



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:53 am GMT

PDB ID : 2H0R  
Title : Structure of the Yeast Nicotinamidase Pnc1p  
Authors : Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.  
Deposited on : 2006-05-15  
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

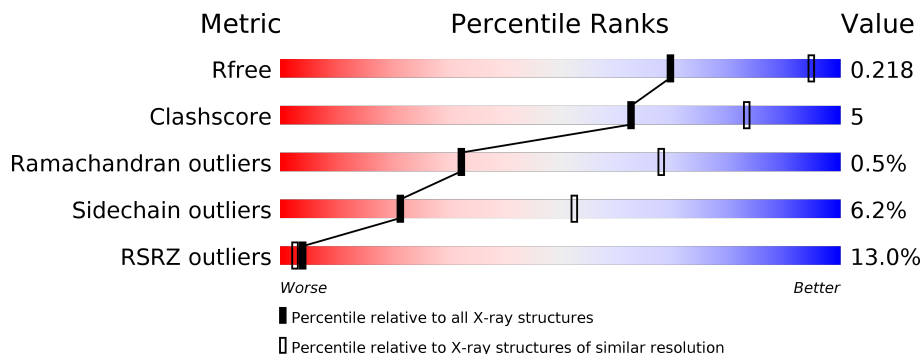
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	216	<div> <div>0%</div> <div>87%</div> <div>13%</div> </div>
1	B	216	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	216	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
1	D	216	<div> <div>11%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	E	216	<div> <div>23%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>
1	F	216	<div> <div>33%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	216	<div><div></div><div>17%</div><div>82%</div><div>17%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12348 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 Nicotinamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	B	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	C	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	D	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	E	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	F	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			
1	G	216	Total	C	N	O	S	0	0	0
			1763	1122	299	335	7			

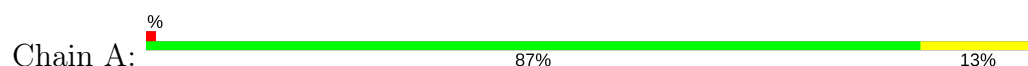
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

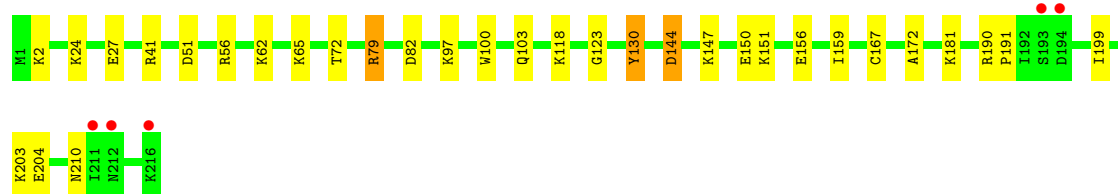
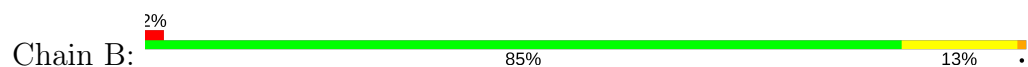
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

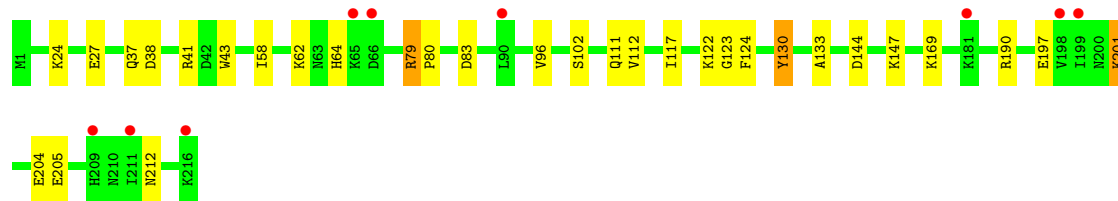
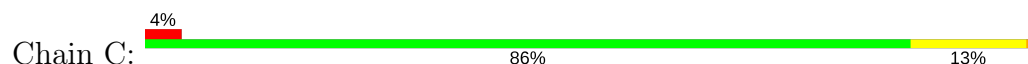
- Molecule 1: Nicotinamidase



