



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 04:19 PM EDT

PDB ID : 5B4N
Title : Structure analysis of function associated loop mutant of substrate recognition domain of Fbs1 ubiquitin ligase
Authors : Nishio, K.; Yoshida, Y.; Tanaka, K.; Mizushima, T.
Deposited on : unknown
Resolution : 2.30 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
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-20029824

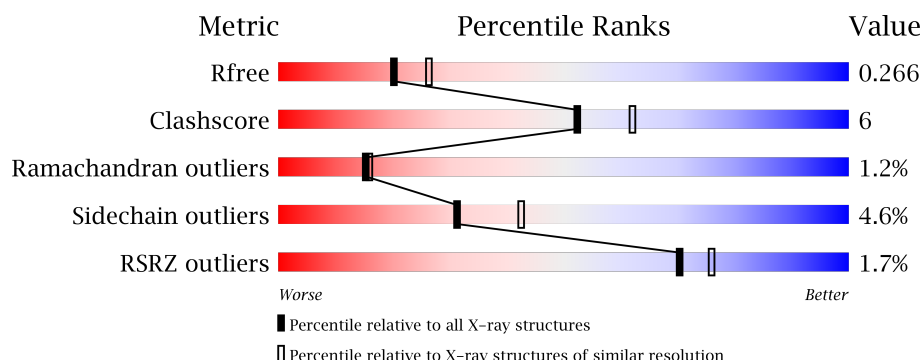
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	203	<div> <div>2%</div> <div>69%</div> <div>15%</div> <div>14%</div> </div>
1	B	203	<div> <div>%</div> <div>73%</div> <div>11%</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2955 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 F-box only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1431	907	245	276	3			
1	B	174	Total	C	N	O	S	0	0	0
			1431	907	245	276	3			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	-	initiating methionine	UNP Q80UW2
A	97	GLY	-	expression tag	UNP Q80UW2
A	98	SER	-	expression tag	UNP Q80UW2
A	99	SER	-	expression tag	UNP Q80UW2
A	100	HIS	-	expression tag	UNP Q80UW2
A	101	HIS	-	expression tag	UNP Q80UW2
A	102	HIS	-	expression tag	UNP Q80UW2
A	103	HIS	-	expression tag	UNP Q80UW2
A	104	HIS	-	expression tag	UNP Q80UW2
A	105	HIS	-	expression tag	UNP Q80UW2
A	106	SER	-	expression tag	UNP Q80UW2
A	107	SER	-	expression tag	UNP Q80UW2
A	108	GLY	-	expression tag	UNP Q80UW2
A	109	LEU	-	expression tag	UNP Q80UW2
A	110	VAL	-	expression tag	UNP Q80UW2
A	111	PRO	-	expression tag	UNP Q80UW2
A	112	ARG	-	expression tag	UNP Q80UW2
A	113	GLY	-	expression tag	UNP Q80UW2
A	114	SER	-	expression tag	UNP Q80UW2
A	115	HIS	-	expression tag	UNP Q80UW2
A	116	MET	-	expression tag	UNP Q80UW2
A	142	LEU	ASP	engineered mutation	UNP Q80UW2
A	143	ASP	VAL	engineered mutation	UNP Q80UW2
A	144	VAL	GLU	engineered mutation	UNP Q80UW2
A	145	ASN	HIS	engineered mutation	UNP Q80UW2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LYS	ARG	engineered mutation	UNP Q80UW2
A	156	SER	PRO	engineered mutation	UNP Q80UW2
A	157	ARG	GLY	engineered mutation	UNP Q80UW2
A	159	GLN	ASN	engineered mutation	UNP Q80UW2
A	160	ARG	GLY	engineered mutation	UNP Q80UW2
A	161	LYS	VAL	engineered mutation	UNP Q80UW2
A	?	-	THR	deletion	UNP Q80UW2
A	164	PRO	GLN	engineered mutation	UNP Q80UW2
A	165	ASN	ASP	engineered mutation	UNP Q80UW2
A	167	GLN	SER	engineered mutation	UNP Q80UW2
A	173	VAL	ALA	engineered mutation	UNP Q80UW2
A	174	THR	SER	engineered mutation	UNP Q80UW2
A	176	TYR	PHE	engineered mutation	UNP Q80UW2
A	177	TYR	GLU	engineered mutation	UNP Q80UW2
A	178	THR	TRP	engineered mutation	UNP Q80UW2
A	214	PRO	THR	engineered mutation	UNP Q80UW2
A	216	CYS	ALA	engineered mutation	UNP Q80UW2
A	219	LYS	LEU	engineered mutation	UNP Q80UW2
A	221	GLN	GLU	engineered mutation	UNP Q80UW2
A	238	GLN	-	insertion	UNP Q80UW2
A	239	PRO	-	insertion	UNP Q80UW2
A	240	ASP	ALA	engineered mutation	UNP Q80UW2
A	241	PRO	THR	engineered mutation	UNP Q80UW2
A	242	ALA	GLY	engineered mutation	UNP Q80UW2
A	243	THR	GLN	engineered mutation	UNP Q80UW2
A	244	ILE	VAL	engineered mutation	UNP Q80UW2
A	245	GLN	ALA	engineered mutation	UNP Q80UW2
A	246	GLN	VAL	engineered mutation	UNP Q80UW2
A	247	LYS	PRO	engineered mutation	UNP Q80UW2
