



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:49 PM EDT

PDB ID : 5MTZ  
Title : Crystal structure of a long form RNase Z from yeast  
Authors : Li de la Sierra-Gallay, I.; Miao, M.; van Tilbeurgh, H.  
Deposited on : 2017-01-11  
Resolution : 2.99 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

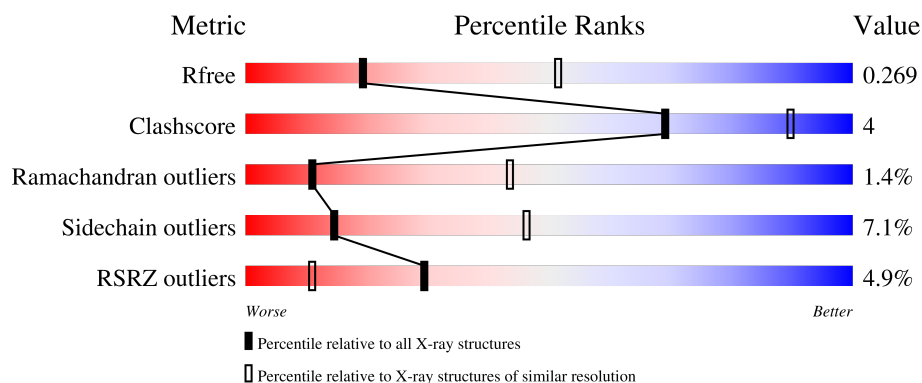
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	874	
1	B	874	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12472 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 Ribonuclease Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	Se	0	0	0
			6284	4020	1046	1192	8	18			
1	B	755	Total	C	N	O	S	Se	0	0	0
			6174	3954	1031	1163	8	18			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MSE	-	initiating methionine	UNP P36159
A	-34	ALA	-	expression tag	UNP P36159
A	-33	HIS	-	expression tag	UNP P36159
A	-32	HIS	-	expression tag	UNP P36159
A	-31	HIS	-	expression tag	UNP P36159
A	-30	HIS	-	expression tag	UNP P36159
A	-29	HIS	-	expression tag	UNP P36159
A	-28	HIS	-	expression tag	UNP P36159
A	-27	VAL	-	expression tag	UNP P36159
A	-26	GLY	-	expression tag	UNP P36159
A	-25	THR	-	expression tag	UNP P36159
A	-24	GLY	-	expression tag	UNP P36159
A	-23	SER	-	expression tag	UNP P36159
A	-22	ASN	-	expression tag	UNP P36159
A	-21	ASP	-	expression tag	UNP P36159
A	-20	ASP	-	expression tag	UNP P36159
A	-19	ASP	-	expression tag	UNP P36159
A	-18	ASP	-	expression tag	UNP P36159
A	-17	LYS	-	expression tag	UNP P36159
A	-16	SER	-	expression tag	UNP P36159
A	-15	PRO	-	expression tag	UNP P36159
A	-14	ASP	-	expression tag	UNP P36159
A	-13	PRO	-	expression tag	UNP P36159
A	-12	ASN	-	expression tag	UNP P36159
A	-11	TRP	-	expression tag	UNP P36159

