



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:39 PM GMT

PDB ID : 4D1S
Title : Pyrrole-3-carboxamides as potent and selective JAK2 inhibitors
Authors : Bertrand, J.; Canevari, G.; Fasolini, M.; Brasca, M.G.; Nesi, M.; Avanzi, N.; Ballinari, D.; Bandiera, T.; Bindi, S.; Carenzi, D.; Casero, D.; Ceriani, L.; Ciomei, M.; Cirila, A.; Colombo, M.; Cribioli, S.; Cristiani, C.; Della Vedova, F.; Fachin, G.; Felder, E.R.; Galvani, A.; Isacchi, A.; Mirizzi, D.; Motto, I.; Panzeri, A.; Pesenti, E.; Vianello, P.; Gnocchi, P.; Donati, D.
Deposited on : 2014-05-05
Resolution : 1.66 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

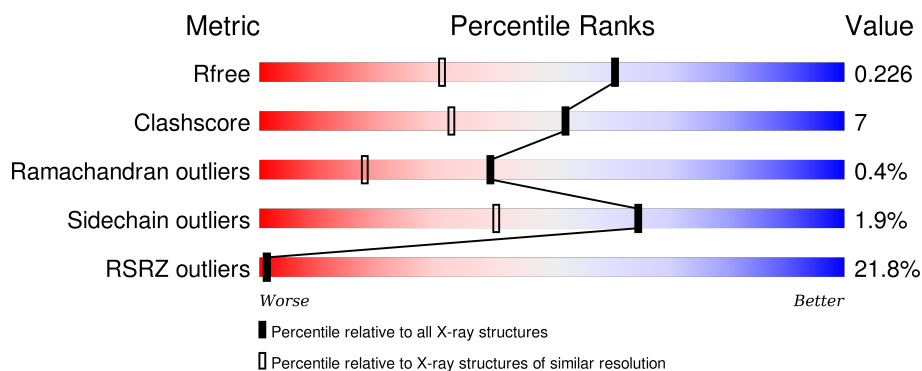
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	298	

2 Entry composition [i](#)

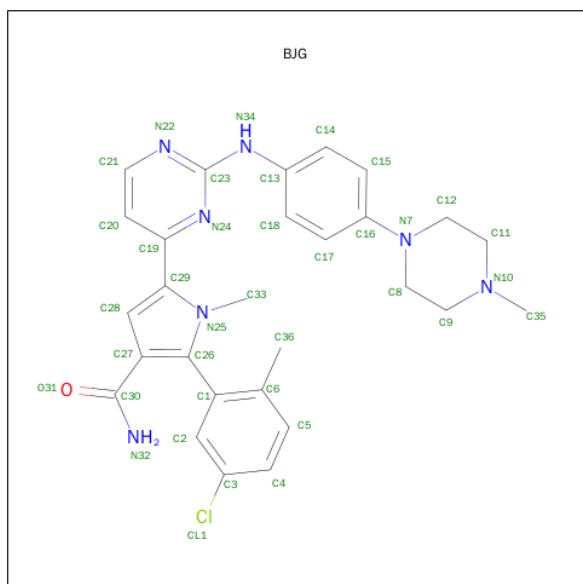
There are 3 unique types of molecules in this entry. The entry contains 2601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	282	2412	1535	420	441	2	14	0	10	0

- Molecule 2 is 2-(5-CHLORO-2-METHYLPHENYL)-1-METHYL-5-(2-{[4-(4-METHYLPIPERAZIN-1-YL)PHENYL]AMINO}PYRIMIDIN-4-YL)-1H-PYRROLE-3-CARBOXAMIDE (three-letter code: BJG) (formula: C₂₈H₃₀ClN₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	37	28	1	7	1	0	0

