Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:19 am BST

PDB ID	:	5JXR
Title	:	Crystal structure of MtISWI
Authors	:	Chen, Z.; Yan, L.
Deposited on	:	2016-05-13
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

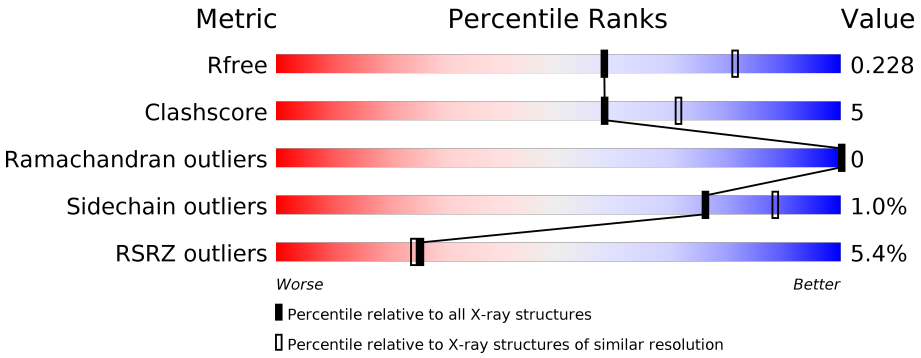
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	723	5% 76% 10% 14%
1	B	723	4% 76% 10% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10454 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 Chromatin-remodeling complex ATPase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			5049	3181	902	947	19			
1	B	625	Total	C	N	O	S	0	0	0
			5049	3181	902	947	19			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

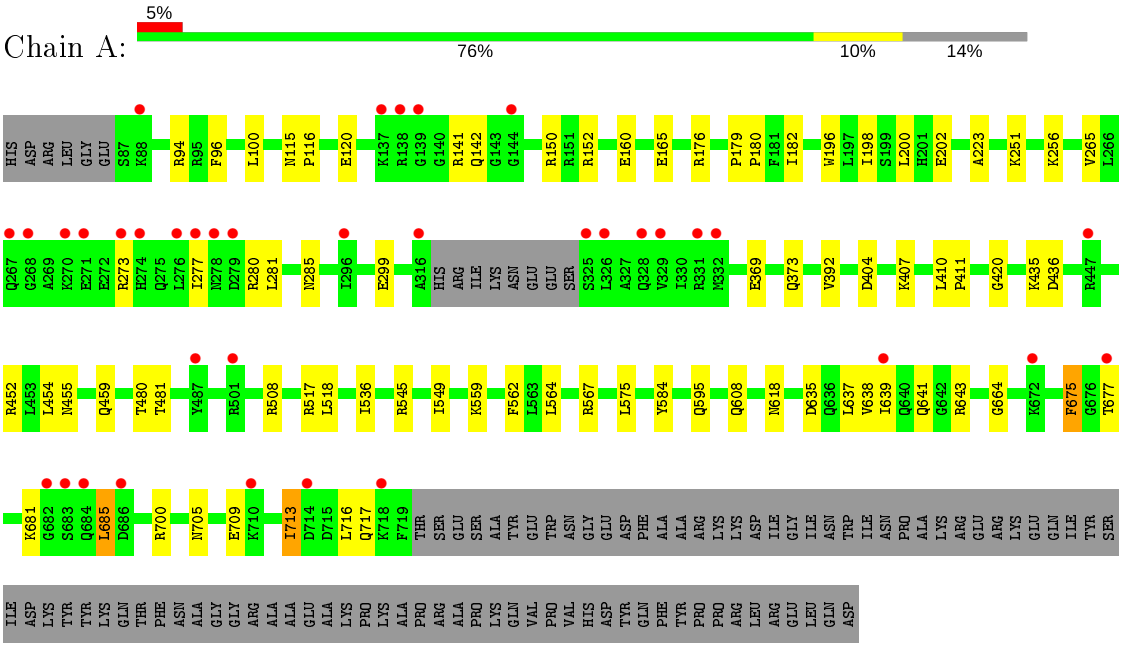
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	172	Total	O	0	0
			172	172		

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.