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLU	-	expression tag	UNP P36159
A	-9	LEU	-	expression tag	UNP P36159
A	-8	VAL	-	expression tag	UNP P36159
A	-7	TYR	-	expression tag	UNP P36159
A	-6	THR	-	expression tag	UNP P36159
A	-5	ALA	-	expression tag	UNP P36159
A	-4	ARG	-	expression tag	UNP P36159
A	-3	LEU	-	expression tag	UNP P36159
A	-2	GLN	-	expression tag	UNP P36159
A	-1	GLU	-	expression tag	UNP P36159
A	0	PHE	-	expression tag	UNP P36159
A	1	MSE	-	expression tag	UNP P36159
B	-35	MSE	-	initiating methionine	UNP P36159
B	-34	ALA	-	expression tag	UNP P36159
B	-33	HIS	-	expression tag	UNP P36159
B	-32	HIS	-	expression tag	UNP P36159
B	-31	HIS	-	expression tag	UNP P36159
B	-30	HIS	-	expression tag	UNP P36159
B	-29	HIS	-	expression tag	UNP P36159
B	-28	HIS	-	expression tag	UNP P36159
B	-27	VAL	-	expression tag	UNP P36159
B	-26	GLY	-	expression tag	UNP P36159
B	-25	THR	-	expression tag	UNP P36159
B	-24	GLY	-	expression tag	UNP P36159
B	-23	SER	-	expression tag	UNP P36159
B	-22	ASN	-	expression tag	UNP P36159
B	-21	ASP	-	expression tag	UNP P36159
B	-20	ASP	-	expression tag	UNP P36159
B	-19	ASP	-	expression tag	UNP P36159
B	-18	ASP	-	expression tag	UNP P36159
B	-17	LYS	-	expression tag	UNP P36159
B	-16	SER	-	expression tag	UNP P36159
B	-15	PRO	-	expression tag	UNP P36159
B	-14	ASP	-	expression tag	UNP P36159
B	-13	PRO	-	expression tag	UNP P36159
B	-12	ASN	-	expression tag	UNP P36159
B	-11	TRP	-	expression tag	UNP P36159
B	-10	GLU	-	expression tag	UNP P36159
B	-9	LEU	-	expression tag	UNP P36159
B	-8	VAL	-	expression tag	UNP P36159
B	-7	TYR	-	expression tag	UNP P36159
B	-6	THR	-	expression tag	UNP P36159

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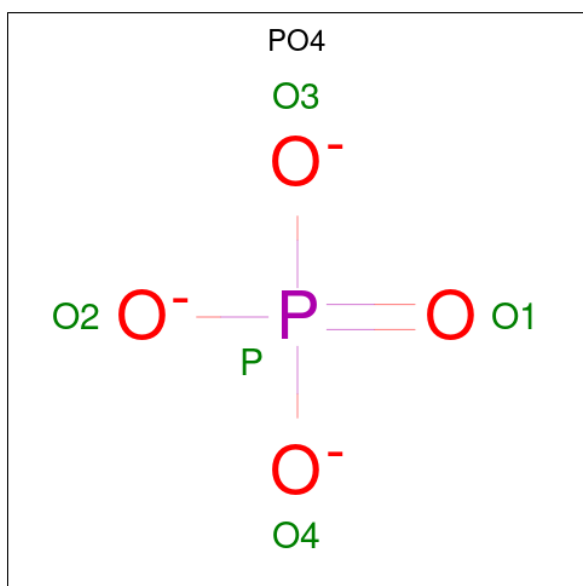
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ALA	-	expression tag	UNP P36159
B	-4	ARG	-	expression tag	UNP P36159
B	-3	LEU	-	expression tag	UNP P36159
B	-2	GLN	-	expression tag	UNP P36159
B	-1	GLU	-	expression tag	UNP P36159
B	0	PHE	-	expression tag	UNP P36159
B	1	MSE	-	expression tag	UNP P36159

