



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:31 PM UTC

PDB ID : 1RXX / pdb_00001rxx
Title : Structure of arginine deiminase
Authors : Galkin, A.; Kulakova, L.; Sarikaya, E.; Lim, K.; Howard, A.; Herzberg, O.;
Structure 2 Function Project (S2F)
Deposited on : 2003-12-18
Resolution : 2.45 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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

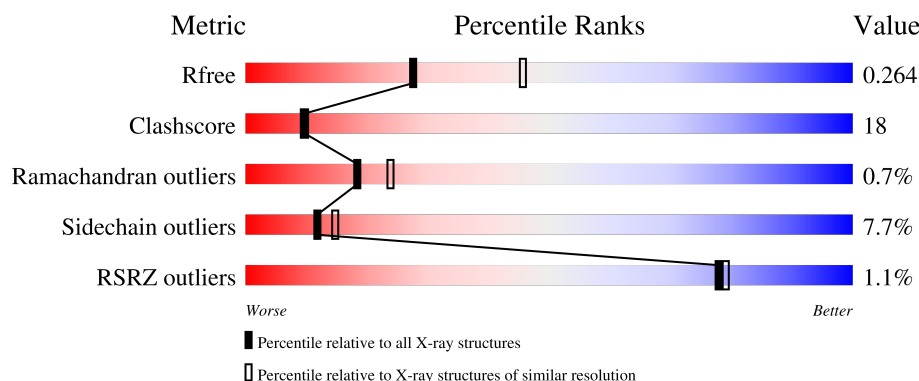
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	421	% 62% 28% 7% .
1	B	421	63% 26% 6% .
1	C	421	% 66% 27% 5% ..
1	D	421	% 62% 28% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13187 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 Arginine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	0	0
			3185	2015	553	600	7	10			
1	B	404	Total	C	N	O	S	Se	0	0	0
			3160	2001	549	593	7	10			
1	C	412	Total	C	N	O	S	Se	0	0	0
			3214	2033	557	607	7	10			
1	D	402	Total	C	N	O	S	Se	0	0	0
			3136	1986	543	590	7	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P13981
A	-1	SER	-	cloning artifact	UNP P13981
A	0	HIS	-	cloning artifact	UNP P13981
A	1	MSE	-	cloning artifact	UNP P13981
A	21	MSE	MET	modified residue	UNP P13981
A	62	MSE	MET	modified residue	UNP P13981
A	72	MSE	MET	modified residue	UNP P13981
A	143	MSE	MET	modified residue	UNP P13981
A	180	MSE	MET	modified residue	UNP P13981
A	229	MSE	MET	modified residue	UNP P13981
A	240	MSE	MET	modified residue	UNP P13981
A	277	MSE	MET	modified residue	UNP P13981
A	316	MSE	MET	modified residue	UNP P13981
A	407	MSE	MET	modified residue	UNP P13981
B	-2	GLY	-	cloning artifact	UNP P13981
B	-1	SER	-	cloning artifact	UNP P13981
B	0	HIS	-	cloning artifact	UNP P13981
B	1	MSE	-	cloning artifact	UNP P13981
B	21	MSE	MET	modified residue	UNP P13981
B	62	MSE	MET	modified residue	UNP P13981
B	72	MSE	MET	modified residue	UNP P13981

