



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:05 PM GMT

PDB ID : 4BFR
Title : Discovery and Optimization of Pyrimidone Indoline Amide PI3Kbeta Inhibitors for the Treatment of Phosphatase and TENsin homologue (PTEN)-Deficient Cancers
Authors : Certal, V.; Carry, J.C.; Halley, F.; Virone-Oddos, A.; Thompson, F.; Filoche-Romme, B.; El-Ahmad, Y.; Karlsson, A.; Charrier, V.; Delorme, C.; Rak, A.; Abecassis, P.Y.; Amara, C.; Vincent, L.; Bonnevaux, H.; Nicolas, J.P.; Mathieu, M.; Bertrand, T.; Marquette, J.P.; Michot, N.; Benard, T.; Perrin, M.A.; Perron, S.; Monget, S.; Gruss-Leleu, F.; Doerflinger, G.; Guizani, H.; Brollo, M.; Delbarre, L.; Bertin, L.; Richepin, P.; Loyau, V.; Garcia-Echeverria, C.; Lengauer, C.; Schio, L.
Deposited on : 2013-03-22
Resolution : 2.80 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)

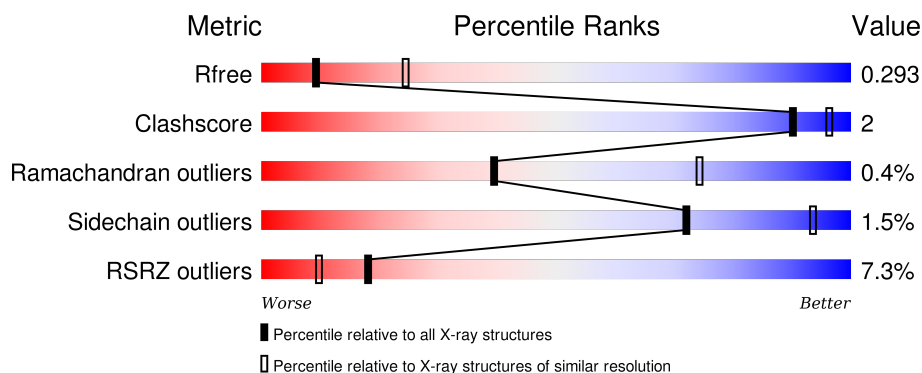
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	952	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>
1	B	952	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13777 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.

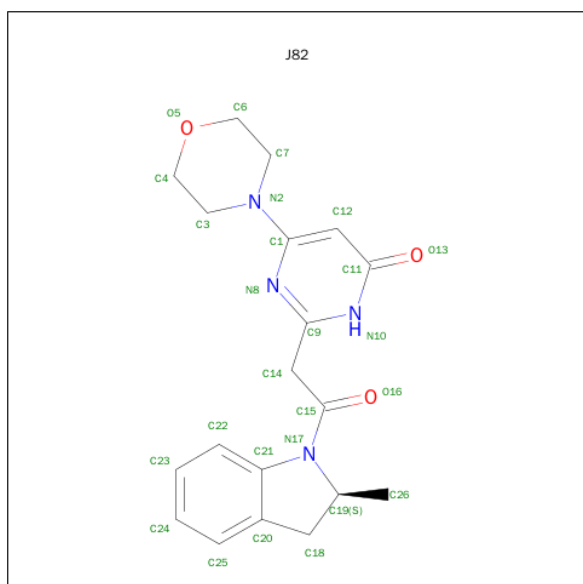
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC S SUBUNIT BETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	855	Total	C	N	O	S	0	0	0
			6902	4436	1165	1259	42			
1	B	836	Total	C	N	O	S	0	0	0
			6743	4339	1138	1225	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	EXPRESSION TAG	UNP Q8BTI9
B	113	GLY	-	EXPRESSION TAG	UNP Q8BTI9

- Molecule 2 is 2-[2-(2-METHYL-2,3-DIHYDRO-INDOL-1-YL)-2-OXO-ETHYL]-6-MORPHOLIN-4-YL-3H-PYRIMIDIN-4-ONE (three-letter code: J82) (formula: C₁₉H₂₂N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	19	4	3		
2	B	1	Total	C	N	O	0	0
			26	19	4	3		