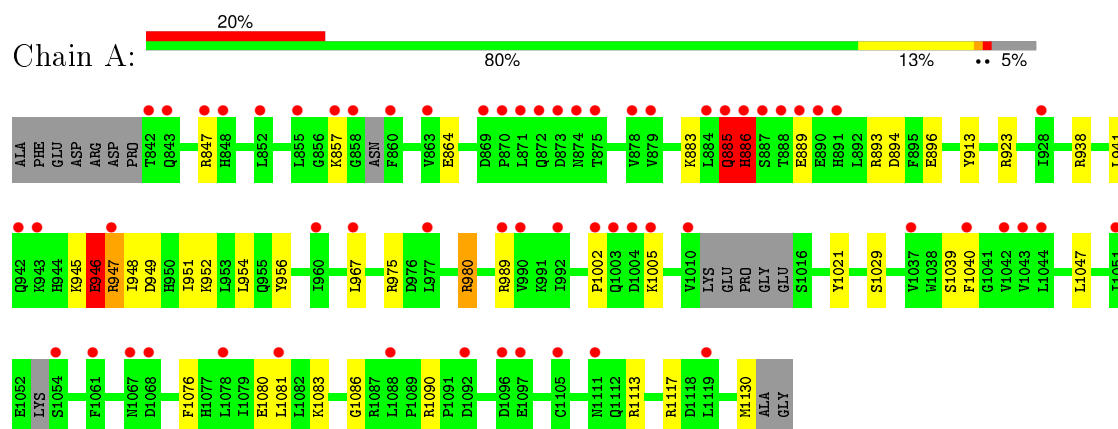
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.78 Å 69.27 Å 50.33 Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	25.16 – 1.66 25.16 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.16-1.66) 95.3 (25.16-1.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.67 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.231 0.195 , 0.226	Depositor DCC
R_{free} test set	2089 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40912 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2601	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BJG, 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	1.20	5/2453 (0.2%)	1.31	23/3292 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	886[A]	HIS	N-CA	8.78	1.64	1.46
1	A	886[B]	HIS	N-CA	8.78	1.64	1.46
1	A	1039	SER	CB-OG	6.29	1.50	1.42
1	A	1029	SER	CA-CB	5.54	1.61	1.52
1	A	896	GLU	CD-OE2	-5.26	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	885	GLN	C-N-CA	11.21	149.73	121.70
1	A	975	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	949	ASP	CB-CG-OD1	9.19	126.57	118.30
1	A	1113	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	956	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	A	886[A]	HIS	CA-C-N	7.13	132.90	117.20
1	A	886[B]	HIS	CA-C-N	7.13	132.90	117.20
1	A	894	ASP	CB-CG-OD2	-6.93	112.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	A	886[A]	HIS	CA-C-O	-6.84	105.72	120.10
1	A	886[B]	HIS	CA-C-O	-6.84	105.72	120.10
1	A	1117	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	967	LEU	CB-CG-CD1	-6.32	100.26	111.00
1	A	1117	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	1113	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	1021	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	980	ARG	CG-CD-NE	-5.94	99.33	111.80
1	A	923	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	1040	PHE	CG-CD1-CE1	-5.65	114.59	120.80
1	A	913	TYR	CG-CD2-CE2	-5.54	116.87	121.30
1	A	975	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	1090	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	1080	GLU	OE1-CD-OE2	-5.17	117.09	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	946	GLU	Peptide

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	2412	0	2413	27	0
2	A	37	0	30	6	0
3	A	152	0	0	3	0
All	All	2601	0	2443	33	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 7.