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Chain	Residue	Modelled	Actual	Comment	Reference
B	143	MSE	MET	modified residue	UNP P13981
B	180	MSE	MET	modified residue	UNP P13981
B	229	MSE	MET	modified residue	UNP P13981
B	240	MSE	MET	modified residue	UNP P13981
B	277	MSE	MET	modified residue	UNP P13981
B	316	MSE	MET	modified residue	UNP P13981
B	407	MSE	MET	modified residue	UNP P13981
C	-2	GLY	-	cloning artifact	UNP P13981
C	-1	SER	-	cloning artifact	UNP P13981
C	0	HIS	-	cloning artifact	UNP P13981
C	1	MSE	-	cloning artifact	UNP P13981
C	21	MSE	MET	modified residue	UNP P13981
C	62	MSE	MET	modified residue	UNP P13981
C	72	MSE	MET	modified residue	UNP P13981
C	143	MSE	MET	modified residue	UNP P13981
C	180	MSE	MET	modified residue	UNP P13981
C	229	MSE	MET	modified residue	UNP P13981
C	240	MSE	MET	modified residue	UNP P13981
C	277	MSE	MET	modified residue	UNP P13981
C	316	MSE	MET	modified residue	UNP P13981
C	407	MSE	MET	modified residue	UNP P13981
D	-2	GLY	-	cloning artifact	UNP P13981
D	-1	SER	-	cloning artifact	UNP P13981
D	0	HIS	-	cloning artifact	UNP P13981
D	1	MSE	-	cloning artifact	UNP P13981
D	21	MSE	MET	modified residue	UNP P13981
D	62	MSE	MET	modified residue	UNP P13981
D	72	MSE	MET	modified residue	UNP P13981
D	143	MSE	MET	modified residue	UNP P13981
D	180	MSE	MET	modified residue	UNP P13981
D	229	MSE	MET	modified residue	UNP P13981
D	240	MSE	MET	modified residue	UNP P13981
D	277	MSE	MET	modified residue	UNP P13981
D	316	MSE	MET	modified residue	UNP P13981
D	407	MSE	MET	modified residue	UNP P13981

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	147	Total O 147 147	0	0

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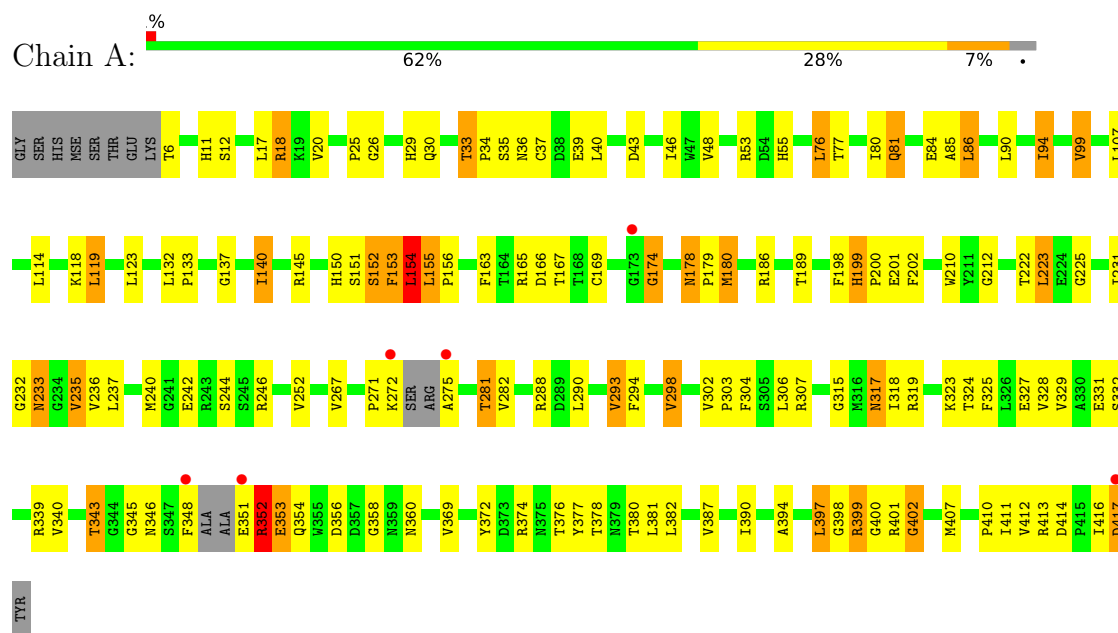
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	144	Total 144	O 144	0	0
2	D	88	Total 88	O 88	0	0

