



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 10:12 am BST

PDB ID : 9QY8 / pdb\_00009qy8  
Title : Crystal structure of apoform human USP18  
Authors : Turnbull, A.P.; Halliwell, T.; Frankling, C.L.  
Deposited on : 2025-04-17  
Resolution : 1.92 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

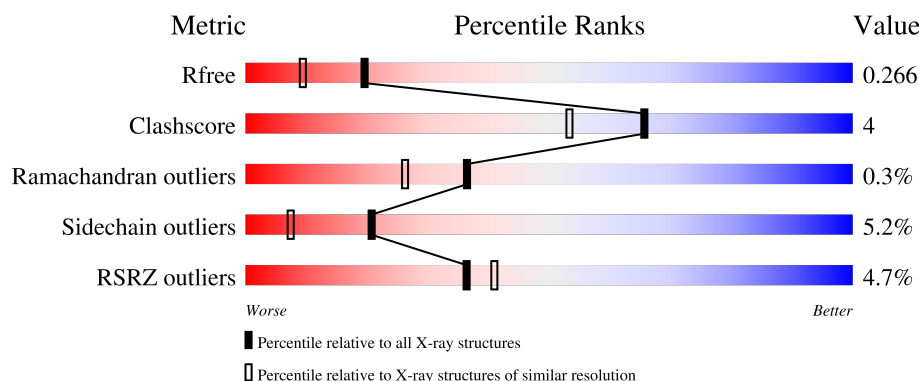
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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  $\geq 3$ , 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	440	 5% 88% 10% •
1	B	440	 5% 82% 15% ••

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6962 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 Ubl carboxyl-terminal hydrolase 18, Response regulator FrzS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	1	0
			3383	2158	571	626	28			
1	B	437	Total	C	N	O	S	0	1	0
			3354	2138	570	619	27			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP Q9UMW8
A	48	PRO	-	expression tag	UNP Q9UMW8
A	401	GLY	-	linker	UNP Q9UMW8
A	402	SER	-	linker	UNP Q9UMW8
A	527	GLY	-	linker	UNP Q1D4U9
A	528	SER	-	linker	UNP Q1D4U9
B	47	GLY	-	expression tag	UNP Q9UMW8
B	48	PRO	-	expression tag	UNP Q9UMW8
B	401	GLY	-	linker	UNP Q9UMW8
B	402	SER	-	linker	UNP Q9UMW8
B	527	GLY	-	linker	UNP Q1D4U9
B	528	SER	-	linker	UNP Q1D4U9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

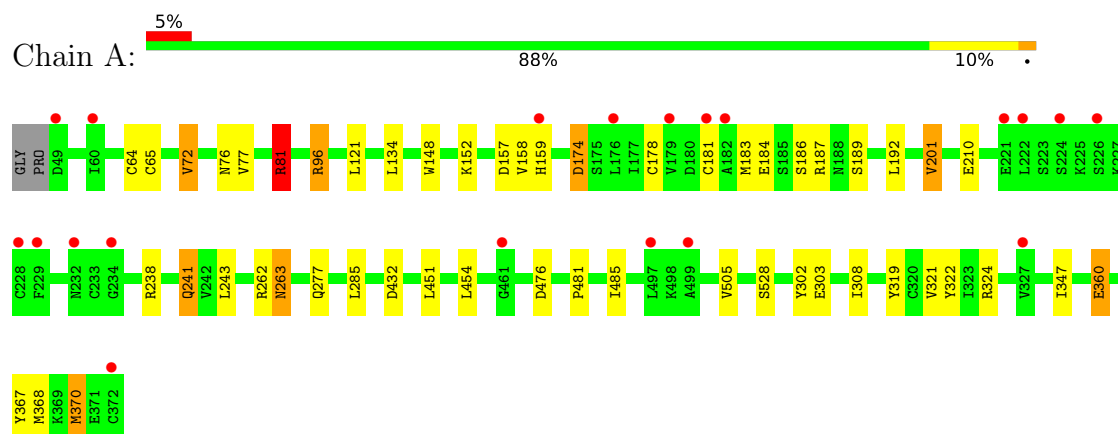
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	102	Total 102	O 102	0	0

