



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:50 AM GMT

PDB ID : 3G8E
Title : Crystal Structure of Rattus norvegicus Visfatin/PBEF/Nampt in Complex with an FK866-based inhibitor
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Deposited on : 2009-02-12
Resolution : 3.00 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 (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

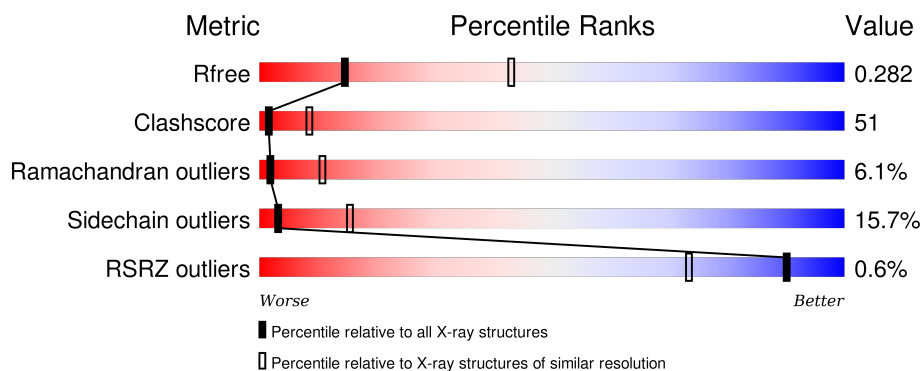
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	491	<div> <div></div> <div> <div></div> <div>31%</div> <div>50%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	491	<div> <div></div> <div> <div></div> <div>34%</div> <div>45%</div> <div>14%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IS1	A	501	-	-	-	X
2	IS1	B	502	-	-	-	X

2 Entry composition [i](#)

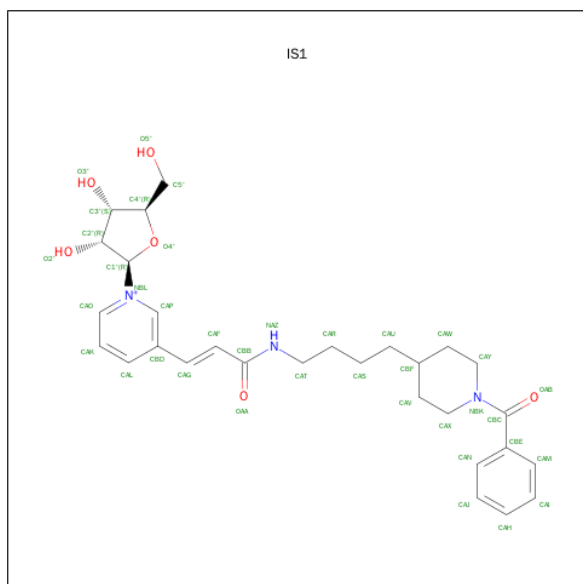
There are 2 unique types of molecules in this entry. The entry contains 7476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is 3-[(1E)-3-OXO-3-({4-[1-(PHENYLCARBONYL)PIPERIDIN-4-YL]BUTYL}AMINO)PROP-1-EN-1-YL]-1-BETA-D-RIBOFURANOSYLPYRIDINIUM (three-letter code: IS1) (formula: C₂₉H₃₈N₃O₆).

