Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 03:32 pm GMT

PDB ID	:	8BXC
Title	:	Crystal structure of JAK2 JH1 in complex with itacitinib
Authors	:	Haikarainen, T.
Deposited on	:	2022-12-08
Resolution	:	1.90 Å(reported)

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

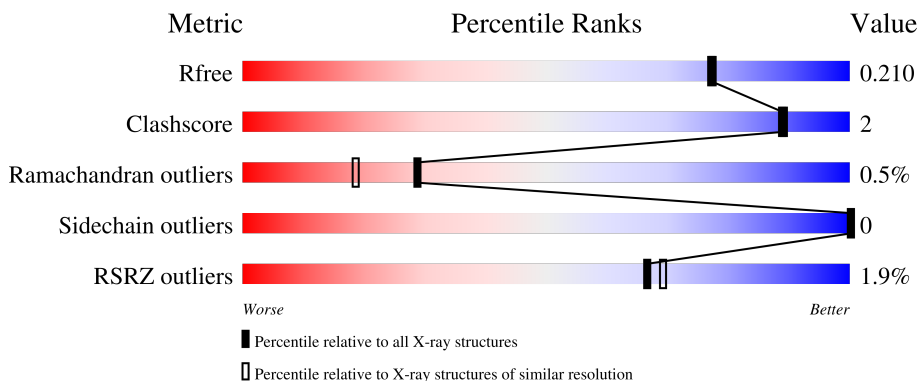|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	Percentile Ranks	Value
Rfree		0.210
Clashscore		2
Ramachandran outliers		0.5%
Sidechain outliers		0
RSRZ outliers		1.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	316	2% — 86% · 7% · 7%
1	B	316	2% — 89% · · 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10047 atoms, of which 4774 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 JAK2.

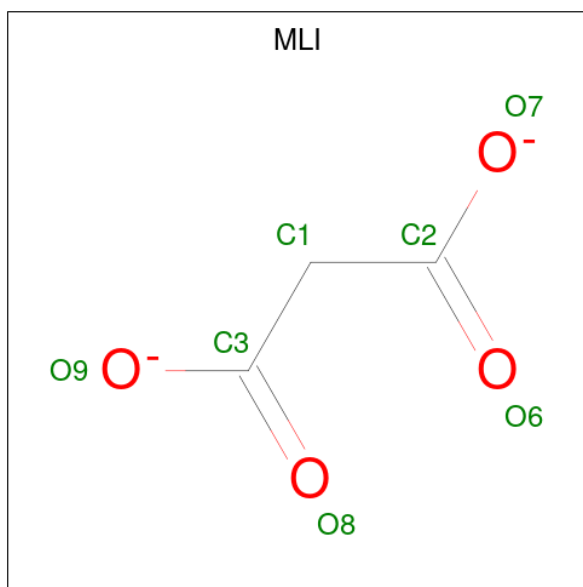| Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	293	Total	C	H	N	O	P	S	0	2	0
			4778	1529	2365	419	449	2	14			
1	B	292	Total	C	H	N	O	P	S	0	1	0
			4759	1523	2361	416	442	2	15			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	MET	-	initiating methionine	UNP O60674
A	818	HIS	-	expression tag	UNP O60674
A	819	HIS	-	expression tag	UNP O60674
A	820	HIS	-	expression tag	UNP O60674
A	821	HIS	-	expression tag	UNP O60674
A	822	HIS	-	expression tag	UNP O60674
A	823	HIS	-	expression tag	UNP O60674
A	824	SER	-	expression tag	UNP O60674
A	825	SER	-	expression tag	UNP O60674
A	826	GLY	-	expression tag	UNP O60674
A	827	VAL	-	expression tag	UNP O60674
A	828	ASP	-	expression tag	UNP O60674
A	829	LEU	-	expression tag	UNP O60674
A	830	GLY	-	expression tag	UNP O60674
A	831	THR	-	expression tag	UNP O60674
A	832	GLU	-	expression tag	UNP O60674
A	833	ASN	-	expression tag	UNP O60674
A	834	LEU	-	expression tag	UNP O60674
A	835	TYR	-	expression tag	UNP O60674
A	836	PHE	-	expression tag	UNP O60674
A	837	GLN	-	expression tag	UNP O60674
A	838	SER	-	expression tag	UNP O60674
A	839	MET	-	expression tag	UNP O60674
B	817	MET	-	initiating methionine	UNP O60674
B	818	HIS	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	819	HIS	-	expression tag	UNP O60674
B	820	HIS	-	expression tag	UNP O60674
B	821	HIS	-	expression tag	UNP O60674
B	822	HIS	-	expression tag	UNP O60674
B	823	HIS	-	expression tag	UNP O60674
B	824	SER	-	expression tag	UNP O60674
B	825	SER	-	expression tag	UNP O60674
B	826	GLY	-	expression tag	UNP O60674
B	827	VAL	-	expression tag	UNP O60674
B	828	ASP	-	expression tag	UNP O60674
B	829	LEU	-	expression tag	UNP O60674
B	830	GLY	-	expression tag	UNP O60674
B	831	THR	-	expression tag	UNP O60674
B	832	GLU	-	expression tag	UNP O60674
B	833	ASN	-	expression tag	UNP O60674
B	834	LEU	-	expression tag	UNP O60674
B	835	TYR	-	expression tag	UNP O60674
B	836	PHE	-	expression tag	UNP O60674
B	837	GLN	-	expression tag	UNP O60674
B	838	SER	-	expression tag	UNP O60674
B	839	MET	-	expression tag	UNP O60674

