Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:50 PM JST

PDB ID	:	7YA7
Title	:	The crystal structure of IpaH1.4 LRR domain
Authors	:	Hiragi, K.; Nishide, A.; Takagi, K.; Iwai, K.; Kim, M.; Mizushima, T.
Deposited on	:	2022-06-27
Resolution	:	1.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

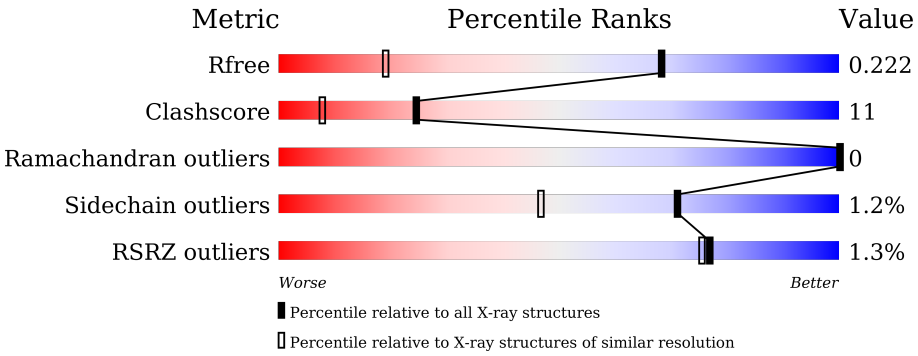
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

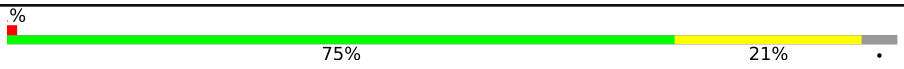
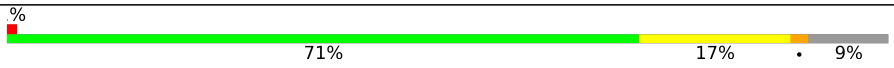
The reported resolution of this entry is 1.40 Å.

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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	243	
1	B	243	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4150 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 RING-type E3 ubiquitin transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1867	1196	321	344	6			
1	B	220	Total	C	N	O	S	0	0	0
			1754	1125	304	320	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP Q9AFJ5
A	40	PRO	-	expression tag	UNP Q9AFJ5
A	41	LEU	-	expression tag	UNP Q9AFJ5
A	42	GLY	-	expression tag	UNP Q9AFJ5
B	39	GLY	-	expression tag	UNP Q9AFJ5
B	40	PRO	-	expression tag	UNP Q9AFJ5
B	41	LEU	-	expression tag	UNP Q9AFJ5
B	42	GLY	-	expression tag	UNP Q9AFJ5

- Molecule 2 is water.

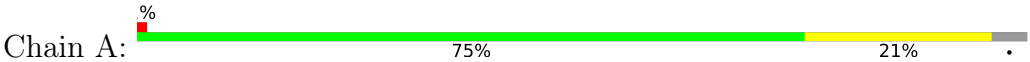
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	292	Total	O	0	0
			292	292		
2	B	237	Total	O	0	0
			237	237		

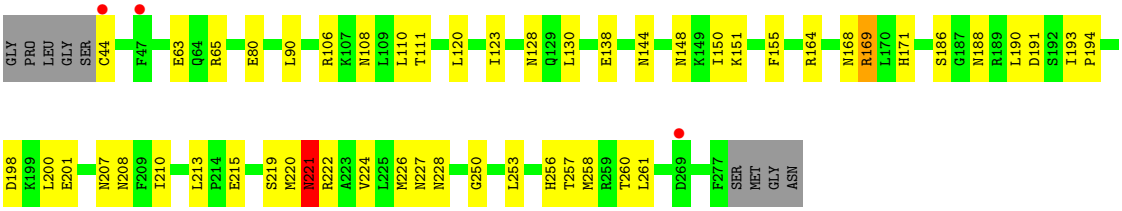
3 Residue-property plots (i)

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: RING-type E3 ubiquitin transferase