A	248	SER	GLU	engineered mutation	UNP Q80UW2
A	250	ALA	GLY	engineered mutation	UNP Q80UW2
A	251	LYS	SER	engineered mutation	UNP Q80UW2
A	253	ARG	MET	engineered mutation	UNP Q80UW2
A	276	VAL	GLN	engineered mutation	UNP Q80UW2
A	278	THR	SER	engineered mutation	UNP Q80UW2
A	279	HIS	VAL	engineered mutation	UNP Q80UW2
A	282	ALA	LYS	engineered mutation	UNP Q80UW2
A	285	TYR	PHE	engineered mutation	UNP Q80UW2
A	287	PRO	ALA	engineered mutation	UNP Q80UW2
B	96	MET	-	initiating methionine	UNP Q80UW2
B	97	GLY	-	expression tag	UNP Q80UW2
B	98	SER	-	expression tag	UNP Q80UW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	SER	-	expression tag	UNP Q80UW2
B	100	HIS	-	expression tag	UNP Q80UW2
B	101	HIS	-	expression tag	UNP Q80UW2
B	102	HIS	-	expression tag	UNP Q80UW2
B	103	HIS	-	expression tag	UNP Q80UW2
B	104	HIS	-	expression tag	UNP Q80UW2
B	105	HIS	-	expression tag	UNP Q80UW2
B	106	SER	-	expression tag	UNP Q80UW2
B	107	SER	-	expression tag	UNP Q80UW2
B	108	GLY	-	expression tag	UNP Q80UW2
B	109	LEU	-	expression tag	UNP Q80UW2
B	110	VAL	-	expression tag	UNP Q80UW2
B	111	PRO	-	expression tag	UNP Q80UW2
B	112	ARG	-	expression tag	UNP Q80UW2
B	113	GLY	-	expression tag	UNP Q80UW2
B	114	SER	-	expression tag	UNP Q80UW2
B	115	HIS	-	expression tag	UNP Q80UW2
B	116	MET	-	expression tag	UNP Q80UW2
B	142	LEU	ASP	engineered mutation	UNP Q80UW2
B	143	ASP	VAL	engineered mutation	UNP Q80UW2
B	144	VAL	GLU	engineered mutation	UNP Q80UW2
B	145	ASN	HIS	engineered mutation	UNP Q80UW2
B	151	LYS	ARG	engineered mutation	UNP Q80UW2
B	156	SER	PRO	engineered mutation	UNP Q80UW2
B	157	ARG	GLY	engineered mutation	UNP Q80UW2
B	159	GLN	ASN	engineered mutation	UNP Q80UW2
B	160	ARG	GLY	engineered mutation	UNP Q80UW2
B	161	LYS	VAL	engineered mutation	UNP Q80UW2
B	?	-	THR	deletion	UNP Q80UW2
B	164	PRO	GLN	engineered mutation	UNP Q80UW2
B	165	ASN	ASP	engineered mutation	UNP Q80UW2
B	167	GLN	SER	engineered mutation	UNP Q80UW2
B	173	VAL	ALA	engineered mutation	UNP Q80UW2
B	174	THR	SER	engineered mutation	UNP Q80UW2
B	176	TYR	PHE	engineered mutation	UNP Q80UW2
B	177	TYR	GLU	engineered mutation	UNP Q80UW2
B	178	THR	TRP	engineered mutation	UNP Q80UW2
B	214	PRO	THR	engineered mutation	UNP Q80UW2
B	216	CYS	ALA	engineered mutation	UNP Q80UW2
B	219	LYS	LEU	engineered mutation	UNP Q80UW2
B	221	GLN	GLU	engineered mutation	UNP Q80UW2
B	238	GLN	-	insertion	UNP Q80UW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	239	PRO	-	insertion	UNP Q80UW2
B	240	ASP	ALA	engineered mutation	UNP Q80UW2
B	241	PRO	THR	engineered mutation	UNP Q80UW2
B	242	ALA	GLY	engineered mutation	UNP Q80UW2
B	243	THR	GLN	engineered mutation	UNP Q80UW2
B	244	ILE	VAL	engineered mutation	UNP Q80UW2
B	245	GLN	ALA	engineered mutation	UNP Q80UW2
B	246	GLN	VAL	engineered mutation	UNP Q80UW2
B	247	LYS	PRO	engineered mutation	UNP Q80UW2
B	248	SER	GLU	engineered mutation	UNP Q80UW2
B	250	ALA	GLY	engineered mutation	UNP Q80UW2
B	251	LYS	SER	engineered mutation	UNP Q80UW2
B	253	ARG	MET	engineered mutation	UNP Q80UW2
B	276	VAL	GLN	engineered mutation	UNP Q80UW2
B	278	THR	SER	engineered mutation	UNP Q80UW2
B	279	HIS	VAL	engineered mutation	UNP Q80UW2
B	282	ALA	LYS	engineered mutation	UNP Q80UW2
B	285	TYR	PHE	engineered mutation	UNP Q80UW2
B	287	PRO	ALA	engineered mutation	UNP Q80UW2