- Molecule 2 is Itacitinib (three-letter code: S4R) (formula: $C_{26}H_{23}F_4N_9O$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 63	C 26	F 4	H 23	N 9	O 1	0	0
2	B	1	Total 63	C 26	F 4	H 23	N 9	O 1	0	0

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 9	C 3	H 2	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total 196	O 196	0	0
4	B	177	Total 179	O 179	0	3

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.
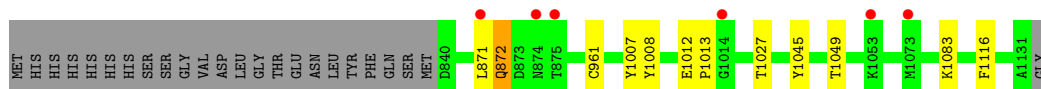
• Molecule 1: Tyrosine-protein kinase JAK2

Chain A:
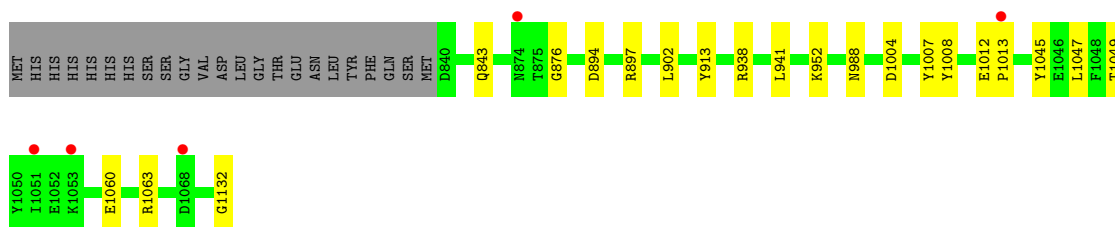
• Molecule 1: Tyrosine-protein kinase JAK2

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.44Å 68.95Å 109.89Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	79.59 – 1.90 79.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.59-1.90) 99.8 (79.59-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.212 0.183 , 0.210	Depositor DCC
R_{free} test set	2794 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 53.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10047	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7350e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: MLI, S4R, PTR

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	0.31	0/2437	0.57	0/3282
1	B	0.29	0/2419	0.58	0/3258
All	All	0.30	0/4856	0.57	0/6540

