



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 11:30 AM EDT

PDB ID : 5K1S
Title : crystal structure of AibC
Authors : Bock, T.; Mueller, R.; Blankenfeldt, W.
Deposited on : 2016-05-18
Resolution : 2.55 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

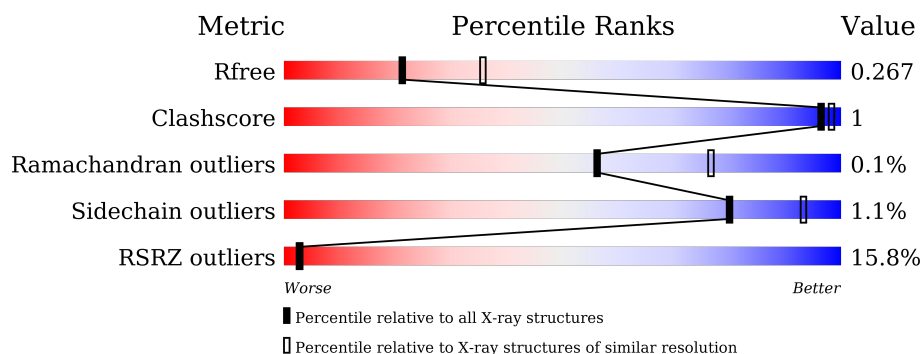
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	362	<div> <div>8%</div> <div>94%</div> <div>5%</div> </div>
1	B	362	<div> <div>24%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
1	C	362	<div> <div>8%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
1	D	362	<div> <div>20%</div> <div>90%</div> <div>.</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	C	402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19587 atoms, of which 9631 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 Oxidoreductase, zinc-binding dehydrogenase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	1	0
			5116	1607	2529	476	488	16			
1	C	358	Total	C	H	N	O	S	0	0	0
			5033	1588	2480	469	480	16			
1	B	333	Total	C	H	N	O	S	0	0	0
			4641	1453	2298	426	449	15			
1	D	333	Total	C	H	N	O	S	0	0	0
			4682	1467	2324	423	452	16			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q1D4I2
A	-15	GLY	-	expression tag	UNP Q1D4I2
A	-14	HIS	-	expression tag	UNP Q1D4I2
A	-13	HIS	-	expression tag	UNP Q1D4I2
A	-12	HIS	-	expression tag	UNP Q1D4I2
A	-11	HIS	-	expression tag	UNP Q1D4I2
A	-10	HIS	-	expression tag	UNP Q1D4I2
A	-9	HIS	-	expression tag	UNP Q1D4I2
A	-8	ALA	-	expression tag	UNP Q1D4I2
A	-7	GLU	-	expression tag	UNP Q1D4I2
A	-6	ASN	-	expression tag	UNP Q1D4I2
A	-5	LEU	-	expression tag	UNP Q1D4I2
A	-4	TYR	-	expression tag	UNP Q1D4I2
A	-3	PHE	-	expression tag	UNP Q1D4I2
A	-2	GLN	-	expression tag	UNP Q1D4I2
A	-1	GLY	-	expression tag	UNP Q1D4I2
A	0	HIS	-	expression tag	UNP Q1D4I2
C	-16	MET	-	initiating methionine	UNP Q1D4I2
C	-15	GLY	-	expression tag	UNP Q1D4I2
C	-14	HIS	-	expression tag	UNP Q1D4I2
C	-13	HIS	-	expression tag	UNP Q1D4I2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q1D4I2
C	-11	HIS	-	expression tag	UNP Q1D4I2
C	-10	HIS	-	expression tag	UNP Q1D4I2
C	-9	HIS	-	expression tag	UNP Q1D4I2
C	-8	ALA	-	expression tag	UNP Q1D4I2
C	-7	GLU	-	expression tag	UNP Q1D4I2
C	-6	ASN	-	expression tag	UNP Q1D4I2
C	-5	LEU	-	expression tag	UNP Q1D4I2
C	-4	TYR	-	expression tag	UNP Q1D4I2
C	-3	PHE	-	expression tag	UNP Q1D4I2
C	-2	GLN	-	expression tag	UNP Q1D4I2
C	-1	GLY	-	expression tag	UNP Q1D4I2
C	0	HIS	-	expression tag	UNP Q1D4I2
B	-16	MET	-	initiating methionine	UNP Q1D4I2
B	-15	GLY	-	expression tag	UNP Q1D4I2
B	-14	HIS	-	expression tag	UNP Q1D4I2
B	-13	HIS	-	expression tag	UNP Q1D4I2
B	-12	HIS	-	expression tag	UNP Q1D4I2
B	-11	HIS	-	expression tag	UNP Q1D4I2
B	-10	HIS	-	expression tag	UNP Q1D4I2
B	-9	HIS	-	expression tag	UNP Q1D4I2
B	-8	ALA	-	expression tag	UNP Q1D4I2
B	-7	GLU	-	expression tag	UNP Q1D4I2
B	-6	ASN	-	expression tag	UNP Q1D4I2
B	-5	LEU	-	expression tag	UNP Q1D4I2
B	-4	TYR	-	expression tag	UNP Q1D4I2
B	-3	PHE	-	expression tag	UNP Q1D4I2
B	-2	GLN	-	expression tag	UNP Q1D4I2
B	-1	GLY	-	expression tag	UNP Q1D4I2
B	0	HIS	-	expression tag	UNP Q1D4I2
D	-16	MET	-	initiating methionine	UNP Q1D4I2
D	-15	GLY	-	expression tag	UNP Q1D4I2
D	-14	HIS	-	expression tag	UNP Q1D4I2
D	-13	HIS	-	expression tag	UNP Q1D4I2
D	-12	HIS	-	expression tag	UNP Q1D4I2
D	-11	HIS	-	expression tag	UNP Q1D4I2
D	-10	HIS	-	expression tag	UNP Q1D4I2
D	-9	HIS	-	expression tag	UNP Q1D4I2
D	-8	ALA	-	expression tag	UNP Q1D4I2
D	-7	GLU	-	expression tag	UNP Q1D4I2
D	-6	ASN	-	expression tag	UNP Q1D4I2
D	-5	LEU	-	expression tag	UNP Q1D4I2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	TYR	-	expression tag	UNP Q1D4I2
D	-3	PHE	-	expression tag	UNP Q1D4I2
D	-2	GLN	-	expression tag	UNP Q1D4I2
D	-1	GLY	-	expression tag	UNP Q1D4I2
D	0	HIS	-	expression tag	UNP Q1D4I2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