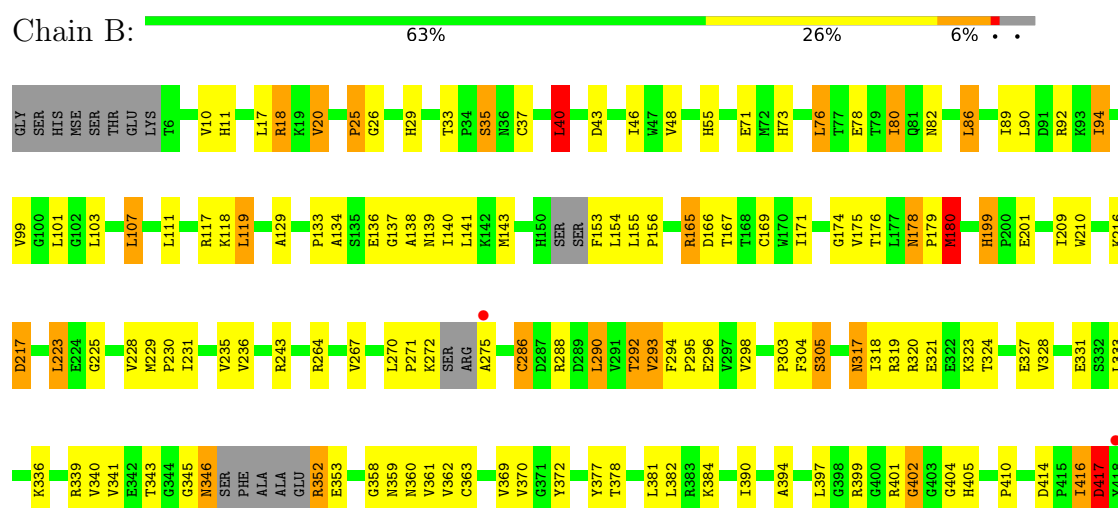
3 Residue-property plots

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.

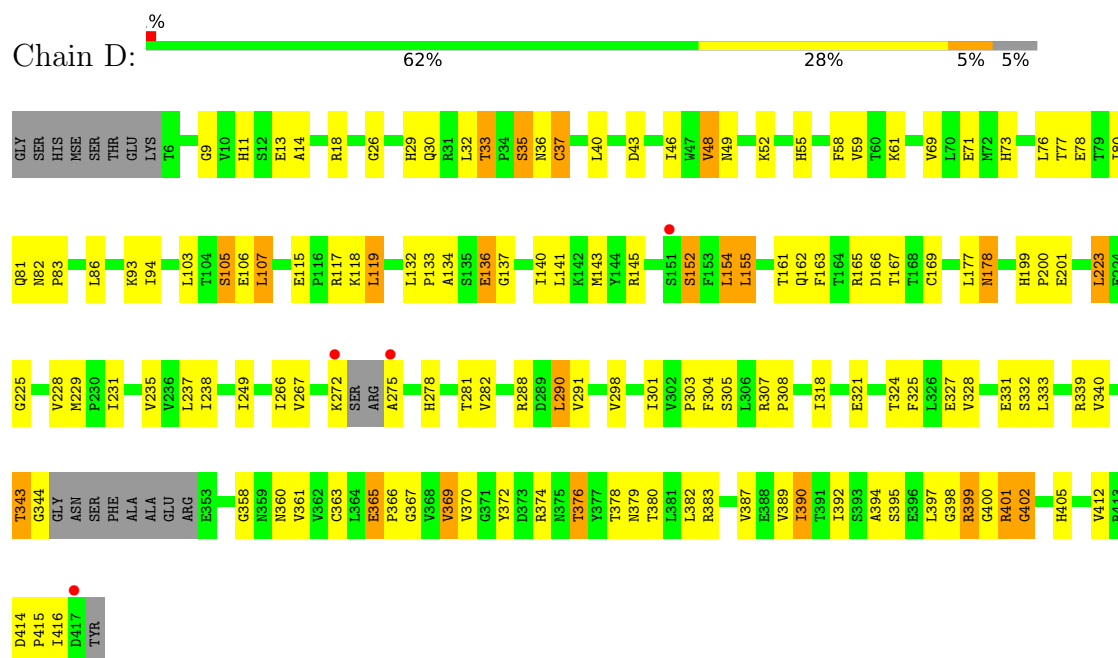
• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.90Å 114.90Å 300.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.45) 99.7 (20.00-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.44Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.264 0.200 , 0.264	Depositor DCC
R_{free} test set	3802 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13187	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.68% 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