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	2413	2365	2368	14	0
1	B	2398	2361	2361	4	0
2	A	40	23	0	0	0
2	B	40	23	0	0	0
3	B	7	2	2	0	0
4	A	196	0	0	4	0
4	B	179	0	0	0	0
All	All	5273	4774	4731	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:A:843[B]:GLN:HG2	4:A:1330:HOH:O	1.99	0.62
1:A:952:LYS:NZ	1:A:988:ASN:OD1	2.38	0.57
1:A:1060:GLU:OE1	1:A:1063:ARG:NH2	2.38	0.54
1:A:876:GLY:HA2	4:A:1446:HOH:O	2.08	0.52
1:A:894:ASP:OD1	1:A:897:ARG:NH2	2.42	0.52
1:A:938:ARG:NH2	4:A:1309:HOH:O	2.47	0.47
1:B:961[B]:CYS:SG	1:B:1116:PHE:O	2.73	0.46
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.16	0.45
1:B:871:LEU:O	1:B:872:GLN:C	2.55	0.44
1:A:1045:TYR:CZ	1:A:1049:THR:HG21	2.52	0.43
1:A:1045:TYR:CE2	1:A:1049:THR:HG21	2.54	0.43
1:B:1027:THR:HG21	1:B:1083:LYS:CE	2.50	0.42
1:A:1132:GLY:OXT	4:A:1301:HOH:O	2.21	0.41
1:A:902:LEU:HG	1:A:913:TYR:HB2	2.01	0.41
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	2.03	0.41
1:A:1012:GLU:N	1:A:1013:PRO:HD3	2.35	0.41
1:A:1004:ASP:OD1	1:A:1004:ASP:N	2.52	0.40
1:B:1045:TYR:O	1:B:1049:THR:HG23	2.21	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	291/316 (92%)	287 (99%)	4 (1%)	0	100	100
1	B	289/316 (92%)	277 (96%)	9 (3%)	3 (1%)	15	6
All	All	580/632 (92%)	564 (97%)	13 (2%)	3 (0%)	29	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	872	GLN
1	B	1012	GLU
1	B	1013	PRO

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	261/286 (91%)	261 (100%)	0	100	100
1	B	259/286 (91%)	259 (100%)	0	100	100
All	All	520/572 (91%)	520 (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 ⓘ

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	B	1007	1	15,16,17	1.36	1 (6%)	19,22,24	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
1	PTR	B	1008	1	15,16,17	1.35	1 (6%)	19,22,24	0.59	0
1	PTR	A	1007	1	15,16,17	1.28	1 (6%)	19,22,24	0.66	0
1	PTR	A	1008	1	15,16,17	1.31	1 (6%)	19,22,24	0.62	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	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1007	PTR	OH-CZ	-4.52	1.30	1.40
1	B	1007	PTR	OH-CZ	-4.49	1.30	1.40
1	B	1008	PTR	OH-CZ	-4.12	1.31	1.40
1	A	1008	PTR	OH-CZ	-4.04	1.31	1.40

There are no bond angle outliers.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	MLI	B	1201	-	6,6,6	1.61	1 (16%)	7,7,7	1.28	0
2	S4R	A	1201	-	35,45,45	2.81	15 (42%)	45,68,68	2.39	18 (40%)
2	S4R	B	1202	-	35,45,45	2.85	13 (37%)	45,68,68	2.24	16 (35%)