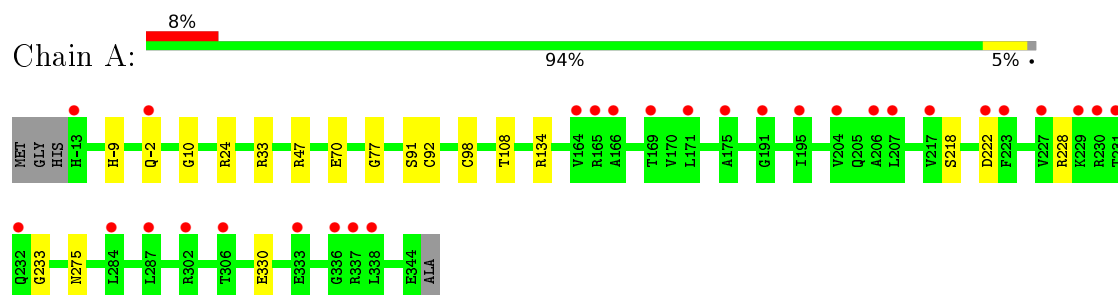
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total 42	O 42	0	0
3	C	35	Total 35	O 35	0	0
3	B	18	Total 18	O 18	0	0
3	D	12	Total 12	O 12	0	0

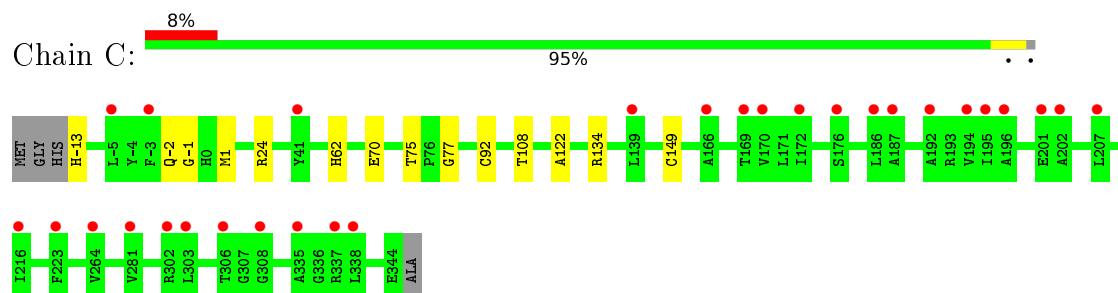
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