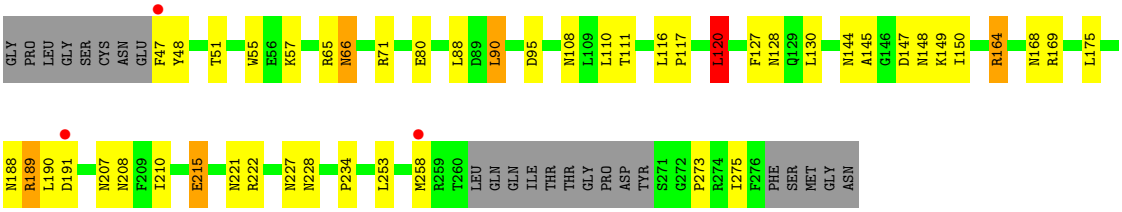
Chain A:





• Molecule 1: RING-type E3 ubiquitin transferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	33.47Å 68.04Å 100.26Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	50.00 – 1.40 33.09 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-1.40) 98.2 (33.09-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.05 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.185 , 0.220 0.186 , 0.222	Depositor DCC
R_{free} test set	4265 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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	1.41	11/1911 (0.6%)	1.27	11/2608 (0.4%)
1	B	1.45	12/1794 (0.7%)	1.30	12/2446 (0.5%)
All	All	1.43	23/3705 (0.6%)	1.29	23/5054 (0.5%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CD-OE2	9.30	1.35	1.25
1	A	215	GLU	CD-OE2	9.29	1.35	1.25
1	A	186	SER	CB-OG	-8.40	1.31	1.42
1	A	221	ASN	CB-CG	6.55	1.66	1.51
1	B	215	GLU	CD-OE2	6.41	1.32	1.25
1	B	145	ALA	CA-CB	-5.80	1.40	1.52
1	B	55	TRP	CD1-NE1	-5.79	1.28	1.38
1	A	155	PHE	CG-CD1	-5.73	1.30	1.38
1	A	215	GLU	CD-OE1	5.67	1.31	1.25
1	B	149	LYS	N-CA	5.52	1.57	1.46
1	B	169	ARG	N-CA	5.47	1.57	1.46
1	A	201	GLU	CD-OE1	-5.41	1.19	1.25
1	B	215	GLU	CD-OE1	5.33	1.31	1.25
1	B	90	LEU	N-CA	-5.30	1.35	1.46
1	A	250	GLY	C-O	5.30	1.32	1.23
1	A	219	SER	CB-OG	-5.28	1.35	1.42
1	A	63	GLU	CD-OE2	5.26	1.31	1.25
1	B	55	TRP	CG-CD1	5.26	1.44	1.36
1	B	127	PHE	C-O	5.21	1.33	1.23
1	B	147	ASP	C-O	5.14	1.33	1.23
1	A	138	GLU	CG-CD	5.09	1.59	1.51
1	A	106	ARG	CZ-NH2	-5.09	1.26	1.33
1	B	65	ARG	CZ-NH1	-5.04	1.26	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	MET	CG-SD-CE	-15.72	75.04	100.20
1	A	169	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	155	PHE	CB-CG-CD2	-8.74	114.68	120.80
1	B	65	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	65	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	55	TRP	CD1-CG-CD2	-7.42	100.36	106.30
1	A	222	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	189	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	164	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	222	ARG	CG-CD-NE	6.53	125.51	111.80
1	A	80	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	B	222	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	198	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	65	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	127	PHE	O-C-N	-5.87	113.31	122.70
1	B	120	LEU	CB-CG-CD2	5.60	120.52	111.00
1	B	189	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	120	LEU	CB-CG-CD1	5.39	120.16	111.00
1	A	200	LEU	CB-CG-CD2	5.37	120.13	111.00
1	A	213	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	95	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	155	PHE	CB-CG-CD1	5.22	124.46	120.80
1	A	65	ARG	NE-CZ-NH1	5.03	122.82	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	1867	0	1898	42	0
1	B	1754	0	1796	38	0
2	A	292	0	0	6	3
2	B	237	0	0	11	1
All	All	4150	0	3694	80	3

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 11.