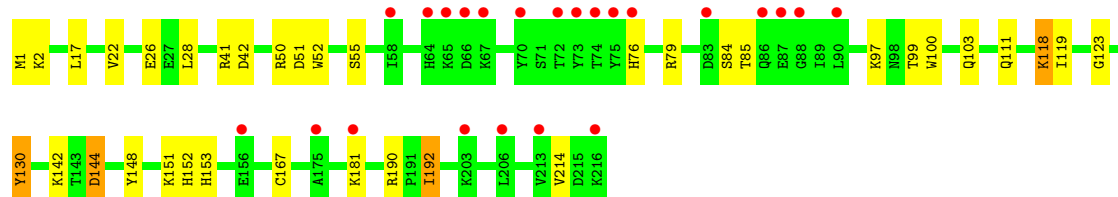
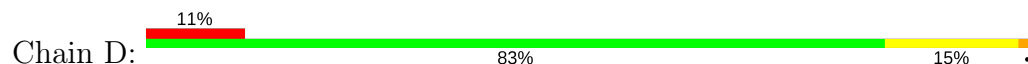
- Molecule 1: Nicotinamidase



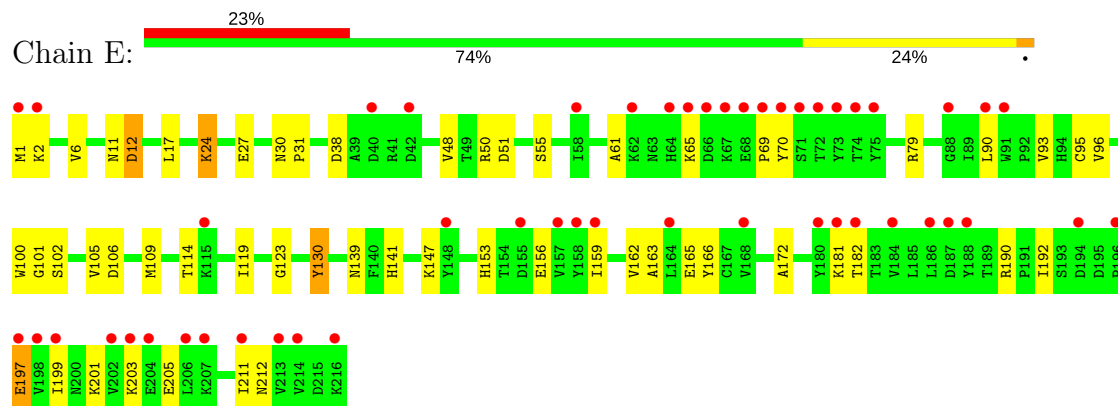
- Molecule 1: Nicotinamidase



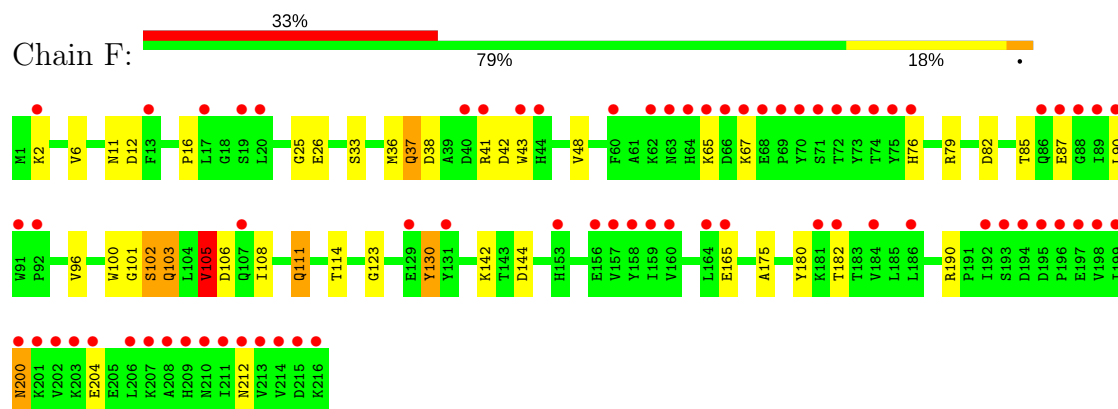
- Molecule 1: Nicotinamidase



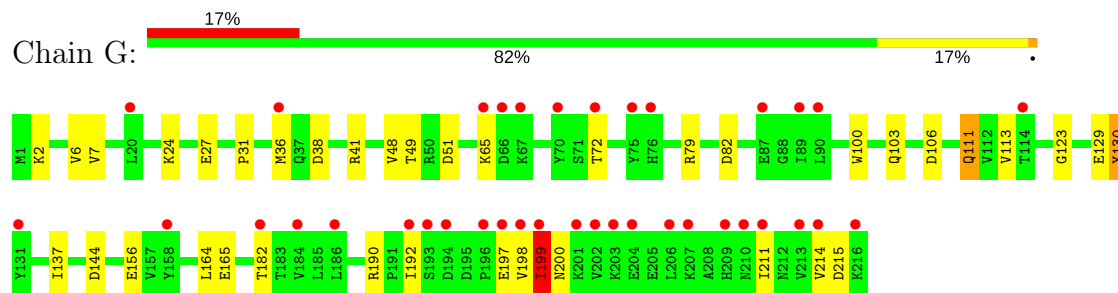
## ● Molecule 1: Nicotinamidase



## ● Molecule 1: Nicotinamidase



## ● Molecule 1: Nicotinamidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	302.04Å 302.04Å 112.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.77 – 2.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.90) 99.8 (48.77-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.220 0.189 , 0.218	Depositor DCC
$R_{free}$ test set	4226 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 93.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.75	1/1809 (0.1%)	0.79	2/2459 (0.1%)
1	B	0.55	1/1809 (0.1%)	0.70	1/2459 (0.0%)
1	C	0.51	0/1809	0.68	0/2459
1	D	0.46	0/1809	0.61	0/2459
1	E	0.59	3/1809 (0.2%)	0.63	1/2459 (0.0%)
1	F	0.71	5/1809 (0.3%)	0.64	1/2459 (0.0%)
1	G	0.59	4/1809 (0.2%)	0.71	2/2459 (0.1%)
All	All	0.60	14/12663 (0.1%)	0.68	7/17213 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	105	VAL	CB-CG1	11.09	1.76	1.52