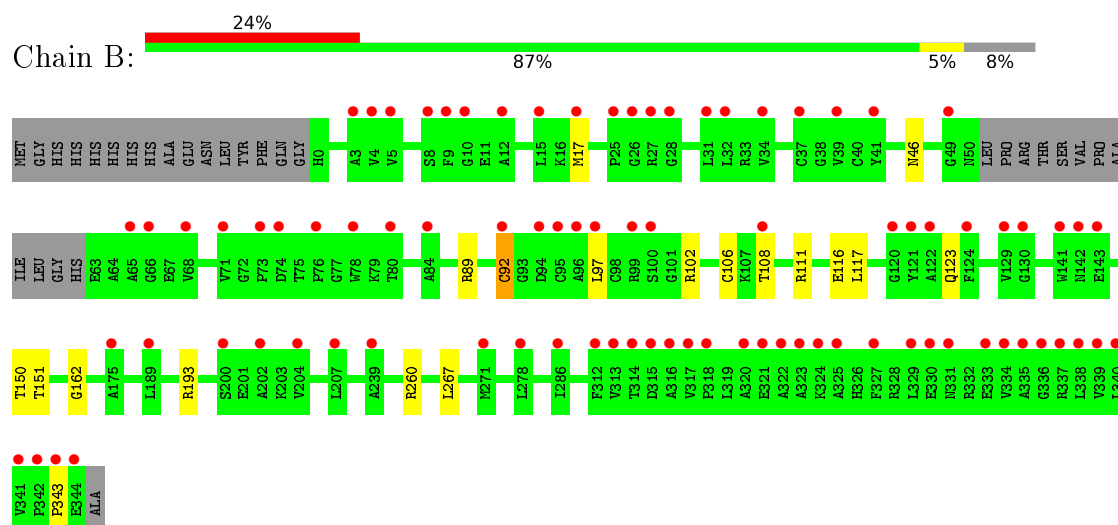
- Molecule 1: Oxidoreductase, zinc-binding dehydrogenase family



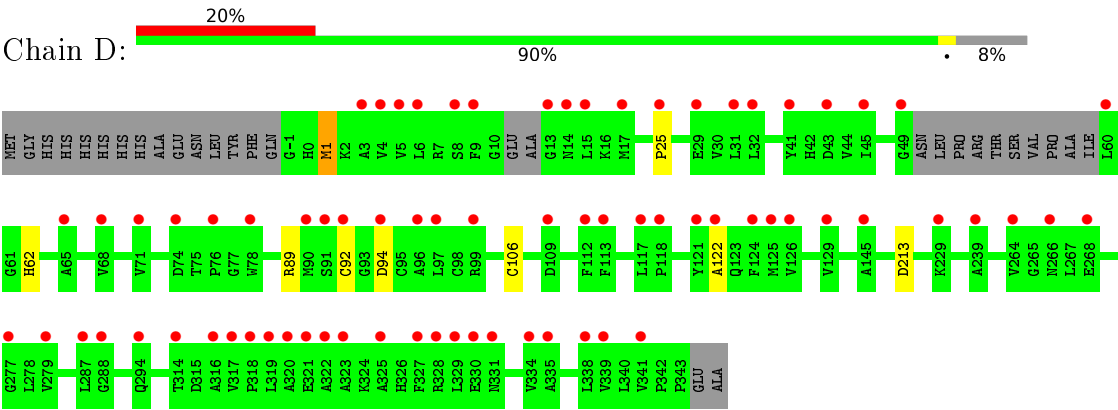
- Molecule 1: Oxidoreductase, zinc-binding dehydrogenase family



- Molecule 1: Oxidoreductase, zinc-binding dehydrogenase family



● Molecule 1: Oxidoreductase, zinc-binding dehydrogenase family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.29Å 77.43Å 309.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 2.55 44.67 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.94-2.55) 100.0 (44.67-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.269 0.228 , 0.267	Depositor DCC
R_{free} test set	3084 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19587	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 3.20% 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](#)

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

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	0.25	0/2633	0.42	0/3582
1	B	0.25	0/2374	0.43	0/3230
1	C	0.25	0/2596	0.42	0/3537
1	D	0.25	0/2390	0.43	0/3248
All	All	0.25	0/9993	0.43	0/13597

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 [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	2587	2529	2543	9	1
1	B	2343	2298	2297	10	0
1	C	2553	2480	2481	6	2
1	D	2358	2324	2323	3	0
2	A	2	0	0	0	1
2	B	2	0	0	0	0
2	C	2	0	0	0	2
2	D	2	0	0	0	0
3	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	35	0	0	1	0
3	D	12	0	0	0	0
All	All	9956	9631	9644	27	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 1.

