



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2017 – 12:23 AM EDT

PDB ID : 3LJ2
Title : IRE1 complexed with JAK Inhibitor I
Authors : Lee, K.P.K.; Sicheri, F.
Deposited on : unknown
Resolution : 3.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

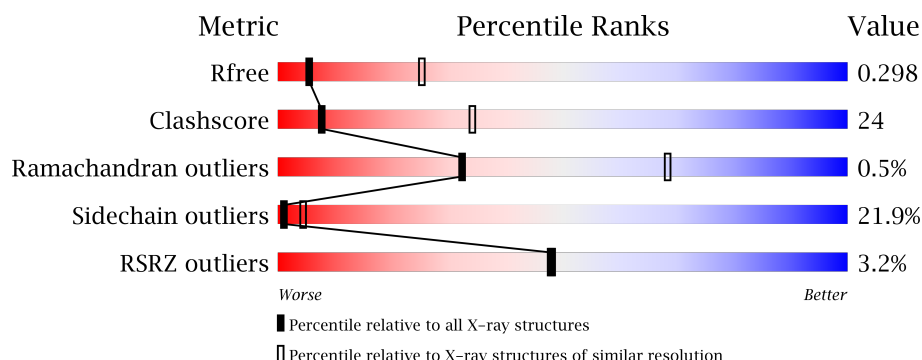
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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}	100719	1167 (3.40-3.28)
Clashscore	112137	1239 (3.40-3.28)
Ramachandran outliers	110173	1219 (3.40-3.28)
Sidechain outliers	110143	1218 (3.40-3.28)
RSRZ outliers	101464	1176 (3.40-3.28)

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	434	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>34%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	434	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>33%</div> <div>8%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6344 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	P	S	0	0	0
			3149	2015	534	581	3	16			
1	B	407	Total	C	N	O	P	S	0	0	0
			3149	2015	534	581	3	16			

There are 48 discrepancies between the modelled and reference sequences:

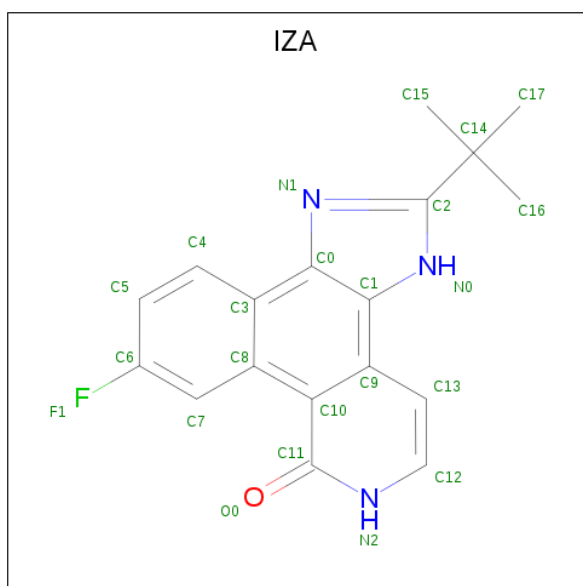
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ARG	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
A	?	-	TYR	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	PRO	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
B	?	-	CYS	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ARG	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
B	?	-	TYR	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	PRO	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361

- Molecule 2 is 2-TERT-BUTYL-9-FLUORO-3,6-DIHYDRO-7H-BENZ[H]-IMIDAZ[4,5-F]IS OQUINOLINE-7-ONE (three-letter code: IZA) (formula: C₁₈H₁₆FN₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			23	18	1	3	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	126.18Å 126.18Å 175.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.50 – 3.33 51.50 – 3.33	Depositor EDS
% Data completeness (in resolution range)	94.6 (51.50-3.33) 94.6 (51.50-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.254 , 0.293 0.254 , 0.298	Depositor DCC
R_{free} test set	1151 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6344	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.333 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: TPO, IZA, SEP

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	0.71	0/3184	0.85	8/4311 (0.2%)
1	B	0.78	1/3184 (0.0%)	0.85	6/4311 (0.1%)
All	All	0.75	1/6368 (0.0%)	0.85	14/8622 (0.2%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	908	CYS	CB-SG	-5.01	1.73	1.81

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	895	ARG	N-CA-CB	-14.35	84.77	110.60
1	B	868	GLN	N-CA-CB	-14.33	84.81	110.60
1	A	894	LYS	N-CA-C	-10.73	82.02	111.00
1	B	867	LEU	N-CA-C	8.67	134.41	111.00
1	B	1076	VAL	C-N-CD	-7.95	103.11	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1003	ASP	Peptide
1	A	1076	VAL	Peptide
1	B	1003	ASP	Peptide
1	B	1076	VAL	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	3149	0	3012	154	2
1	B	3149	0	3012	147	0
2	A	23	0	16	1	0
2	B	23	0	16	1	0
All	All	6344	0	6056	301	2

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 24.