1	E	106	ASP	C-O	9.56	1.41	1.23
1	F	105	VAL	CB-CG2	9.37	1.72	1.52
1	F	103	GLN	C-N	8.41	1.53	1.34
1	G	106	ASP	C-O	8.32	1.39	1.23
1	G	41	ARG	CZ-NH1	7.94	1.43	1.33
1	F	102	SER	CB-OG	7.74	1.52	1.42
1	E	106	ASP	C-N	6.57	1.49	1.34
1	G	31	PRO	N-CD	6.30	1.56	1.47
1	G	41	ARG	CZ-NH2	6.15	1.41	1.33
1	E	105	VAL	C-O	5.91	1.34	1.23
1	F	102	SER	C-O	5.36	1.33	1.23
1	B	203	LYS	CD-CE	5.36	1.64	1.51
1	A	62	LYS	CD-CE	5.29	1.64	1.51

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	41	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	A	130	TYR	CB-CA-C	-6.82	96.75	110.40
1	G	41	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	144	ASP	N-CA-CB	-5.98	99.83	110.60
1	B	144	ASP	N-CA-CB	-5.46	100.77	110.60
1	F	105	VAL	CA-CB-CG1	-5.40	102.80	110.90
1	E	106	ASP	C-N-CA	-5.19	108.73	121.70

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	1763	0	1723	13	0
1	B	1763	0	1723	15	0
1	C	1763	0	1723	18	0
1	D	1763	0	1723	16	0
1	E	1763	0	1723	28	0
1	F	1763	0	1723	25	0
1	G	1763	0	1723	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
All	All	12348	0	12061	123	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 5.

