Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 01:07 PM EDT

PDB ID	:	6FI9
Title	:	Crystal Structure of a zinc-responsive MarR family member, Lactococcus lactis ZitR
Authors	:	Varela, P.F.; Legrand, P.
Deposited on	:	2018-01-17
Resolution	:	2.80 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:

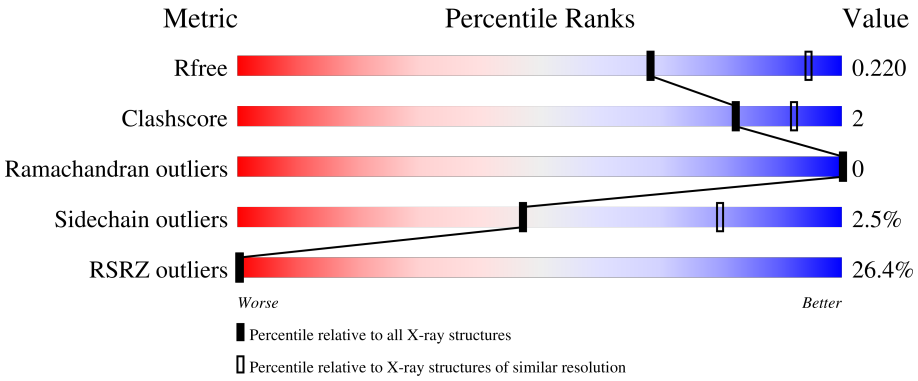
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	144	6% 91% 9%
1	B	144	8% 94% 6%
1	C	144	8% 89% 10%
1	D	144	4% 92% 8%
1	E	144	31% 86% 14%

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Mol	Chain	Length	Quality of chain
1	F	144	62% 92% 8%
1	G	144	69% 94% 6%
1	H	144	24% 88% 12%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	G	202	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9168 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 Transcriptional regulator ZitR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	B	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	C	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	D	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	E	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	F	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	G	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			
1	H	144	Total	C	N	O	S	0	0	0
			1144	720	197	224	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP A2RNS2
A	4	ARG	ALA	engineered mutation	UNP A2RNS2
A	8	GLU	ASP	engineered mutation	UNP A2RNS2
B	2	ALA	SER	engineered mutation	UNP A2RNS2
B	4	ARG	ALA	engineered mutation	UNP A2RNS2
B	8	GLU	ASP	engineered mutation	UNP A2RNS2
C	2	ALA	SER	engineered mutation	UNP A2RNS2
C	4	ARG	ALA	engineered mutation	UNP A2RNS2
C	8	GLU	ASP	engineered mutation	UNP A2RNS2
D	2	ALA	SER	engineered mutation	UNP A2RNS2
D	4	ARG	ALA	engineered mutation	UNP A2RNS2
D	8	GLU	ASP	engineered mutation	UNP A2RNS2
E	2	ALA	SER	engineered mutation	UNP A2RNS2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ARG	ALA	engineered mutation	UNP A2RNS2
E	8	GLU	ASP	engineered mutation	UNP A2RNS2
F	2	ALA	SER	engineered mutation	UNP A2RNS2
F	4	ARG	ALA	engineered mutation	UNP A2RNS2
F	8	GLU	ASP	engineered mutation	UNP A2RNS2
G	2	ALA	SER	engineered mutation	UNP A2RNS2
G	4	ARG	ALA	engineered mutation	UNP A2RNS2
G	8	GLU	ASP	engineered mutation	UNP A2RNS2
H	2	ALA	SER	engineered mutation	UNP A2RNS2
H	4	ARG	ALA	engineered mutation	UNP A2RNS2
H	8	GLU	ASP	engineered mutation	UNP A2RNS2

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

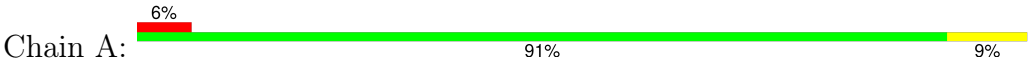
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

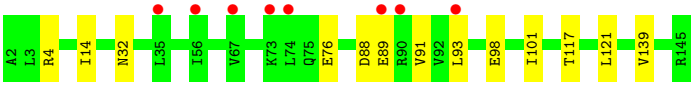
3 Residue-property plots (i)

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: Transcriptional regulator ZitR