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

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

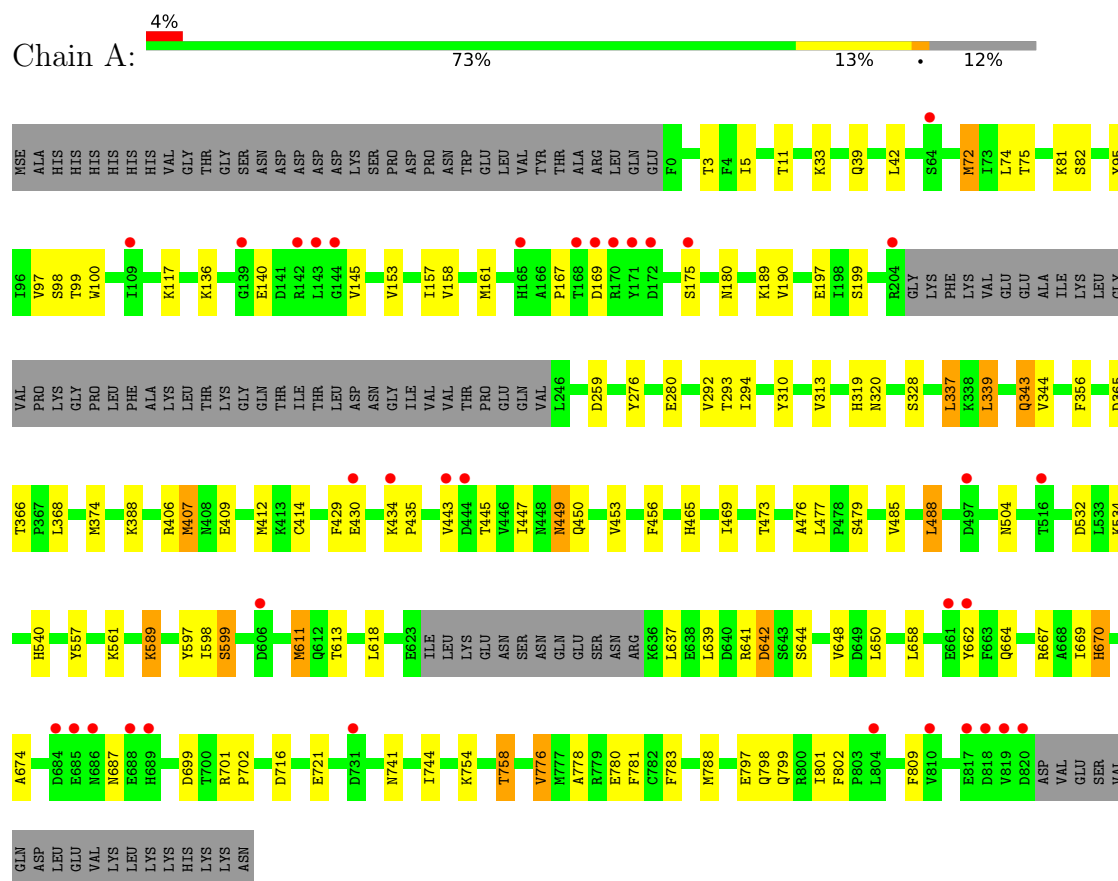


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

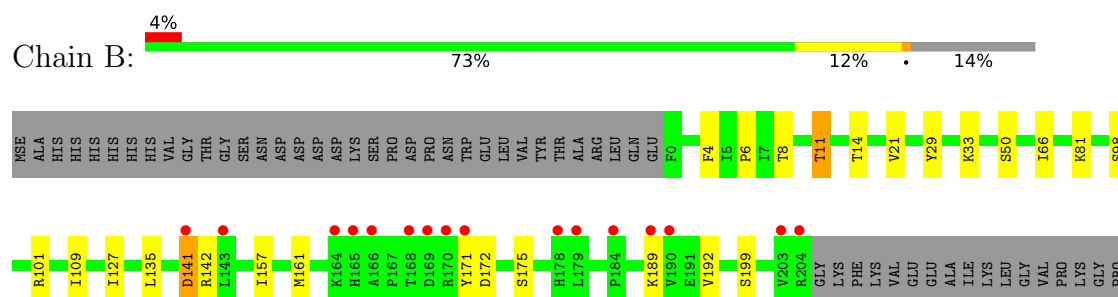
### 3 Residue-property plots [i](#)

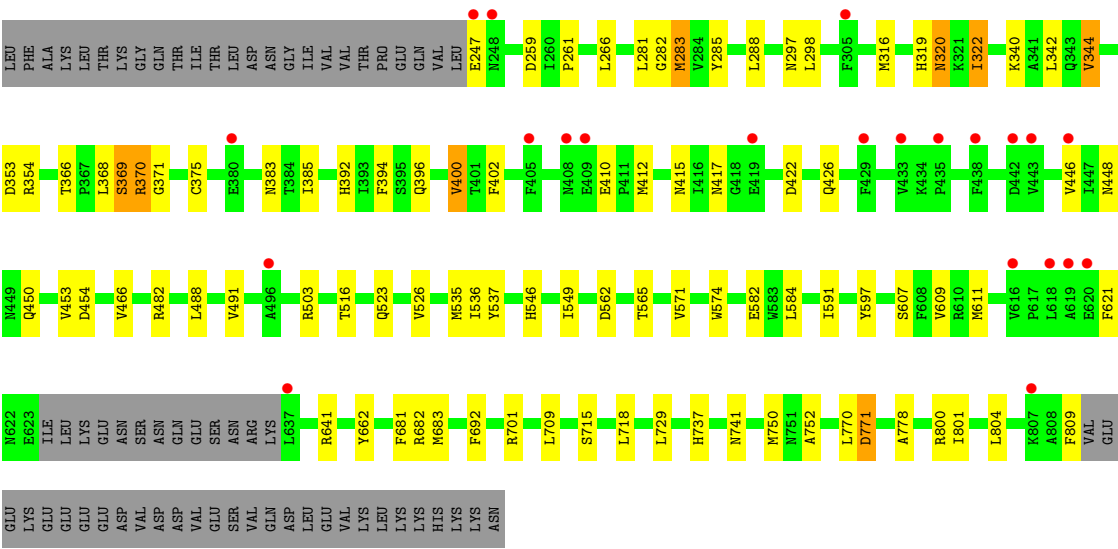
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribonuclease Z