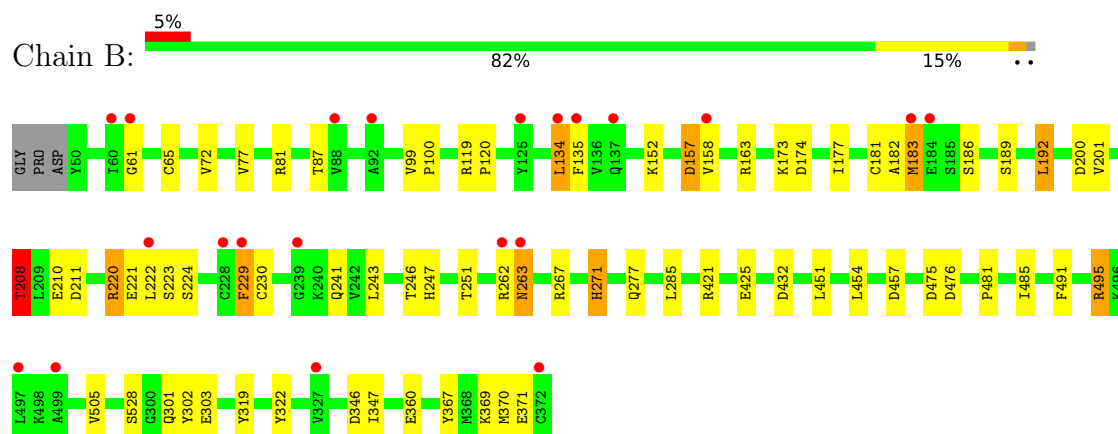
### 3 Residue-property plots

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: Ubl carboxyl-terminal hydrolase 18, Response regulator FrzS



- Molecule 1: Ubl carboxyl-terminal hydrolase 18, Response regulator FrzS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.87Å 71.78Å 73.06Å 79.32° 76.28° 89.88°	Depositor
Resolution (Å)	39.59 – 1.92 39.59 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.4 (39.59-1.92) 97.5 (39.59-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.205 , 0.260 0.213 , 0.266	Depositor DCC
$R_{free}$ test set	2020 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.67	0/3453	1.16	10/4683 (0.2%)
1	B	0.66	0/3423	1.18	19/4645 (0.4%)
All	All	0.66	0/6876	1.17	29/9328 (0.3%)

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	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	GLU	CB-CA-C	-7.47	97.31	109.72
1	B	271	HIS	CB-CA-C	7.34	123.04	109.54
1	B	360	GLU	CB-CA-C	-7.28	97.64	109.72
1	A	174	ASP	CB-CA-C	7.10	121.84	110.19
1	B	120	PRO	N-CA-CB	-6.15	97.95	102.25
1	A	174	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	208	THR	N-CA-CB	-5.92	100.59	111.37
1	B	371	GLU	CB-CA-C	5.92	121.26	112.03
1	A	210	GLU	CB-CG-CD	5.89	122.61	112.60
1	B	251	THR	CA-CB-OG1	-5.86	100.82	109.60
1	B	229	PHE	CA-CB-CG	5.76	119.56	113.80
1	B	476	ASP	CA-CB-CG	5.71	118.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	454	LEU	N-CA-CB	-5.64	101.92	110.77
1	B	346	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	476	ASP	CB-CA-C	-5.57	101.39	110.85
1	B	475	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	476	ASP	CB-CA-C	-5.44	101.59	110.85
1	A	243	LEU	N-CA-CB	-5.37	101.66	110.68
1	B	158	VAL	N-CA-CB	5.37	119.83	110.65
1	A	476	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	183	MET	CG-SD-CE	5.25	112.45	100.90
1	B	210	GLU	CB-CG-CD	5.20	121.45	112.60
1	B	243	LEU	N-CA-CB	-5.20	101.95	110.68
1	B	454	LEU	N-CA-CB	-5.13	103.05	110.84
1	B	457	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	200	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	201	VAL	CB-CA-C	-5.06	105.41	112.04
1	A	158	VAL	N-CA-CB	5.04	117.39	110.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	324	ARG	Sidechain
1	A	81	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	224	SER	Peptide

## 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	3383	0	3297	21	0
1	B	3354	0	3278	30	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	121	0	0	3	0
3	B	102	0	0	4	0
All	All	6962	0	6575	51	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 4.