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
3	MLI	B	1201	-	-	0/4/4/4	-
2	S4R	A	1201	-	-	0/14/52/52	0/6/6/6
2	S4R	B	1202	-	-	6/14/52/52	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1202	S4R	C11-C12	6.46	1.54	1.46
2	A	1201	S4R	C11-C12	6.32	1.54	1.46
2	A	1201	S4R	C30-C28	6.04	1.59	1.50
2	B	1202	S4R	C36-C32	6.02	1.60	1.51
2	B	1202	S4R	C30-C28	6.01	1.59	1.50
2	A	1201	S4R	C36-C32	5.55	1.60	1.51
2	A	1201	S4R	C28-N03	5.27	1.46	1.34
2	A	1201	S4R	C24-N23	4.78	1.43	1.34
2	B	1202	S4R	C24-N23	4.75	1.43	1.34
2	B	1202	S4R	C28-N03	4.74	1.45	1.34
2	B	1202	S4R	C04-N03	4.20	1.54	1.47
2	B	1202	S4R	C32-N33	3.85	1.37	1.33
2	A	1201	S4R	C32-N33	3.74	1.37	1.33
2	B	1202	S4R	C02-N03	3.58	1.53	1.47
2	B	1202	S4R	C30-C31	3.56	1.45	1.38
2	A	1201	S4R	C04-N03	3.54	1.53	1.47
2	A	1201	S4R	C30-C31	3.41	1.44	1.38
2	B	1202	S4R	C19-N27	3.28	1.36	1.32
2	A	1201	S4R	C15-N14	3.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	S4R	C19-N27	3.10	1.35	1.32
2	B	1202	S4R	C26-N27	3.04	1.39	1.33
2	B	1202	S4R	C31-C32	3.04	1.43	1.38
2	A	1201	S4R	C26-N27	3.03	1.39	1.33
2	A	1201	S4R	C31-C32	2.93	1.43	1.38
2	B	1202	S4R	C15-N14	2.82	1.38	1.35
2	A	1201	S4R	C05-C06	2.78	1.59	1.52
3	B	1201	MLI	C1-C3	2.60	1.55	1.51
2	A	1201	S4R	C01-C06	2.29	1.58	1.52
2	A	1201	S4R	C26-N25	2.11	1.35	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	S4R	C05-C06-N07	-7.97	91.82	112.52
2	A	1201	S4R	C05-C06-N07	-7.30	93.56	112.52
2	A	1201	S4R	C31-C32-N33	5.34	123.29	118.35
2	B	1202	S4R	C36-C32-C31	-4.41	118.63	122.64
2	A	1201	S4R	C11-C12-N13	-4.32	172.40	178.11
2	B	1202	S4R	C31-C32-N33	4.15	122.19	118.35
2	A	1201	S4R	C01-C02-N03	4.13	117.10	110.82
2	A	1201	S4R	C04-N03-C02	-4.05	104.82	112.62
2	A	1201	S4R	C36-C32-C31	-3.84	119.15	122.64
2	A	1201	S4R	C30-C31-C32	-3.56	117.84	123.08
2	A	1201	S4R	C01-C06-N07	3.51	121.62	112.52
2	A	1201	S4R	C20-C19-N27	-3.38	120.82	123.04
2	B	1202	S4R	C20-C19-N27	-3.08	121.02	123.04
2	B	1202	S4R	C36-C32-N33	2.98	119.18	112.74
2	B	1202	S4R	C30-C31-C32	-2.90	118.81	123.08
2	B	1202	S4R	C31-C30-C28	-2.84	117.99	124.81
2	B	1202	S4R	C35-C30-C28	2.79	124.81	119.26
2	B	1202	S4R	C05-C04-N03	2.78	115.04	110.82
2	B	1202	S4R	C02-C01-C06	-2.77	105.54	110.81
2	B	1202	S4R	C11-C12-N13	-2.74	174.48	178.11
2	B	1202	S4R	C05-C06-C01	2.61	117.22	111.19
2	A	1201	S4R	C15-N14-N18	-2.55	110.17	111.69
2	B	1202	S4R	N25-C26-N27	-2.45	124.85	128.68
2	A	1201	S4R	C04-N03-C28	2.41	130.40	122.78
2	A	1201	S4R	N25-C26-N27	-2.36	124.99	128.68
2	A	1201	S4R	C30-C28-N03	2.27	121.92	118.28
2	A	1201	S4R	C36-C32-N33	2.23	117.56	112.74
2	A	1201	S4R	C16-C19-C20	2.21	124.93	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1202	S4R	C15-N14-N18	-2.19	110.38	111.69
2	A	1201	S4R	C35-C34-N33	-2.12	121.33	123.96
2	B	1202	S4R	C01-C06-N07	2.10	117.98	112.52
2	A	1201	S4R	C17-N18-N14	2.09	106.41	104.23
2	B	1202	S4R	C30-C28-N03	2.07	121.59	118.28
2	A	1201	S4R	C26-N25-C24	2.05	118.25	113.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1202	S4R	N33-C32-C36-F37
2	B	1202	S4R	N33-C32-C36-F38
2	B	1202	S4R	N33-C32-C36-F39
2	B	1202	S4R	C31-C32-C36-F37
2	B	1202	S4R	C31-C32-C36-F39
2	B	1202	S4R	C31-C32-C36-F38

