



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:02 PM UTC

PDB ID : 6JG5 / pdb_00006jg5
Title : Crystal structure of AimR
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Deposited on : 2019-02-13
Resolution : 2.22 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

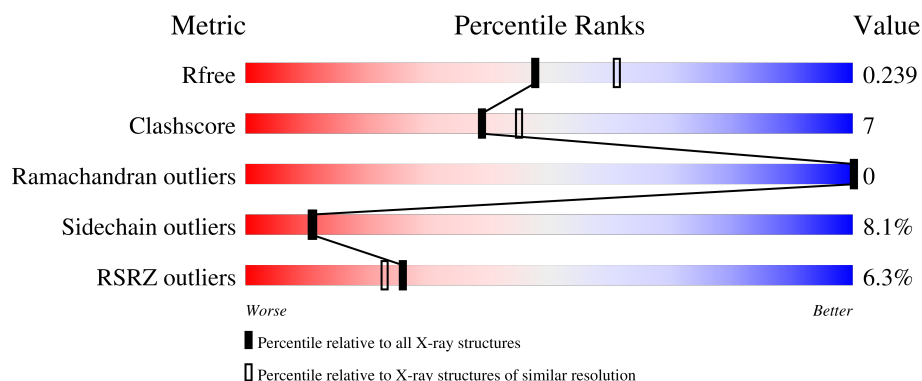
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 $\leq 5\%$. 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	395	11% 80% 16% ..
1	B	395	2% 80% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6753 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 AimR transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3214	2051	534	608	21			
1	B	390	Total	C	N	O	S	0	0	0
			3210	2048	533	608	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O64094
A	387	LEU	-	expression tag	UNP O64094
A	388	GLU	-	expression tag	UNP O64094
A	389	HIS	-	expression tag	UNP O64094
A	390	HIS	-	expression tag	UNP O64094
A	391	HIS	-	expression tag	UNP O64094
A	392	HIS	-	expression tag	UNP O64094
A	393	HIS	-	expression tag	UNP O64094
A	394	HIS	-	expression tag	UNP O64094
B	0	MET	-	initiating methionine	UNP O64094
B	387	LEU	-	expression tag	UNP O64094
B	388	GLU	-	expression tag	UNP O64094
B	389	HIS	-	expression tag	UNP O64094
B	390	HIS	-	expression tag	UNP O64094
B	391	HIS	-	expression tag	UNP O64094
B	392	HIS	-	expression tag	UNP O64094
B	393	HIS	-	expression tag	UNP O64094
B	394	HIS	-	expression tag	UNP O64094

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		

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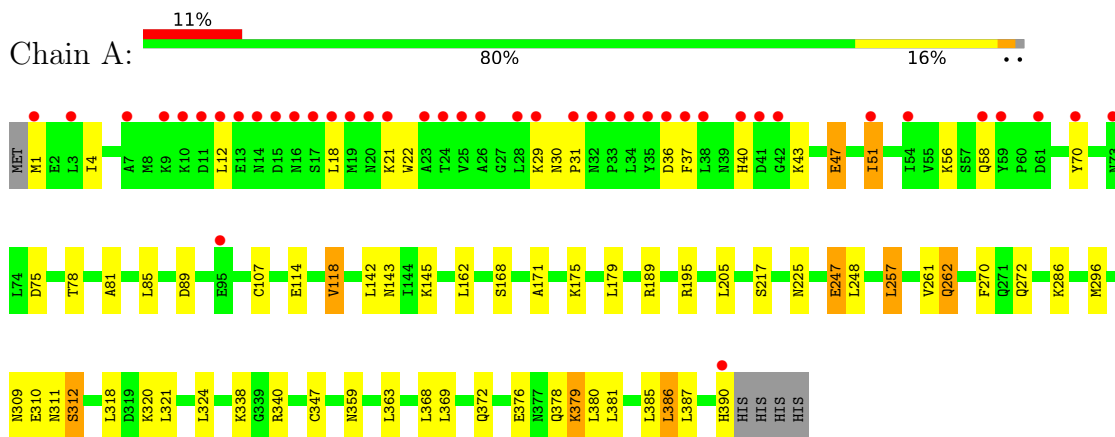
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	175	Total	O	0	0
			175	175		

