



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:51 PM GMT

PDB ID : 3FNS  
Title : Crystal structure of histo-aspartic protease (HAP) from Plasmodium Falciparum  
Authors : Bhaumik, P.; Gustchina, A.; Wlodawer, A.  
Deposited on : 2008-12-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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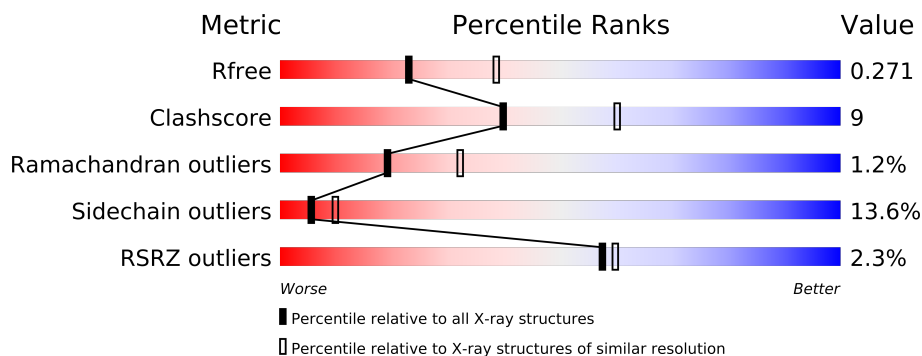
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	332	
1	B	332	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5290 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HAP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2590	1679	401	502	8			
1	B	325	Total	C	N	O	S	0	0	0
			2590	1679	401	502	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is water.

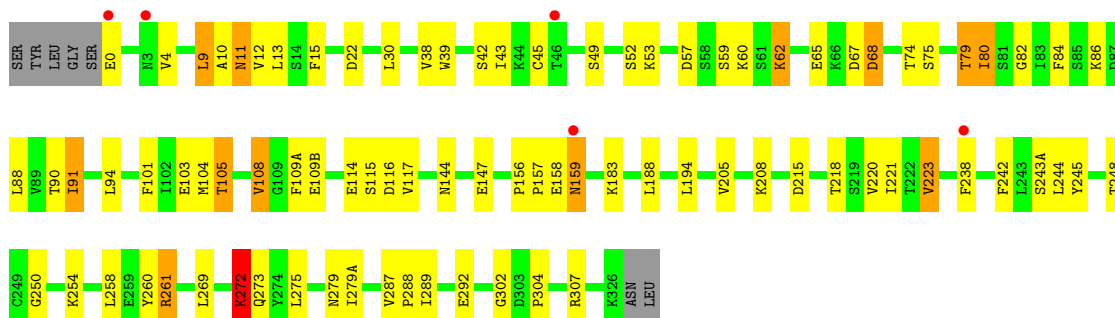
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	45	Total	O	0	0
			45	45		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

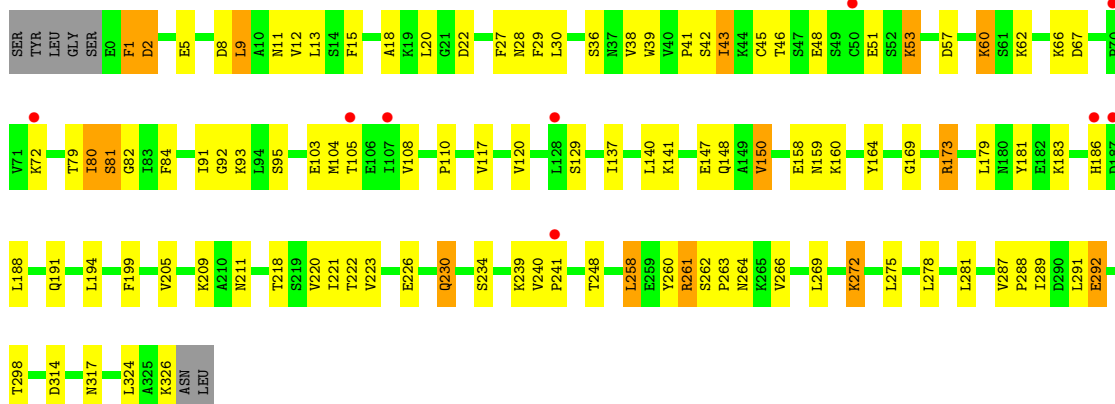
#### • Molecule 1: HAP protein

Chain A: 