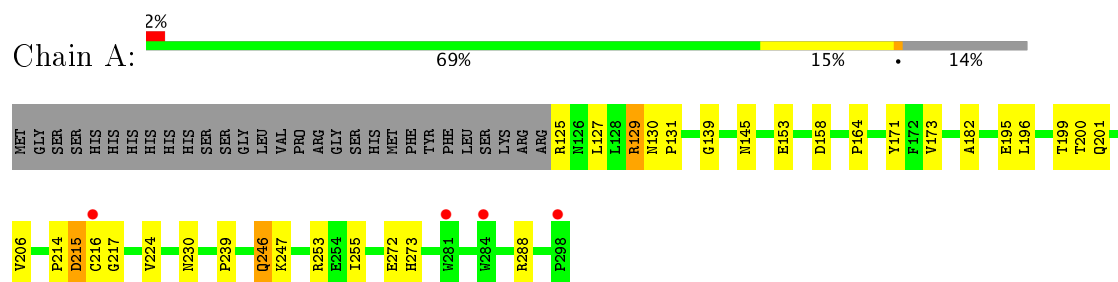
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	48	Total O 48 48	0	0
2	B	45	Total O 45 45	0	0

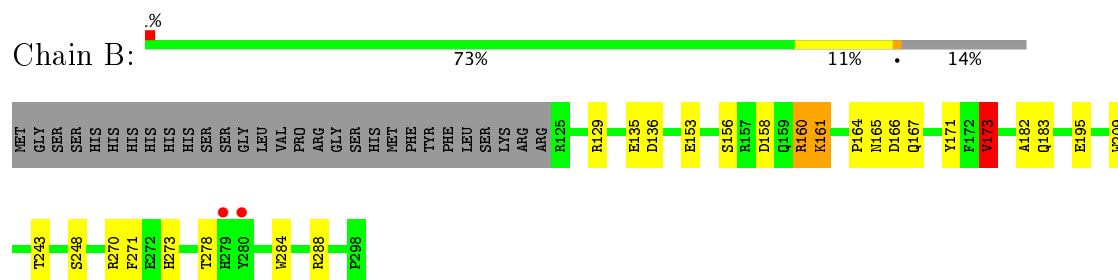
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: F-box only protein 2



- Molecule 1: F-box only protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.54Å 96.20Å 44.68Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	39.80 – 2.30 39.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.80-2.30) 99.9 (39.70-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.185 , 0.266 0.185 , 0.266	Depositor DCC
R_{free} test set	831 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 15.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.146 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2955	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.86	0/1473	0.95	4/2003 (0.2%)
1	B	0.81	0/1473	0.87	2/2003 (0.1%)
All	All	0.84	0/2946	0.91	6/4006 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	CG-CD-NE	-6.53	98.09	111.80
1	A	288	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	270	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	253	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	173	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	253	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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	1431	0	1339	21	0
1	B	1431	0	1339	14	0
2	A	48	0	0	1	0
2	B	45	0	0	1	0
All	All	2955	0	2678	35	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 6.

