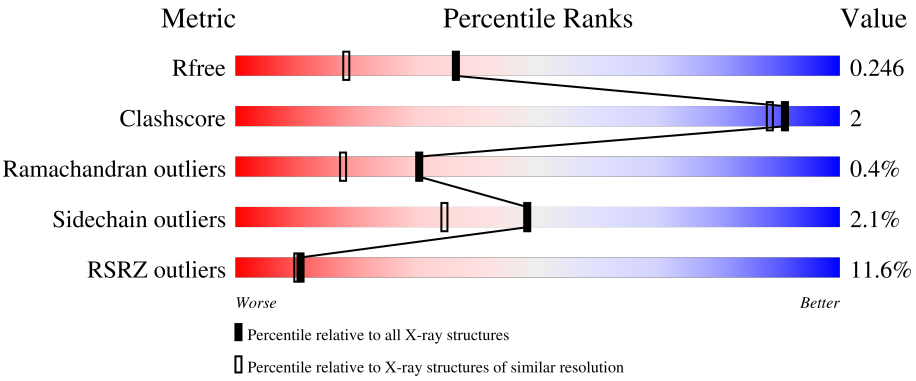
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 <=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	302	9% 94%
2	B	301	13% 90% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5173 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 JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	297	2448	1554	416	460	2	16	90	5	0

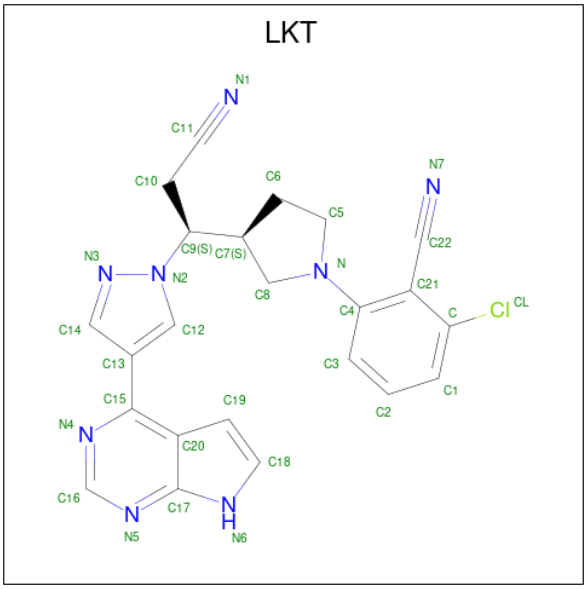
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	expression tag	UNP P23458

- Molecule 2 is a protein called Tyrosine-protein kinase JAK1.

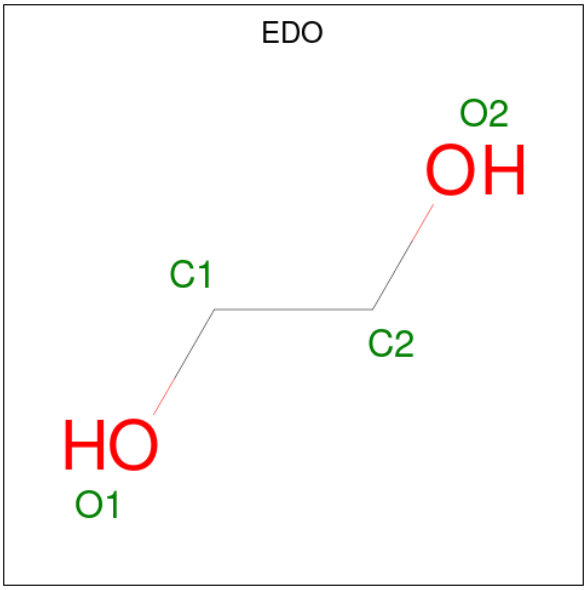
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	284	2398	1525	410	445	2	16	37	11	0

- Molecule 3 is 2-chloranyl-6-[(3 {S})-3-[(1 {S})-2-cyano-1-[4-(7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl)pyrazol-1-yl]ethyl]pyrrolidin-1-yl]benzenecarbonitrile (three-letter code: LKT) (formula: $C_{23}H_{19}ClN_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			32	23	1	8		
3	B	1	Total	C	Cl	N	0	0
			32	23	1	8		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