#### • Molecule 1: Ribonuclease Z





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.00Å 136.00Å 115.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 2.99 49.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.61-2.99) 99.8 (49.61-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.181 , 0.262 0.191 , 0.269	Depositor DCC
$R_{free}$ test set	2135 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4

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	0.52	0/6410	0.74	1/8638 (0.0%)
1	B	0.53	1/6300 (0.0%)	0.73	0/8491
All	All	0.53	1/12710 (0.0%)	0.73	1/17129 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLU	CD-OE1	5.59	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LEU	CA-CB-CG	5.02	126.84	115.30

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	6284	0	6147	49	0
1	B	6174	0	6048	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
All	All	12472	0	12195	90	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 (90) 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:A:365:ASP:O	1:A:366:THR:HG22	1.78	0.83
1:A:157:ILE:HG22	1:A:161:MSE:HE2	1.65	0.79
1:B:681:PHE:HB2	1:B:683:MSE:CE	2.20	0.72
1:B:681:PHE:HB2	1:B:683:MSE:HE1	1.73	0.71
1:A:343:GLN:HE22	1:A:798:GLN:HE21	1.38	0.70
1:B:283:MSE:HE1	1:B:400:VAL:HG21	1.75	0.68
1:A:98:SER:HA	1:A:161:MSE:HE1	1.78	0.65
1:A:158:VAL:HA	1:A:161:MSE:HE3	1.78	0.64
1:B:98:SER:HA	1:B:161:MSE:HE1	1.82	0.61
1:A:280:GLU:HA	1:A:412:MSE:HE1	1.84	0.59
1:A:445:THR:HA	1:A:449:ASN:HD21	1.66	0.59
1:B:426:GLN:NE2	1:B:448:ASN:OD1	2.35	0.59
1:A:754:LYS:HE2	1:A:780:GLU:OE1	2.03	0.58
1:B:157:ILE:HG22	1:B:161:MSE:HE3	1.85	0.58
1:B:523:GLN:HA	1:B:526:VAL:HG12	1.86	0.58
1:A:153:VAL:HG21	1:A:618:LEU:HD11	1.87	0.57
1:B:718:LEU:HB2	1:B:750:MSE:HE1	1.86	0.57
1:A:343:GLN:NE2	1:A:798:GLN:HE21	2.02	0.56
1:A:788:MSE:HE1	1:A:798:GLN:HE22	1.69	0.56
1:A:741:ASN:HA	1:A:744:ILE:HG22	1.88	0.56
1:B:266:LEU:HD21	1:B:298:LEU:HA	1.88	0.55
1:A:337:LEU:HD11	1:A:447:ILE:HD11	1.89	0.55
1:B:342:LEU:HB3	1:B:801:ILE:HD13	1.89	0.55
1:A:356:PHE:HB2	1:A:368:LEU:HD21	1.88	0.55
1:A:598:ILE:O	1:A:599:SER:CB	2.54	0.54
1:B:536:ILE:HD11	1:B:549:ILE:HG12	1.90	0.54
1:A:799:GLN:HA	1:A:802:PHE:CD1	2.43	0.53
1:A:598:ILE:HD13	1:A:650:LEU:HD23	1.92	0.50
1:B:50:SER:HA	1:B:81:LYS:HE2	1.93	0.50
1:A:33:LYS:HE2	1:A:259:ASP:OD2	2.11	0.50
1:B:11:THR:HG23	1:B:14:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ASN:O	1:A:744:ILE:HG22	2.12	0.50