All (51) 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:177:ILE:HD11	1:B:421:ARG:NH1	2.01	0.73
1:A:178:CYS:O	1:A:181:CYS:O	2.05	0.73
1:B:491:PHE:O	1:B:495:ARG:HG3	1.94	0.67
1:A:159:HIS:ND1	3:A:701:HOH:O	2.28	0.65
1:B:208:THR:HG22	1:B:211:ASP:H	1.64	0.63
1:A:184:GLU:HG3	1:A:432:ASP:OD1	1.99	0.62
1:B:425:GLU:OE2	3:B:701:HOH:O	2.16	0.60
1:B:322:TYR:CD2	1:B:347:ILE:CD1	2.85	0.60
1:A:184:GLU:HB3	3:A:785:HOH:O	2.01	0.59
1:B:134:LEU:HD13	1:B:135:PHE:CE2	2.37	0.59
1:B:163:ARG:HH11	1:B:163:ARG:HG3	1.68	0.58
1:B:491:PHE:O	1:B:495:ARG:CG	2.54	0.56
1:B:302:TYR:HB3	1:B:367:TYR:HB3	1.88	0.56
1:B:77:VAL:O	1:B:81:ARG:HG3	2.06	0.56
1:A:76:ASN:ND2	1:A:368:MET:HE1	2.22	0.55
1:B:267:ARG:HH21	1:B:267:ARG:HG2	1.71	0.55
1:A:302:TYR:HB3	1:A:367:TYR:HB3	1.87	0.55
1:B:177:ILE:HD11	1:B:421:ARG:CZ	2.37	0.54
1:B:65:CYS:HB3	1:B:319:TYR:CD2	2.42	0.54
1:A:322:TYR:CD2	1:A:347:ILE:CD1	2.93	0.51
1:A:262:ARG:O	1:A:263:ASN:C	2.54	0.51
1:B:451:LEU:HD12	1:B:481:PRO:HB2	1.94	0.49
1:B:262:ARG:O	1:B:263:ASN:C	2.56	0.49
1:B:229:PHE:O	1:B:230:CYS:C	2.56	0.49
1:A:65:CYS:HB3	1:A:319:TYR:CD2	2.50	0.47
1:B:369:LYS:HE2	3:B:762:HOH:O	2.15	0.46
1:A:322:TYR:CG	1:A:347:ILE:HD12	2.51	0.46
1:A:360:GLU:HG3	3:A:789:HOH:O	2.15	0.45
1:B:134:LEU:HD13	1:B:135:PHE:CD2	2.52	0.45
1:A:174:ASP:O	1:A:186:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:HD12	1:A:481:PRO:HB2	1.99	0.45
1:B:192:LEU:HD22	3:B:716:HOH:O	2.17	0.44
1:A:174:ASP:OD1	1:A:241:GLN:NE2	2.51	0.44
1:B:221:GLU:O	1:B:223:SER:N	2.51	0.44
1:B:267:ARG:HG2	1:B:267:ARG:NH2	2.32	0.44
1:A:303:GLU:HG2	1:A:370:MET:SD	2.58	0.43
1:A:76:ASN:ND2	1:A:368:MET:CE	2.81	0.43
1:B:303:GLU:HG3	1:B:370:MET:SD	2.58	0.43
1:B:181:CYS:O	1:B:182:ALA:HB3	2.20	0.42
1:B:119:ARG:NE	3:B:709:HOH:O	2.46	0.42
1:B:322:TYR:CG	1:B:347:ILE:HD12	2.54	0.42
1:A:72:VAL:HG12	1:A:321:VAL:HG21	2.03	0.41
1:A:148:TRP:CZ3	1:A:152:LYS:HD3	2.55	0.41
1:A:77:VAL:O	1:A:81:ARG:HG3	2.19	0.41
1:B:174:ASP:O	1:B:186:SER:HA	2.20	0.41
1:B:61:GLY:HA2	1:B:135:PHE:CE1	2.55	0.41
1:B:246:THR:OG1	1:B:247:HIS:HD2	2.03	0.41
1:B:99:VAL:N	1:B:100:PRO:HD2	2.35	0.41
1:A:485:ILE:HA	1:A:505:VAL:O	2.21	0.41
1:A:485:ILE:HG22	1:A:505:VAL:HB	2.03	0.41
1:B:485:ILE:HA	1:B:505:VAL:O	2.21	0.41