All (80) 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:144:ASN:HB3	2:B:487:HOH:O	1.61	0.99
1:A:44:CYS:N	2:A:301:HOH:O	2.11	0.81
1:B:128:ASN:HB2	1:B:148:ASN:HD21	1.50	0.76
1:A:150:ILE:H	1:A:168:ASN:HD22	1.34	0.74
1:A:258:MET:HA	1:A:258:MET:HE2	1.70	0.74
1:A:208:ASN:HB2	1:A:228:ASN:HD21	1.54	0.72
1:B:108:ASN:HB2	1:B:128:ASN:HD21	1.54	0.72
1:A:120:LEU:HD21	1:A:123:ILE:HG12	1.72	0.71
1:A:128:ASN:HB2	1:A:148:ASN:HD21	1.55	0.71
1:A:108:ASN:HB2	1:A:128:ASN:HD21	1.56	0.71
1:A:256:HIS:O	1:A:260:THR:HG23	1.92	0.70
1:B:210:ILE:H	1:B:228:ASN:HD22	1.38	0.69
1:B:57:LYS:NZ	2:B:304:HOH:O	2.25	0.69
1:B:208:ASN:HB2	1:B:228:ASN:HD21	1.57	0.68
1:A:148:ASN:HB2	1:A:168:ASN:HD21	1.59	0.68
1:A:130:LEU:H	1:A:148:ASN:HD22	1.41	0.66
1:A:151:LYS:HE3	1:A:169:ARG:HD2	1.79	0.64
1:B:150:ILE:H	1:B:168:ASN:HD22	1.45	0.64
1:B:207:ASN:HD21	1:B:227:ASN:HD22	1.45	0.63
1:A:90:LEU:H	1:A:108:ASN:HD22	1.47	0.62
1:A:207:ASN:HD21	1:A:227:ASN:HD22	1.47	0.61
1:B:190:LEU:H	1:B:208:ASN:HD22	1.48	0.61
1:A:210:ILE:H	1:A:228:ASN:HD22	1.50	0.60
1:B:66:ASN:H	1:B:66:ASN:HD22	1.48	0.60
1:A:144:ASN:ND2	1:A:164:ARG:HE	1.99	0.59
1:A:221:ASN:ND2	2:A:304:HOH:O	2.33	0.59
1:A:144:ASN:HD22	1:A:164:ARG:HE	1.51	0.58
1:B:144:ASN:HD21	1:B:164:ARG:HH11	1.52	0.57
1:B:148:ASN:HB2	1:B:168:ASN:HD21	1.69	0.57
1:A:110:LEU:H	1:A:128:ASN:HD22	1.51	0.56
1:A:130:LEU:H	1:A:148:ASN:ND2	2.03	0.56
1:B:90:LEU:H	1:B:108:ASN:HD22	1.53	0.56
1:B:189:ARG:HD3	2:B:302:HOH:O	2.05	0.56
1:A:188:ASN:HB2	1:A:208:ASN:HD21	1.71	0.54
2:A:304:HOH:O	1:B:71:ARG:HG2	2.07	0.54
1:A:253:LEU:HD13	1:A:258:MET:HE1	1.90	0.53
1:B:130:LEU:H	1:B:148:ASN:HD22	1.58	0.52
1:A:258:MET:HE2	1:A:261:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HA	1:A:258:MET:CE	2.38	0.52
1:B:66:ASN:HD22	1:B:66:ASN:N	2.08	0.51
1:B:117:PRO:HD2	1:B:120:LEU:HD22	1.92	0.51
1:A:191:ASP:OD1	1:A:191:ASP:C	2.47	0.51
1:A:207:ASN:ND2	1:A:227:ASN:HD22	2.10	0.50
1:B:188:ASN:HB2	1:B:208:ASN:HD21	1.77	0.49
1:B:144:ASN:HD22	1:B:164:ARG:HB2	1.77	0.49
1:B:175:LEU:HD12	2:B:357:HOH:O	2.13	0.49
1:A:258:MET:CE	1:A:261:LEU:HD12	2.43	0.49
1:B:273:PRO:HG2	1:B:275:ILE:HD11	1.95	0.48
1:A:90:LEU:H	1:A:108:ASN:ND2	2.11	0.48
1:A:171:HIS:HD2	2:A:433:HOH:O	1.97	0.48
1:A:128:ASN:CB	1:A:148:ASN:HD21	2.25	0.47
1:B:228:ASN:O	2:B:301:HOH:O	2.20	0.47
1:A:190:LEU:H	1:A:208:ASN:HD22	1.61	0.47
1:A:111:THR:HG23	2:A:386:HOH:O	2.15	0.47
1:B:111:THR:HG23	2:B:362:HOH:O	2.16	0.45
1:B:253:LEU:O	1:B:258:MET:HE3	2.17	0.45
1:A:253:LEU:HD13	1:A:258:MET:CE	2.46	0.45
1:A:120:LEU:HD21	1:A:123:ILE:CG1	2.44	0.45
1:B:234:PRO:HA	2:B:313:HOH:O	2.15	0.45
1:B:144:ASN:HB3	2:B:392:HOH:O	2.15	0.45
1:A:257:THR:HG22	1:A:258:MET:HE3	1.99	0.45
1:A:120:LEU:CD2	1:A:123:ILE:CG1	2.96	0.44
1:A:44:CYS:CA	2:A:301:HOH:O	2.64	0.44
1:B:207:ASN:ND2	1:B:227:ASN:HD22	2.14	0.44
1:B:144:ASN:ND2	1:B:164:ARG:HH11	2.14	0.44
1:B:90:LEU:H	1:B:108:ASN:ND2	2.15	0.43
1:A:120:LEU:CD2	1:A:123:ILE:HG12	2.46	0.43
1:A:193:ILE:HG13	1:A:194:PRO:HD2	1.99	0.43
1:B:128:ASN:CB	1:B:148:ASN:HD21	2.27	0.43
1:A:224:VAL:HG13	1:A:226:MET:SD	2.59	0.42
1:A:253:LEU:CD1	1:A:258:MET:HE1	2.50	0.42
1:B:110:LEU:H	1:B:128:ASN:HD22	1.68	0.41
1:B:221:ASN:HB2	2:B:306:HOH:O	2.19	0.41
1:B:48:TYR:O	1:B:51:THR:HG22	2.20	0.41
1:B:116:LEU:HA	1:B:117:PRO:HD3	2.00	0.41
1:A:120:LEU:HD23	1:A:123:ILE:HD11	2.03	0.40
1:A:221:ASN:HB2	2:B:491:HOH:O	2.21	0.40
1:B:190:LEU:H	1:B:208:ASN:ND2	2.15	0.40
1:B:215:GLU:HG2	2:B:461:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:H	1:B:108:ASN:HD21	1.70	0.40

