WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2024 – 03:27 AM EDT

PDB ID	:	4ELO
Title	:	Ferric binding protein in apo form 1
Authors	:	Wang, Q.; Liu, X.Q.; Wang, X.Q.
Deposited on	:	2012-04-11
Resolution	:	1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) 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 ⓘ

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

The reported resolution of this entry is 1.91 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.
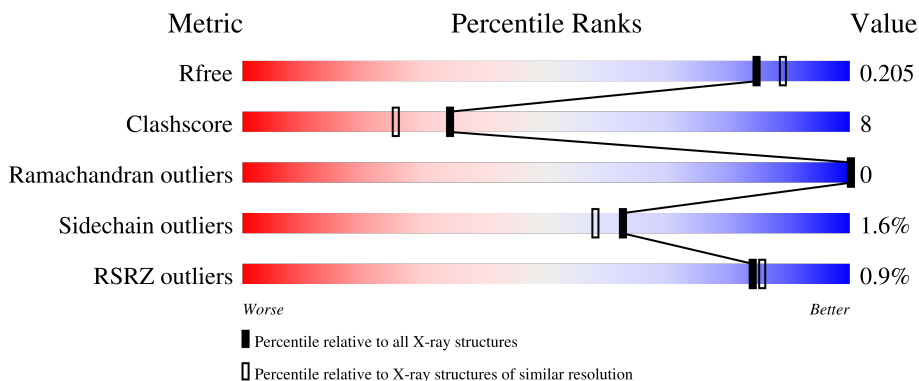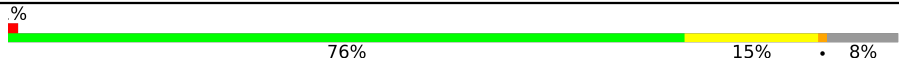

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	336	
1	B	336	
1	C	336	
1	D	336	
1	E	336	

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Mol	Chain	Length	Quality of chain
1	F	336	76% 15% 8%

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 15969 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 Iron ABC transporter, periplasmic iron-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1530	419	434	5			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1530	419	434	5			
1	C	308	Total	C	N	O	S	8	1	0
			2396	1535	422	434	5			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1530	419	434	5			
1	E	308	Total	C	N	O	S	0	0	0
			2388	1530	419	434	5			
1	F	308	Total	C	N	O	S	0	0	0
			2388	1530	419	434	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	HIS	-	expression tag	UNP Q5SHV2
A	332	HIS	-	expression tag	UNP Q5SHV2
A	333	HIS	-	expression tag	UNP Q5SHV2
A	334	HIS	-	expression tag	UNP Q5SHV2
A	335	HIS	-	expression tag	UNP Q5SHV2
A	336	HIS	-	expression tag	UNP Q5SHV2
B	331	HIS	-	expression tag	UNP Q5SHV2
B	332	HIS	-	expression tag	UNP Q5SHV2
B	333	HIS	-	expression tag	UNP Q5SHV2
B	334	HIS	-	expression tag	UNP Q5SHV2
B	335	HIS	-	expression tag	UNP Q5SHV2
B	336	HIS	-	expression tag	UNP Q5SHV2
C	331	HIS	-	expression tag	UNP Q5SHV2
C	332	HIS	-	expression tag	UNP Q5SHV2
C	333	HIS	-	expression tag	UNP Q5SHV2
C	334	HIS	-	expression tag	UNP Q5SHV2
C	335	HIS	-	expression tag	UNP Q5SHV2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	336	HIS	-	expression tag	UNP Q5SHV2
D	331	HIS	-	expression tag	UNP Q5SHV2
D	332	HIS	-	expression tag	UNP Q5SHV2
D	333	HIS	-	expression tag	UNP Q5SHV2
D	334	HIS	-	expression tag	UNP Q5SHV2
D	335	HIS	-	expression tag	UNP Q5SHV2
D	336	HIS	-	expression tag	UNP Q5SHV2
E	331	HIS	-	expression tag	UNP Q5SHV2
E	332	HIS	-	expression tag	UNP Q5SHV2
E	333	HIS	-	expression tag	UNP Q5SHV2
E	334	HIS	-	expression tag	UNP Q5SHV2
E	335	HIS	-	expression tag	UNP Q5SHV2
E	336	HIS	-	expression tag	UNP Q5SHV2
F	331	HIS	-	expression tag	UNP Q5SHV2
F	332	HIS	-	expression tag	UNP Q5SHV2
F	333	HIS	-	expression tag	UNP Q5SHV2
F	334	HIS	-	expression tag	UNP Q5SHV2
F	335	HIS	-	expression tag	UNP Q5SHV2
F	336	HIS	-	expression tag	UNP Q5SHV2

- Molecule 2 is water.