1:B:683:MSE:HE3	1:B:692:PHE:HB3	1.92	0.49
1:A:42:LEU:HD12	1:A:72:MSE:HE1	1.94	0.49
1:B:33:LYS:HE2	1:B:259:ASP:OD2	2.13	0.49
1:A:97:VAL:HG23	1:A:158:VAL:HG22	1.95	0.49
1:A:366:THR:O	1:A:366:THR:HG23	2.13	0.48
1:B:283:MSE:CE	1:B:400:VAL:HG21	2.42	0.48
1:A:557:TYR:O	1:A:561:LYS:HB2	2.14	0.48
1:A:473:THR:HA	1:A:758:THR:HG22	1.97	0.47
1:B:340:LYS:O	1:B:344:VAL:N	2.49	0.46
1:A:95:TYR:O	1:A:99:THR:HG23	2.16	0.46
1:A:180:ASN:HD22	1:A:613:THR:HB	1.81	0.46
1:A:456:PHE:CE1	1:A:469:ILE:HD11	2.51	0.46
1:A:670:HIS:CD2	1:A:699:ASP:HB2	2.50	0.46
1:B:157:ILE:HG22	1:B:161:MSE:CE	2.44	0.46
1:A:11:THR:HG21	1:A:328:SER:OG	2.17	0.45
1:B:535:MSE:HE3	1:B:537:TYR:HB2	1.99	0.45
1:B:574:TRP:HA	1:B:597:TYR:OH	2.17	0.44
1:A:98:SER:HA	1:A:161:MSE:CE	2.46	0.44
1:A:294:ILE:HD11	1:A:319:HIS:ND1	2.32	0.44
1:A:429:PHE:CD1	1:A:443:VAL:HG22	2.53	0.44
1:A:450:GLN:NE2	1:A:453:VAL:HG11	2.33	0.44
1:B:701:ARG:NH1	1:B:737:HIS:O	2.49	0.44
1:A:406:ARG:O	1:A:407:MSE:C	2.57	0.43
1:B:6:PRO:HB3	1:B:394:PHE:CZ	2.53	0.43
1:B:282:GLY:HA2	1:B:412:MSE:HE1	2.01	0.43
1:A:669:ILE:HB	1:A:701:ARG:HB3	1.99	0.43
1:B:750:MSE:HE2	1:B:752:ALA:HB2	2.00	0.43
1:A:744:ILE:HD11	1:A:776:VAL:HG13	2.01	0.43
1:B:584:LEU:HD13	1:B:591:ILE:HB	2.01	0.43
1:A:534:LYS:HB3	1:A:658:LEU:HD22	2.01	0.42
1:A:611:MSE:HE2	1:A:639:LEU:HB2	2.01	0.42
1:B:319:HIS:HB3	1:B:322:ILE:HB	2.01	0.42
1:B:340:LYS:HG3	1:B:344:VAL:HG12	2.01	0.42
1:B:283:MSE:HE3	1:B:402:PHE:CZ	2.55	0.42
1:A:339:LEU:HD13	1:A:809:PHE:HZ	1.85	0.42
1:B:135:LEU:HG	1:B:192:VAL:HG12	2.01	0.42
1:B:369:SER:O	1:B:371:GLY:N	2.53	0.42
1:A:642:ASP:OD2	1:B:50:SER:OG	2.38	0.41
1:B:8:THR:HA	1:B:396:GLN:HE21	1.84	0.41
1:B:546:HIS:HB2	1:B:549:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:OE2	1:A:276:TYR:OH	2.33	0.41
1:A:701:ARG:HG3	1:A:702:PRO:HD2	2.02	0.41
1:B:101:ARG:NH2	1:B:582:GLU:OE1	2.54	0.41
1:B:715:SER:OG	1:B:750:MSE:HE3	2.20	0.41
1:A:598:ILE:O	1:A:599:SER:HB3	2.20	0.41
1:B:741:ASN:HD21	1:B:771:ASP:HB2	1.86	0.41
1:A:488:LEU:HD21	1:A:504:ASN:HB3	2.01	0.41
1:B:415:ASN:HD21	1:B:417:ASN:HB2	1.85	0.41
1:B:450:GLN:HA	1:B:453:VAL:HG12	2.02	0.41
1:A:540:HIS:HB3	1:A:674:ALA:HA	2.03	0.41
1:B:21:VAL:HG22	1:B:29:TYR:HB2	2.03	0.41
1:B:285:TYR:CE1	1:B:316:MSE:HG2	2.56	0.41
1:B:320:ASN:O	1:B:354:ARG:NH1	2.54	0.41
1:A:310:TYR:CD1	1:A:310:TYR:N	2.89	0.40
1:A:776:VAL:HG11	1:A:781:PHE:CE1	2.56	0.40
1:A:783:PHE:O	1:A:788:MSE:HE1	2.20	0.40
1:A:434:LYS:HB3	1:A:435:PRO:HD3	2.04	0.40
1:B:4:PHE:HB2	1:B:400:VAL:HG13	2.02	0.40