All (3) 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)
2:A:458:HOH:O	2:B:481:HOH:O[1_455]	2.09	0.11
2:A:315:HOH:O	2:A:540:HOH:O[1_545]	2.10	0.10
2:A:305:HOH:O	2:A:401:HOH:O[2_656]	2.11	0.09

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	232/243 (96%)	219 (94%)	13 (6%)	0	100	100
1	B	216/243 (89%)	202 (94%)	14 (6%)	0	100	100
All	All	448/486 (92%)	421 (94%)	27 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	214/220 (97%)	213 (100%)	1 (0%)	88	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	201/220 (91%)	197 (98%)	4 (2%)	55 23
All	All	415/440 (94%)	410 (99%)	5 (1%)	71 47

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	47	PHE
1	B	66	ASN
1	B	120	LEU
1	B	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	128	ASN
1	A	144	ASN
1	A	148	ASN
1	A	159	ASN
1	A	168	ASN
1	A	171	HIS
1	A	207	ASN
1	A	208	ASN
1	A	228	ASN
1	A	243	ASN
1	A	262	GLN
1	B	66	ASN
1	B	79	GLN
1	B	108	ASN
1	B	128	ASN
1	B	144	ASN
1	B	148	ASN
1	B	168	ASN
1	B	207	ASN
1	B	208	ASN
1	B	228	ASN

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 monosaccharides 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

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	234/243 (96%)	-0.01	3 (1%)	77	75	6, 13, 27, 38	0
1	B	220/243 (90%)	0.13	3 (1%)	75	74	8, 18, 31, 41	0
All	All	454/486 (93%)	0.06	6 (1%)	77	75	6, 15, 30, 41	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	PHE	4.3
1	A	44	CYS	3.3
1	A	269	ASP	2.9
1	B	258	MET	2.9
1	A	47	PHE	2.5
1	B	191	ASP	2.5

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.