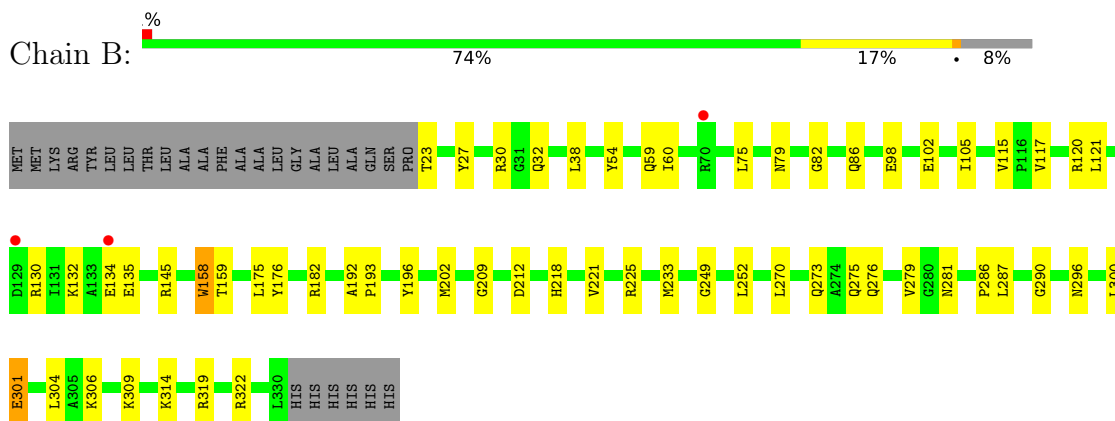| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	293	Total 293	O 293	0	0
2	B	248	Total 248	O 248	0	0
2	C	331	Total 331	O 331	0	0
2	D	252	Total 252	O 252	0	0
2	E	252	Total 252	O 252	0	0
2	F	257	Total 257	O 257	0	0

3 Residue-property plots ⓘ

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: Iron ABC transporter, periplasmic iron-binding protein

Chain A:

- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein

Chain B:

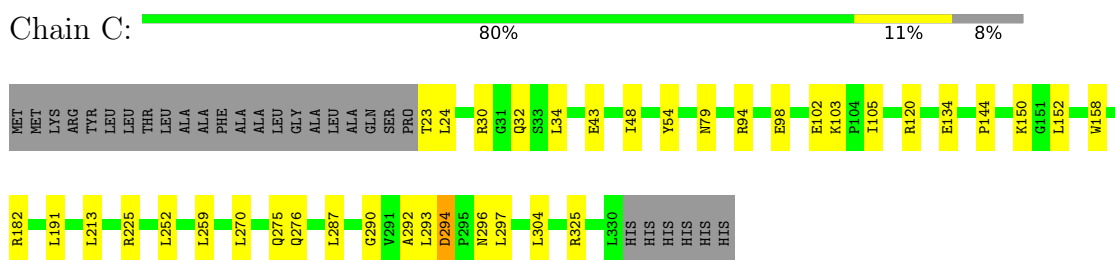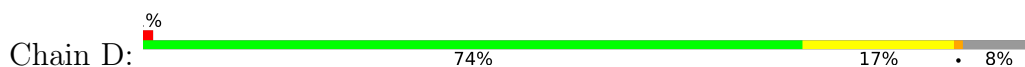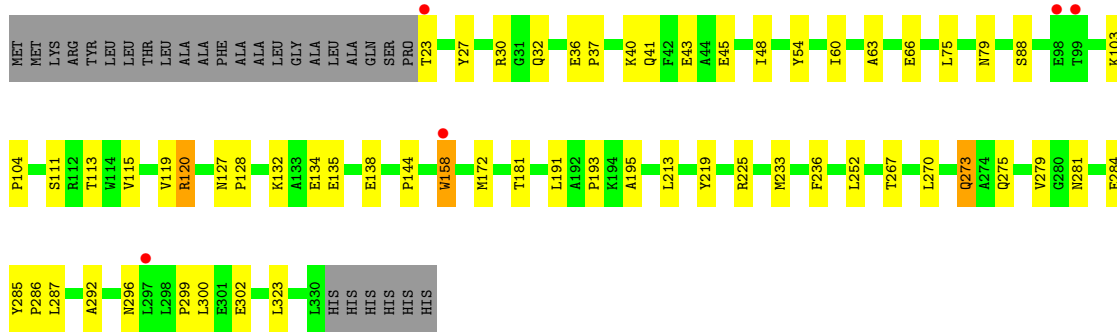- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein

Chain C:

- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein

Chain D:

MET MET LYS ARG TYR LEU LEU THR LEU ALA ALA PHE ALA ALA LEU GLY ALA LEU ALA GLN SER PRO T23 Y27 R30 G31 Q32 E36 P37 K40 Q41 F42 E43 A44 E45 I48 Y54 I60 A63 E66 L75 N79 S88 E98 T99 K103

P104 S111 R112 T113 W114 V115 V119 R120 N127 P128 K132 A133 E134 E135 E138 P144 W158 M172 T181 L191 A192 P193 K194 A195 L213 Y219 R225 M233 F236 L252 T267 L270 Q273 A274 Q275 V279 G280 N281 E284

Y285 P286 L287 A292 N296 L297 L298 P299 L300 E301 E302 L323 L330 HIS HIS HIS HIS HIS

• Molecule 1: Iron ABC transporter, periplasmic iron-binding protein

Chain E:

%

78% 13% 8%

MET MET LYS ARG TYR LEU LEU THR LEU ALA ALA PHE ALA ALA LEU GLY ALA LEU ALA GLN SER PRO T23 G29 Q32 S33 L34 V39 E43 Y54 S55 L61 Q65 S71 P72 A73 D74 T99 L100 I105 A110 S111 R112 R120 L121 W158

L175 E179 G209 H218 R225 R230 D238 A241 S256 Q275 Q276 V279 G280 N281 P286 L287 A292 N296 E301 E302 K306 S307 P308 D318 L324 R325 E326 L330 HIS HIS HIS HIS HIS
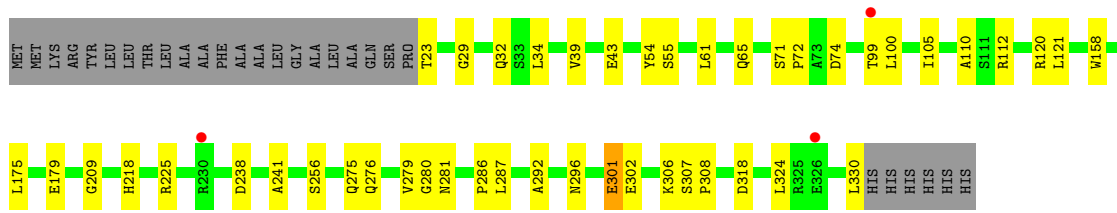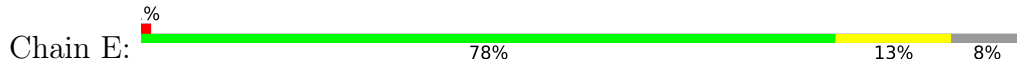
• Molecule 1: Iron ABC transporter, periplasmic iron-binding protein

Chain F:

%

76% 15% • 8%

MET MET LYS ARG TYR LEU LEU THR LEU ALA ALA PHE ALA ALA LEU GLY ALA LEU ALA GLN SER PRO T23 R30 G31 Q32 E45 T46 Y54 Q65 N79 A106 F107 V115 P116 V117 R120 V123 R130 L141 K150 R155 W158 T159 K180