#### • Molecule 1: HAP protein

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.80Å 89.80Å 198.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 39.36 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.50) 99.7 (39.36-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, $R_{free}$	0.225 , 0.274 0.232 , 0.271	Depositor DCC
$R_{free}$ test set	1040 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34639 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.63	0/2655	0.74	1/3603 (0.0%)
1	B	0.67	0/2655	0.74	1/3603 (0.0%)
All	All	0.65	0/5310	0.74	2/7206 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	258	LEU	CA-CB-CG	5.67	128.34	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2590	0	2541	41	1
1	B	2590	0	2541	61	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
3	A	59	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	0	2	1
All	All	5290	0	5082	97	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:THR:HG22	1:A:108:VAL:HG12	1.58	0.83
1:B:79:THR:HB	1:B:108:VAL:HG12	1.67	0.75
1:A:109(A):PHE:HB3	3:A:382:HOH:O	1.92	0.68
1:B:179:LEU:HD13	1:B:181:TYR:CE1	2.30	0.67
1:A:238:PHE:HZ	3:A:384:HOH:O	1.77	0.66
1:B:80:ILE:HD11	1:B:104:MET:HG2	1.76	0.65
1:B:42:SER:HB3	1:B:103:GLU:HB3	1.78	0.65
1:B:48:GLU:O	1:B:51:GLU:HG3	1.97	0.65
1:A:80:ILE:HD11	1:A:104:MET:HG2	1.79	0.65
1:A:39:TRP:CZ3	1:A:80:ILE:HD12	2.31	0.64
1:A:82:GLY:HA2	1:A:105:THR:HB	1.80	0.63
1:B:186:HIS:HB3	1:B:188:LEU:HD23	1.81	0.62
1:B:158:GLU:HB3	1:B:160:LYS:HG3	1.82	0.62
1:B:22:ASP:OD1	1:B:62:LYS:HG2	2.00	0.61
1:A:279(A):ILE:HD13	1:B:117:VAL:CG2	2.31	0.60
1:A:279:ASN:OD1	1:A:279(A):ILE:HG23	2.02	0.59
1:B:314:ASP:CG	1:B:317:ASN:HD22	2.06	0.59
1:B:179:LEU:CD1	1:B:181:TYR:CE1	2.86	0.58
1:A:39:TRP:HZ3	1:A:80:ILE:HD12	1.68	0.58
1:A:114:GLU:HG2	1:B:158:GLU:HG3	1.85	0.57
1:B:262:SER:HB2	1:B:263:PRO:CD	2.35	0.57
1:B:5:GLU:HG2	1:B:164:TYR:CE1	2.40	0.56
1:B:223:VAL:O	1:B:288:PRO:HA	2.06	0.56
1:A:65:GLU:HB2	1:A:86:LYS:HB3	1.89	0.56
1:A:9:LEU:HB2	1:A:15:PHE:CE2	2.40	0.55
1:B:80:ILE:HD13	1:B:80:ILE:C	2.28	0.55
1:B:148:GLN:HB2	1:B:150:VAL:HG22	1.89	0.54
1:A:279:ASN:HB2	1:B:15:PHE:HZ	1.72	0.54
1:B:241:PRO:HA	3:B:355:HOH:O	2.08	0.53
1:B:278:LEU:HD12	1:B:281:LEU:HB2	1.91	0.53
1:B:261:ARG:HB3	1:B:266:VAL:HG22	1.91	0.53
1:A:79:THR:HG22	1:A:108:VAL:CG1	2.34	0.53
1:B:194:LEU:HD13	1:B:260:TYR:HB3	1.91	0.52
1:A:80:ILE:HD13	1:A:80:ILE:C	2.30	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:THR:HG22	1:A:250:GLY:H	1.75	0.52
1:A:307:ARG:HD3	3:A:351:HOH:O	2.09	0.52
1:A:38:VAL:HG22	1:A:101:PHE:CB	2.41	0.51
1:B:18:ALA:HB3	1:B:29:PHE:CE1	2.46	0.51