All (123) 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:F:105:VAL:CB	1:F:105:VAL:CG1	1.76	1.62
1:D:2:LYS:HE2	1:D:41:ARG:O	1.74	0.85
1:G:100:TRP:HA	1:G:103:GLN:NE2	1.95	0.82
1:F:105:VAL:CA	1:F:105:VAL:CG1	2.62	0.76
1:F:25:GLY:HA2	1:F:190:ARG:HG3	1.68	0.76
1:F:12:ASP:OD2	1:F:101:GLY:HA3	1.87	0.74
1:G:27:GLU:HB2	1:G:190:ARG:HH12	1.54	0.73
1:C:201:LYS:O	1:C:205:GLU:HB2	1.88	0.73
1:E:6:VAL:HB	1:E:48:VAL:HG12	1.74	0.69
1:E:12:ASP:OD2	1:E:101:GLY:HA3	1.93	0.68
1:G:129:GLU:HB3	1:G:137:ILE:HD13	1.74	0.67
1:D:1:MET:HB2	1:D:153:HIS:O	1.99	0.62
1:D:76:HIS:HA	1:D:85:THR:HG22	1.81	0.61
1:G:100:TRP:HA	1:G:103:GLN:HE22	1.67	0.58
1:C:123:GLY:HA2	1:C:130:TYR:CD1	2.39	0.57
1:E:50:ARG:HE	1:E:119:ILE:HG21	1.69	0.57
1:E:50:ARG:HH21	1:E:119:ILE:HD13	1.70	0.56
1:F:33:SER:O	1:F:37:GLN:NE2	2.38	0.56
1:E:69:PRO:O	1:E:70:TYR:HB2	2.05	0.56
1:E:156:GLU:HB3	1:E:181:LYS:HB2	1.88	0.56
1:G:36:MET:HE1	1:G:111:GLN:HG2	1.88	0.55
1:E:96:VAL:O	1:E:102:SER:HB3	2.06	0.55
1:E:30:ASN:HB2	1:E:31:PRO:HD3	1.89	0.55
1:D:22:VAL:HG22	1:D:192:ILE:HG13	1.89	0.54
1:E:24:LYS:HB2	1:E:190:ARG:HD2	1.90	0.54
1:G:2:LYS:HG3	1:G:156:GLU:HG3	1.90	0.53
1:G:36:MET:CE	1:G:111:GLN:HG2	2.38	0.53
1:C:169:LYS:HD2	1:C:205:GLU:OE1	2.08	0.53
1:F:36:MET:CE	1:F:111:GLN:HG2	2.39	0.53
1:F:6:VAL:HB	1:F:48:VAL:HG12	1.91	0.53
1:G:6:VAL:HB	1:G:48:VAL:HG12	1.90	0.53
1:D:50:ARG:NH1	1:D:52:TRP:CZ3	2.77	0.52
1:F:100:TRP:HA	1:F:103:GLN:OE1	2.09	0.52
1:A:27:GLU:OE1	1:A:190:ARG:NH1	2.42	0.52
1:B:118:LYS:NZ	1:B:144:ASP:OD2	2.31	0.52
1:B:27:GLU:HB2	1:B:190:ARG:HH12	1.74	0.52
1:C:197:GLU:OE2	1:C:201:LYS:HG3	2.10	0.51
1:E:165:GLU:HG2	1:E:166:TYR:CD2	2.46	0.51
1:C:58:ILE:O	1:C:64:HIS:HE1	1.94	0.51
1:B:156:GLU:HB3	1:B:181:LYS:HB3	1.93	0.50
1:E:162:VAL:HB	1:E:163:ALA:HA	1.93	0.50
1:B:2:LYS:HG3	1:B:156:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:MET:HE2	1:F:111:GLN:HG2	1.94	0.49
1:E:182:THR:HB	1:E:211:ILE:HG12	1.93	0.49
1:E:123:GLY:HA2	1:E:130:TYR:CD1	2.48	0.49
1:F:76:HIS:HA	1:F:85:THR:HG22	1.94	0.49
1:D:100:TRP:O	1:D:103:GLN:HB2	2.12	0.48
1:D:118:LYS:HD3	1:D:148:TYR:CD2	2.49	0.48
1:B:151:LYS:HD3	1:D:17:LEU:CD2	2.44	0.48
1:B:27:GLU:HB2	1:B:190:ARG:NH1	2.29	0.48
1:C:27:GLU:HB2	1:C:190:ARG:HH12	1.78	0.48
1:B:100:TRP:O	1:B:103:GLN:HB2	2.14	0.48
1:C:96:VAL:O	1:C:102:SER:HB3	2.14	0.47
1:B:123:GLY:HA2	1:B:130:TYR:CD1	2.48	0.47
1:E:11:ASN:HB3	1:E:100:TRP:CH2	2.49	0.47
1:D:148:TYR:CE2	1:D:152:HIS:NE2	2.82	0.47
1:F:175:ALA:O	1:F:180:TYR:HB2	2.14	0.47
1:G:164:LEU:HD22	1:G:199:ILE:HG23	1.95	0.47
1:D:50:ARG:HE	1:D:119:ILE:HG21	1.79	0.47
1:B:2:LYS:CE	1:B:41:ARG:O	2.63	0.47
1:B:147:LYS:HD3	1:B:147:LYS:HA	1.70	0.47
1:A:164:LEU:HA	1:A:168:VAL:HB	1.97	0.47
1:F:200:ASN:N	1:F:200:ASN:OD1	2.48	0.46
1:G:123:GLY:HA2	1:G:130:TYR:CD1	2.51	0.46
1:D:118:LYS:NZ	1:D:144:ASP:OD2	2.30	0.46
1:C:83:ASP:N	1:C:83:ASP:OD1	2.49	0.46
1:E:27:GLU:HB2	1:E:190:ARG:HH12	1.80	0.46
1:E:141:HIS:NE2	1:F:106:ASP:OD2	2.47	0.46
1:A:203:LYS:O	1:A:207:LYS:HG3	2.16	0.46
1:A:1:MET:HB3	1:A:1:MET:HE2	1.81	0.45
1:D:151:LYS:HE3	1:E:17:LEU:CD2	2.46	0.45
1:E:51:ASP:O	1:E:95:CYS:HB3	2.16	0.45