A192 P193 K194 A195 Y196 M202 G209 L213 H218 V221 R225 R230 M233 R237 D240 G249 L252 R264 L270 Q275 Q276 V279 G280 N281 P286 L287 V291 A292 L293 D294 P295 N296 P308 K309 L330 HIS HIS HIS HIS

HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.12Å 139.35Å 326.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.15 – 1.91 36.15 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.8 (36.15-1.91) 95.6 (36.15-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.95 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.163 , 0.207 0.161 , 0.205	Depositor DCC
R_{free} test set	7178 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.0	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15969	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.37	0/2438	0.53	0/3311
1	B	0.33	0/2438	0.50	0/3311
1	C	0.39	0/2449	0.55	1/3325 (0.0%)
1	D	0.34	0/2438	0.52	0/3311
1	E	0.32	0/2438	0.48	0/3311
1	F	0.34	0/2438	0.52	2/3311 (0.1%)
All	All	0.35	0/14639	0.52	3/19880 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	30	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	30	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	182	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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	2388	0	2449	36	0
1	B	2388	0	2449	46	0
1	C	2396	0	2462	27	0
1	D	2388	0	2449	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2388	0	2449	37	0
1	F	2388	0	2449	53	0
2	A	293	0	0	8	0
2	B	248	0	0	8	0
2	C	331	0	0	2	0
2	D	252	0	0	2	0
2	E	252	0	0	6	0
2	F	257	0	0	4	0
All	All	15969	0	14707	244	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 8.

The worst 5 of 244 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:D:120:ARG:HG3	1:D:120:ARG:HH11	1.13	1.09
1:F:123:VAL:HG21	1:F:233:MET:HE2	1.43	0.99
1:D:120:ARG:HD2	1:D:219:TYR:CE2	2.01	0.96
1:F:23:THR:HG22	2:F:581:HOH:O	1.67	0.94
1:D:120:ARG:HD3	1:D:284:GLU:OE2	1.70	0.91

There are no symmetry-related clashes.

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	306/336 (91%)	299 (98%)	7 (2%)	0	100	100
1	B	306/336 (91%)	304 (99%)	2 (1%)	0	100	100
1	C	307/336 (91%)	305 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	306/336 (91%)	304 (99%)	2 (1%)	0	100	100
1	E	306/336 (91%)	305 (100%)	1 (0%)	0	100	100
1	F	306/336 (91%)	304 (99%)	2 (1%)	0	100	100
All	All	1837/2016 (91%)	1821 (99%)	16 (1%)	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	247/268 (92%)	242 (98%)	5 (2%)	55	49
1	B	247/268 (92%)	243 (98%)	4 (2%)	62	58
1	C	248/268 (92%)	245 (99%)	3 (1%)	71	69
1	D	247/268 (92%)	242 (98%)	5 (2%)	55	49
1	E	247/268 (92%)	244 (99%)	3 (1%)	71	69
1	F	247/268 (92%)	243 (98%)	4 (2%)	62	58
All	All	1483/1608 (92%)	1459 (98%)	24 (2%)	62	58

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	273	GLN
1	E	120	ARG
1	D	323	LEU
1	E	158	TRP
1	B	158	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	281	ASN
1	F	296	ASN
1	E	296	ASN
1	F	275	GLN
1	B	296	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, 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(Å²)	Q<0.9
1	A	308/336 (91%)	-0.19	3 (0%)	82	84	9, 17, 42, 59	0
1	B	308/336 (91%)	-0.17	3 (0%)	82	84	11, 23, 46, 66	0
1	C	308/336 (91%)	-0.36	0	100	100	7, 15, 33, 49	0
1	D	308/336 (91%)	-0.12	5 (1%)	72	74	12, 23, 48, 64	0
1	E	308/336 (91%)	-0.18	3 (0%)	82	84	12, 23, 47, 65	0
1	F	308/336 (91%)	-0.22	2 (0%)	89	90	12, 22, 45, 58	0
All	All	1848/2016 (91%)	-0.21	16 (0%)	84	85	7, 21, 45, 66	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	326	GLU	3.5
1	A	298	LEU	3.0
1	F	23	THR	2.8
1	E	230	ARG	2.7
1	D	99	THR	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 ⓘ

There are no such residues in this entry.