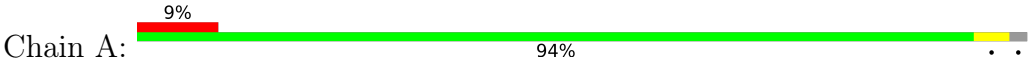
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	142	Total	O	0	1
			143	143		

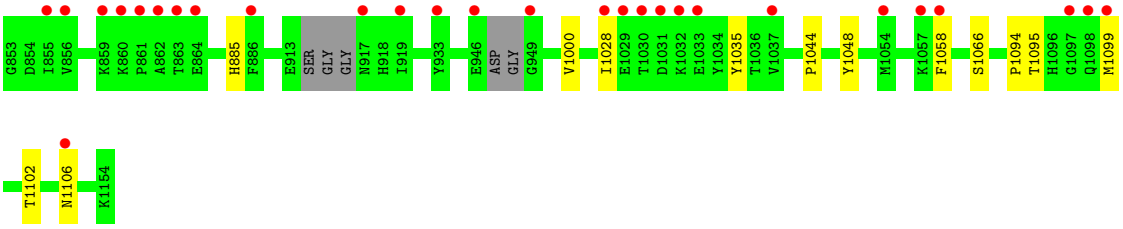
3 Residue-property plots (i)

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 JAK1

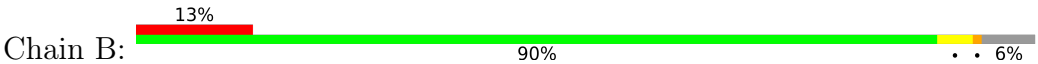
Chain A:

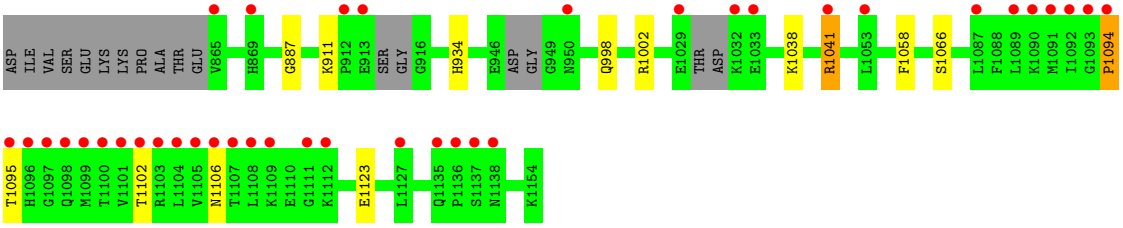




• Molecule 2: Tyrosine-protein kinase JAK1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.19Å 174.06Å 44.96Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	35.48 – 1.85 35.48 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.48-1.85) 99.8 (35.48-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 1.86Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.212 , 0.241 0.213 , 0.246	Depositor DCC
R_{free} test set	2481 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, PTR, LKT

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	0.49	0/2465	0.62	0/3317
2	B	0.52	0/2412	0.62	0/3241
All	All	0.51	0/4877	0.62	0/6558

There are no bond length outliers.

There are no bond angle outliers.