1:C:112:VAL:HA	1:C:117:ILE:HD12	1.98	0.45
1:G:198:VAL:C	1:G:200:ASN:H	2.20	0.45
1:F:2:LYS:HE2	1:F:41:ARG:O	2.15	0.45
1:A:123:GLY:HA2	1:A:130:TYR:CD1	2.51	0.45
1:D:123:GLY:HA2	1:D:130:TYR:CD1	2.51	0.45
1:C:41:ARG:HB3	1:C:43:TRP:CE2	2.53	0.44
1:E:199:ILE:O	1:E:203:LYS:HB2	2.17	0.44
1:A:99:THR:O	1:A:100:TRP:C	2.55	0.44
1:F:67:LYS:HE3	1:F:90:LEU:HD11	2.00	0.44
1:E:197:GLU:OE2	1:E:201:LYS:HG3	2.18	0.44
1:A:110:ASP:O	1:A:114:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:CD1	1:B:172:ALA:HA	2.48	0.43
1:C:38:ASP:O	1:C:41:ARG:HB2	2.17	0.43
1:A:23:PRO:HG2	1:A:194:ASP:HB3	2.01	0.43
1:A:187:ASP:HB2	1:A:215:ASP:O	2.18	0.43
1:F:123:GLY:HA2	1:F:130:TYR:CD1	2.53	0.43
1:G:182:THR:HB	1:G:211:ILE:HG12	2.00	0.43
1:B:159:ILE:HD13	1:B:172:ALA:HA	2.01	0.43
1:F:11:ASN:HB3	1:F:100:TRP:CH2	2.54	0.43
1:E:1:MET:HG3	1:E:153:HIS:HB2	2.01	0.43
1:E:130:TYR:N	1:E:130:TYR:CD1	2.87	0.43
1:C:62:LYS:HG2	1:C:62:LYS:O	2.19	0.42
1:A:100:TRP:CE3	1:C:147:LYS:HG3	2.54	0.42
1:D:28:LEU:HD11	1:D:190:ARG:HG2	2.02	0.42
1:E:201:LYS:O	1:E:205:GLU:HB2	2.20	0.42
1:G:7:VAL:HA	1:G:49:THR:OG1	2.19	0.42
1:C:130:TYR:N	1:C:130:TYR:CD1	2.88	0.42
1:A:199:ILE:O	1:A:203:LYS:HB2	2.20	0.42
1:E:147:LYS:HE3	1:F:100:TRP:HB3	2.02	0.42
1:F:87:GLU:OE1	1:F:87:GLU:HA	2.20	0.41
1:A:118:LYS:HD3	1:A:148:TYR:CD2	2.55	0.41
1:C:41:ARG:HA	1:C:41:ARG:HD3	1.77	0.41
1:D:130:TYR:N	1:D:130:TYR:CD1	2.89	0.41
1:F:37:GLN:HE21	1:F:37:GLN:N	2.18	0.41
1:F:96:VAL:O	1:F:102:SER:HB3	2.20	0.41
1:B:191:PRO:HG3	1:B:199:ILE:HD11	2.01	0.41
1:B:79:ARG:HB3	1:B:82:ASP:HB3	2.02	0.41
1:E:159:ILE:HD13	1:E:172:ALA:HA	2.01	0.41
1:E:163:ALA:HB1	1:E:192:ILE:HG13	2.02	0.41
1:F:37:GLN:H	1:F:37:GLN:HE21	1.68	0.41
1:C:122:LYS:HD3	1:C:133:ALA:HA	2.03	0.41
1:C:79:ARG:HA	1:C:80:PRO:HD3	1.93	0.41
1:D:99:THR:O	1:D:100:TRP:C	2.58	0.41
1:G:199:ILE:H	1:G:199:ILE:HG13	1.53	0.41
1:B:2:LYS:HE3	1:B:41:ARG:O	2.20	0.41
1:E:50:ARG:NE	1:E:119:ILE:HG21	2.36	0.41
1:F:105:VAL:HG23	1:F:108:ILE:HG13	2.02	0.41
1:F:16:PRO:HD3	1:F:26:GLU:OE1	2.21	0.41
1:A:106:ASP:HB3	1:C:124:PHE:CD2	2.56	0.40
1:E:61:ALA:HB2	1:E:90:LEU:HB3	2.03	0.40
1:F:43:TRP:HA	1:F:43:TRP:CE3	2.57	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	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
1	B	214/216 (99%)	200 (94%)	14 (6%)	0	100	100
1	C	214/216 (99%)	198 (92%)	16 (8%)	0	100	100
1	D	214/216 (99%)	203 (95%)	10 (5%)	1 (0%)	32	68
1	E	214/216 (99%)	195 (91%)	17 (8%)	2 (1%)	20	54
1	F	214/216 (99%)	195 (91%)	18 (8%)	1 (0%)	32	68
1	G	214/216 (99%)	195 (91%)	16 (8%)	3 (1%)	13	41
All	All	1498/1512 (99%)	1391 (93%)	100 (7%)	7 (0%)	32	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	SER
1	E	38	ASP
1	G	199	ILE
1	F	38	ASP
1	G	215	ASP
1	G	38	ASP
1	E	93	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	199/199 (100%)	192 (96%)	7 (4%)	41	75
1	B	199/199 (100%)	186 (94%)	13 (6%)	20	49
1	C	199/199 (100%)	190 (96%)	9 (4%)	32	66
1	D	199/199 (100%)	184 (92%)	15 (8%)	16	42
1	E	199/199 (100%)	187 (94%)	12 (6%)	22	54
1	F	199/199 (100%)	183 (92%)	16 (8%)	14	38
1	G	199/199 (100%)	184 (92%)	15 (8%)	16	42
All	All	1393/1393 (100%)	1306 (94%)	87 (6%)	21	52