1:A:74:THR:HG22	1:A:79:THR:OG1	2.11	0.51
1:A:223:VAL:O	1:A:288:PRO:HA	2.11	0.50
1:B:36:SER:HB3	1:B:129:SER:HB3	1.92	0.50
1:B:22:ASP:OD1	1:B:62:LYS:CG	2.59	0.50
1:B:18:ALA:HB3	1:B:29:PHE:CD1	2.47	0.50
1:A:272:LYS:HE2	1:A:273:GLN:HE21	1.75	0.50
1:A:45:CYS:HA	1:A:105:THR:O	2.10	0.50
1:B:67:ASP:HB3	1:B:84:PHE:O	2.10	0.50
1:B:27:PHE:HE2	1:B:41:PRO:HD2	1.77	0.50
1:B:186:HIS:HB3	1:B:188:LEU:CD2	2.41	0.50
1:A:38:VAL:HG22	1:A:101:PHE:HB3	1.94	0.50
1:A:244:LEU:HD23	1:A:245:TYR:CE2	2.48	0.49
1:B:2:ASP:OD1	1:B:92:GLY:HA3	2.12	0.49
1:A:4:VAL:HB	1:A:91:ILE:CD1	2.42	0.49
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.95	0.49
1:A:91:ILE:HG13	1:A:91:ILE:O	2.13	0.48
1:B:291:LEU:O	1:B:292:GLU:HB2	2.13	0.48
1:A:215:ASP:O	1:A:302:GLY:HA2	2.14	0.48
1:B:199:PHE:CG	1:B:258:LEU:HD13	2.49	0.48
1:B:262:SER:HB2	1:B:263:PRO:HD2	1.96	0.48
1:B:5:GLU:HG2	1:B:164:TYR:HE1	1.79	0.48
1:B:141:LYS:HE3	1:B:147:GLU:O	2.14	0.47
1:A:221:ILE:HG12	1:A:304:PRO:HG2	1.95	0.47
1:B:53:LYS:HE2	1:B:117:VAL:O	2.13	0.47
1:B:137:ILE:HA	1:B:140:LEU:HD12	1.97	0.47
1:B:158:GLU:O	1:B:160:LYS:N	2.36	0.47
1:B:199:PHE:CD1	1:B:258:LEU:HD13	2.50	0.47
1:B:72:LYS:HB3	1:B:81:SER:HB3	1.97	0.47
1:A:10:ALA:O	1:A:11:ASN:HB2	2.14	0.47
1:B:82:GLY:HA3	1:B:103:GLU:O	2.15	0.46
1:A:90:THR:HG23	1:A:94:LEU:O	2.15	0.46
1:B:194:LEU:CD2	1:B:262:SER:HB3	2.46	0.46
1:B:211:ASN:O	1:B:298:THR:HA	2.15	0.46
1:A:272:LYS:HG2	1:B:110:PRO:HD3	1.97	0.45
1:B:28:ASN:HB2	1:B:117:VAL:HA	1.99	0.45
1:B:264:ASN:HB2	3:B:362:HOH:O	2.16	0.45
1:B:186:HIS:HB2	1:B:191:GLN:HE21	1.80	0.45
1:B:173:ARG:O	1:B:326:LYS:HE3	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ASP:HB3	1:A:84:PHE:O	2.16	0.44
1:B:57:ASP:OD2	1:B:60:LYS:HG2	2.18	0.44
1:B:39:TRP:CZ3	1:B:80:ILE:HD12	2.52	0.43
1:A:156:PRO:HA	1:A:157:PRO:HD3	1.85	0.43
1:A:22:ASP:OD1	1:A:62:LYS:HB3	2.18	0.43
1:A:272:LYS:HE2	1:A:273:GLN:NE2	2.33	0.43
1:B:1:PHE:CD1	1:B:169:GLY:HA3	2.53	0.43
1:A:194:LEU:HD13	1:A:260:TYR:HB3	2.01	0.43
1:A:242:PHE:HB3	1:A:243(A):SER:O	2.19	0.42
1:B:43:ILE:HA	1:B:43:ILE:HD13	1.91	0.42
1:B:9:LEU:HB2	1:B:15:PHE:CE2	2.55	0.41
1:A:272:LYS:HE3	1:B:110:PRO:HG3	2.01	0.41
1:B:158:GLU:C	1:B:160:LYS:H	2.22	0.41
1:B:230:GLN:HE21	1:B:230:GLN:HB3	1.60	0.41
1:B:262:SER:CB	1:B:263:PRO:CD	2.98	0.41
1:A:57:ASP:OD2	1:A:59:SER:OG	2.39	0.41
1:B:240:VAL:HA	1:B:241:PRO:HD3	1.91	0.41
1:A:67:ASP:O	1:A:68:ASP:HB2	2.20	0.41
1:B:45:CYS:HA	1:B:105:THR:O	2.19	0.41
1:B:226:GLU:O	1:B:230:GLN:HG2	2.22	0.40
1:B:221:ILE:HD13	1:B:221:ILE:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:ARG:NH1	3:B:366:HOH:O[4_454]	1.67	0.53