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	2448	0	2428	6	0
2	B	2398	0	2386	8	0
3	A	32	0	0	1	0
3	B	32	0	0	1	0
4	B	8	0	12	3	0
5	A	112	0	0	1	0
5	B	143	0	0	0	0
All	All	5173	0	4826	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:934:HIS:HE2	4:B:1203:EDO:H22	1.62	0.64
3:A:1201:LKT:C5	3:A:1201:LKT:C22	2.79	0.60
3:B:1201:LKT:C5	3:B:1201:LKT:C22	2.80	0.59
1:A:1048:TYR:CE2	1:A:1058:PHE:HZ	2.25	0.55
2:B:934:HIS:HE2	4:B:1203:EDO:C2	2.19	0.55
2:B:934:HIS:NE2	4:B:1203:EDO:H22	2.24	0.52
2:B:1002[B]:ARG:HA	2:B:1058:PHE:CZ	2.46	0.51
1:A:1048:TYR:CZ	1:A:1058:PHE:HZ	2.29	0.50
1:A:1095:THR:O	2:B:1041:ARG:HG2	2.11	0.50
1:A:1000:VAL:HG13	1:A:1028:ILE:HD11	2.00	0.43
2:B:1002[A]:ARG:HA	2:B:1058:PHE:CZ	2.53	0.43
1:A:885:HIS:HE1	5:A:1307:HOH:O	2.02	0.42
2:B:1094:PRO:HB2	2:B:1095:THR:H	1.69	0.41
1:A:1044:PRO:HD2	1:A:1048:TYR:CZ	2.57	0.40
2:B:887:GLY:O	2:B:911:LYS:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/302 (97%)	289 (98%)	4 (1%)	1 (0%)	37	25
2	B	285/301 (95%)	279 (98%)	5 (2%)	1 (0%)	30	18
All	All	579/603 (96%)	568 (98%)	9 (2%)	2 (0%)	30	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1094	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1094	PRO

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	270/267 (101%)	264 (98%)	6 (2%)	47	32
2	B	264/267 (99%)	256 (97%)	8 (3%)	36	21
All	All	534/534 (100%)	520 (97%)	14 (3%)	48	26

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1066[A]	SER
1	A	1066[B]	SER
1	A	1099[A]	MET
1	A	1099[B]	MET
1	A	1102	THR
1	A	1106	ASN
2	B	998	GLN
2	B	1038	LYS
2	B	1041	ARG
2	B	1066[A]	SER
2	B	1066[B]	SER
2	B	1102	THR
2	B	1106	ASN
2	B	1123	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	885	HIS
2	B	998	GLN
2	B	1106	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	PTR	A	1034	1	15,16,17	0.47	0	19,22,24	0.58	0
2	PTR	B	1035	2	15,16,17	0.51	0	19,22,24	0.96	0
1	PTR	A	1035	1	15,16,17	0.57	0	19,22,24	0.98	1 (5%)
2	PTR	B	1034	2	15,16,17	0.45	0	19,22,24	0.53	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
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1
2	PTR	B	1035	2	-	0/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/10/11/13	0/1/1/1
2	PTR	B	1034	2	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1035	PTR	O3P-P-OH	2.04	111.62	105.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	EDO	B	1203	-	3,3,3	0.36	0	2,2,2	0.45	0
3	LKT	B	1201	-	32,36,36	1.53	3 (9%)	30,51,51	1.38	3 (10%)
3	LKT	A	1201	-	32,36,36	1.71	3 (9%)	30,51,51	1.38	5 (16%)
4	EDO	B	1202	-	3,3,3	0.66	0	2,2,2	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1203	-	-	1/1/1/1	-
3	LKT	B	1201	-	-	0/12/30/30	0/5/5/5
3	LKT	A	1201	-	-	1/12/30/30	0/5/5/5
4	EDO	B	1202	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	LKT	C4-C21	8.28	1.50	1.41
3	B	1201	LKT	C4-C21	6.47	1.48	1.41
3	B	1201	LKT	C13-C15	-3.73	1.44	1.49
3	A	1201	LKT	C13-C15	-2.96	1.45	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	LKT	C15-N4	2.22	1.35	1.32
3	A	1201	LKT	C15-N4	2.13	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1201	LKT	C20-C15-N4	-4.33	120.19	123.04
3	A	1201	LKT	C12-N2-C9	3.94	128.97	125.48
3	B	1201	LKT	C12-N2-C9	3.80	128.85	125.48
3	A	1201	LKT	C20-C15-N4	-3.69	120.61	123.04
3	B	1201	LKT	C5-N-C4	2.68	129.17	121.48
3	A	1201	LKT	C13-C15-N4	2.41	118.95	115.32
3	A	1201	LKT	C4-C21-C22	2.29	123.43	119.53
3	A	1201	LKT	C5-N-C4	2.09	127.48	121.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1202	EDO	O1-C1-C2-O2
4	B	1203	EDO	O1-C1-C2-O2
3	A	1201	LKT	C4-C21-C22-N7

There are no ring outliers.