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	51	ASP
1	A	72	THR
1	A	79	ARG
1	A	130	TYR
1	A	167	CYS
1	A	204	GLU
1	B	24	LYS
1	B	51	ASP
1	B	56	ARG
1	B	62	LYS
1	B	65	LYS
1	B	72	THR
1	B	79	ARG
1	B	97	LYS
1	B	130	TYR
1	B	150	GLU
1	B	167	CYS
1	B	204	GLU
1	B	210	ASN
1	C	24	LYS
1	C	37	GLN
1	C	79	ARG
1	C	111	GLN
1	C	130	TYR
1	C	144	ASP
1	C	201	LYS
1	C	204	GLU
1	C	212	ASN

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Mol	Chain	Res	Type
1	D	26	GLU
1	D	42	ASP
1	D	51	ASP
1	D	55	SER
1	D	79	ARG
1	D	97	LYS
1	D	111	GLN
1	D	118	LYS
1	D	130	TYR
1	D	142	LYS
1	D	144	ASP
1	D	167	CYS
1	D	181	LYS
1	D	192	ILE
1	D	214	VAL
1	E	2	LYS
1	E	12	ASP
1	E	24	LYS
1	E	55	SER
1	E	65	LYS
1	E	79	ARG
1	E	109	MET
1	E	114	THR
1	E	130	TYR
1	E	139	ASN
1	E	197	GLU
1	E	212	ASN
1	F	37	GLN
1	F	42	ASP
1	F	65	LYS
1	F	79	ARG
1	F	82	ASP
1	F	105	VAL
1	F	111	GLN
1	F	114	THR
1	F	130	TYR
1	F	142	LYS
1	F	144	ASP
1	F	165	GLU
1	F	182	THR
1	F	200	ASN
1	F	204	GLU