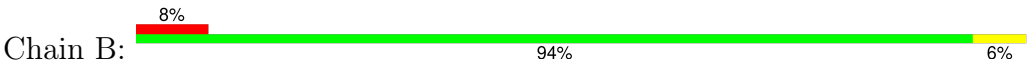
Chain A:

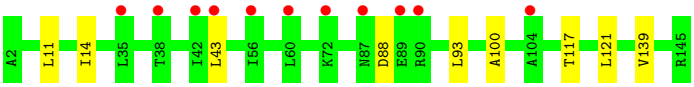




• Molecule 1: Transcriptional regulator ZitR

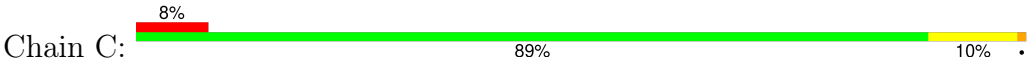
Chain B:

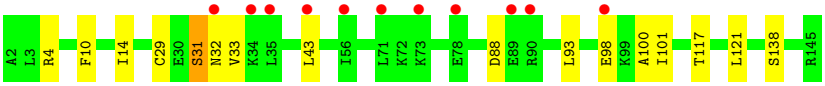




• Molecule 1: Transcriptional regulator ZitR

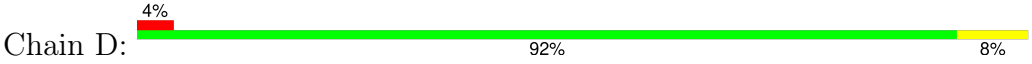
Chain C:

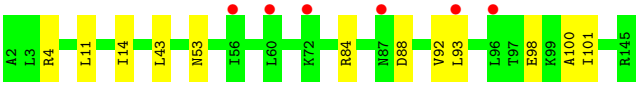




• Molecule 1: Transcriptional regulator ZitR

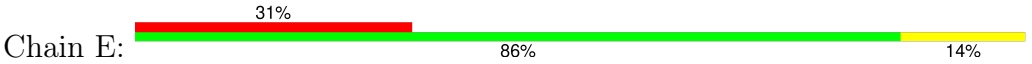
Chain D:

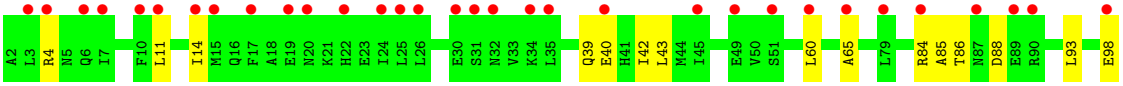


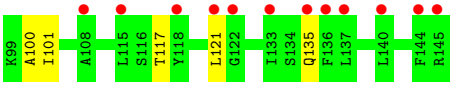


• Molecule 1: Transcriptional regulator ZitR

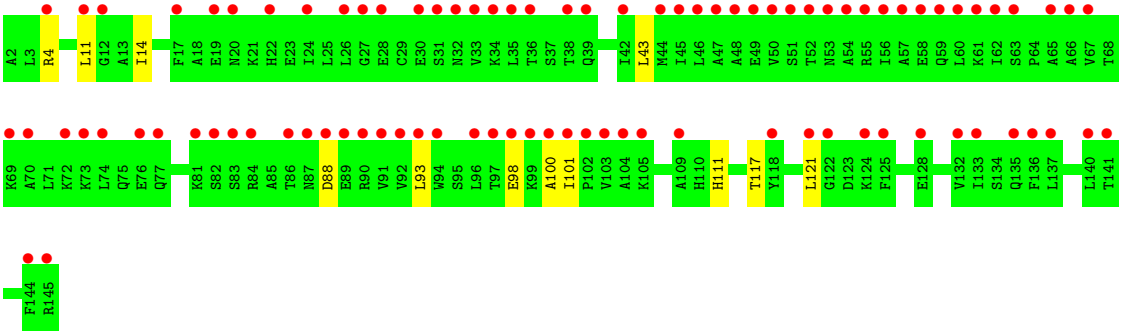
Chain E:



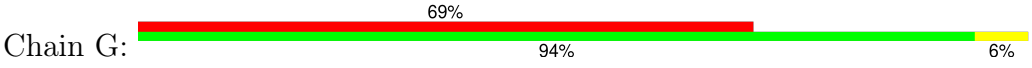


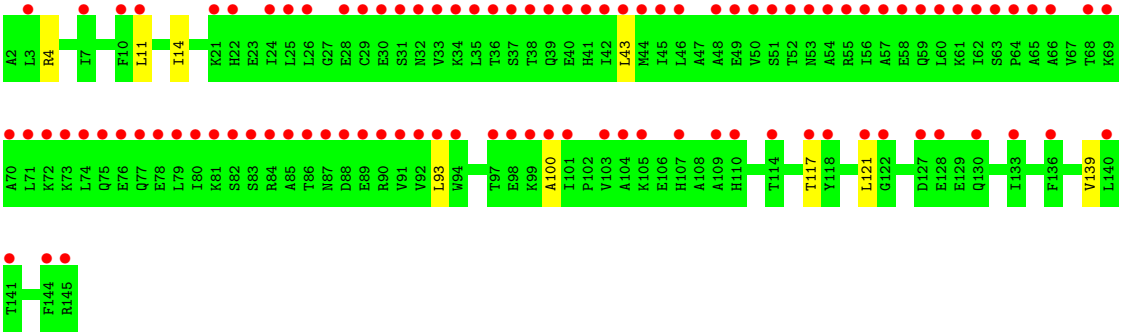


• Molecule 1: Transcriptional regulator ZitR

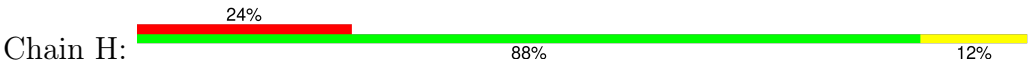


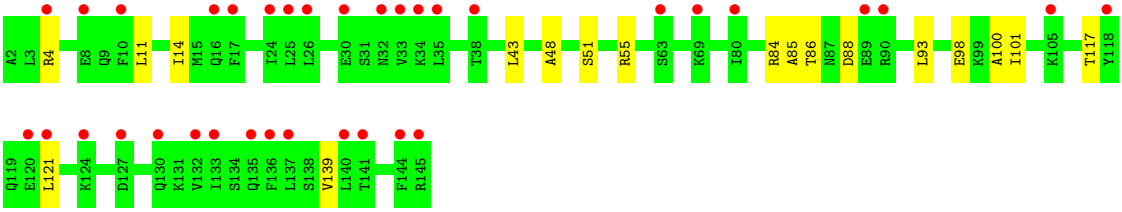
• Molecule 1: Transcriptional regulator ZitR





• Molecule 1: Transcriptional regulator ZitR





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	128.52Å 128.52Å 88.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.15 – 2.80 48.14 – 2.87	Depositor EDS
% Data completeness (in resolution range)	60.9 (48.15-2.80) 65.6 (48.14-2.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.236 , 0.251 0.212 , 0.220	Depositor DCC
R_{free} test set	1028 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 96.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.319 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9168	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 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	0.40	0/1158	0.58	0/1560
1	B	0.40	0/1158	0.59	0/1560
1	C	0.41	0/1158	0.59	0/1560
1	D	0.41	0/1158	0.59	0/1560
1	E	0.39	0/1158	0.57	0/1560
1	F	0.40	0/1158	0.56	0/1560
1	G	0.39	0/1158	0.56	0/1560
1	H	0.38	0/1158	0.56	0/1560
All	All	0.40	0/9264	0.57	0/12480

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	1144	0	1165	8	0
1	B	1144	0	1165	6	0
1	C	1144	0	1165	7	0
1	D	1144	0	1164	5	0
1	E	1144	0	1165	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1144	0	1165	6	0
1	G	1144	0	1165	4	0
1	H	1144	0	1165	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
All	All	9168	0	9319	46	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 2.