All (27) 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:89:ARG:NH2	1:B:106:CYS:O	2.10	0.84
1:C:75:THR:O	3:C:501:HOH:O	2.01	0.79
1:A:10:GLY:O	1:A:47:ARG:NH1	2.16	0.78
1:C:77:GLY:O	1:C:134:ARG:NH1	2.21	0.73
1:C:24:ARG:NH2	1:C:70:GLU:OE2	2.27	0.67
1:A:77:GLY:O	1:A:134:ARG:NH2	2.29	0.64
1:A:47:ARG:NH2	1:A:330:GLU:OE2	2.33	0.61
1:B:123:GLN:NE2	1:B:343:PRO:O	2.35	0.60
1:A:24:ARG:NH2	1:A:70:GLU:OE2	2.41	0.53
1:B:92:CYS:SG	1:B:108:THR:OG1	2.67	0.52
1:B:97:LEU:O	1:B:102:ARG:N	2.44	0.50
1:B:111:ARG:HD2	1:B:117:LEU:HD21	1.95	0.49
1:D:89:ARG:NH2	1:D:106:CYS:O	2.46	0.48
1:B:116:GLU:N	1:B:116:GLU:OE1	2.42	0.48
1:B:193:ARG:NH2	1:D:213:ASP:OD1	2.42	0.47
1:C:-2:GLN:OE1	1:C:24:ARG:NH1	2.49	0.46
1:C:1:MET:CE	1:C:122:ALA:HB1	2.45	0.46
1:A:228:ARG:O	1:A:233:GLY:N	2.45	0.46
1:B:162:GLY:O	1:B:260:ARG:NH1	2.50	0.45
1:C:92:CYS:SG	1:C:108:THR:OG1	2.76	0.43
1:A:218:SER:OG	1:A:222:ASP:OD1	2.30	0.42
1:D:1:MET:SD	1:D:122:ALA:HB1	2.59	0.42
1:A:-2:GLN:OE1	1:A:24:ARG:NH1	2.46	0.42
1:A:92:CYS:SG	1:A:108:THR:OG1	2.78	0.42
1:B:150:THR:OG1	1:B:151:THR:N	2.53	0.41
1:A:91:SER:OG	1:A:98:CYS:SG	2.79	0.41
1:B:117:LEU:HD23	1:B:117:LEU:N	2.36	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)
1:C:62:HIS:HE2	2:C:402:ZN:ZN[3_545]	1.43	0.17
1:C:149:CYS:HG	2:C:402:ZN:ZN[3_545]	1.54	0.06
1:A:-9:HIS:HE2	2:A:402:ZN:ZN[4_556]	1.56	0.04

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	357/362 (99%)	340 (95%)	17 (5%)	0	100	100
1	B	329/362 (91%)	312 (95%)	17 (5%)	0	100	100
1	C	356/362 (98%)	339 (95%)	16 (4%)	1 (0%)	46	66
1	D	327/362 (90%)	309 (94%)	17 (5%)	1 (0%)	46	66
All	All	1369/1448 (94%)	1300 (95%)	67 (5%)	2 (0%)	56	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	GLY
1	D	25	PRO

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	261/277 (94%)	259 (99%)	2 (1%)	86	96
1	B	232/277 (84%)	228 (98%)	4 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	251/277 (91%)	250 (100%)	1 (0%)	93	98
1	D	236/277 (85%)	232 (98%)	4 (2%)	68	88
All	All	980/1108 (88%)	969 (99%)	11 (1%)	80	93

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

Mol	Chain	Res	Type
1	A	33	ARG
1	A	275	ASN
1	C	-13	HIS
1	B	17	MET
1	B	46	ASN
1	B	92	CYS
1	B	267	LEU
1	D	1	MET
1	D	62	HIS
1	D	92	CYS
1	D	94	ASP