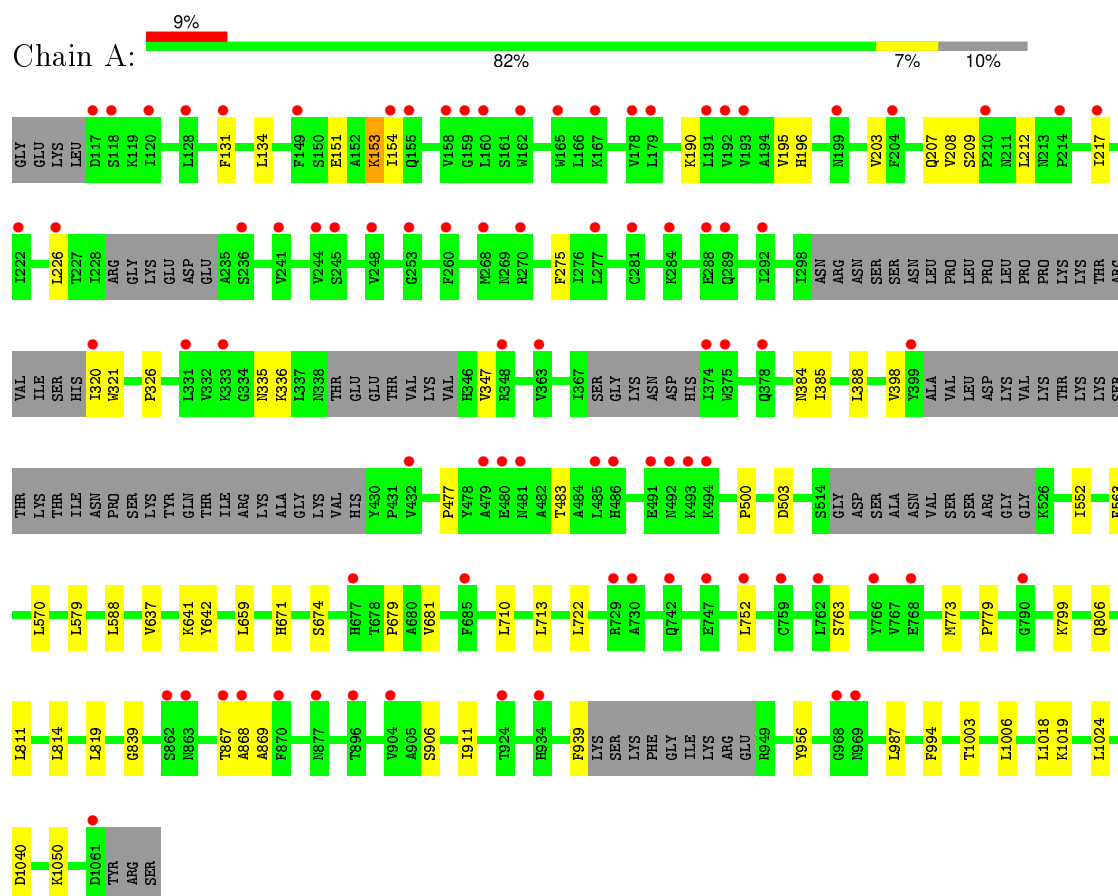
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	47	Total	O	0	0
			47	47		

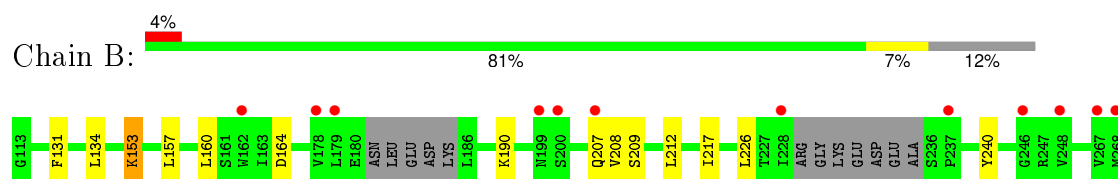
3 Residue-property plots

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 ($RSRZ > 2$). 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: PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT BETA ISOFORM



- Molecule 1: PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT BETA ISOFORM





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.31Å 129.03Å 154.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.00 – 2.80 77.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.00-2.80) 99.7 (77.45-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.260 , 0.275 0.280 , 0.293	Depositor DCC
R_{free} test set	3084 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.4	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 60849 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13777	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: J82

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	0.38	0/7047	0.53	0/9524
1	B	0.38	0/6879	0.52	0/9287
All	All	0.38	0/13926	0.53	0/18811