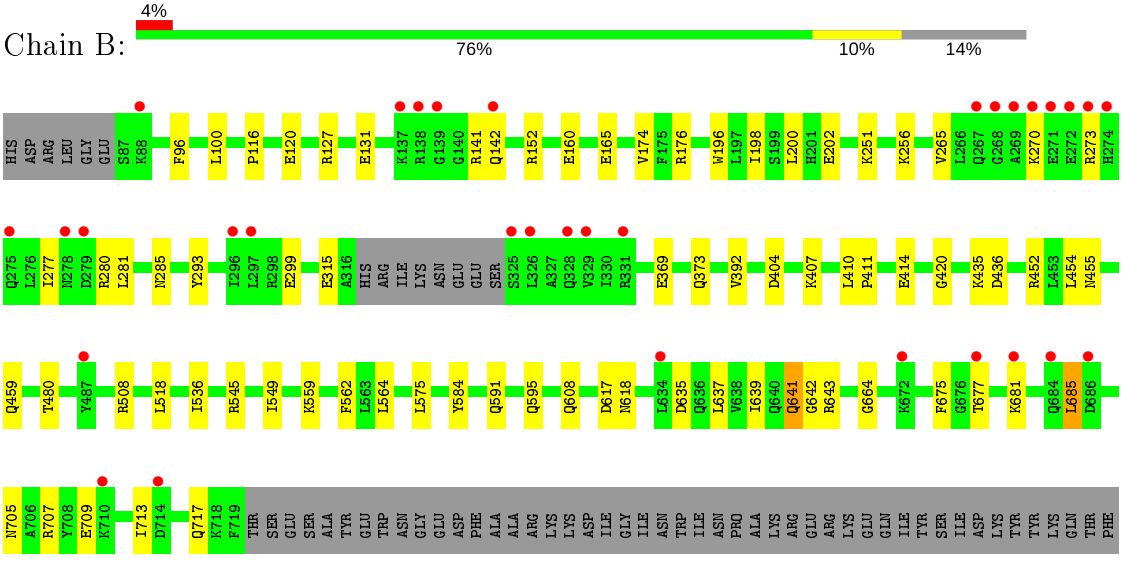
- Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain A:



- Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain B:



ASN ALA GLY GLY ARG ALA ALA GLU ALA LYS PRO LYS ALA PRO ARG ALA PRO LYS GLN VAL PRO VAL HIS ASP TYR GLN PHE TYR PRO PRO ARG LEU ARG GLU LEU GLN ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	127.77Å 127.77Å 106.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.91 – 2.40 32.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.91-2.40) 94.6 (32.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.195 , 0.226 0.196 , 0.228	Depositor DCC
R_{free} test set	3770 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.031 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10454	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.26	0/5134	0.45	0/6914
1	B	0.26	0/5134	0.44	0/6914
All	All	0.26	0/10268	0.44	0/13828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5049	0	5066	55	0
1	B	5049	0	5066	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	182	0	0	6	0
3	B	172	0	0	7	0
All	All	10454	0	10132	97	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 5.