All (46) 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:C:32:ASN:HB2	1:F:88:ASP:HB2	1.72	0.70
1:E:84:ARG:H	1:H:86:THR:HG22	1.71	0.56
1:F:11:LEU:HA	1:F:14:ILE:HD12	1.89	0.55
1:A:76:GLU:HA	1:E:65:ALA:HB2	1.90	0.52
1:A:121:LEU:HD22	1:B:139:VAL:HG12	1.93	0.50
1:G:139:VAL:HG12	1:H:121:LEU:HD22	1.93	0.50
1:H:117:THR:O	1:H:121:LEU:HG	2.13	0.49
1:D:53:ASN:HB2	1:D:92:VAL:HG23	1.95	0.49
1:G:117:THR:O	1:G:121:LEU:HG	2.13	0.49
1:A:117:THR:O	1:A:121:LEU:HG	2.14	0.48
1:E:117:THR:O	1:E:121:LEU:HG	2.14	0.48
1:C:117:THR:O	1:C:121:LEU:HG	2.13	0.47
1:B:117:THR:O	1:B:121:LEU:HG	2.13	0.47
1:E:86:THR:HG22	1:H:84:ARG:H	1.79	0.47
1:A:139:VAL:HG12	1:B:121:LEU:HD22	1.95	0.47
1:E:85:ALA:HA	1:H:85:ALA:HA	1.98	0.46
1:E:43:LEU:HD22	1:E:100:ALA:HB1	1.97	0.45
1:A:89:GLU:H	1:A:91:VAL:HG12	1.82	0.45
1:D:84:ARG:HB3	1:D:88:ASP:OD2	2.17	0.44
1:F:117:THR:O	1:F:121:LEU:HG	2.18	0.44
1:C:32:ASN:HB2	1:F:88:ASP:CB	2.43	0.44
1:A:32:ASN:HB2	1:H:48:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:LEU:HD22	1:H:100:ALA:HB1	2.00	0.43
1:C:29:CYS:SG	1:C:31:SER:HB2	2.58	0.43
1:C:43:LEU:HD22	1:C:100:ALA:HB1	2.01	0.43
1:E:39:GLN:HA	1:E:42:ILE:HD12	2.01	0.43
1:E:135:GLN:HG2	1:H:139:VAL:HG13	1.99	0.43
1:B:43:LEU:HD22	1:B:100:ALA:HB1	2.00	0.42
1:D:11:LEU:HA	1:D:14:ILE:HD12	2.01	0.42
1:G:43:LEU:HD22	1:G:100:ALA:HB1	2.01	0.42
1:A:14:ILE:HD13	1:B:14:ILE:HD13	2.00	0.42
1:H:11:LEU:HA	1:H:14:ILE:HD12	2.02	0.42
1:C:98:GLU:HA	1:C:101:ILE:HD12	2.02	0.42
1:E:40:GLU:HA	1:E:43:LEU:HD12	2.02	0.42
1:E:11:LEU:HA	1:E:14:ILE:HD12	2.02	0.42
1:G:11:LEU:HA	1:G:14:ILE:HD12	2.02	0.41
1:C:10:PHE:CZ	1:C:14:ILE:HD11	2.55	0.41
1:B:11:LEU:HA	1:B:14:ILE:HD12	2.01	0.41
1:H:98:GLU:HA	1:H:101:ILE:HD12	2.02	0.41
1:F:98:GLU:HA	1:F:101:ILE:HD12	2.02	0.41
1:D:98:GLU:HA	1:D:101:ILE:HD12	2.02	0.41
1:A:98:GLU:HA	1:A:101:ILE:HD12	2.02	0.41
1:F:43:LEU:HD22	1:F:100:ALA:HB1	2.02	0.41
1:H:51:SER:HB2	1:H:55:ARG:HH11	1.86	0.40
1:D:43:LEU:HD22	1:D:100:ALA:HB1	2.02	0.40
1:E:98:GLU:HA	1:E:101:ILE:HD12	2.02	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	142/144 (99%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	C	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	D	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	E	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	F	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
1	G	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	H	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
All	All	1136/1152 (99%)	1113 (98%)	23 (2%)	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	126/126 (100%)	123 (98%)	3 (2%)	49	81
1	B	126/126 (100%)	124 (98%)	2 (2%)	62	88
1	C	126/126 (100%)	120 (95%)	6 (5%)	25	58
1	D	126/126 (100%)	124 (98%)	2 (2%)	62	88
1	E	126/126 (100%)	122 (97%)	4 (3%)	39	73
1	F	126/126 (100%)	123 (98%)	3 (2%)	49	81
1	G	126/126 (100%)	124 (98%)	2 (2%)	62	88
1	H	126/126 (100%)	123 (98%)	3 (2%)	49	81
All	All	1008/1008 (100%)	983 (98%)	25 (2%)	47	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	88	ASP