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	437/440 (99%)	425 (97%)	11 (2%)	1 (0%)	43	34
1	B	436/440 (99%)	423 (97%)	11 (2%)	2 (0%)	24	14
All	All	873/880 (99%)	848 (97%)	22 (2%)	3 (0%)	36	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ASN
1	A	64	CYS
1	B	222	LEU

### 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	359/390 (92%)	342 (95%)	17 (5%)	23	9
1	B	357/390 (92%)	337 (94%)	20 (6%)	19	6
All	All	716/780 (92%)	679 (95%)	37 (5%)	21	7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	81	ARG
1	A	96	ARG
1	A	121	LEU
1	A	134	LEU
1	A	157	ASP
1	A	183	MET
1	A	189	SER
1	A	192	LEU
1	A	201	VAL
1	A	241	GLN
1	A	263	ASN
1	A	277	GLN
1	A	285	LEU
1	A	528	SER
1	A	308	ILE
1	A	370	MET
1	B	72	VAL
1	B	87	THR
1	B	134	LEU

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Mol	Chain	Res	Type
1	B	152	LYS
1	B	157	ASP
1	B	173	LYS
1	B	183	MET
1	B	189	SER
1	B	192	LEU
1	B	201	VAL
1	B	208	THR
1	B	220	ARG
1	B	241	GLN
1	B	271	HIS
1	B	277	GLN
1	B	285	LEU
1	B	432	ASP
1	B	495	ARG
1	B	528	SER
1	B	301	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	188	ASN
1	A	232	ASN
1	A	241	GLN
1	A	247	HIS
1	A	263	ASN
1	A	271	HIS
1	B	95	GLN
1	B	131	ASN
1	B	241	GLN
1	B	247	HIS
1	B	301	GLN

### 5.3.3 RNA ⓘ

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](#)

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	438/440 (99%)	0.34	20 (4%) 37 42	28, 54, 94, 134	1 (0%)
1	B	437/440 (99%)	0.47	21 (4%) 35 40	28, 58, 100, 141	1 (0%)
All	All	875/880 (99%)	0.41	41 (4%) 36 41	28, 56, 99, 141	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	5.1
1	B	135	PHE	4.6
1	A	179	VAL	4.4
1	B	60	ILE	3.9
1	B	229	PHE	3.4
1	A	499	ALA	3.4
1	A	49	ASP	3.3
1	B	134	LEU	3.2
1	A	182	ALA	3.1
1	A	222	LEU	3.0
1	B	499	ALA	3.0
1	B	497	LEU	3.0
1	B	228	CYS	3.0
1	A	228	CYS	2.9
1	B	263	ASN	2.9
1	B	125	TYR	2.7
1	B	183	MET	2.5
1	A	221	GLU	2.5
1	A	224	SER	2.5
1	B	88	VAL	2.4
1	A	226	SER	2.4
1	A	229	PHE	2.4
1	B	61	GLY	2.3
1	B	262	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.3
1	B	372	CYS	2.3
1	A	232	ASN	2.3
1	A	60	ILE	2.3
1	A	372	CYS	2.3
1	A	176	LEU	2.3
1	A	181	CYS	2.2
1	A	497	LEU	2.2
1	B	222	LEU	2.2
1	A	327	VAL	2.2
1	B	158	VAL	2.2
1	A	461	GLY	2.2
1	B	92	ALA	2.2
1	B	327	VAL	2.1
1	B	137	GLN	2.1
1	B	239	GLY	2.1
1	A	159	HIS	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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	A	601	1/1	0.95	0.08	75,75,75,75	0
2	ZN	B	601	1/1	0.97	0.10	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.