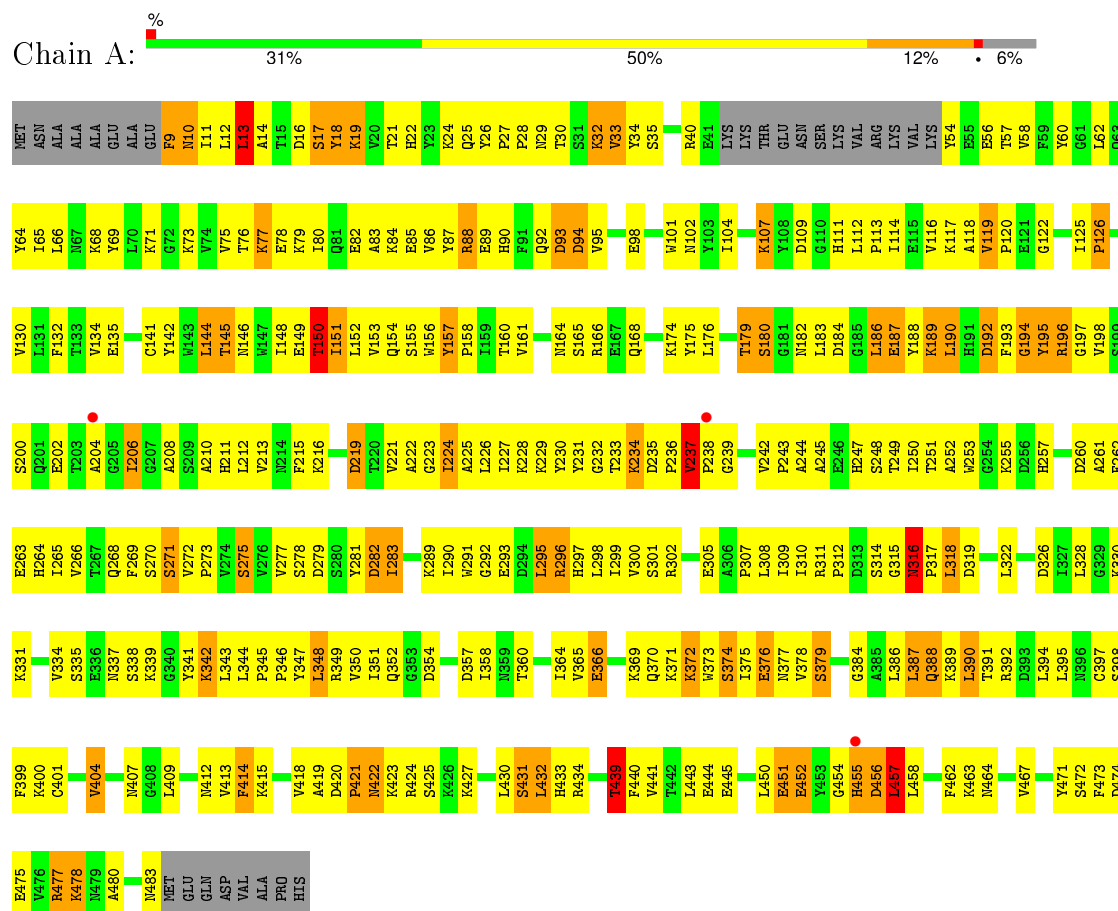


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	29	3	6		
2	B	1	Total	C	N	O	0	0
			38	29	3	6		

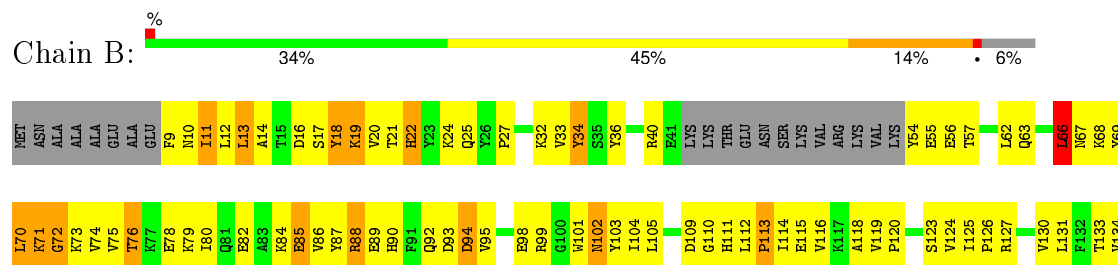
3 Residue-property plots

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: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase



K423	K424	R425	S425	K426	K427	G428	R429	L430	S431	L432	H433	T439	F440	L443	E444	E445	G446	K447	G448	D449	L450	E451	E452	Y453	G454	H455	D456	L457	L458	F462	K463	N464	K469	S470	Y471	S472	F473	D474	E475	Q481	L482	N483	MET	GLU	GLN	ASP	VAL	ALA	PRO	HIS			
K354	K355	I358	I359	T360	I364	V365	E366	G367	K368	K371	K372	W373	S374	I375	E376	I377	G378	S379	F380	G381	G384	A385	L386	D387	Q388	K389	L390	T391	R392	D393	L394	L395	S398	F399	K400	V404	V405	T406	N407	G408	L409	G410	V411	N412	V413	F414	K415	V418	A419	D420	P421	N422	
E135	M136	T137	D138	P139	E140	G141	Y142	W143	L144	T145	N146	W147	L148	E149	T150	I151	L152	V153	Q154	S155	W156	Y157	P158	V161	M164	S165	R166	E167	Q168	K169	K170	I171	L172	A173	K174	Y175	L176	T179	S180	G181	N182	L186	E187	Y188	K189	L190	Y195	R196	G197	V198	Q201	E202	T203
A204	G205	I206	H211	L212	D219	T220	V221	I224	A225	L226	I227	Y231	G232	T233	K234	D235	P236	Y237	P238	G239	V242	P243	A244	T249	I250	T251	A252	W253	K259	F262	E263	H264	I265	V266	T267	Q268	P269	V272	P273	V274	S275	V276	V277	S278	Y281	D282	I283						
A286	C287	E288	K289	I290	W291	G292	E293	D294	L295	R296	I299	V300	T304	E305	A306	P307	L308	I309	I310	R311	P312	D313	S314	L318	V321	L322	K323	V324	L325	D326	I327	L328	K331	F332	P333	V334	N337	S338	K339	G340	Y341	K342	L343	L344	P345	P346	Y347	L348	R349	V350	I351	Q352	G353

