wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 01:35 PM EDT

PDB ID	:	5FFJ
Title	:	Structure of a nuclease-deletion mutant of the Type ISP restriction-modification enzyme LlaGI in complex with a DNA substrate mimic
Authors	:	Saikrishnan, K.; Kulkarni, M.; Nirwan, N.
Deposited on	:	2015-12-18
Resolution	:	2.84 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

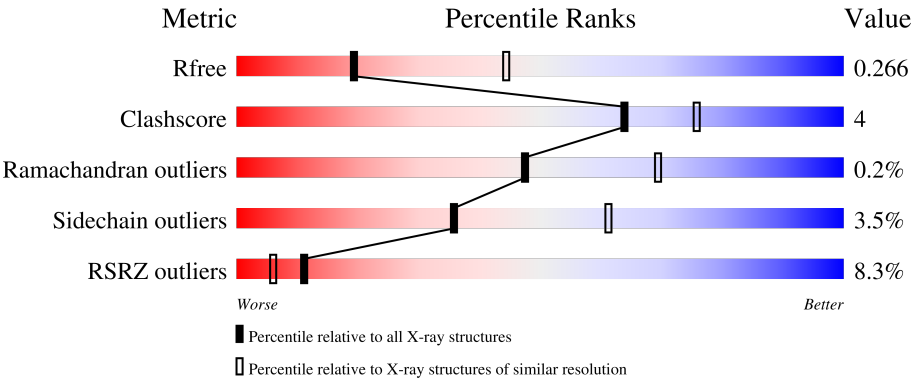
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	1406	7% 64% 10% 26%
1	B	1406	7% 78% 9% 12%
2	D	23	83% 13%
2	E	23	4% 96%
3	C	23	78% 17%

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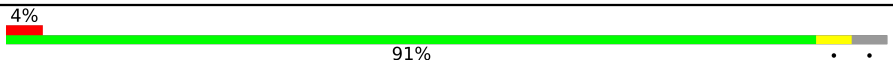
Mol	Chain	Length	Quality of chain
3	F	23	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36361 atoms, of which 17133 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 Endonuclease and methylase LlaGI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1044	Total	C	H	N	O	S	0	0	0
			15492	5077	7466	1364	1568	17			
1	B	1232	Total	C	H	N	O	S	0	0	0
			18040	5927	8659	1589	1845	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	expression tag	UNP Q93R01
B	165	MET	-	expression tag	UNP Q93R01

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP *AP*GP*TP*CP*TP*AP*TP*TP*AP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	22	Total	C	H	N	O	P	0	0	0
			688	212	251	70	134	21			
2	E	23	Total	C	H	N	O	P	0	0	0
			721	222	263	75	139	22			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*GP*CP*TP*AP*AP*TP*AP*GP *AP*CP*TP*GP*GP*AP*TP*GP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	22	Total	C	H	N	O	P	0	0	0
			709	218	248	91	130	22			
3	F	22	Total	C	H	N	O	P	0	0	0
			703	218	246	91	127	21			

- Molecule 4 is water.