The worst 5 of 301 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:829:PHE:HA	1:A:832:CYS:SG	1.81	1.20
1:B:829:PHE:HA	1:B:832:CYS:SG	1.86	1.15
1:B:865:ASN:CB	1:B:868:GLN:OE1	1.96	1.13
1:A:861:LEU:HD23	1:A:861:LEU:N	1.52	1.10
1:A:860:LEU:C	1:A:861:LEU:HD23	1.79	1.01

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:LEU:CD1	1:A:1063:MET:SD[3_455]	1.89	0.31
1:A:933:ARG:NH2	1:A:1010:MET:SD[6_565]	2.13	0.07

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	399/434 (92%)	373 (94%)	24 (6%)	2 (0%)	32	68
1	B	399/434 (92%)	373 (94%)	24 (6%)	2 (0%)	32	68
All	All	798/868 (92%)	746 (94%)	48 (6%)	4 (0%)	32	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1077	PRO
1	B	1077	PRO
1	A	1004	PRO
1	B	1004	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	324/395 (82%)	251 (78%)	73 (22%)	1	4
1	B	324/395 (82%)	255 (79%)	69 (21%)	1	5
All	All	648/790 (82%)	506 (78%)	142 (22%)	1	4

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1069	ILE
1	B	720	THR

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Mol	Chain	Res	Type
1	B	1052	LEU
1	A	1080	PHE
1	A	1113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1036	ASN
1	A	1090	ASN
1	B	787	HIS
1	A	866	ASN
1	B	727	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	SEP	A	840	1	9,9,10	2.05	3 (33%)	9,12,14	2.28	2 (22%)
1	SEP	A	841	1	9,9,10	1.82	2 (22%)	9,12,14	1.58	2 (22%)
1	TPO	A	844	1	9,10,11	1.11	1 (11%)	10,14,16	1.64	2 (20%)
1	SEP	B	840	1	9,9,10	2.30	4 (44%)	9,12,14	2.18	1 (11%)
1	SEP	B	841	1	9,9,10	1.94	4 (44%)	9,12,14	1.56	2 (22%)
1	TPO	B	844	1	9,10,11	1.42	1 (11%)	10,14,16	1.36	1 (10%)

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	SEP	A	840	1	-	0/5/8/10	0/0/0/0
1	SEP	A	841	1	-	0/5/8/10	0/0/0/0
1	TPO	A	844	1	-	1/8/11/13	0/0/0/0
1	SEP	B	840	1	-	0/5/8/10	0/0/0/0
1	SEP	B	841	1	-	0/5/8/10	0/0/0/0
1	TPO	B	844	1	-	1/8/11/13	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	SEP	P-O2P	2.06	1.63	1.54
1	A	841	SEP	P-O3P	2.06	1.63	1.54
1	B	841	SEP	CA-C	2.09	1.53	1.50
1	B	841	SEP	P-O2P	2.10	1.63	1.54
1	A	844	TPO	CA-C	2.13	1.53	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	840	SEP	P-OG-CB	-5.44	103.31	118.30
1	A	840	SEP	P-OG-CB	-4.42	106.13	118.30
1	B	841	SEP	P-OG-CB	-3.06	109.88	118.30
1	A	841	SEP	O3P-P-OG	2.02	112.10	106.73
1	A	844	TPO	O3P-P-O2P	2.22	116.56	107.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	844	TPO	OG1-CB-CA-N
1	B	844	TPO	OG1-CB-CA-N

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	840	SEP	1	0
1	A	841	SEP	1	0
1	A	844	TPO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	840	SEP	1	0
1	B	841	SEP	2	0
1	B	844	TPO	3	0

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	IZA	A	1	-	21,26,26	1.74	5 (23%)	26,41,41	1.51	3 (11%)
2	IZA	B	1	-	21,26,26	1.97	8 (38%)	26,41,41	1.23	3 (11%)

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	IZA	A	1	-	-	0/6/6/6	0/4/4/4
2	IZA	B	1	-	-	0/6/6/6	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	IZA	C14-C2	-3.24	1.48	1.53
2	A	1	IZA	C9-C1	-2.90	1.39	1.45
2	B	1	IZA	C3-C0	-2.59	1.39	1.45
2	B	1	IZA	C9-C1	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	IZA	C3-C0	-2.06	1.41	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	IZA	C13-C12-N2	-3.47	120.21	123.80
2	B	1	IZA	C5-C6-C7	-2.69	120.17	123.22
2	A	1	IZA	C12-N2-C11	2.51	122.29	116.60
2	B	1	IZA	C12-N2-C11	3.02	123.47	116.60
2	B	1	IZA	C6-C7-C8	3.08	121.34	119.40

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	1	IZA	1	0
2	B	1	IZA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	404/434 (93%)	0.59	18 (4%) 34 34	39, 40, 41, 41	0
1	B	404/434 (93%)	0.52	8 (1%) 65 66	39, 40, 41, 42	0
All	All	808/868 (93%)	0.55	26 (3%) 48 48	39, 40, 41, 42	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	838	GLY	4.7
1	A	818	GLY	4.0
1	A	838	GLY	3.6
1	A	1018	PHE	3.3
1	B	708	PHE	3.2

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. 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
1	TPO	B	844	11/12	0.91	0.17	-	40,40,41,42	0
1	SEP	B	840	10/11	0.71	0.34	-	40,41,41,43	0
1	TPO	A	844	11/12	0.86	0.26	-	40,40,41,42	0
1	SEP	A	841	10/11	0.77	0.16	-	40,40,41,42	0
1	SEP	B	841	10/11	0.84	0.20	-	40,40,41,42	0
1	SEP	A	840	10/11	0.76	0.23	-	40,41,41,43	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	IZA	B	1	23/23	0.97	0.37	0.76	37,41,44,46	0
2	IZA	A	1	23/23	0.95	0.31	-0.10	41,44,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.