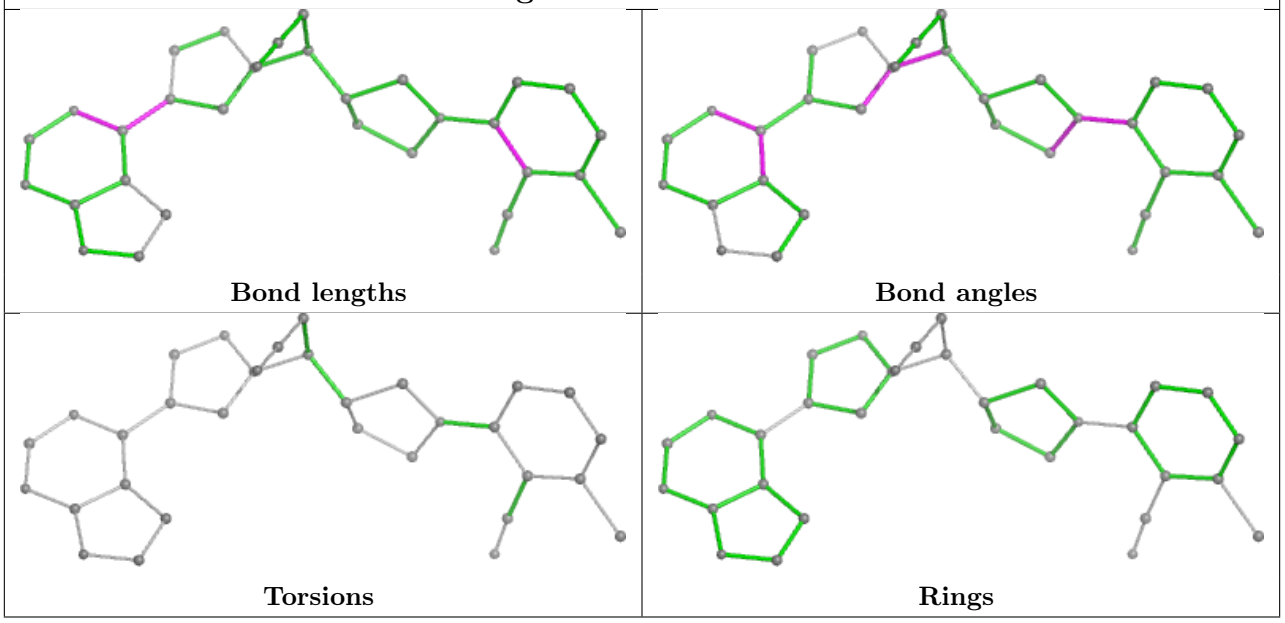
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1203	EDO	3	0
3	B	1201	LKT	1	0
3	A	1201	LKT	1	0