All (97) 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:638:VAL:HG12	1:B:641:GLN:HG3	1.52	0.90
1:A:641:GLN:NE2	1:B:641:GLN:OE1	2.06	0.88
1:B:411:PRO:O	1:B:608:GLN:NE2	2.25	0.68
1:A:411:PRO:O	1:A:608:GLN:NE2	2.28	0.67
1:B:414:GLU:OE1	3:B:1101:HOH:O	2.12	0.66
1:A:256:LYS:NZ	3:A:1103:HOH:O	2.29	0.65
1:B:641:GLN:HG2	1:B:642:GLY:N	2.12	0.64
1:B:280:ARG:HA	1:B:285:ASN:HB3	1.80	0.64
1:A:94:ARG:NH2	3:A:1107:HOH:O	2.33	0.61
1:A:280:ARG:HA	1:A:285:ASN:HB3	1.82	0.61
1:B:435:LYS:NZ	3:B:1108:HOH:O	2.34	0.61
1:A:639:ILE:O	1:A:643:ARG:HG3	2.02	0.60
1:A:435:LYS:NZ	3:A:1109:HOH:O	2.33	0.60
1:A:508:ARG:NH1	1:A:559:LYS:O	2.32	0.59
1:A:595:GLN:NE2	3:A:1106:HOH:O	2.35	0.58
1:A:176:ARG:NH2	1:A:635:ASP:OD1	2.36	0.58
1:B:518:LEU:HD21	1:B:584:TYR:CD1	2.38	0.58
1:A:369:GLU:OE2	1:A:373:GLN:NE2	2.35	0.58
1:B:707:ARG:NH1	3:B:1114:HOH:O	2.37	0.58
1:B:369:GLU:OE2	1:B:373:GLN:NE2	2.37	0.56
1:B:176:ARG:NH2	1:B:635:ASP:OD1	2.39	0.56
1:B:595:GLN:NE2	3:B:1105:HOH:O	2.39	0.56
1:A:436:ASP:OD2	1:A:452:ARG:NH2	2.39	0.56
1:A:641:GLN:HG3	1:A:713:ILE:HD13	1.86	0.56
1:A:641:GLN:HG2	1:A:713:ILE:HG21	1.87	0.55
1:B:251:LYS:HE2	1:B:265:VAL:HG21	1.89	0.55
1:B:518:LEU:HD21	1:B:584:TYR:CE1	2.41	0.54
1:B:436:ASP:OD2	1:B:452:ARG:NH2	2.40	0.54
1:A:713:ILE:HG23	1:B:637:LEU:HD13	1.90	0.54
1:B:152:ARG:O	3:B:1102:HOH:O	2.19	0.51
1:A:251:LYS:HE2	1:A:265:VAL:HG21	1.93	0.51
1:A:142:GLN:HB2	1:A:480:THR:HG22	1.93	0.51
1:B:277:ILE:HA	1:B:281:LEU:HB3	1.93	0.51
1:A:517:ARG:NH1	3:A:1118:HOH:O	2.43	0.50
1:A:165:GLU:HB3	1:A:454:LEU:HD22	1.94	0.49
1:A:455:ASN:O	1:A:459:GLN:HG2	2.13	0.49
1:B:639:ILE:O	1:B:643:ARG:HG3	2.13	0.49
1:B:681:LYS:HB3	1:B:685:LEU:HD23	1.95	0.49
1:A:277:ILE:HA	1:A:281:LEU:HB3	1.95	0.48
1:B:273:ARG:NE	1:B:299:GLU:OE2	2.46	0.48
1:A:518:LEU:HD11	1:A:584:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ARG:NH1	1:B:160:GLU:OE1	2.33	0.48
1:B:455:ASN:O	1:B:459:GLN:HG2	2.14	0.48
1:A:549:ILE:HD12	1:A:575:LEU:HD21	1.96	0.48
1:A:196:TRP:CH2	1:A:200:LEU:HD11	2.49	0.48
1:A:273:ARG:NE	1:A:299:GLU:OE2	2.46	0.48
1:A:681:LYS:HB3	1:A:685:LEU:HD23	1.96	0.48
1:B:705:ASN:O	1:B:709:GLU:HG2	2.15	0.47
1:B:536:ILE:HB	1:B:564:LEU:HD23	1.95	0.47
1:B:142:GLN:HB2	1:B:480:THR:HG22	1.95	0.47
1:B:549:ILE:HD12	1:B:575:LEU:HD21	1.97	0.47
1:A:705:ASN:O	1:A:709:GLU:HG2	2.15	0.47
1:A:635:ASP:O	1:A:639:ILE:HG12	2.15	0.46
1:A:410:LEU:HD12	1:A:410:LEU:H	1.80	0.46
1:B:508:ARG:NH1	1:B:559:LYS:O	2.39	0.46
1:B:713:ILE:O	1:B:717:GLN:HG2	2.15	0.46
1:A:567:ARG:HD2	3:A:1259:HOH:O	2.15	0.46
1:B:198:ILE:O	1:B:202:GLU:HG2	2.16	0.46
1:A:637:LEU:HD13	1:B:713:ILE:HG23	1.98	0.46
1:B:410:LEU:H	1:B:410:LEU:HD12	1.81	0.46
1:B:141:ARG:NH2	3:B:1116:HOH:O	2.41	0.45
1:A:675:PHE:HE2	1:B:618:ASN:HB2	1.81	0.45
1:A:713:ILE:O	1:A:717:GLN:HG2	2.16	0.45
1:B:174:VAL:H	1:B:591:GLN:NE2	2.13	0.45
1:B:256:LYS:NZ	3:B:1117:HOH:O	2.41	0.45
1:A:545:ARG:O	1:A:549:ILE:HG12	2.17	0.45
1:A:152:ARG:NH1	1:A:160:GLU:OE1	2.38	0.44
1:B:635:ASP:O	1:B:639:ILE:HG12	2.18	0.44
1:A:618:ASN:O	1:B:664:GLY:HA3	2.18	0.44
1:A:664:GLY:HA3	1:B:618:ASN:O	2.18	0.43
1:B:116:PRO:O	1:B:120:GLU:HG2	2.18	0.43
1:B:165:GLU:HB3	1:B:454:LEU:HD22	2.00	0.43
1:A:700:ARG:NH1	1:B:617:ASP:OD2	2.33	0.43
1:A:536:ILE:HB	1:A:564:LEU:HD23	1.99	0.43
1:B:545:ARG:O	1:B:549:ILE:HG12	2.18	0.43
1:B:404:ASP:O	1:B:407:LYS:HG2	2.19	0.42
1:A:641:GLN:CG	1:A:713:ILE:HG21	2.50	0.42
1:A:116:PRO:O	1:A:120:GLU:HG2	2.19	0.42
1:A:713:ILE:HA	1:A:716:LEU:HB3	2.02	0.42
1:A:115:ASN:HA	1:A:116:PRO:HD2	1.90	0.42
1:A:179:PRO:HA	1:A:180:PRO:HD3	1.88	0.42
1:A:198:ILE:O	1:A:202:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:O	1:A:277:ILE:HG13	2.19	0.42
1:A:420:GLY:H	1:B:677:THR:HB	1.85	0.42
1:B:127:ARG:NH1	1:B:131:GLU:OE2	2.52	0.42
1:A:404:ASP:O	1:A:407:LYS:HG2	2.19	0.41
1:A:182:ILE:HD11	1:A:223:ALA:HA	2.02	0.41
1:A:518:LEU:HD11	1:A:584:TYR:CD1	2.55	0.41
1:A:96:PHE:O	1:A:100:LEU:HG	2.21	0.41
1:B:96:PHE:O	1:B:100:LEU:HG	2.21	0.41
1:A:141:ARG:HB3	1:A:481:THR:HG23	2.02	0.41
1:A:677:THR:HB	1:B:420:GLY:H	1.84	0.41
1:A:685:LEU:HD13	1:A:685:LEU:HA	1.86	0.41
1:B:270:LYS:HG2	1:B:273:ARG:HH22	1.85	0.41
1:B:293:TYR:OH	1:B:315:GLU:O	2.39	0.41
1:B:273:ARG:O	1:B:277:ILE:HG13	2.21	0.40
1:B:196:TRP:CH2	1:B:200:LEU:HD11	2.57	0.40