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 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 S4R A 1201

Bond lengths

Bond angles

Torsions

Rings

Ligand S4R B 1202

Bond lengths

Bond angles

Torsions

Rings
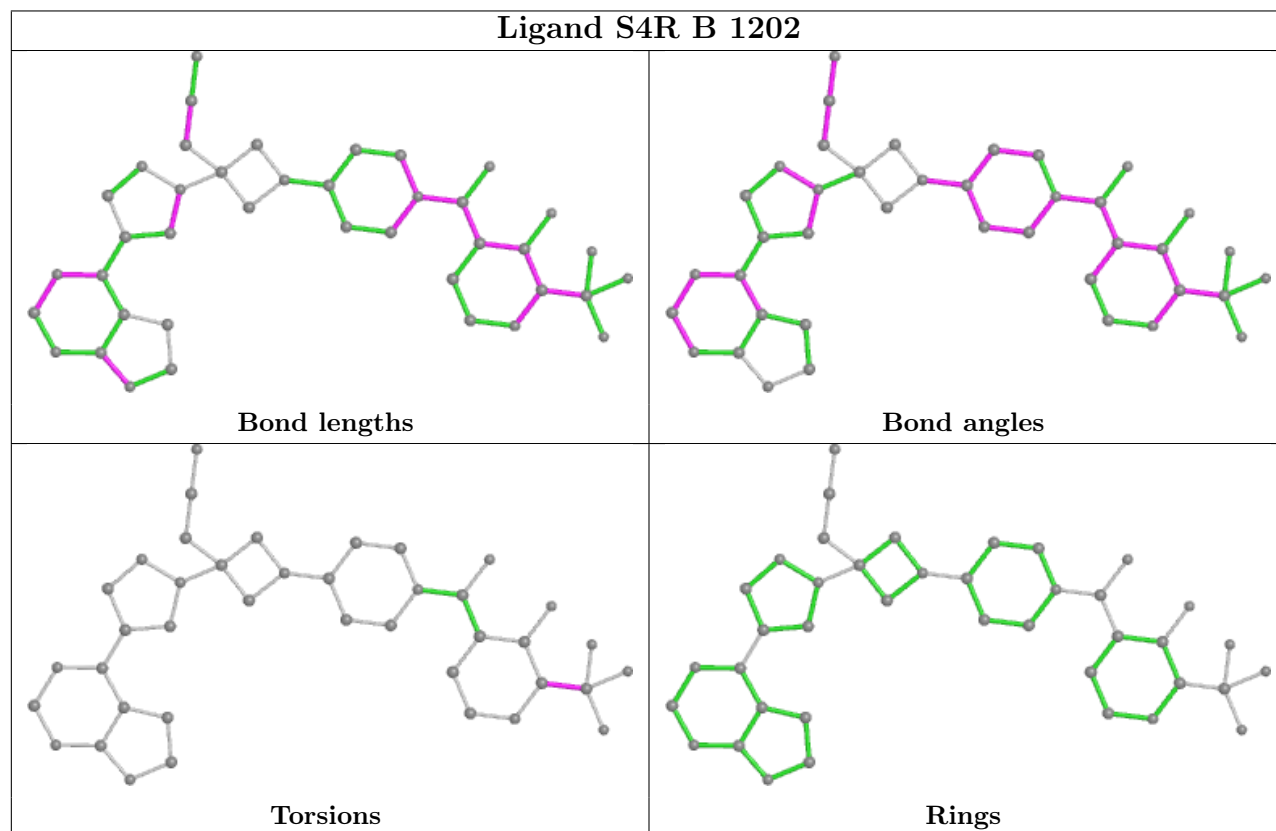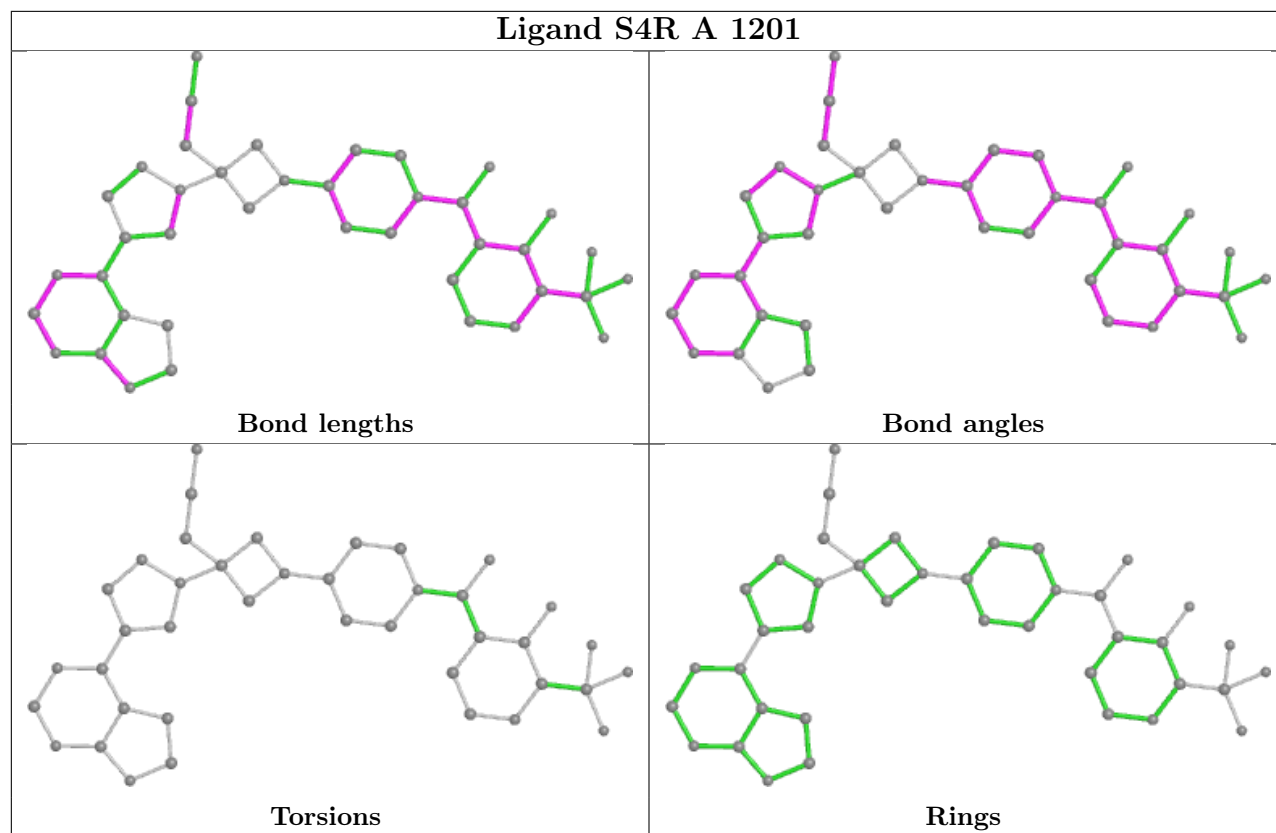
5.7 Other polymers (i)