All (35) 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:246:GLN:H	1:A:246:GLN:CD	1.81	0.84
1:A:215:ASP:O	2:A:301:HOH:O	2.05	0.74
1:A:129:ARG:HG2	1:A:139:GLY:HA3	1.72	0.72
1:A:216:CYS:HA	1:A:246:GLN:HB3	1.74	0.68
1:A:246:GLN:N	1:A:246:GLN:CD	2.48	0.66
1:A:182:ALA:HB2	1:A:272:GLU:HG3	1.78	0.64
1:A:216:CYS:SG	1:A:217:GLY:N	2.71	0.63
1:B:173:VAL:HG13	1:B:288:ARG:HG2	1.85	0.59
1:A:195:GLU:O	1:A:199:THR:HB	2.03	0.58
1:A:206:VAL:HG11	1:A:224:VAL:HG11	1.86	0.57
1:A:214:PRO:O	1:A:215:ASP:HB2	2.05	0.56
1:B:129:ARG:H	1:B:183:GLN:HE22	1.52	0.56
1:B:160:ARG:HH21	1:B:160:ARG:HG3	1.70	0.55
1:A:216:CYS:HA	1:A:246:GLN:CB	2.41	0.50
1:B:209:TRP:NE1	2:B:301:HOH:O	2.23	0.48
1:A:196:LEU:O	1:A:200:THR:HB	2.14	0.47
1:A:145:ASN:H	1:A:145:ASN:HD22	1.63	0.47
1:B:160:ARG:HG3	1:B:160:ARG:NH2	2.30	0.47
1:B:161:LYS:NZ	1:B:161:LYS:CB	2.78	0.47
1:A:246:GLN:O	1:A:247:LYS:HG2	2.16	0.46
1:B:165:ASN:C	1:B:167:GLN:H	2.19	0.46
1:A:239:PRO:HG3	1:A:255:ILE:HD11	1.98	0.45
1:A:130:ASN:N	1:A:131:PRO:HD3	2.31	0.45
1:A:171:TYR:HE2	1:A:173:VAL:CG2	2.30	0.44
1:B:135:GLU:O	1:B:136:ASP:HB2	2.18	0.43
1:B:158:ASP:HA	1:B:161:LYS:HD3	2.01	0.43
1:B:156:SER:O	1:B:160:ARG:HG2	2.19	0.42
1:B:182:ALA:HA	1:B:271:PHE:O	2.19	0.42
1:A:171:TYR:CE2	1:A:173:VAL:CG2	3.03	0.42
1:A:125:ARG:HD2	1:A:125:ARG:HH11	1.74	0.42
1:B:153:GLU:HB2	1:B:171:TYR:CZ	2.55	0.41
1:B:243:THR:HG23	1:B:284:TRP:CZ3	2.55	0.41
1:A:246:GLN:O	1:A:247:LYS:HE3	2.21	0.41
1:A:153:GLU:HB2	1:A:171:TYR:CZ	2.57	0.40
1:B:161:LYS:HZ3	1:B:161:LYS:HB3	1.86	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	172/203 (85%)	161 (94%)	9 (5%)	2 (1%)	15	16
1	B	172/203 (85%)	159 (92%)	11 (6%)	2 (1%)	15	16
All	All	344/406 (85%)	320 (93%)	20 (6%)	4 (1%)	15	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ASP
1	B	164	PRO
1	A	164	PRO
1	B	166	ASP

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	153/179 (86%)	146 (95%)	7 (5%)	31	42
1	B	153/179 (86%)	146 (95%)	7 (5%)	31	42
All	All	306/358 (86%)	292 (95%)	14 (5%)	31	42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	129	ARG

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Mol	Chain	Res	Type
1	A	158	ASP
1	A	201	GLN
1	A	230	ASN
1	A	246	GLN
1	A	273	HIS
1	B	160	ARG
1	B	161	LYS
1	B	173	VAL
1	B	195	GLU
1	B	248	SER
1	B	273	HIS
1	B	278	THR

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	145	ASN
1	B	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	174/203 (85%)	-0.24	4 (2%) 61 67	14, 27, 60, 82	0
1	B	174/203 (85%)	-0.29	2 (1%) 80 84	15, 27, 53, 80	0
All	All	348/406 (85%)	-0.27	6 (1%) 70 76	14, 27, 56, 82	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	PRO	5.1
1	A	216	CYS	2.7
1	A	281	TRP	2.6
1	A	284	TRP	2.4
1	B	279	HIS	2.4
1	B	280	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.