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	762/874 (87%)	686 (90%)	66 (9%)	10 (1%)	12	45
1	B	749/874 (86%)	669 (89%)	69 (9%)	11 (2%)	10	42
All	All	1511/1748 (86%)	1355 (90%)	135 (9%)	21 (1%)	11	43

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ASP
1	B	370	ARG
1	A	145	VAL
1	A	167	PRO
1	A	407	MSE
1	A	599	SER
1	A	778	ALA
1	A	136	LYS
1	A	476	ALA
1	B	368	LEU
1	B	562	ASP
1	A	589	LYS
1	A	670	HIS
1	B	142	ARG
1	B	171	TYR
1	B	261	PRO
1	A	797	GLU
1	B	778	ALA
1	B	322	ILE
1	B	109	ILE
1	B	344	VAL

### 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	707/783 (90%)	655 (93%)	52 (7%)	13	44
1	B	694/783 (89%)	646 (93%)	48 (7%)	15	48
All	All	1401/1566 (90%)	1301 (93%)	100 (7%)	14	46

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	ILE
1	A	39	GLN

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Mol	Chain	Res	Type
1	A	72	MSE
1	A	75	THR
1	A	81	LYS
1	A	82	SER
1	A	100	TRP
1	A	117	LYS
1	A	140	GLU
1	A	169	ASP
1	A	175	SER
1	A	189	LYS
1	A	190	VAL
1	A	199	SER
1	A	292	VAL
1	A	293	THR
1	A	313	VAL
1	A	320	ASN
1	A	337	LEU
1	A	339	LEU
1	A	343	GLN
1	A	344	VAL
1	A	374	MSE
1	A	388	LYS
1	A	409	GLU
1	A	414	CYS
1	A	430	GLU
1	A	449	ASN
1	A	465	HIS
1	A	477	LEU
1	A	479	SER
1	A	485	VAL
1	A	488	LEU
1	A	532	ASP
1	A	589	LYS
1	A	597	TYR
1	A	611	MSE
1	A	637	LEU
1	A	641	ARG
1	A	642	ASP
1	A	644	SER
1	A	648	VAL
1	A	662	TYR
1	A	664	GLN

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Mol	Chain	Res	Type
1	A	667	ARG
1	A	687	ASN
1	A	716	ASP
1	A	721	GLU
1	A	758	THR
1	A	776	VAL
1	A	801	ILE
1	B	11	THR
1	B	66	ILE
1	B	127	ILE
1	B	141	ASP
1	B	172	ASP
1	B	175	SER
1	B	189	LYS
1	B	199	SER
1	B	281	LEU
1	B	283	MSE
1	B	288	LEU
1	B	297	ASN
1	B	320	ASN
1	B	353	ASP
1	B	366	THR
1	B	369	SER
1	B	370	ARG
1	B	375	CYS
1	B	383	ASN
1	B	385	ILE
1	B	392	HIS
1	B	400	VAL
1	B	410	GLU
1	B	422	ASP
1	B	446	VAL
1	B	454	ASP
1	B	466	VAL
1	B	482	ARG
1	B	488	LEU
1	B	491	VAL
1	B	503	ARG
1	B	516	THR
1	B	565	THR
1	B	571	VAL
1	B	607	SER