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	6902	0	6937	31	0
1	B	6743	0	6808	30	0
2	A	26	0	22	1	0
2	B	26	0	22	1	0
3	A	33	0	0	0	0
3	B	47	0	0	0	0
All	All	13777	0	13789	63	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 (63) 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:153:LYS:HD2	1:B:659:LEU:HB3	1.61	0.82
1:A:153:LYS:HD2	1:A:659:LEU:HB3	1.60	0.82
1:A:868:ALA:N	1:A:869:ALA:HA	1.94	0.81
1:A:868:ALA:H	1:A:869:ALA:HA	1.50	0.71
1:B:914:ARG:HB2	1:B:953:ILE:HD13	1.80	0.63
1:B:911:ILE:HG22	1:B:914:ARG:HD3	1.83	0.59
1:B:618:VAL:HG21	1:B:649:ALA:HB1	1.87	0.57
1:A:208:VAL:HG21	1:A:217:ILE:HG12	1.90	0.54
1:A:320:ILE:HG12	1:A:500:PRO:HD3	1.89	0.54
1:B:208:VAL:HG21	1:B:217:ILE:HG12	1.89	0.54
1:B:641:LYS:HG2	1:B:681:VAL:HG11	1.91	0.53
1:A:641:LYS:HG2	1:A:681:VAL:HG11	1.92	0.52
1:B:385:ILE:HA	1:B:388:LEU:HD12	1.91	0.52
1:B:240:TYR:HB3	1:B:277:LEU:HD22	1.92	0.52
1:A:477:PRO:HG2	1:A:679:PRO:HB2	1.92	0.52
1:B:994:PHE:HB3	1:B:1018:LEU:HD21	1.91	0.52
1:A:385:ILE:HA	1:A:388:LEU:HD12	1.91	0.51
1:A:994:PHE:HB3	1:A:1018:LEU:HD21	1.91	0.51
1:B:477:PRO:HG2	1:B:679:PRO:HB2	1.92	0.50
1:B:160:LEU:HG	1:B:164:ASP:HB3	1.94	0.49
1:A:1019:LYS:HA	1:A:1024:LEU:HD12	1.94	0.49
1:B:339:THR:HG23	1:B:343:VAL:HG22	1.95	0.49
1:A:637:VAL:HG11	1:A:671:HIS:HB3	1.96	0.48
1:B:1019:LYS:HA	1:B:1024:LEU:HD12	1.95	0.48
1:B:291:MET:HA	1:B:294:ILE:HD12	1.96	0.47
1:A:151:GLU:HA	1:A:154:ILE:HD12	1.97	0.47
1:A:326:PRO:HA	1:A:384:ASN:HA	1.96	0.47
1:B:346:HIS:HB3	1:B:366:GLU:HG2	1.98	0.46
1:A:196:HIS:HB3	1:A:203:VAL:HG12	1.97	0.46
1:B:956:TYR:HA	1:B:959:ILE:HD12	1.97	0.46
1:A:195:VAL:HG22	1:A:275:PHE:HB2	1.97	0.46
1:B:326:PRO:HA	1:B:384:ASN:HA	1.96	0.46
1:B:294:ILE:HG12	1:B:697:VAL:HB	1.98	0.45
1:A:209:SER:HB3	1:A:212:LEU:HD12	1.99	0.45
2:B:2000:J82:H19	2:B:2000:J82:H142	1.88	0.45
1:A:811:LEU:HA	1:A:814:LEU:HD12	1.98	0.44
1:B:811:LEU:HA	1:B:814:LEU:HD12	1.98	0.44
1:A:642:TYR:HB2	1:A:1003:THR:HG21	1.98	0.44
1:A:336:LYS:HB2	1:A:483:THR:HA	1.99	0.44
1:B:642:TYR:HB2	1:B:1003:THR:HG21	1.98	0.44
1:B:435:VAL:HG21	1:B:453:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HD3	1:A:207:GLN:HB3	2.01	0.43
1:B:209:SER:HB3	1:B:212:LEU:HD12	2.00	0.43
1:A:320:ILE:HG23	1:A:321:TRP:H	1.83	0.43
1:B:347:VAL:HG22	1:B:398:VAL:HG22	2.01	0.43
1:B:190:LYS:HD3	1:B:207:GLN:HB3	2.01	0.42
1:B:906:SER:HA	1:B:911:ILE:HD12	2.00	0.42
1:A:347:VAL:HG22	1:A:398:VAL:HG22	2.01	0.42
1:A:806:GLN:HE21	1:A:1006:LEU:HG	1.85	0.42
2:A:2000:J82:H19	2:A:2000:J82:H142	1.90	0.42
1:A:956:TYR:HB3	1:A:1050:LYS:HD2	2.02	0.42
1:B:710:LEU:HA	1:B:713:LEU:HD12	2.03	0.41
1:A:552:ILE:HG22	1:A:570:LEU:HD12	2.03	0.41
1:A:773:MET:HB3	1:A:779:PRO:HD2	2.03	0.41
1:A:906:SER:HA	1:A:911:ILE:HD12	2.02	0.41
1:B:552:ILE:HG22	1:B:570:LEU:HD12	2.03	0.41
1:B:637:VAL:HG11	1:B:671:HIS:HB3	2.03	0.41
1:A:779:PRO:HB3	1:A:799:LYS:HG2	2.03	0.40
1:A:131:PHE:HA	1:A:134:LEU:HD12	2.03	0.40
1:A:710:LEU:HA	1:A:713:LEU:HD12	2.03	0.40
1:A:674:SER:HA	1:A:839:GLY:HA2	2.03	0.40
1:B:131:PHE:HA	1:B:134:LEU:HD12	2.04	0.40
1:B:445:GLN:HA	1:B:498:TYR:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	839/952 (88%)	813 (97%)	23 (3%)	3 (0%)	39	74
1	B	814/952 (86%)	787 (97%)	24 (3%)	3 (0%)	39	74
All	All	1653/1904 (87%)	1600 (97%)	47 (3%)	6 (0%)	39	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	THR
1	A	763	SER
1	B	763	SER
1	B	931	ASP
1	A	335	ASN
1	B	426	GLY