All (33) 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:A:1141:BJG:H332	2:A:1141:BJG:H18	1.50	0.91
1:A:889:GLU:HG3	1:A:893:ARG:HE	1.50	0.76
1:A:946:GLU:HA	1:A:948:ILE:H	1.64	0.62
1:A:1002:PRO:HG2	1:A:1005:LYS:HB2	1.82	0.60
1:A:951:ILE:HD13	1:A:1130:MET:CE	2.32	0.60
1:A:938:ARG:NH1	3:A:2060:HOH:O	2.35	0.59
1:A:864:GLU:OE2	1:A:883:LYS:NZ	2.30	0.54
1:A:885:GLN:O	1:A:886[A]:HIS:CG	2.60	0.54
1:A:951:ILE:HD13	1:A:1130:MET:HE2	1.91	0.51
2:A:1141:BJG:H363	2:A:1141:BJG:C33	2.41	0.50
1:A:889:GLU:O	1:A:893:ARG:HG3	2.12	0.50
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	1.93	0.49
1:A:1081[B]:LEU:HD22	1:A:1086:GLY:HA3	1.95	0.48
2:A:1141:BJG:N24	2:A:1141:BJG:H18	2.29	0.48
1:A:951:ILE:HD13	1:A:1130:MET:HE3	1.95	0.47
1:A:989[B]:ARG:HH11	1:A:989[B]:ARG:HG3	1.79	0.47
1:A:889:GLU:HG3	1:A:893:ARG:NE	2.25	0.46
2:A:1141:BJG:N24	2:A:1141:BJG:C33	2.78	0.46
2:A:1141:BJG:N24	2:A:1141:BJG:H332	2.31	0.46
2:A:1141:BJG:H18	2:A:1141:BJG:C33	2.36	0.46
1:A:885:GLN:C	1:A:886[A]:HIS:CG	2.90	0.45
1:A:1083:LYS:NZ	3:A:2102:HOH:O	2.51	0.43
1:A:954:LEU:HA	1:A:954:LEU:HD23	1.83	0.43
1:A:947:ARG:O	1:A:952:LYS:NZ	2.50	0.43
1:A:889:GLU:CG	1:A:893:ARG:HH21	2.31	0.42
1:A:885:GLN:C	1:A:886[A]:HIS:CD2	2.92	0.42
1:A:1081[B]:LEU:CD2	1:A:1086:GLY:HA3	2.50	0.41
1:A:945:LYS:HB2	1:A:945:LYS:HE2	1.94	0.41
1:A:885:GLN:O	1:A:886[A]:HIS:CD2	2.74	0.41
1:A:847:ARG:HG2	3:A:2015:HOH:O	2.21	0.41
1:A:889:GLU:CG	1:A:893:ARG:HE	2.26	0.40
1:A:954:LEU:HD12	1:A:1130:MET:CE	2.52	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	282/298 (95%)	270 (96%)	10 (4%)	2 (1%)	26 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	886[A]	HIS
1	A	886[B]	HIS

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	267/269 (99%)	262 (98%)	5 (2%)	65 40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	857	LYS
1	A	885	GLN
1	A	946	GLU
1	A	947	ARG
1	A	980	ARG

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

Mol	Chain	Res	Type
1	A	909	ASN
1	A	1070	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	1007	1	14,16,17	1.00	1 (7%)	18,22,24	1.61	4 (22%)
1	PTR	A	1008	1	14,16,17	0.73	0	18,22,24	2.04	9 (50%)

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	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1007	PTR	CE2-CD2	2.19	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	OH-CZ-CE1	-3.04	109.86	119.22
1	A	1008	PTR	CB-CG-CD1	-2.99	114.65	120.90
1	A	1008	PTR	CE1-CD1-CG	-2.26	117.94	121.04
1	A	1007	PTR	CB-CG-CD1	-2.22	116.25	120.90
1	A	1008	PTR	CE2-CD2-CG	-2.20	118.03	121.04
1	A	1008	PTR	O2P-P-OH	-2.02	97.96	105.22
1	A	1007	PTR	CD2-CG-CD1	2.40	121.97	118.13
1	A	1007	PTR	O3P-P-O2P	2.55	117.10	107.38
1	A	1008	PTR	O3P-P-O2P	2.72	117.75	107.38
1	A	1007	PTR	O3P-P-O1P	2.85	119.76	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	OH-CZ-CE2	3.00	128.46	119.22
1	A	1008	PTR	CD2-CG-CD1	3.02	122.97	118.13
1	A	1008	PTR	P-OH-CZ	3.14	132.79	123.76

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	BJG	A	1141	-	39,41,41	2.55	14 (35%)	50,59,59	3.09	21 (42%)