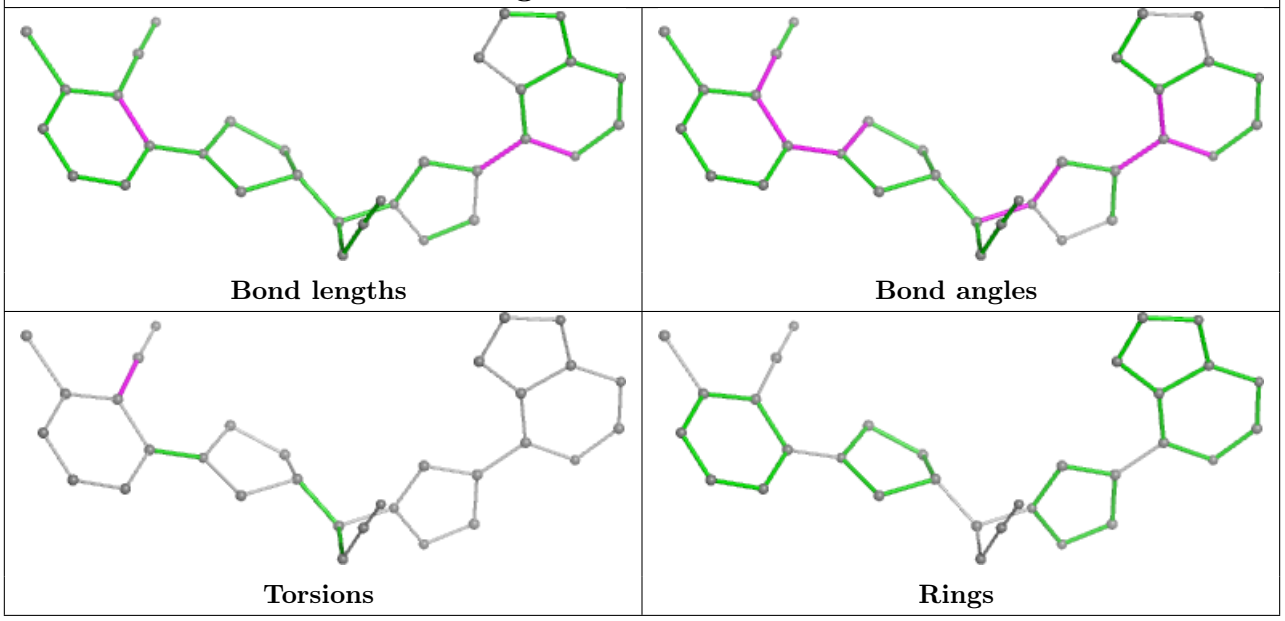
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand LKT B 1201



Ligand LKT A 1201



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^{th} 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	295/302 (97%)	0.47	28 (9%)	15	15	14, 38, 79, 96	34 (11%)
2	B	282/301 (93%)	0.48	39 (13%)	8	7	8, 37, 96, 155	22 (7%)
All	All	577/603 (95%)	0.48	67 (11%)	11	10	8, 37, 86, 155	56 (9%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1099[A]	MET	7.1
2	B	1098	GLN	6.5
2	B	1092	ILE	5.8
1	A	1058	PHE	5.2
2	B	1097	GLY	4.9
2	B	1094	PRO	4.7
2	B	1096	HIS	4.7
1	A	855	ILE	4.5
2	B	1101	VAL	4.3
2	B	1112	LYS	4.3
1	A	862	ALA	4.1
2	B	1095	THR	4.0
1	A	886	PHE	3.8
2	B	1138	ASN	3.8
2	B	1091	MET	3.4
2	B	1106	ASN	3.4
1	A	860	LYS	3.3
2	B	1136	PRO	3.3
2	B	1103	ARG	3.3
2	B	1104	LEU	3.2
1	A	1030	THR	3.2
2	B	865	VAL	3.2
2	B	1093	GLY	3.2
2	B	1137	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	861	PRO	3.1
1	A	1032	LYS	3.1
1	A	1028	ILE	3.0
2	B	1100	THR	3.0
2	B	1029	GLU	3.0
2	B	913	GLU	2.9
1	A	919	ILE	2.9
1	A	933	TYR	2.9
2	B	1107	THR	2.9
2	B	1053	LEU	2.8
2	B	1102	THR	2.8
1	A	917	ASN	2.7
2	B	869	HIS	2.7
1	A	1029	GLU	2.7
1	A	1054	MET	2.7
2	B	1109	LYS	2.6
2	B	1108	LEU	2.6
2	B	1105	VAL	2.5
1	A	1106	ASN	2.5
2	B	1111	GLY	2.5
1	A	856	VAL	2.5
1	A	863	THR	2.5
1	A	1098	GLN	2.5
2	B	1089	LEU	2.4
1	A	1099[A]	MET	2.4
2	B	1090	LYS	2.4
1	A	946	GLU	2.4
2	B	1041	ARG	2.3
1	A	1097	GLY	2.3
2	B	950	ASN	2.3
1	A	1037	VAL	2.3
1	A	1031	ASP	2.3
2	B	1135	GLN	2.3
2	B	912	PRO	2.2
1	A	864	GLU	2.2
1	A	1033	GLU	2.2
2	B	1032	LYS	2.1
2	B	1087	LEU	2.1
2	B	1033	GLU	2.1
1	A	859	LYS	2.0
1	A	949	GLY	2.0
1	A	1057	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1127	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
2	PTR	B	1034	16/17	0.87	0.12	62,80,98,98	0
1	PTR	A	1034	16/17	0.88	0.12	71,81,92,93	0
1	PTR	A	1035	16/17	0.92	0.11	66,69,75,75	0
2	PTR	B	1035	16/17	0.94	0.10	49,52,56,56	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