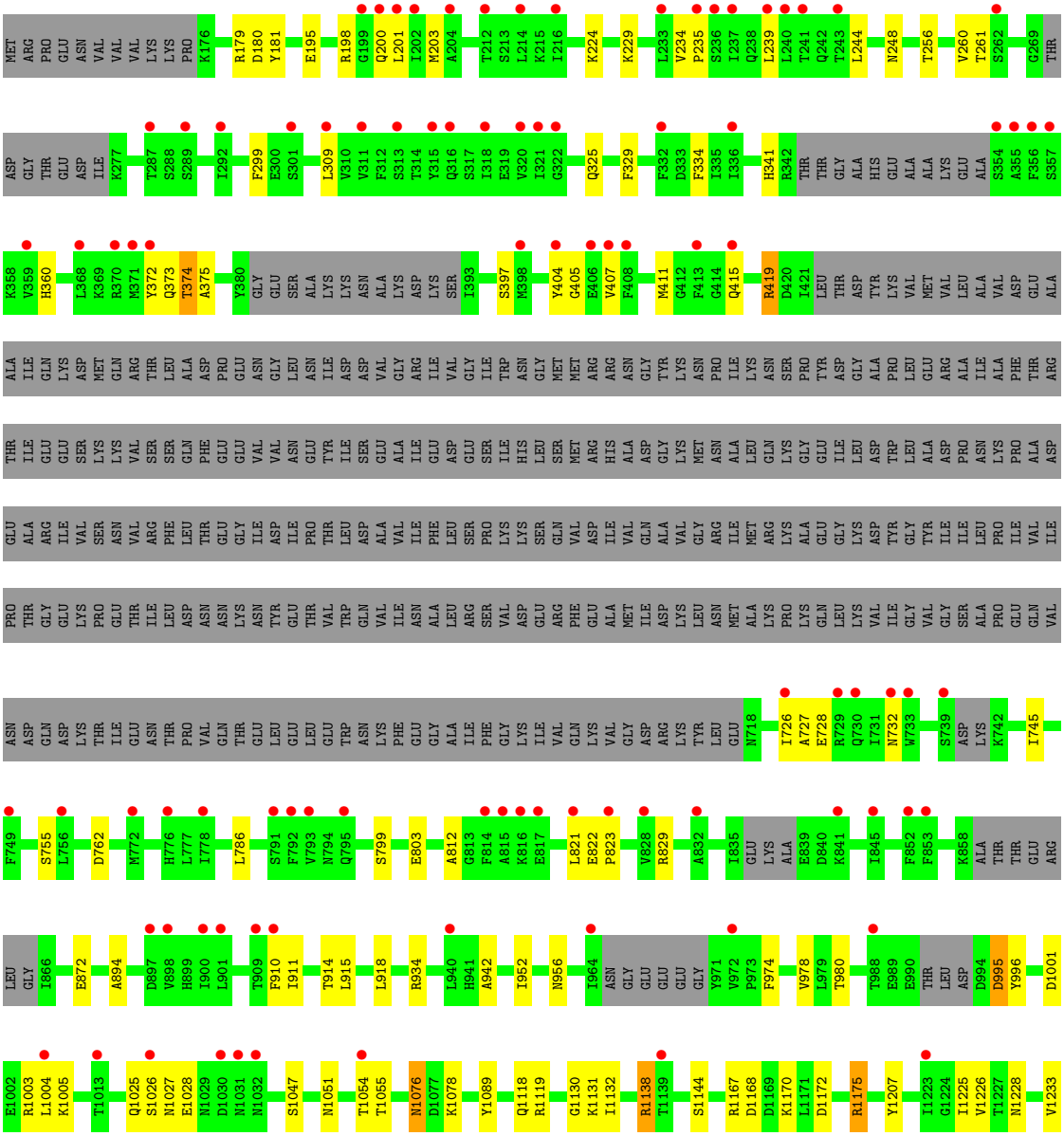
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	1	Total O 1 1	0	0

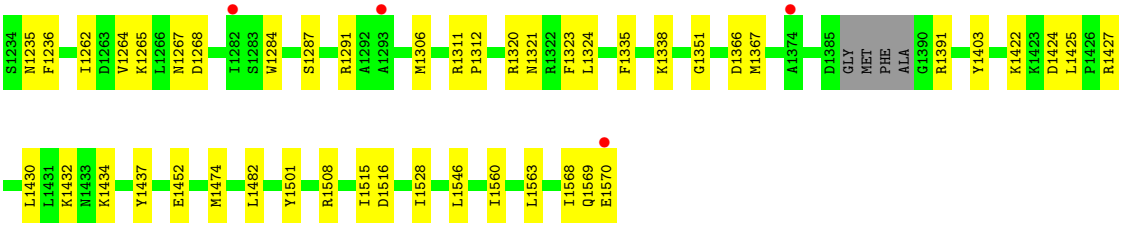
3 Residue-property plots (i)

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: Endonuclease and methylase LlaGI