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Mol	Chain	Res	Type
1	A	93	LEU
1	B	88	ASP
1	B	93	LEU
1	C	4	ARG
1	C	31	SER
1	C	33	VAL
1	C	88	ASP
1	C	93	LEU
1	C	138	SER
1	D	4	ARG
1	D	93	LEU
1	E	4	ARG
1	E	60	LEU
1	E	88	ASP
1	E	93	LEU
1	F	4	ARG
1	F	93	LEU
1	F	111	HIS
1	G	4	ARG
1	G	93	LEU
1	H	4	ARG
1	H	88	ASP
1	H	93	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	E	39	GLN
1	E	107	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 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, 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	144/144 (100%)	0.57	8 (5%) 24 16	55, 110, 147, 165	0
1	B	144/144 (100%)	0.70	11 (7%) 13 7	54, 112, 155, 181	0
1	C	144/144 (100%)	0.69	11 (7%) 13 7	47, 98, 161, 170	0
1	D	144/144 (100%)	0.66	6 (4%) 36 26	47, 96, 145, 179	0
1	E	144/144 (100%)	1.75	44 (30%) 0 0	135, 198, 249, 264	0
1	F	144/144 (100%)	3.73	90 (62%) 0 0	175, 270, 293, 296	0
1	G	144/144 (100%)	5.63	99 (68%) 0 0	163, 274, 287, 288	0
1	H	144/144 (100%)	1.55	35 (24%) 0 0	109, 174, 245, 267	0
All	All	1152/1152 (100%)	1.91	304 (26%) 0 0	47, 148, 284, 296	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	35	LEU	30.8
1	G	59	GLN	25.9
1	G	82	SER	25.7
1	G	92	VAL	23.0
1	G	58	GLU	21.7
1	G	60	LEU	19.7
1	G	70	ALA	19.7
1	G	87	ASN	19.4
1	G	42	ILE	18.3
1	F	56	ILE	17.1
1	G	100	ALA	16.4
1	F	92	VAL	15.7
1	G	99	LYS	15.1
1	F	54	ALA	15.0
1	E	90	ARG	14.9
1	F	66	ALA	14.6

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Mol	Chain	Res	Type	RSRZ
1	G	98	GLU	14.1
1	F	104	ALA	13.0
1	G	34	LYS	12.6
1	G	45	ILE	12.6
1	G	33	VAL	12.6
1	F	34	LYS	12.5
1	G	97	THR	12.5
1	E	25	LEU	12.3
1	G	56	ILE	12.2
1	F	96	LEU	12.1
1	G	53	ASN	12.0
1	G	93	LEU	11.7
1	G	80	ILE	11.6
1	G	91	VAL	11.3
1	G	43	LEU	10.8
1	G	76	GLU	10.8
1	E	24	ILE	10.7
1	F	63	SER	10.6
1	G	26	LEU	10.4
1	F	51	SER	10.4
1	G	101	ILE	10.4
1	E	26	LEU	10.3
1	G	77	GLN	9.9
1	G	40	GLU	9.8
1	G	24	ILE	9.8
1	F	31	SER	9.8
1	G	41	HIS	9.7
1	F	91	VAL	9.5
1	G	36	THR	9.4
1	G	85	ALA	9.3
1	F	128	GLU	9.3
1	G	86	THR	9.0
1	G	89	GLU	8.8
1	G	144	PHE	8.8
1	G	84	ARG	8.5
1	E	89	GLU	8.4
1	F	65	ALA	8.4
1	F	35	LEU	8.1
1	G	22	HIS	8.1
1	G	69	LYS	8.0
1	F	100	ALA	8.0
1	H	130	GLN	7.9