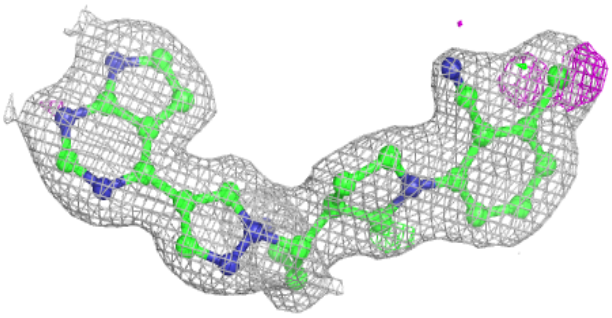
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

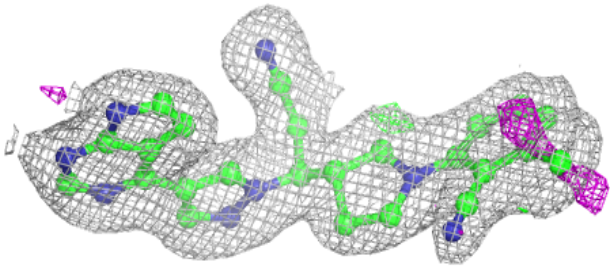
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	1202	4/4	0.82	0.14	50,51,52,55	0
4	EDO	B	1203	4/4	0.86	0.21	38,39,39,41	0
3	LKT	A	1201	32/32	0.92	0.09	23,28,37,44	0
3	LKT	B	1201	32/32	0.97	0.05	12,16,24,28	0

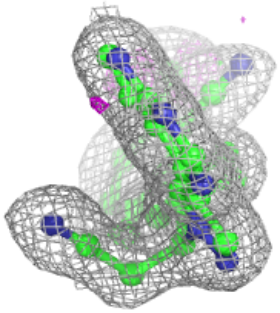
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LKT 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)

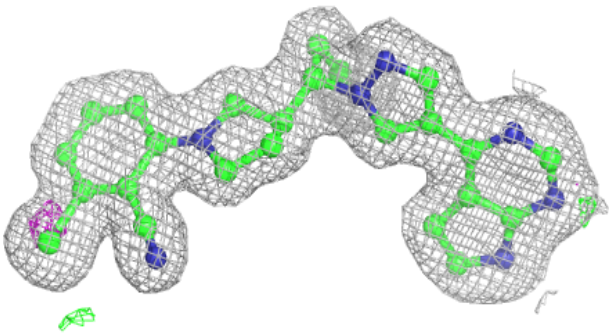


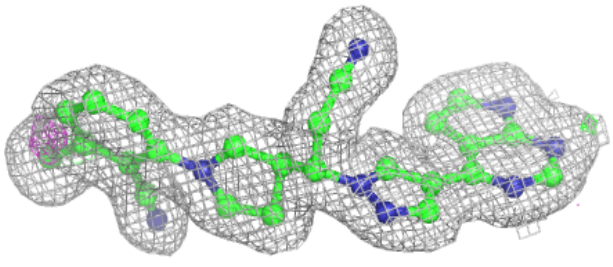


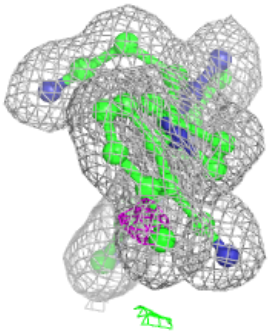


Electron density around LKT B 1201:

$2mF_o$-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 (i)

There are no such residues in this entry.