## 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	323/332 (97%)	302 (94%)	18 (6%)	3 (1%)	25	42
1	B	323/332 (97%)	291 (90%)	27 (8%)	5 (2%)	15	25
All	All	646/664 (97%)	593 (92%)	45 (7%)	8 (1%)	19	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	B	1	PHE
1	A	272	LYS
1	B	159	ASN
1	B	239	LYS
1	B	272	LYS
1	B	292	GLU
1	A	292	GLU

### 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	295/301 (98%)	253 (86%)	42 (14%)	5	8
1	B	295/301 (98%)	257 (87%)	38 (13%)	6	11
All	All	590/602 (98%)	510 (86%)	80 (14%)	5	10

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	GLU
1	A	9	LEU
1	A	11	ASN
1	A	12	VAL
1	A	13	LEU
1	A	30	LEU
1	A	43	ILE
1	A	49	SER
1	A	52	SER
1	A	53	LYS
1	A	60	LYS
1	A	62	LYS
1	A	68	ASP
1	A	75	SER
1	A	79	THR
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	91	ILE
1	A	105	THR
1	A	108	VAL
1	A	109(B)	GLU
1	A	115	SER
1	A	116	ASP
1	A	117	VAL
1	A	144	ASN
1	A	147	GLU
1	A	158	GLU
1	A	159	ASN
1	A	183	LYS
1	A	188	LEU
1	A	205	VAL
1	A	208	LYS
1	A	218	THR
1	A	220	VAL
1	A	223	VAL
1	A	254	LYS
1	A	261	ARG
1	A	269	LEU
1	A	272	LYS
1	A	275	LEU
1	A	287	VAL
1	A	289	ILE
1	B	2	ASP
1	B	8	ASP
1	B	9	LEU
1	B	11	ASN
1	B	12	VAL
1	B	13	LEU
1	B	20	LEU
1	B	30	LEU
1	B	38	VAL
1	B	43	ILE
1	B	46	THR
1	B	53	LYS
1	B	60	LYS
1	B	66	LYS
1	B	80	ILE
1	B	81	SER

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Mol	Chain	Res	Type
1	B	91	ILE
1	B	93	LYS
1	B	95	SER
1	B	120	VAL
1	B	150	VAL
1	B	173	ARG
1	B	183	LYS
1	B	205	VAL
1	B	209	LYS
1	B	218	THR
1	B	220	VAL
1	B	222	THR
1	B	230	GLN
1	B	234	SER
1	B	248	THR
1	B	261	ARG
1	B	269	LEU
1	B	272	LYS
1	B	275	LEU
1	B	287	VAL
1	B	289	ILE
1	B	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	203	ASN
1	A	230	GLN
1	A	264	ASN
1	B	144	ASN
1	B	191	GLN
1	B	203	ASN
1	B	230	GLN
1	B	264	ASN
1	B	317	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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.

## 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	325/332 (97%)	-0.00	5 (1%) 70 72	26, 51, 72, 86	1 (0%)
1	B	325/332 (97%)	0.09	9 (2%) 50 53	28, 53, 72, 86	1 (0%)
All	All	650/664 (97%)	0.05	14 (2%) 57 61	26, 52, 72, 86	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ASN	3.9
1	A	238	PHE	3.7
1	A	46	THR	3.3
1	B	241	PRO	2.8
1	A	0	GLU	2.6
1	B	128	LEU	2.6
1	B	105	THR	2.6
1	B	50	CYS	2.3
1	A	3	ASN	2.2
1	B	72	LYS	2.1
1	B	107	ILE	2.1
1	B	70	PRO	2.1
1	B	187	ASP	2.1
1	B	186	HIS	2.0

### 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 carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	330	1/1	0.07	-	65,65,65,65	1
2	ZN	A	332	1/1	0.05	-	71,71,71,71	1
2	ZN	B	329	1/1	0.11	-	49,49,49,49	0
2	ZN	A	331	1/1	0.26	-	71,71,71,71	1
2	ZN	A	330	1/1	0.13	-	49,49,49,49	1
2	ZN	A	329	1/1	0.08	-	36,36,36,36	0

## 6.5 Other polymers

There are no such residues in this entry.