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 [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	358/362 (98%)	0.74	29 (8%) 15 16	35, 61, 99, 127	0
1	B	333/362 (91%)	1.55	86 (25%) 1 1	41, 85, 141, 180	0
1	C	358/362 (98%)	0.74	29 (8%) 15 16	41, 64, 106, 132	0
1	D	333/362 (91%)	1.36	74 (22%) 1 1	36, 79, 133, 166	0
All	All	1382/1448 (95%)	1.09	218 (15%) 3 3	35, 69, 124, 180	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	12.9
1	D	320	ALA	11.4
1	B	329	LEU	8.8
1	B	327	PHE	8.3
1	D	327	PHE	8.0
1	D	325	ALA	7.8
1	B	28	GLY	7.7
1	B	325	ALA	6.7
1	B	316	ALA	6.5
1	B	66	GLY	6.5
1	D	122	ALA	6.2
1	B	322	ALA	6.0
1	B	340	LEU	6.0
1	D	335	ALA	5.9
1	D	8	SER	5.7
1	B	27	ARG	5.6
1	B	99	ARG	5.6
1	B	314	THR	5.5
1	B	323	ALA	5.4
1	B	335	ALA	5.4
1	D	6	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	339	VAL	5.3
1	D	338	LEU	5.3
1	B	320	ALA	5.1
1	D	314	THR	5.1
1	B	12	ALA	5.0
1	B	3	ALA	4.9
1	B	333	GLU	4.8
1	B	41	TYR	4.8
1	B	331	ASN	4.8
1	B	4	VAL	4.8
1	B	94	ASP	4.6
1	B	76	PRO	4.6
1	D	317	VAL	4.6
1	B	65	ALA	4.5
1	C	195	ILE	4.5
1	B	129	VAL	4.5
1	B	96	ALA	4.4
1	B	317	VAL	4.4
1	D	334	VAL	4.3
1	D	323	ALA	4.3
1	D	118	PRO	4.2
1	B	341	VAL	4.2
1	D	328	ARG	4.2
1	D	4	VAL	4.1
1	D	322	ALA	4.1
1	D	17	MET	4.1
1	B	124	PHE	4.1
1	C	216	ILE	4.0
1	A	165	ARG	4.0
1	C	176	SER	3.9
1	D	316	ALA	3.9
1	B	338	LEU	3.9
1	B	39	VAL	3.9
1	D	97	LEU	3.8
1	A	166	ALA	3.8
1	B	34	VAL	3.7
1	B	8	SER	3.7
1	D	13	GLY	3.7
1	B	37	CYS	3.7
1	A	191	GLY	3.6
1	D	15	LEU	3.6
1	D	287	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	266	ASN	3.6
1	D	49	GLY	3.6
1	C	306	THR	3.5
1	A	195	ILE	3.5
1	D	318	PRO	3.5
1	D	45	ILE	3.4
1	B	15	LEU	3.4
1	B	343	PRO	3.4
1	B	324	LYS	3.4
1	A	171	LEU	3.4
1	D	5	VAL	3.3
1	C	303	LEU	3.3
1	B	313	VAL	3.3
1	B	312	PHE	3.3
1	A	227	VAL	3.3
1	B	32	LEU	3.3
1	C	223	PHE	3.3
1	D	29	GLU	3.2
1	B	202	ALA	3.2
1	C	202	ALA	3.1
1	C	201	GLU	3.1
1	D	99	ARG	3.1
1	D	329	LEU	3.1
1	A	336	GLY	3.1
1	B	49	GLY	3.1
1	D	330	GLU	3.1
1	A	229	LYS	3.1
1	D	3	ALA	3.0
1	B	9	PHE	3.0
1	D	74	ASP	3.0
1	C	194	VAL	3.0
1	A	206	ALA	3.0
1	B	73	PRO	3.0
1	B	74	ASP	3.0
1	B	207	LEU	3.0
1	A	217	VAL	2.9
1	C	169	THR	2.9
1	C	187	ALA	2.9
1	B	68	VAL	2.9
1	D	339	VAL	2.9
1	B	342	PRO	2.9
1	C	335	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	117	LEU	2.8
1	D	113	PHE	2.8
1	C	166	ALA	2.8
1	B	71	VAL	2.8