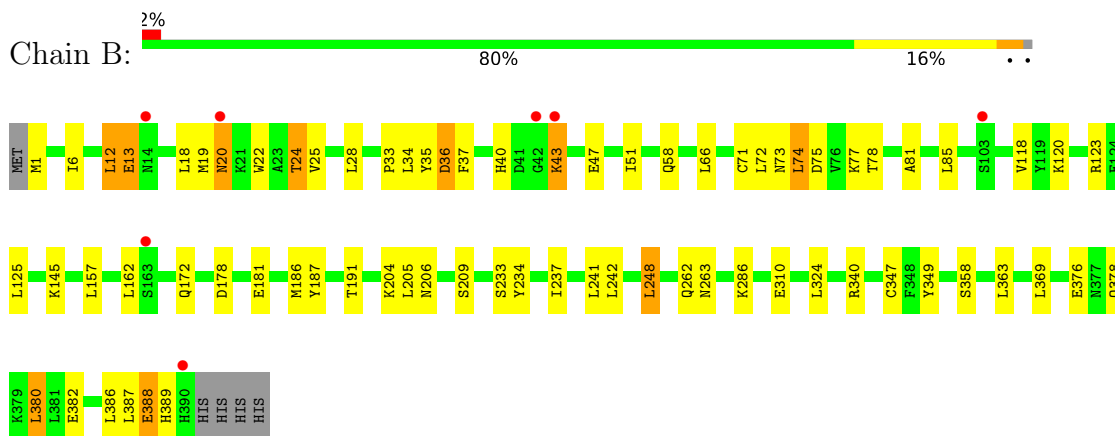
3 Residue-property plots [i](#)

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: AimR transcriptional regulator



- Molecule 1: AimR transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 219.43Å 33.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 2.22 49.54 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.54-2.22) 98.9 (49.54-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.14rc3_3206: ???)	Depositor
R, R_{free}	0.196 , 0.239 0.198 , 0.239	Depositor DCC
R_{free} test set	2119 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6753	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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	0.45	3/3272 (0.1%)	0.55	1/4402 (0.0%)
1	B	0.37	1/3268 (0.0%)	0.55	0/4398
All	All	0.41	4/6540 (0.1%)	0.55	1/8800 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	ASN	C-O	-5.86	1.17	1.24
1	A	312	SER	C-O	-5.72	1.17	1.24
1	A	347	CYS	CB-SG	5.59	1.99	1.81
1	B	347	CYS	CB-SG	5.35	1.98	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	GLU	CB-CA-C	5.27	120.02	112.12

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	3214	0	3205	49	1
1	B	3210	0	3194	41	1
2	A	154	0	0	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	175	0	0	12	2
All	All	6753	0	6399	87	4

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 7.