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Mol	Chain	Res	Type
1	F	212	ASN
1	G	24	LYS
1	G	51	ASP
1	G	65	LYS
1	G	72	THR
1	G	79	ARG
1	G	82	ASP
1	G	111	GLN
1	G	113	VAL
1	G	130	TYR
1	G	144	ASP
1	G	165	GLU
1	G	192	ILE
1	G	197	GLU
1	G	199	ILE
1	G	214	VAL

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

Mol	Chain	Res	Type
1	A	141	HIS
1	C	44	HIS
1	C	64	HIS
1	C	111	GLN
1	E	37	GLN
1	E	139	ASN
1	E	212	ASN
1	F	37	GLN
1	F	111	GLN
1	F	209	HIS
1	G	103	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	216/216 (100%)	0.40	2 (0%) 84 83	67, 75, 86, 95	0
1	B	216/216 (100%)	0.47	5 (2%) 61 57	66, 75, 90, 96	0
1	C	216/216 (100%)	0.56	9 (4%) 37 32	67, 76, 89, 93	0
1	D	216/216 (100%)	0.75	23 (10%) 7 5	66, 77, 84, 92	0
1	E	216/216 (100%)	1.33	50 (23%) 1 0	70, 77, 89, 92	0
1	F	216/216 (100%)	1.66	71 (32%) 0 0	70, 77, 90, 91	0
1	G	216/216 (100%)	0.94	37 (17%) 2 1	70, 77, 90, 92	0
All	All	1512/1512 (100%)	0.87	197 (13%) 4 3	66, 76, 89, 96	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	213	VAL	7.5
1	F	75	TYR	6.9
1	E	213	VAL	6.7
1	F	89	ILE	6.6
1	E	204	GLU	6.6
1	E	182	THR	6.4
1	G	201	LYS	6.4
1	F	211	ILE	6.2
1	G	199	ILE	6.1
1	E	70	TYR	6.0
1	E	216	LYS	6.0
1	E	74	THR	5.9
1	F	214	VAL	5.8
1	F	63	ASN	5.6
1	F	164	LEU	5.5
1	F	194	ASP	5.5
1	F	203	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	72	THR	5.4
1	F	64	HIS	5.4
1	F	72	THR	5.2
1	F	184	VAL	5.2
1	F	196	PRO	5.2
1	G	90	LEU	5.2
1	G	198	VAL	5.2
1	G	75	TYR	5.0
1	F	199	ILE	5.0
1	E	71	SER	5.0
1	E	206	LEU	5.0
1	F	88	GLY	4.8
1	F	67	LYS	4.7
1	E	73	TYR	4.7
1	F	70	TYR	4.7
1	F	17	LEU	4.7
1	F	192	ILE	4.6
1	D	67	LYS	4.6
1	B	216	LYS	4.6
1	F	90	LEU	4.6
1	F	209	HIS	4.5
1	F	91	TRP	4.5
1	F	206	LEU	4.5
1	F	197	GLU	4.4
1	E	199	ILE	4.4
1	G	216	LYS	4.4
1	G	213	VAL	4.4
1	E	211	ILE	4.3
1	F	204	GLU	4.3
1	D	66	ASP	4.3
1	E	68	GLU	4.3
1	F	158	TYR	4.3
1	F	198	VAL	4.3
1	F	71	SER	4.2
1	F	159	ILE	4.1
1	D	216	LYS	4.1
1	F	207	LYS	4.1
1	F	216	LYS	4.0
1	F	200	ASN	4.0
1	D	73	TYR	4.0
1	F	73	TYR	3.9
1	E	42	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	40	ASP	3.9
1	E	69	PRO	3.9
1	D	72	THR	3.9
1	E	198	VAL	3.9
1	E	62	LYS	3.8
1	E	181	LYS	3.8
1	E	164	LEU	3.8
1	E	158	TYR	3.8
1	E	67	LYS	3.8
1	F	86	GLN	3.7
1	F	43	TRP	3.7
1	E	1	MET	3.7
1	E	196	PRO	3.6
1	E	188	TYR	3.6
1	E	90	LEU	3.6
1	F	195	ASP	3.6
1	D	75	TYR	3.5
1	E	75	TYR	3.5
1	E	88	GLY	3.5
1	F	201	LYS	3.4
1	F	156	GLU	3.4
1	F	186	LEU	3.4