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	763/849 (90%)	751 (98%)	12 (2%)	70	93
1	B	747/849 (88%)	737 (99%)	10 (1%)	76	94
All	All	1510/1698 (89%)	1488 (98%)	22 (2%)	72	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LYS
1	A	226	LEU
1	A	503	ASP
1	A	563	PHE
1	A	579	LEU
1	A	588	LEU
1	A	722	LEU
1	A	752	LEU
1	A	819	LEU
1	A	939	PHE
1	A	987	LEU
1	A	1040	ASP
1	B	153	LYS
1	B	157	LEU
1	B	226	LEU
1	B	324	ASN
1	B	563	PHE

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Mol	Chain	Res	Type
1	B	579	LEU
1	B	588	LEU
1	B	590	GLN
1	B	752	LEU
1	B	819	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	HIS
1	A	590	GLN
1	A	671	HIS
1	A	806	GLN
1	A	929	HIS
1	B	590	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	J82	A	2000	-	27,29,29	1.28	3 (11%)	33,41,41	1.90	4 (12%)
2	J82	B	2000	-	27,29,29	1.24	3 (11%)	33,41,41	1.92	4 (12%)

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	J82	A	2000	-	-	0/12/32/32	0/4/4/4
2	J82	B	2000	-	-	0/12/32/32	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	J82	C19-N17	2.13	1.53	1.48
2	A	2000	J82	C19-N17	2.16	1.53	1.48
2	B	2000	J82	C11-N10	3.08	1.38	1.33
2	A	2000	J82	C11-N10	3.17	1.39	1.33
2	B	2000	J82	C9-N10	4.55	1.40	1.33
2	A	2000	J82	C9-N10	4.75	1.41	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	J82	C12-C11-N10	-7.50	114.96	124.05
2	A	2000	J82	C12-C11-N10	-7.48	114.98	124.05
2	A	2000	J82	N10-C9-N8	-2.40	122.72	126.18
2	B	2000	J82	N10-C9-N8	-2.38	122.75	126.18
2	A	2000	J82	C11-C12-C1	4.46	121.91	116.33
2	B	2000	J82	C11-C12-C1	4.54	122.01	116.33
2	A	2000	J82	C9-N8-C1	4.56	119.48	115.68
2	B	2000	J82	C9-N8-C1	4.62	119.53	115.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	J82	1	0
2	B	2000	J82	1	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	855/952 (89%)	0.89	85 (9%)	9 4	46, 81, 113, 138	0
1	B	836/952 (87%)	0.71	39 (4%)	35 24	49, 70, 95, 138	0
All	All	1691/1904 (88%)	0.80	124 (7%)	18 10	46, 74, 109, 138	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	TYR	7.3
1	A	863	ASN	6.6
1	A	117	ASP	6.0
1	A	492	ASN	5.7
1	A	162	TRP	4.9
1	A	226	LEU	4.8
1	B	514	SER	4.7
1	A	160	LEU	4.4
1	A	862	SER	4.3
1	A	494	LYS	4.3
1	A	292	ILE	4.2