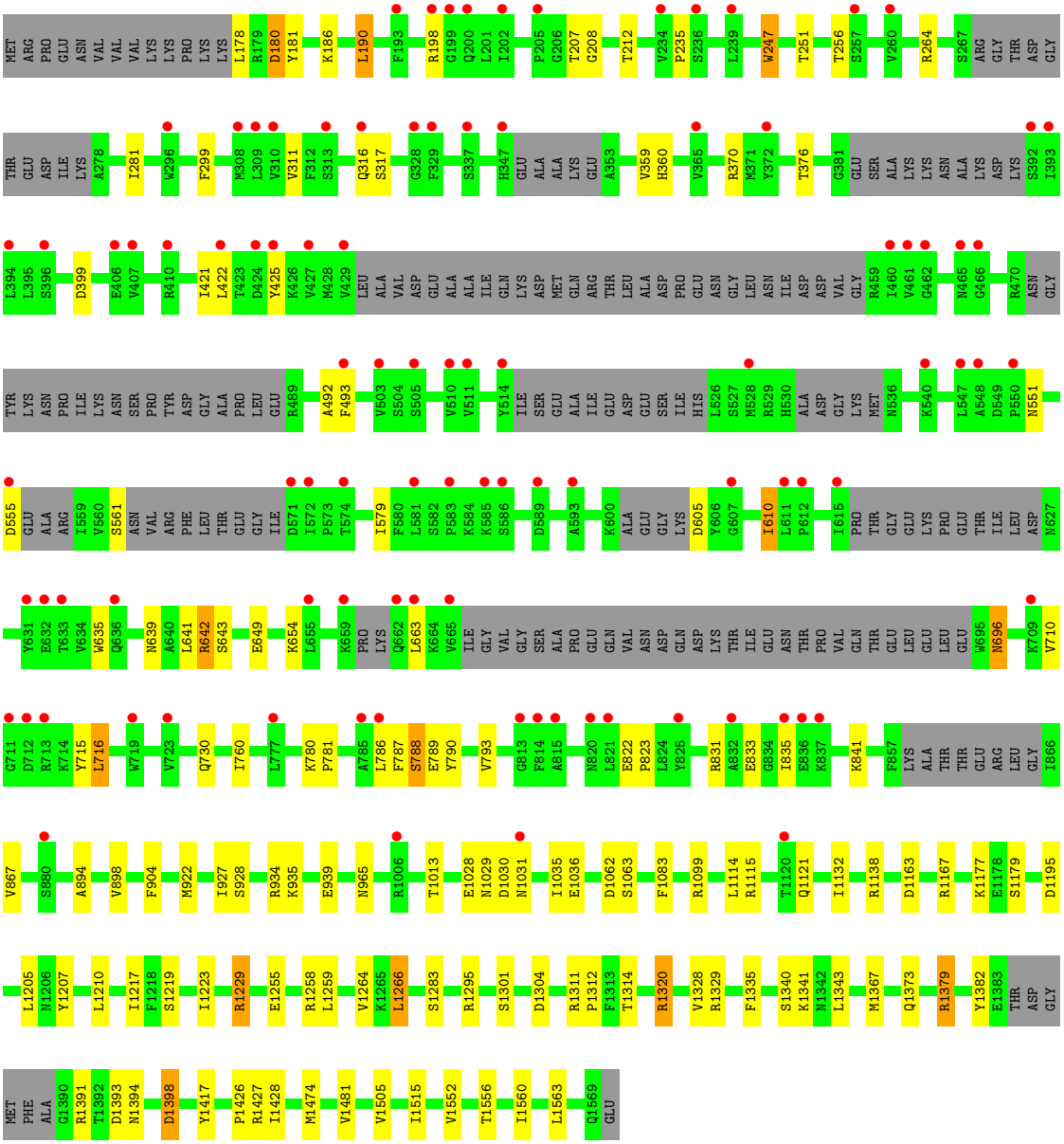
Chain A:





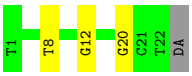
• Molecule 1: Endonuclease and methylase LlaGI

Chain B:



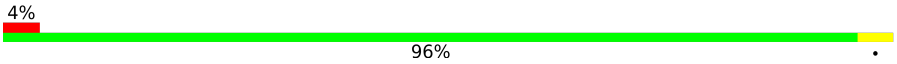
• Molecule 2: DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP*AP*GP*TP*CP*TP*AP*TP*TP*AP*GP*CP*T)-3')