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Mol	Chain	Res	Type	RSRZ
1	F	24	ILE	7.9
1	F	62	ILE	7.9
1	H	145	ARG	7.9
1	G	81	LYS	7.8
1	G	103	VAL	7.8
1	H	89	GLU	7.8
1	G	75	GLN	7.7
1	F	30	GLU	7.7
1	F	118	TYR	7.7
1	G	78	GLU	7.5
1	G	55	ARG	7.5
1	G	39	GLN	7.5
1	F	87	ASN	7.5
1	E	118	TYR	7.3
1	H	136	PHE	7.3
1	F	53	ASN	7.2
1	F	67	VAL	6.9
1	F	33	VAL	6.9
1	F	57	ALA	6.9
1	G	88	ASP	6.8
1	F	60	LEU	6.7
1	F	83	SER	6.6
1	G	79	LEU	6.6
1	G	49	GLU	6.5
1	E	144	PHE	6.4
1	G	63	SER	6.4
1	F	144	PHE	6.4
1	G	71	LEU	6.4
1	G	121	LEU	6.3
1	C	89	GLU	6.3
1	G	83	SER	6.1
1	F	90	ARG	6.0
1	F	77	GLN	5.9
1	F	74	LEU	5.8
1	G	64	PRO	5.7
1	H	24	ILE	5.7
1	F	82	SER	5.7
1	H	90	ARG	5.7
1	G	48	ALA	5.6
1	G	94	TRP	5.6
1	G	32	ASN	5.6
1	F	32	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	52	THR	5.5
1	G	65	ALA	5.4
1	B	90	ARG	5.4
1	F	89	GLU	5.3
1	H	144	PHE	5.3
1	E	137	LEU	5.3
1	G	127	ASP	5.2
1	G	30	GLU	5.2
1	E	136	PHE	5.1
1	F	76	GLU	5.1
1	E	4	ARG	5.1
1	F	135	GLN	5.0
1	H	34	LYS	5.0
1	H	137	LEU	5.0
1	F	88	ASP	5.0
1	F	38	THR	5.0
1	G	110	HIS	4.9
1	F	102	PRO	4.9
1	H	118	TYR	4.9
1	H	16	GLN	4.9
1	F	103	VAL	4.9
1	G	90	ARG	4.9
1	H	26	LEU	4.9
1	F	61	LYS	4.8
1	H	4	ARG	4.8
1	F	72	LYS	4.8
1	H	133	ILE	4.7
1	G	38	THR	4.7
1	H	135	GLN	4.7
1	F	69	LYS	4.7
1	B	60	LEU	4.7
1	H	140	LEU	4.7
1	G	44	MET	4.6
1	G	109	ALA	4.6
1	G	21	LYS	4.6
1	E	17	PHE	4.5
1	F	4	ARG	4.5
1	G	46	LEU	4.5
1	F	42	ILE	4.5
1	H	141	THR	4.5
1	E	3	LEU	4.5
1	E	7	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	73	LYS	4.4
1	G	133	ILE	4.4
1	H	17	PHE	4.4
1	G	61	LYS	4.4
1	F	46	LEU	4.4
1	F	45	ILE	4.4
1	F	44	MET	4.3
1	E	35	LEU	4.3
1	F	55	ARG	4.3
1	E	32	ASN	4.2
1	H	33	VAL	4.2
1	F	93	LEU	4.2
1	F	101	ILE	4.2
1	F	48	ALA	4.1
1	G	104	ALA	4.1
1	F	97	THR	4.1
1	F	36	THR	4.0
1	G	114	THR	4.0
1	G	57	ALA	4.0
1	G	66	ALA	4.0
1	A	35	LEU	4.0
1	B	89	GLU	4.0
1	E	60	LEU	3.9
1	E	34	LYS	3.9
1	F	98	GLU	3.9
1	E	10	PHE	3.9
1	F	22	HIS	3.9
1	E	98	GLU	3.9
1	H	121	LEU	3.9
1	E	22	HIS	3.8
1	G	105	LYS	3.8
1	F	99	LYS	3.7
1	G	72	LYS	3.7
1	F	94	TRP	3.7
1	H	8	GLU	3.7
1	F	27	GLY	3.7
1	F	26	LEU	3.7
1	F	84	ARG	3.7
1	F	70	ALA	3.7
1	E	14	ILE	3.7
1	F	132	VAL	3.6
1	F	28	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	11	LEU	3.6
1	F	140	LEU	3.6
1	B	56	ILE	3.5
1	F	47	ALA	3.5
1	E	40	GLU	3.5
1	D	93	LEU	3.5
1	G	145	ARG	3.5
1	E	115	LEU	3.4
1	E	15	MET	3.4
1	G	52	THR	3.4
1	G	51	SER	3.4
1	D	56	ILE	3.3
1	E	30	GLU	3.3
1	B	43	LEU	3.3
1	C	73	LYS	3.3
1	G	62	ILE	3.3
1	G	28	GLU	3.3
1	G	54	ALA	3.2
1	G	25	LEU	3.2
1	F	86	THR	3.2
1	E	133	ILE	3.2