1	D	321	GLU	2.8
1	D	341	VAL	2.8
1	B	100	SER	2.8
1	B	175	ALA	2.7
1	B	143	GLU	2.7
1	B	84	ALA	2.7
1	D	92	CYS	2.7
1	D	71	VAL	2.7
1	C	172	ILE	2.7
1	D	43	ASP	2.7
1	B	121	TYR	2.7
1	B	330	GLU	2.7
1	B	5	VAL	2.7
1	C	207	LEU	2.7
1	D	121	TYR	2.7
1	A	302	ARG	2.7
1	A	223	PHE	2.7
1	D	32	LEU	2.7
1	D	112	PHE	2.7
1	A	207	LEU	2.6
1	B	122	ALA	2.6
1	B	315	ASP	2.6
1	D	68	VAL	2.6
1	B	78	TRP	2.6
1	D	41	TYR	2.6
1	D	109	ASP	2.6
1	A	232	GLN	2.6
1	B	336	GLY	2.6
1	C	196	ALA	2.6
1	D	76	PRO	2.6
1	D	78	TRP	2.6
1	D	331	ASN	2.6
1	D	31	LEU	2.5
1	A	337	ARG	2.5
1	C	338	LEU	2.5
1	A	-13	HIS	2.5
1	D	94	ASP	2.5
1	D	288	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	THR	2.5
1	B	97	LEU	2.5
1	B	344	GLU	2.5
1	A	333	GLU	2.5
1	B	95	CYS	2.5
1	C	186	LEU	2.4
1	B	108	THR	2.4
1	A	164	VAL	2.4
1	A	204	VAL	2.4
1	B	92	CYS	2.4
1	D	129	VAL	2.4
1	A	222	ASP	2.4
1	B	204	VAL	2.4
1	D	91	SER	2.4
1	D	125	MET	2.4
1	D	277	GLY	2.4
1	C	302	ARG	2.4
1	A	284	LEU	2.4
1	C	139	LEU	2.4
1	B	26	GLY	2.4
1	D	65	ALA	2.4
1	C	-5	LEU	2.4
1	D	319	LEU	2.4
1	B	142	ASN	2.3
1	A	338	LEU	2.3
1	C	308	GLY	2.3
1	B	10	GLY	2.3
1	D	124	PHE	2.3
1	C	337	ARG	2.3
1	B	337	ARG	2.3
1	D	14	ASN	2.3
1	B	130	GLY	2.3
1	B	321	GLU	2.3
1	A	287	LEU	2.3
1	D	25	PRO	2.3
1	D	268	GLU	2.3
1	C	281	VAL	2.3
1	D	279	VAL	2.3
1	B	271	MET	2.3
1	B	189	LEU	2.2
1	A	-2	GLN	2.2
1	C	170	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	200	SER	2.2
1	C	-3	PHE	2.2
1	B	80	THR	2.2
1	B	25	PRO	2.2
1	D	145	ALA	2.2
1	B	17	MET	2.2
1	D	9	PHE	2.2
1	C	264	VAL	2.1
1	B	141	TRP	2.1
1	D	60	LEU	2.1
1	D	96	ALA	2.1
1	D	126	VAL	2.1
1	A	231	THR	2.1
1	B	318	PRO	2.1
1	B	278	LEU	2.1
1	B	286	ILE	2.1
1	B	31	LEU	2.1
1	A	230	ARG	2.1
1	A	306	THR	2.1
1	C	41	TYR	2.1
1	D	239	ALA	2.1
1	A	175	ALA	2.1
1	B	239	ALA	2.1
1	B	120	GLY	2.1
1	D	90	MET	2.0
1	C	192	ALA	2.0
1	D	264	VAL	2.0
1	D	294	GLN	2.0
1	D	229	LYS	2.0

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	C	402	1/1	0.97	0.23	1.04	89,89,89,89	0
2	ZN	A	401	1/1	0.97	0.18	0.48	67,67,67,67	0
2	ZN	B	401	1/1	0.94	0.24	0.06	108,108,108,108	0
2	ZN	C	401	1/1	0.99	0.16	-0.13	61,61,61,61	0
2	ZN	A	402	1/1	0.99	0.17	-0.55	70,70,70,70	0
2	ZN	D	401	1/1	0.85	0.16	-0.79	117,117,117,117	0
2	ZN	B	402	1/1	0.92	0.05	-2.38	107,107,107,107	0
2	ZN	D	402	1/1	0.86	0.06	-3.10	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.