1	F	202	VAL	3.4
1	G	214	VAL	3.3
1	D	87	GLU	3.3
1	F	68	GLU	3.3
1	E	40	ASP	3.3
1	E	187	ASP	3.3
1	D	65	LYS	3.3
1	G	193	SER	3.2
1	E	203	LYS	3.2
1	E	184	VAL	3.2
1	G	207	LYS	3.2
1	E	202	VAL	3.1
1	F	181	LYS	3.1
1	F	20	LEU	3.1
1	F	157	VAL	3.0
1	G	206	LEU	3.0
1	C	66	ASP	3.0
1	G	70	TYR	3.0
1	G	36	MET	3.0
1	E	214	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	208	ALA	3.0
1	E	91	TRP	3.0
1	E	157	VAL	2.9
1	G	211	ILE	2.9
1	C	216	LYS	2.9
1	D	203	LYS	2.9
1	G	203	LYS	2.9
1	G	184	VAL	2.9
1	E	2	LYS	2.9
1	F	65	LYS	2.9
1	F	212	ASN	2.8
1	F	69	PRO	2.8
1	E	186	LEU	2.8
1	E	159	ILE	2.8
1	F	66	ASP	2.8
1	F	165	GLU	2.8
1	F	193	SER	2.8
1	B	212	ASN	2.8
1	G	186	LEU	2.8
1	F	87	GLU	2.7
1	C	209	HIS	2.7
1	E	66	ASP	2.7
1	G	72	THR	2.7
1	B	194	ASP	2.7
1	F	2	LYS	2.7
1	D	83	ASP	2.7
1	D	206	LEU	2.7
1	G	20	LEU	2.7
1	G	114	THR	2.7
1	F	44	HIS	2.7
1	D	181	LYS	2.6
1	E	194	ASP	2.6
1	F	62	LYS	2.6
1	F	131	TYR	2.6
1	G	66	ASP	2.6
1	F	210	ASN	2.6
1	C	198	VAL	2.6
1	G	87	GLU	2.6
1	C	65	LYS	2.6
1	G	194	ASP	2.5
1	G	89	ILE	2.5
1	G	204	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	90	LEU	2.5
1	G	65	LYS	2.4
1	F	76	HIS	2.4
1	G	131	TYR	2.4
1	E	64	HIS	2.4
1	E	65	LYS	2.4
1	B	211	ILE	2.4
1	D	74	THR	2.4
1	A	65	LYS	2.4
1	E	58	ILE	2.4
1	G	209	HIS	2.3
1	C	211	ILE	2.3
1	G	192	ILE	2.3
1	F	160	VAL	2.3
1	F	13	PHE	2.3
1	F	19	SER	2.3
1	D	175	ALA	2.3
1	A	216	LYS	2.2
1	G	67	LYS	2.2
1	E	155	ASP	2.2
1	F	129	GLU	2.2
1	D	58	ILE	2.2
1	E	207	LYS	2.2
1	F	92	PRO	2.2
1	D	156	GLU	2.2
1	G	76	HIS	2.2
1	E	148	TYR	2.2
1	D	88	GLY	2.2
1	B	193	SER	2.2
1	E	168	VAL	2.2
1	C	90	LEU	2.1
1	E	115	LYS	2.1
1	F	153	HIS	2.1
1	C	199	ILE	2.1
1	F	74	THR	2.1
1	F	182	THR	2.1
1	F	41	ARG	2.1
1	F	60	PHE	2.1
1	G	158	TYR	2.1
1	G	202	VAL	2.1
1	D	64	HIS	2.1
1	G	182	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	197	GLU	2.1
1	D	76	HIS	2.1
1	E	197	GLU	2.1
1	C	181	LYS	2.1
1	F	215	ASP	2.0
1	D	213	VAL	2.0
1	D	70	TYR	2.0
1	E	180	TYR	2.0
1	G	210	ASN	2.0
1	D	86	GLN	2.0
1	G	196	PRO	2.0
1	F	107	GLN	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	F	301	1/1	0.93	0.15	-1.03	92,92,92,92	0
2	ZN	E	301	1/1	0.94	0.12	-2.33	97,97,97,97	0
2	ZN	D	301	1/1	0.90	0.05	-2.87	87,87,87,87	0
2	ZN	G	301	1/1	0.93	0.04	-3.46	88,88,88,88	0
2	ZN	C	301	1/1	0.97	0.08	-5.36	90,90,90,90	0
2	ZN	B	301	1/1	0.95	0.12	-	87,87,87,87	0
2	ZN	A	301	1/1	0.99	0.20	-	84,84,84,84	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.