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	0.87	1/3242 (0.0%)	1.27	38/4379 (0.9%)
1	B	0.89	2/3216 (0.1%)	1.22	28/4342 (0.6%)
1	C	0.85	0/3273	1.29	33/4422 (0.7%)
1	D	0.78	0/3192	1.22	19/4313 (0.4%)
All	All	0.85	3/12923 (0.0%)	1.25	118/17456 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	MSE	SE-CE	-14.56	1.51	1.95
1	B	370	VAL	CA-CB	-5.61	1.47	1.54
1	A	252	VAL	CA-CB	5.16	1.60	1.54

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	SER	N-CA-C	11.54	135.38	110.80
1	C	346	ASN	N-CA-C	11.29	127.68	109.85
1	D	154	LEU	N-CA-C	-10.17	100.19	111.07
1	B	167	THR	N-CA-C	10.11	124.97	112.23
1	A	43	ASP	N-CA-C	9.78	121.94	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	144	TYR	Sidechain
1	C	348	PHE	Sidechain

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	3185	0	3161	124	0
1	B	3160	0	3139	117	0
1	C	3214	0	3186	102	0
1	D	3136	0	3119	109	0
2	A	113	0	0	15	0
2	B	147	0	0	16	0
2	C	144	0	0	20	0
2	D	88	0	0	13	0
All	All	13187	0	12605	444	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 18.

The worst 5 of 444 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:352:ARG:HG3	1:B:352:ARG:HH11	1.13	1.11
1:A:343:THR:HG21	1:A:358:GLY:H	1.15	1.08
1:B:343:THR:HG21	1:B:358:GLY:H	1.21	1.04
1:D:343:THR:HG21	1:D:358:GLY:H	1.20	1.02
1:B:363:CYS:HB2	2:B:517:HOH:O	1.61	1.01

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	402/421 (96%)	381 (95%)	18 (4%)	3 (1%)	18	24
1	B	396/421 (94%)	373 (94%)	21 (5%)	2 (0%)	24	32
1	C	408/421 (97%)	385 (94%)	18 (4%)	5 (1%)	10	11
1	D	396/421 (94%)	371 (94%)	23 (6%)	2 (0%)	24	32
All	All	1602/1684 (95%)	1510 (94%)	80 (5%)	12 (1%)	18	24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	GLY
1	C	347	SER
1	C	402	GLY
1	D	152	SER
1	A	402	GLY

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	347/346 (100%)	316 (91%)	31 (9%)	9	10
1	B	343/346 (99%)	311 (91%)	32 (9%)	8	9
1	C	349/346 (101%)	328 (94%)	21 (6%)	17	26
1	D	342/346 (99%)	320 (94%)	22 (6%)	16	22
All	All	1381/1384 (100%)	1275 (92%)	106 (8%)	12	15

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	369	VAL
1	C	119	LEU

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Mol	Chain	Res	Type
1	D	343	THR
1	B	384	LYS
1	C	33	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	ASN
1	C	187	GLN
1	C	162	GLN
1	C	359	ASN
1	A	187	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	398/421 (94%)	-0.38	6 (1%) 72 74	26, 41, 70, 91	0
1	B	394/421 (93%)	-0.50	2 (0%) 87 88	22, 38, 66, 97	0
1	C	402/421 (95%)	-0.46	6 (1%) 72 74	23, 39, 69, 99	0
1	D	392/421 (93%)	-0.26	4 (1%) 79 80	31, 46, 73, 89	0
All	All	1586/1684 (94%)	-0.40	18 (1%) 78 79	22, 42, 71, 99	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	PHE	3.7
1	A	348	PHE	3.6
1	C	347	SER	3.5
1	A	417	ASP	3.4
1	B	275	ALA	3.2

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.