1	A	968	GLY	4.1
1	B	494	LYS	4.0
1	B	968	GLY	4.0
1	A	281	CYS	3.8
1	B	199	ASN	3.7
1	A	374	ILE	3.7
1	A	154	ILE	3.7
1	B	1044	ARG	3.6
1	A	289	GLN	3.6
1	B	849	SER	3.6
1	B	492	ASN	3.5
1	A	167	LYS	3.5
1	B	402	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	874	ALA	3.4
1	A	969	ASN	3.3
1	B	246	GLY	3.2
1	A	432	VAL	3.2
1	A	485	LEU	3.2
1	A	333	LYS	3.2
1	B	344	LYS	3.2
1	B	725	VAL	3.1
1	B	1043	LEU	3.0
1	A	331	LEU	3.0
1	A	868	ALA	3.0
1	A	284	LYS	3.0
1	A	236	SER	3.0
1	A	131	PHE	3.0
1	A	729	ARG	3.0
1	A	210	PRO	2.9
1	A	480	GLU	2.9
1	A	479	ALA	2.9
1	B	370	LYS	2.9
1	A	191	LEU	2.9
1	A	204	PHE	2.8
1	A	867	THR	2.8
1	B	179	LEU	2.8
1	A	363	VAL	2.8
1	A	685	PHE	2.8
1	A	493	LYS	2.8
1	A	730	ALA	2.7
1	B	759	CYS	2.7
1	B	969	ASN	2.7
1	A	214	PRO	2.7
1	A	199	ASN	2.6
1	A	924	THR	2.6
1	A	165	TRP	2.6
1	B	590	GLN	2.6
1	B	248	VAL	2.6
1	B	429	HIS	2.6
1	B	336	LYS	2.6
1	A	747	GLU	2.5
1	B	753	GLN	2.5
1	B	268	MET	2.5
1	A	270	ARG	2.5
1	A	1061	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	877	ASN	2.5
1	B	289	GLN	2.4
1	B	296	ALA	2.4
1	B	965	GLY	2.4
1	A	128	LEU	2.4
1	A	192	VAL	2.4
1	A	244	VAL	2.4
1	A	277	LEU	2.4
1	B	360	LYS	2.4
1	B	207	GLN	2.4
1	A	253	GLY	2.4
1	A	491	GLU	2.4
1	A	378	GLN	2.3
1	A	155	GLN	2.3
1	B	267	VAL	2.3
1	A	320	ILE	2.3
1	A	762	LEU	2.3
1	A	486	HIS	2.3
1	B	237	PRO	2.3
1	A	752	LEU	2.3
1	A	768	GLU	2.3
1	A	677	HIS	2.3
1	A	159	GLY	2.3
1	B	277	LEU	2.3
1	B	178	VAL	2.3
1	A	375	TRP	2.2
1	B	970	THR	2.2
1	A	870	PHE	2.2
1	B	162	TRP	2.2
1	A	178	VAL	2.2
1	B	200	SER	2.2
1	A	348	ARG	2.2
1	A	193	VAL	2.2
1	A	268	MET	2.2
1	A	222	ILE	2.2
1	B	761	ILE	2.2
1	A	241	VAL	2.2
1	A	934	HIS	2.2
1	A	120	ILE	2.1
1	B	854	ILE	2.1
1	A	904	VAL	2.1
1	A	149	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	260	PHE	2.1
1	A	759	CYS	2.1
1	A	742	GLN	2.1
1	A	118	SER	2.0
1	A	245	SER	2.0
1	A	217	ILE	2.0
1	A	158	VAL	2.0
1	A	179	LEU	2.0
1	A	248	VAL	2.0
1	A	790	GLY	2.0
1	B	228	ILE	2.0
1	A	766	TYR	2.0
1	A	481	ASN	2.0
1	A	896	THR	2.0
1	B	748	ALA	2.0
1	A	288	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	J82	A	2000	26/26	0.94	0.27	0.77	48,49,51,51	0
2	J82	B	2000	26/26	0.93	0.24	-0.08	50,50,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.