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Mol	Chain	Res	Type
1	B	609	VAL
1	B	611	MSE
1	B	621	PHE
1	B	641	ARG
1	B	662	TYR
1	B	682	ARG
1	B	709	LEU
1	B	729	LEU
1	B	770	LEU
1	B	771	ASP
1	B	800	ARG
1	B	804	LEU
1	B	809	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN
1	A	614	GLN
1	A	798	GLN
1	B	396	GLN
1	B	415	ASN
1	B	449	ASN
1	B	523	GLN
1	B	653	GLN
1	B	664	GLN
1	B	751	ASN
1	B	762	GLN

### 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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	B	903	2	4,4,4	0.78	0	6,6,6	0.97	0
3	PO4	A	903	2	4,4,4	0.97	0	6,6,6	0.56	0

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

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, 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	750/874 (85%)	0.29	35 (4%)	31 11	50, 80, 121, 166	0
1	B	737/874 (84%)	0.27	38 (5%)	27 10	51, 80, 134, 171	0
All	All	1487/1748 (85%)	0.28	73 (4%)	29 11	50, 80, 128, 171	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ARG	6.0
1	A	688	GLU	5.3
1	B	169	ASP	5.1
1	A	689	HIS	4.6
1	A	169	ASP	4.4
1	B	618	LEU	4.2
1	A	170	ARG	4.2
1	B	164	LYS	4.1
1	B	248	ASN	4.0
1	B	204	ARG	3.9
1	B	247	GLU	3.9
1	B	203	VAL	3.8
1	A	820	ASP	3.8
1	B	165	HIS	3.7
1	A	818	ASP	3.6
1	A	171	TYR	3.5
1	B	143	LEU	3.4
1	B	405	PHE	3.4
1	A	168	THR	3.4
1	B	408	ASN	3.3
1	B	168	THR	3.3
1	A	143	LEU	3.3
1	B	190	VAL	3.2
1	A	142	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	165	HIS	3.0
1	B	616	VAL	3.0
1	A	443	VAL	2.9
1	A	606	ASP	2.8
1	A	817	GLU	2.8
1	A	819	VAL	2.8
1	B	179	LEU	2.8
1	A	685	GLU	2.7
1	A	204	ARG	2.7
1	A	661	GLU	2.6
1	B	433	VAL	2.6
1	A	172	ASP	2.6
1	A	144	GLY	2.6
1	B	141	ASP	2.6
1	B	166	ALA	2.6
1	B	620	GLU	2.5
1	B	807	LYS	2.5
1	B	178	HIS	2.5
1	B	443	VAL	2.5
1	A	497	ASP	2.5
1	B	409	GLU	2.5
1	B	189	LYS	2.4
1	A	444	ASP	2.4
1	A	434	LYS	2.4
1	A	662	TYR	2.4
1	B	619	ALA	2.4
1	B	435	PRO	2.4
1	A	731	ASP	2.3
1	A	810	VAL	2.3
1	B	438	PHE	2.3
1	B	442	ASP	2.2
1	B	637	LEU	2.2
1	A	516	THR	2.2
1	A	109	ILE	2.2
1	B	446	VAL	2.2
1	B	496	ALA	2.2
1	A	175	SER	2.2
1	B	419	GLU	2.1
1	A	804	LEU	2.1
1	A	430	GLU	2.1
1	B	380	GLU	2.1
1	B	171	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	686	ASN	2.0
1	B	305	PHE	2.0
1	B	429	PHE	2.0
1	B	184	PRO	2.0
1	A	684	ASP	2.0
1	A	139	GLY	2.0
1	A	64	SER	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<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	B	901	1/1	0.98	0.07	73,73,73,73	0
3	PO4	A	903	5/5	0.98	0.11	77,89,95,102	0
3	PO4	B	903	5/5	0.98	0.14	75,78,85,86	0
2	ZN	B	902	1/1	0.99	0.15	68,68,68,68	0
2	ZN	A	902	1/1	0.99	0.12	73,73,73,73	0
2	ZN	A	901	1/1	0.99	0.07	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.