1	G	68	THR	3.2
1	H	25	LEU	3.2
1	F	137	LEU	3.1
1	E	145	ARG	3.1
1	G	141	THR	3.1
1	G	3	LEU	3.1
1	H	132	VAL	3.1
1	G	140	LEU	3.1
1	G	10	PHE	3.1
1	E	51	SER	3.1
1	F	39	GLN	3.1
1	G	29	CYS	3.1
1	G	7	ILE	3.1
1	G	31	SER	3.0
1	F	105	LYS	3.0
1	G	117	THR	3.0
1	F	121	LEU	3.0
1	F	125	PHE	3.0
1	C	90	ARG	3.0
1	E	140	LEU	2.9
1	F	136	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	49	GLU	2.9
1	C	71	LEU	2.9
1	B	42	ILE	2.9
1	H	124	LYS	2.9
1	A	73	LYS	2.8
1	F	133	ILE	2.8
1	E	84	ARG	2.8
1	C	35	LEU	2.8
1	G	50	VAL	2.8
1	E	19	GLU	2.7
1	F	141	THR	2.7
1	F	58	GLU	2.7
1	G	74	LEU	2.7
1	H	35	LEU	2.6
1	H	32	ASN	2.6
1	B	104	ALA	2.6
1	F	109	ALA	2.6
1	H	38	THR	2.6
1	F	49	GLU	2.6
1	G	118	TYR	2.6
1	B	35	LEU	2.5
1	C	43	LEU	2.5
1	C	34	LYS	2.5
1	A	93	LEU	2.5
1	D	60	LEU	2.5
1	H	127	ASP	2.5
1	F	12	GLY	2.5
1	E	20	ASN	2.4
1	C	56	ILE	2.4
1	F	124	LYS	2.4
1	G	136	PHE	2.4
1	F	59	GLN	2.4
1	E	31	SER	2.4
1	A	67	VAL	2.3
1	F	81	LYS	2.3
1	E	87	ASN	2.3
1	F	122	GLY	2.3
1	A	89	GLU	2.3
1	E	122	GLY	2.3
1	H	120	GLU	2.3
1	A	90	ARG	2.3
1	C	32	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	10	PHE	2.3
1	D	87	ASN	2.2
1	F	145	ARG	2.2
1	B	72	LYS	2.2
1	G	128	GLU	2.2
1	A	74	LEU	2.2
1	F	20	ASN	2.2
1	F	11	LEU	2.2
1	G	11	LEU	2.2
1	E	108	ALA	2.2
1	H	105	LYS	2.2
1	C	78	GLU	2.2
1	C	98	GLU	2.2
1	F	50	VAL	2.2
1	B	87	ASN	2.2
1	E	45	ILE	2.1
1	G	37	SER	2.1
1	H	30	GLU	2.1
1	E	79	LEU	2.1
1	F	17	PHE	2.1
1	E	65	ALA	2.1
1	H	80	ILE	2.1
1	B	38	THR	2.1
1	E	121	LEU	2.1
1	G	122	GLY	2.1
1	G	107	HIS	2.1
1	D	96	LEU	2.1
1	H	69	LYS	2.1
1	E	6	GLN	2.0
1	A	56	ILE	2.0
1	D	72	LYS	2.0
1	F	73	LYS	2.0
1	F	19	GLU	2.0
1	H	63	SER	2.0
1	E	135	GLN	2.0
1	G	130	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 monosaccharides 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	ZN	G	201	1/1	0.62	0.28	300,300,300,300	0
2	ZN	G	202	1/1	0.79	0.41	300,300,300,300	0
2	ZN	F	201	1/1	0.84	0.12	234,234,234,234	0
2	ZN	E	202	1/1	0.91	0.09	154,154,154,154	0
2	ZN	E	201	1/1	0.91	0.08	167,167,167,167	0
2	ZN	H	201	1/1	0.91	0.15	165,165,165,165	0
2	ZN	H	202	1/1	0.92	0.08	142,142,142,142	0
2	ZN	F	202	1/1	0.93	0.04	257,257,257,257	0
2	ZN	A	202	1/1	0.94	0.16	121,121,121,121	0
2	ZN	C	201	1/1	0.97	0.11	84,84,84,84	0
2	ZN	B	202	1/1	0.98	0.12	145,145,145,145	0
2	ZN	C	202	1/1	0.98	0.11	124,124,124,124	0
2	ZN	D	201	1/1	0.98	0.15	73,73,73,73	0
2	ZN	D	202	1/1	0.98	0.17	114,114,114,114	0
2	ZN	B	201	1/1	0.99	0.11	89,89,89,89	0
2	ZN	A	201	1/1	0.99	0.14	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.