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	291/316 (92%)	0.14	5 (1%)	70	72	13, 24, 57, 80	0
1	B	290/316 (91%)	0.16	6 (2%)	63	66	14, 23, 55, 84	0
All	All	581/632 (91%)	0.15	11 (1%)	66	69	13, 24, 56, 84	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1053	LYS	6.8
1	B	1014	GLY	4.7
1	B	874	ASN	3.6
1	A	874	ASN	3.1
1	A	1051	ILE	3.1
1	B	875	THR	2.9
1	B	1053	LYS	2.4
1	B	871	LEU	2.2
1	B	1073	MET	2.2
1	A	1068	ASP	2.1
1	A	1013	PRO	2.1

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

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(Å^2)	Q<0.9
1	PTR	B	1008	16/17	0.89	0.16	25,38,72,78	0
1	PTR	A	1008	16/17	0.91	0.15	23,37,77,95	0
1	PTR	A	1007	16/17	0.93	0.10	28,42,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PTR	B	1007	16/17	0.94	0.11	28,40,69,77	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, 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.

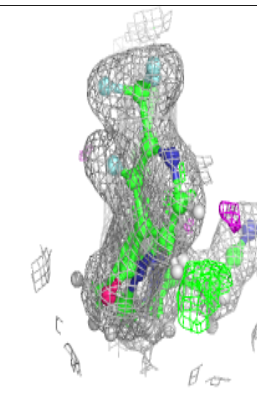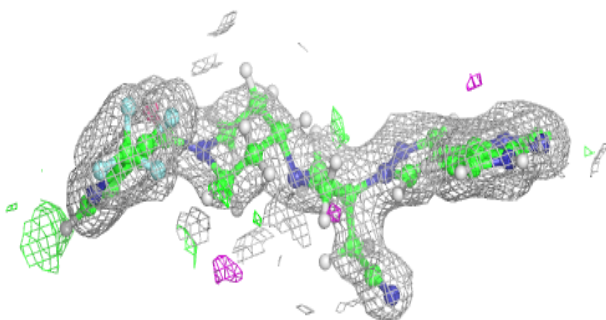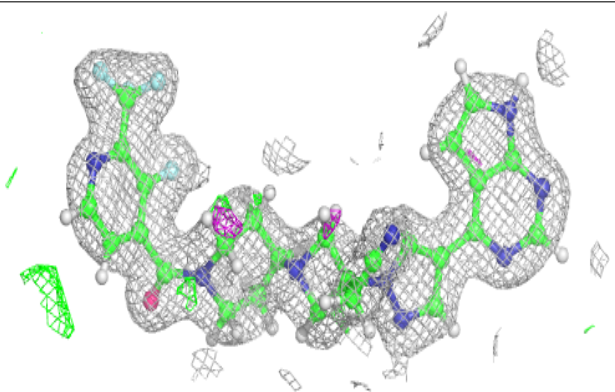| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	S4R	B	1202	40/40	0.93	0.13	14,25,62,68	0
2	S4R	A	1201	40/40	0.94	0.11	15,22,37,44	0
3	MLI	B	1201	7/7	0.94	0.16	22,25,31,31	0

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 S4R B 1202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
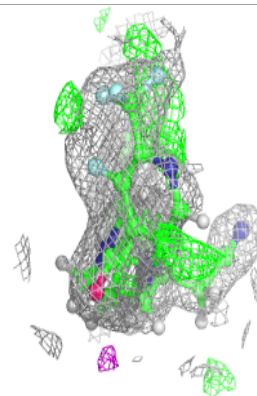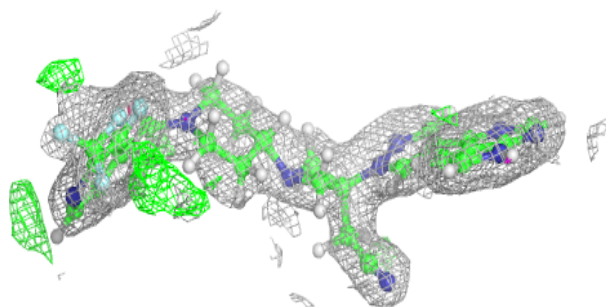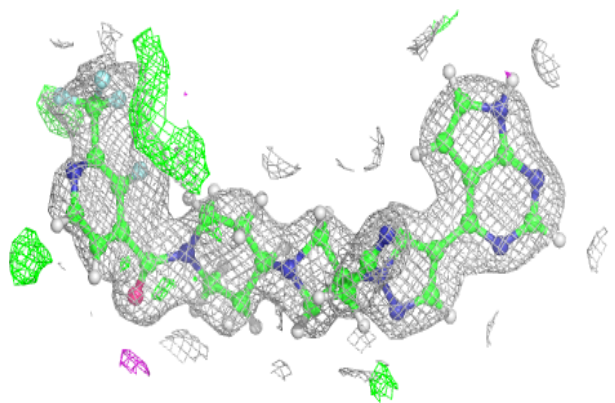
Electron density around S4R A 1201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.