All (87) 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:31:PRO:HB2	2:A:403:HOH:O	1.18	1.32
1:B:13:GLU:HG3	2:B:401:HOH:O	1.41	1.19
1:B:13:GLU:N	2:B:401:HOH:O	1.86	1.07
1:B:37:PHE:HA	1:B:43:LYS:HE3	1.43	0.98
1:A:40:HIS:O	2:A:401:HOH:O	1.81	0.95
1:B:234:TYR:OH	2:B:403:HOH:O	1.87	0.93
1:B:123:ARG:NH1	2:B:406:HOH:O	2.03	0.90
1:A:390:HIS:O	2:A:402:HOH:O	1.94	0.86
1:A:43:LYS:HB3	2:A:401:HOH:O	1.77	0.82
1:A:320:LYS:NZ	2:A:404:HOH:O	2.10	0.82
1:B:36:ASP:OD2	2:B:404:HOH:O	1.98	0.81
1:B:209:SER:OG	2:B:402:HOH:O	1.86	0.81
1:B:204:LYS:NZ	2:B:408:HOH:O	2.08	0.80
1:B:181:GLU:OE2	2:B:405:HOH:O	2.03	0.77
1:A:31:PRO:O	2:A:403:HOH:O	2.05	0.74
1:B:178:ASP:OD2	2:B:407:HOH:O	2.06	0.74
1:A:78:THR:HG23	1:A:81:ALA:H	1.55	0.71
1:A:75:ASP:O	1:A:78:THR:HG22	1.96	0.65
1:B:40:HIS:HB2	1:B:43:LYS:NZ	2.14	0.63
1:A:56:LYS:HE2	1:A:225:ASN:O	1.99	0.62
1:B:12:LEU:HD11	1:B:19:MET:HE2	1.81	0.62
1:A:4:ILE:HG22	2:A:431:HOH:O	1.99	0.62
1:A:56:LYS:NZ	2:A:407:HOH:O	2.33	0.61
1:B:1:MET:HE3	1:B:6:ILE:HG12	1.83	0.61
1:A:143:ASN:OD1	1:A:145:LYS:NZ	2.33	0.61
1:B:71:CYS:HA	1:B:74:LEU:HD22	1.84	0.60
1:A:380:LEU:HD21	1:B:380:LEU:HD21	1.84	0.60
1:B:28:LEU:HD13	1:B:33:PRO:HG2	1.85	0.59
1:A:31:PRO:C	2:A:403:HOH:O	2.42	0.59
1:A:247:GLU:H	1:A:247:GLU:CD	2.11	0.57
1:B:349:TYR:OH	1:B:376:GLU:OE1	2.09	0.57
1:B:43:LYS:NZ	1:B:43:LYS:HB3	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:OD2	1:A:195:ARG:NH2	2.39	0.55
1:B:36:ASP:O	1:B:43:LYS:NZ	2.29	0.55
1:A:37:PHE:HA	1:A:43:LYS:HG2	1.88	0.55
1:B:78:THR:HG23	1:B:81:ALA:H	1.72	0.55
1:A:43:LYS:CB	2:A:401:HOH:O	2.42	0.54
1:A:22:TRP:HE1	1:A:58:GLN:HG3	1.72	0.54
1:A:114:GLU:O	1:A:118:VAL:HG13	2.08	0.54
1:B:22:TRP:NE1	1:B:58:GLN:OE1	2.35	0.52
1:A:379:LYS:NZ	2:A:412:HOH:O	2.43	0.52
1:A:40:HIS:C	2:A:401:HOH:O	2.42	0.51
1:B:36:ASP:HB3	1:B:43:LYS:HD3	1.93	0.50
1:A:40:HIS:HB2	2:A:401:HOH:O	2.12	0.50
1:B:37:PHE:CA	1:B:43:LYS:HE3	2.30	0.50
1:B:19:MET:HE3	1:B:35:TYR:CZ	2.46	0.49
1:B:18:LEU:HD13	1:B:58:GLN:HE22	1.77	0.49
1:A:272:GLN:HB3	1:A:296:MET:HE2	1.94	0.48
1:B:78:THR:CG2	1:B:81:ALA:H	2.27	0.48
1:B:263:ASN:HB2	2:B:440:HOH:O	2.14	0.47
1:A:168:SER:HA	1:A:359:ASN:HD22	1.79	0.47
1:B:241:LEU:HD13	1:B:248:LEU:HB3	1.96	0.46
1:B:187:TYR:O	1:B:191:THR:HG23	2.16	0.46
1:A:257:LEU:HD13	1:A:270:PHE:HB2	1.97	0.46
1:B:75:ASP:O	1:B:78:THR:HG22	2.16	0.46
1:B:20:ASN:O	1:B:24:THR:HG22	2.16	0.46
1:B:40:HIS:HB2	1:B:43:LYS:HZ3	1.78	0.46
1:A:22:TRP:NE1	1:A:58:GLN:HG3	2.30	0.46
1:B:13:GLU:CG	2:B:401:HOH:O	2.25	0.45
1:A:368:LEU:HD11	1:A:385:LEU:HD21	1.98	0.44
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.82	0.43
1:A:386:LEU:HD11	1:B:389:HIS:CD2	2.53	0.43
1:B:388:GLU:HG2	1:B:389:HIS:N	2.33	0.43
1:A:262:GLN:H	1:A:262:GLN:CD	2.25	0.43
1:A:171:ALA:O	1:A:175:LYS:HG3	2.19	0.43
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.56	0.43
1:A:37:PHE:HA	1:A:43:LYS:CG	2.47	0.43
1:A:29:LYS:O	1:A:30:ASN:HB3	2.19	0.42
1:A:51:ILE:H	1:A:51:ILE:HG13	1.39	0.42
1:A:30:ASN:HA	1:A:31:PRO:HD3	1.87	0.42
1:B:186:MET:HA	1:B:186:MET:HE2	2.01	0.42
1:A:47:GLU:OE1	1:A:47:GLU:HA	2.17	0.42
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:SER:O	1:B:237:ILE:HG13	2.20	0.42
1:A:1:MET:N	2:A:415:HOH:O	2.52	0.42
1:A:51:ILE:HD13	1:A:70:TYR:CE2	2.55	0.42
1:B:47:GLU:HA	2:B:413:HOH:O	2.20	0.42
1:A:36:ASP:HB3	1:A:43:LYS:HE2	2.01	0.41
1:A:378:GLN:HG3	2:A:426:HOH:O	2.19	0.41
1:B:378:GLN:O	1:B:382:GLU:HG3	2.20	0.41
1:B:77:LYS:NZ	1:B:77:LYS:HB2	2.35	0.41
1:A:318:LEU:HD23	1:A:321:LEU:HD12	2.02	0.41
1:A:387:LEU:HB3	1:B:387:LEU:HB3	2.03	0.41
1:A:18:LEU:HD23	1:A:21:LYS:HD2	2.03	0.41
1:A:22:TRP:HE1	1:A:58:GLN:CG	2.33	0.41
1:A:372:GLN:HG3	1:A:381:LEU:HD13	2.02	0.41
1:A:376:GLU:HG3	1:A:380:LEU:HD12	2.03	0.40