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	BJG	A	1141	-	-	0/17/30/30	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1141	BJG	C27-C30	-10.30	1.38	1.50
2	A	1141	BJG	C1-C26	-4.90	1.41	1.48
2	A	1141	BJG	C29-C19	-3.17	1.41	1.48
2	A	1141	BJG	C36-C6	-3.00	1.44	1.51
2	A	1141	BJG	C27-C26	-2.73	1.33	1.39
2	A	1141	BJG	C35-N10	2.10	1.52	1.46
2	A	1141	BJG	C9-C8	2.31	1.60	1.51
2	A	1141	BJG	C19-N24	2.32	1.38	1.34
2	A	1141	BJG	C21-N22	2.42	1.39	1.34
2	A	1141	BJG	C4-C3	2.43	1.42	1.38
2	A	1141	BJG	C8-N7	2.90	1.51	1.46
2	A	1141	BJG	C2-C3	2.99	1.43	1.38
2	A	1141	BJG	C30-N32	3.11	1.39	1.33
2	A	1141	BJG	C1-C6	3.44	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1141	BJG	C20-C21-N22	-7.35	115.51	123.90
2	A	1141	BJG	C35-N10-C11	-6.48	100.52	110.63
2	A	1141	BJG	C2-C1-C6	-5.33	115.21	119.00
2	A	1141	BJG	N22-C23-N24	-4.73	121.63	126.67
2	A	1141	BJG	C2-C3-CL1	-4.41	113.66	119.14
2	A	1141	BJG	C35-N10-C9	-3.90	104.55	110.63
2	A	1141	BJG	C5-C4-C3	-3.42	115.43	119.23
2	A	1141	BJG	C20-C19-N24	-3.37	117.35	122.01
2	A	1141	BJG	C27-C26-N25	-2.52	105.75	108.24
2	A	1141	BJG	C36-C6-C5	-2.33	115.57	120.33
2	A	1141	BJG	C17-C16-N7	-2.24	118.37	121.38
2	A	1141	BJG	C14-C13-N34	-2.05	113.98	120.66
2	A	1141	BJG	C14-C15-C16	-2.05	117.72	120.36
2	A	1141	BJG	N34-C23-N24	2.00	123.00	116.91
2	A	1141	BJG	C4-C3-C2	2.46	124.82	121.53
2	A	1141	BJG	C28-C27-C26	2.49	109.93	106.49
2	A	1141	BJG	C21-C20-C19	5.63	122.64	117.26
2	A	1141	BJG	C19-N24-C23	5.82	120.84	116.49
2	A	1141	BJG	C5-C6-C1	6.20	123.57	118.14
2	A	1141	BJG	C12-N7-C8	6.67	125.59	111.59
2	A	1141	BJG	C21-N22-C23	7.41	121.92	115.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1141	BJG	6	0

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	280/298 (93%)	1.28	61 (21%) 1 1	9, 18, 41, 55	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	872	GLN	7.7
1	A	860	PHE	7.5
1	A	871	LEU	6.4
1	A	1003	GLN	6.0
1	A	875	THR	5.7
1	A	842	THR	5.6
1	A	874	ASN	4.4
1	A	1002	PRO	4.2
1	A	885	GLN	4.2
1	A	1051	ILE	4.0
1	A	1004	ASP	4.0
1	A	873	ASP	3.9
1	A	1068	ASP	3.8
1	A	886[A]	HIS	3.7
1	A	1096	ASP	3.6
1	A	889	GLU	3.6
1	A	890	GLU	3.5
1	A	858	GLY	3.3
1	A	843	GLN	3.2
1	A	1042	VAL	2.9
1	A	887	SER	2.9
1	A	1092	ASP	2.8
1	A	857	LYS	2.8
1	A	943	LYS	2.7
1	A	1088	LEU	2.7
1	A	848	HIS	2.6
1	A	942	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	847	ARG	2.6
1	A	891	HIS	2.6
1	A	852	LEU	2.5
1	A	1005	LYS	2.5
1	A	870	PRO	2.5
1	A	1043	VAL	2.5
1	A	989[A]	ARG	2.5
1	A	1054	SER	2.4
1	A	869	ASP	2.4
1	A	992	ILE	2.4
1	A	1081[A]	LEU	2.4
1	A	977	LEU	2.4
1	A	1044	LEU	2.4
1	A	1067	ASN	2.3
1	A	990	VAL	2.3
1	A	1078	LEU	2.3
1	A	1037	VAL	2.3
1	A	1010	VAL	2.3
1	A	855	LEU	2.2
1	A	960	ILE	2.2
1	A	1040	PHE	2.2
1	A	878	VAL	2.2
1	A	1119	LEU	2.2
1	A	967	LEU	2.1
1	A	928	ILE	2.1
1	A	1097	GLU	2.1
1	A	884	LEU	2.1
1	A	863	VAL	2.1
1	A	879	VAL	2.1
1	A	1105	CYS	2.0
1	A	1111	ASN	2.0
1	A	947	ARG	2.0
1	A	1061	PHE	2.0
1	A	888	THR	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	PTR	A	1007	16/17	0.77	0.22	-	19,30,52,53	0
1	PTR	A	1008	16/17	0.83	0.19	-	19,28,56,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	BJG	A	1141	37/37	0.81	0.16	0.10	13,21,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.