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	621/723 (86%)	604 (97%)	17 (3%)	0	100	100
1	B	621/723 (86%)	604 (97%)	17 (3%)	0	100	100
All	All	1242/1446 (86%)	1208 (97%)	34 (3%)	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	541/624 (87%)	535 (99%)	6 (1%)	73 87
1	B	541/624 (87%)	536 (99%)	5 (1%)	78 90
All	All	1082/1248 (87%)	1071 (99%)	11 (1%)	76 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	392	VAL
1	A	562	PHE
1	A	675	PHE
1	A	685	LEU
1	A	713	ILE
1	B	392	VAL
1	B	562	PHE
1	B	641	GLN
1	B	675	PHE
1	B	685	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	625/723 (86%)	0.30	36 (5%)	23	22	19, 50, 103, 152	0
1	B	625/723 (86%)	0.29	32 (5%)	28	26	20, 50, 103, 155	0
All	All	1250/1446 (86%)	0.29	68 (5%)	25	24	19, 50, 103, 155	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	HIS	7.3
1	A	273	ARG	6.4
1	A	278	ASN	6.3
1	A	274	HIS	6.0
1	B	270	LYS	5.9
1	B	710	LYS	5.5
1	B	273	ARG	5.4
1	B	268	GLY	5.3
1	A	684	GLN	4.4
1	A	268	GLY	4.4
1	B	275	GLN	4.3
1	B	138	ARG	4.2
1	B	684	GLN	4.1
1	B	88	LYS	4.0
1	A	279	ASP	4.0
1	B	329	VAL	3.9
1	B	271	GLU	3.9
1	B	279	ASP	3.8
1	A	137	LYS	3.6
1	A	329	VAL	3.6
1	A	714	ASP	3.6
1	A	270	LYS	3.6
1	A	677	THR	3.6
1	A	710	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	686	ASP	3.5
1	A	325	SER	3.5
1	A	88	LYS	3.3
1	A	326	LEU	3.3
1	A	672	LYS	3.3
1	A	682	GLY	3.3
1	B	672	LYS	3.2
1	A	138	ARG	3.2
1	B	272	GLU	3.2
1	A	683	SER	3.1
1	A	267	GLN	3.0
1	B	686	ASP	3.0
1	B	331	ARG	3.0
1	B	677	THR	2.9
1	A	139	GLY	2.9
1	A	271	GLU	2.9
1	B	267	GLN	2.9
1	B	142	GLN	2.8
1	A	276	LEU	2.7
1	A	447	ARG	2.7
1	A	296	ILE	2.7
1	B	137	LYS	2.7
1	B	681	LYS	2.7
1	B	296	ILE	2.6
1	B	269	ALA	2.6
1	A	718	LYS	2.6
1	B	297	LEU	2.5
1	A	277	ILE	2.5
1	B	278	ASN	2.5
1	A	639	ILE	2.5
1	A	144	GLY	2.4
1	A	328	GLN	2.4
1	A	487	TYR	2.4
1	A	501	ARG	2.3
1	B	487	TYR	2.3
1	A	331	ARG	2.3
1	A	316	ALA	2.3
1	B	634	LEU	2.3
1	B	326	LEU	2.3
1	A	332	MET	2.2
1	B	325	SER	2.2
1	B	139	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	714	ASP	2.0
1	B	328	GLN	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 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	CL	B	1000	1/1	0.98	0.13	39,39,39,39	0
2	CL	A	1000	1/1	0.99	0.08	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.