All (4) 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:443:HOH:O	2:A:513:HOH:O[1_556]	2.05	0.15
1:B:120:LYS:NZ	2:B:407:HOH:O[1_556]	2.06	0.14
1:A:142:LEU:O	1:A:312:SER:OG[4_554]	2.18	0.02
2:B:517:HOH:O	2:B:571:HOH:O[2_555]	2.18	0.02

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	388/395 (98%)	379 (98%)	9 (2%)	0	100	100
1	B	388/395 (98%)	380 (98%)	8 (2%)	0	100	100
All	All	776/790 (98%)	759 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	363/369 (98%)	339 (93%)	24 (7%)	15	17
1	B	362/369 (98%)	327 (90%)	35 (10%)	8	7
All	All	725/738 (98%)	666 (92%)	59 (8%)	11	11

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	51	ILE
1	A	85	LEU
1	A	107	CYS
1	A	118	VAL
1	A	162	LEU
1	A	179	LEU
1	A	189	ARG
1	A	205	LEU
1	A	217	SER
1	A	247	GLU
1	A	248	LEU
1	A	257	LEU
1	A	261	VAL
1	A	262	GLN
1	A	286	LYS
1	A	309	ASN
1	A	324	LEU
1	A	338	LYS
1	A	340	ARG
1	A	363	LEU
1	A	369	LEU
1	A	379	LYS
1	A	386	LEU
1	B	12	LEU

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Mol	Chain	Res	Type
1	B	13	GLU
1	B	20	ASN
1	B	24	THR
1	B	25	VAL
1	B	34	LEU
1	B	36	ASP
1	B	43	LYS
1	B	51	ILE
1	B	66	LEU
1	B	72	LEU
1	B	73	ASN
1	B	74	LEU
1	B	85	LEU
1	B	118	VAL
1	B	125	LEU
1	B	145	LYS
1	B	157	LEU
1	B	162	LEU
1	B	172	GLN
1	B	205	LEU
1	B	206	ASN
1	B	242	LEU
1	B	248	LEU
1	B	262	GLN
1	B	286	LYS
1	B	310	GLU
1	B	324	LEU
1	B	340	ARG
1	B	358	SER
1	B	363	LEU
1	B	369	LEU
1	B	380	LEU
1	B	386	LEU
1	B	388	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	32	ASN
1	A	127	ASN
1	A	160	HIS

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Mol	Chain	Res	Type
1	A	197	HIS
1	A	265	ASN
1	A	343	GLN
1	A	359	ASN
1	A	372	GLN
1	A	378	GLN
1	B	46	ASN
1	B	160	HIS
1	B	197	HIS
1	B	206	ASN
1	B	252	ASN
1	B	262	GLN
1	B	278	ASN

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 oligosaccharides 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, 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	390/395 (98%)	0.20	42 (10%) 11 8	16, 35, 95, 131	0
1	B	390/395 (98%)	-0.02	7 (1%) 67 65	16, 33, 61, 93	0
All	All	780/790 (98%)	0.09	49 (6%) 26 23	16, 34, 80, 131	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	TYR	5.2
1	B	390	HIS	4.0
1	A	29	LYS	3.9
1	A	18	LEU	3.6
1	A	12	LEU	3.5
1	A	14	ASN	3.5
1	A	40	HIS	3.4
1	A	61	ASP	3.4
1	B	42	GLY	3.3
1	A	390	HIS	3.3
1	A	20	ASN	3.2
1	A	1	MET	3.2
1	A	15	ASP	3.1
1	A	9	LYS	3.0
1	A	38	LEU	3.0
1	A	17	SER	3.0
1	A	51	ILE	2.9
1	A	31	PRO	2.8
1	A	16	ASN	2.7
1	A	7	ALA	2.6
1	B	14	ASN	2.6
1	A	59	TYR	2.6
1	A	11	ASP	2.5
1	B	43	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	ASP	2.5
1	A	23	ALA	2.4
1	A	26	ALA	2.4
1	A	21	LYS	2.4
1	A	34	LEU	2.4
1	A	42	GLY	2.4
1	A	24	THR	2.4
1	A	95	GLU	2.3
1	A	33	PRO	2.3
1	A	19	MET	2.3
1	A	3	LEU	2.3
1	B	163	SER	2.2
1	A	41	ASP	2.2
1	A	54	ILE	2.2
1	A	32	ASN	2.2
1	A	13	GLU	2.2
1	A	28	LEU	2.1
1	B	103	SER	2.1
1	A	70	TYR	2.1
1	A	73	ASN	2.1
1	B	20	ASN	2.1
1	A	25	VAL	2.1
1	A	37	PHE	2.1
1	A	58	GLN	2.1
1	A	10	LYS	2.0

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 oligosaccharides 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.