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 107.41Å 120.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 40.04 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 99.0 (40.04-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.299 0.269 , 0.282	Depositor DCC
R_{free} test set	1119 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	5 of 22195 reflections (0.023%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7476	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 56.75 % 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 2.6152e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IS1

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	0.53	2/3788 (0.1%)	0.81	4/5136 (0.1%)
1	B	0.45	0/3788	0.78	3/5136 (0.1%)
All	All	0.49	2/7576 (0.0%)	0.80	7/10272 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	LEU	CG-CD1	-7.57	1.23	1.51
1	A	432	LEU	C-O	-6.38	1.11	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	348	LEU	CA-CB-CG	5.68	128.38	115.30
1	B	66	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	455	HIS	N-CA-C	5.50	125.84	111.00
1	A	270	SER	N-CA-C	-5.41	96.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3700	0	3665	397	0
1	B	3700	0	3665	390	0
2	A	38	0	37	15	0
2	B	38	0	37	8	0
All	All	7476	0	7404	753	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 51.

The worst 5 of 753 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:432:LEU:O	1:A:457:LEU:CD1	1.90	1.19
1:A:19:LYS:HG3	1:A:22:HIS:CD2	1.80	1.15
1:A:432:LEU:O	1:A:457:LEU:HD13	1.46	1.12
1:A:148:ILE:HD13	1:A:152:LEU:HD12	1.32	1.11
1:B:179:THR:HG21	1:B:374:SER:HA	1.13	1.08

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	459/491 (94%)	372 (81%)	58 (13%)	29 (6%)	2 9
1	B	459/491 (94%)	371 (81%)	61 (13%)	27 (6%)	2 11
All	All	918/982 (94%)	743 (81%)	119 (13%)	56 (6%)	2 11

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	271	SER
1	A	282	ASP
1	B	71	LYS
1	B	72	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	408/431 (95%)	345 (85%)	63 (15%)	3	16
1	B	408/431 (95%)	343 (84%)	65 (16%)	3	15
All	All	816/862 (95%)	688 (84%)	128 (16%)	3	15

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	SER
1	B	85	GLU
1	B	429	ARG
1	A	451	GLU
1	B	18	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN
1	B	111	HIS
1	B	455	HIS
1	B	102	ASN
1	B	129	ASN

5.3.3 RNA ⓘ

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	IS1	A	501	-	38,41,41	1.43	6 (15%)	48,55,55	2.62	10 (20%)
2	IS1	B	502	-	38,41,41	1.30	6 (15%)	48,55,55	2.05	9 (18%)

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	IS1	A	501	-	-	0/23/53/53	0/4/4/4
2	IS1	B	502	-	-	0/23/53/53	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IS1	O4'-C4'	-4.99	1.33	1.45
2	B	502	IS1	CAF-CBB	-4.66	1.38	1.48
2	A	501	IS1	CAF-CBB	-4.23	1.39	1.48
2	B	502	IS1	CBD-CAG	-2.75	1.39	1.47
2	A	501	IS1	CBD-CAG	-2.59	1.39	1.47

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	501	IS1	C2'-C3'-C4'	-4.73	92.90	102.61
2	A	501	IS1	C4'-O4'-C1'	-3.45	105.92	109.72
2	A	501	IS1	CBD-CAG-CAF	-3.27	118.21	126.91
2	B	502	IS1	C4'-O4'-C1'	-3.24	106.16	109.72
2	B	502	IS1	CBD-CAG-CAF	-2.37	120.60	126.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IS1	15	0
2	B	502	IS1	8	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	463/491 (94%)	-0.05	3 (0%) 90 73	7, 33, 56, 78	0
1	B	463/491 (94%)	-0.07	3 (0%) 90 73	10, 32, 55, 79	0
All	All	926/982 (94%)	-0.06	6 (0%) 90 73	7, 33, 56, 79	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	2.8
1	A	455	HIS	2.5
1	A	238	PRO	2.3
1	A	204	ALA	2.2
1	B	294	ASP	2.1

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(\AA^2)	Q<0.9
2	IS1	A	501	38/38	0.74	0.41	4.63	54,64,87,89	0
2	IS1	B	502	38/38	0.75	0.40	4.23	56,62,78,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.