Chain D:



• Molecule 2: DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP*AP*GP*TP*CP*TP*AP*TP*TP*AP*GP*CP*T)-3')

Chain E:

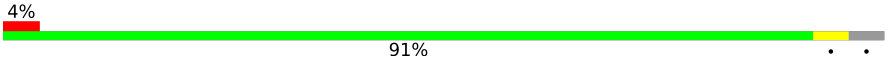


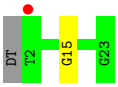
• Molecule 3: DNA (5'-D(P*TP*AP*GP*CP*TP*AP*AP*TP*AP*GP*AP*CP*TP*GP*GP*AP*TP*GP*GP*AP*GP*G)-3')

Chain C:

• Molecule 3: DNA (5'-D(P*TP*AP*GP*CP*TP*AP*AP*TP*AP*GP*AP*CP*TP*GP*GP*AP*TP*GP*GP*AP*GP*G)-3')

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.40Å 222.29Å 117.41Å 90.00° 105.14° 90.00°	Depositor
Resolution (Å)	50.00 – 2.84 84.37 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.84) 99.9 (84.37-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.229 , 0.262 0.234 , 0.266	Depositor DCC
R_{free} test set	5109 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	36361	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.24	0/8178	0.44	0/11106
1	B	0.24	0/9548	0.43	0/12967
2	D	0.67	0/486	1.05	0/746
2	E	0.66	0/510	1.05	0/783
3	C	0.58	0/519	0.99	0/801
3	F	0.59	0/515	0.98	0/796
All	All	0.30	0/19756	0.54	0/27199

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	GLN	Peptide
1	A	1026	SER	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	8026	7466	7460	77	0
1	B	9381	8659	8658	71	0
2	D	437	251	252	3	0
2	E	458	263	263	1	0
3	C	461	248	248	6	0
3	F	457	246	246	1	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
All	All	19228	17133	17127	150	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 4.

The worst 5 of 150 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:1320:ARG:NH2	1:B:1335:PHE:O	2.13	0.82
1:B:1255:GLU:OE1	1:B:1258:ARG:NH2	2.17	0.77
1:B:922:MET:HA	1:B:927:ILE:HG22	1.65	0.77
1:A:1089:TYR:OH	1:A:1144:SER:OG	2.06	0.73
1:A:198:ARG:NH1	1:A:360:HIS:O	2.25	0.70

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	1022/1406 (73%)	966 (94%)	55 (5%)	1 (0%)	51 75
1	B	1200/1406 (85%)	1152 (96%)	44 (4%)	4 (0%)	41 61
All	All	2222/2812 (79%)	2118 (95%)	99 (4%)	5 (0%)	47 69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1030	ASP
1	A	235	PRO
1	B	710	VAL
1	B	235	PRO
1	B	760	ILE

5.3.2 Protein sidechains (i)

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	826/1256 (66%)	804 (97%)	22 (3%)	44	69
1	B	949/1256 (76%)	908 (96%)	41 (4%)	29	54
All	All	1775/2512 (71%)	1712 (96%)	63 (4%)	36	61

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	311	VAL
1	B	1328	VAL
1	B	663	LEU
1	B	1320	ARG
1	B	1391	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	1044/1406 (74%)	0.72	98 (9%) 8 4	38, 84, 121, 139	0
1	B	1232/1406 (87%)	0.72	97 (7%) 12 8	34, 74, 134, 150	0
2	D	22/23 (95%)	0.55	0 100 100	44, 57, 92, 100	0
2	E	23/23 (100%)	0.77	1 (4%) 35 27	37, 54, 102, 144	0
3	C	22/23 (95%)	0.57	0 100 100	46, 53, 86, 91	0
3	F	22/23 (95%)	0.64	1 (4%) 33 25	39, 56, 89, 121	0
All	All	2365/2904 (81%)	0.72	197 (8%) 11 6	34, 76, 126, 150	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	SER	9.5
1	B	547	LEU	8.9
1	B	631	TYR	7.1
1	B	615	ILE	6.6
1	B	427	VAL	6.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.