



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:56 PM UTC

PDB ID : 2H0R / pdb_00002h0r
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

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
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

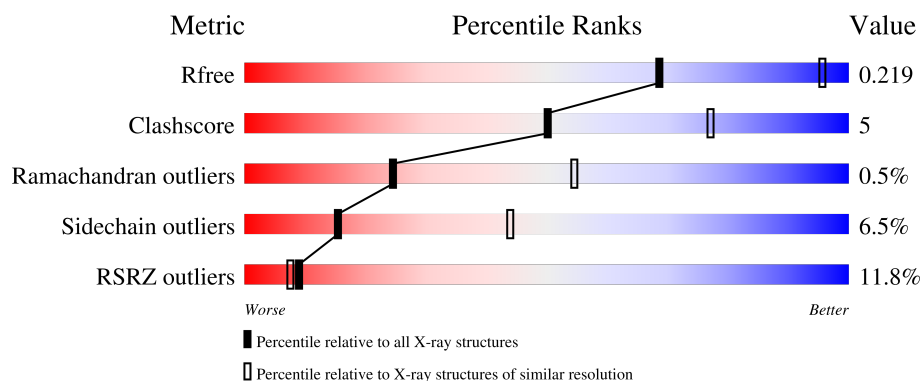
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	216	84% 15% .
1	B	216	23% 82% 16% .
1	C	216	16% 84% 14% .
1	D	216	3% 83% 15% .
1	E	216	9% 73% 25% .

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Mol	Chain	Length	Quality of chain
1	F	216	10% 76% 20% • •
1	G	216	20% 81% 17% ••

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			

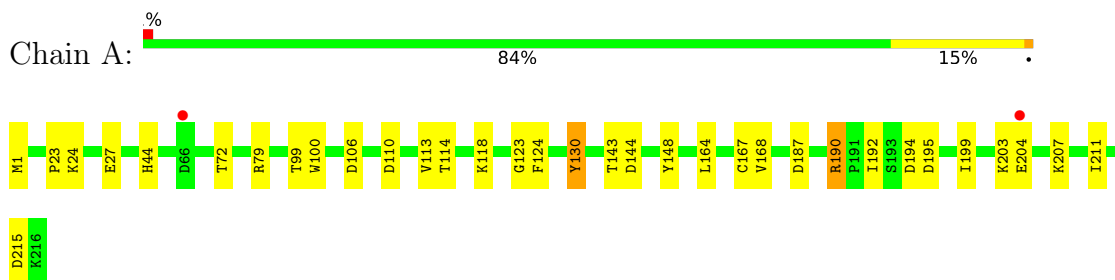
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

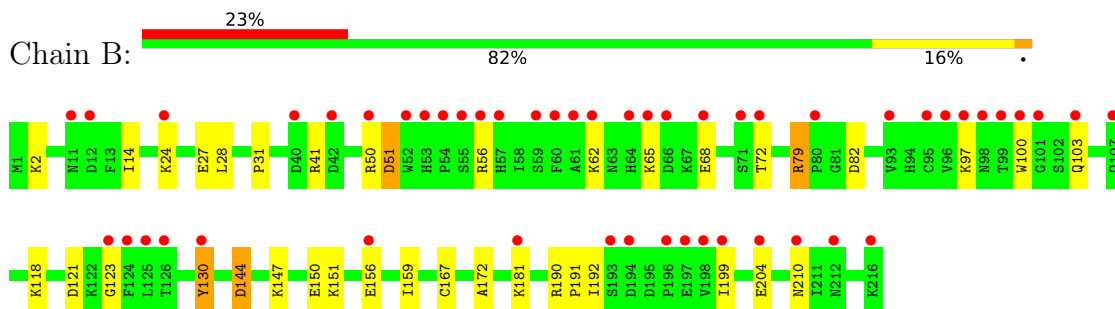
3 Residue-property plots [i](#)

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.

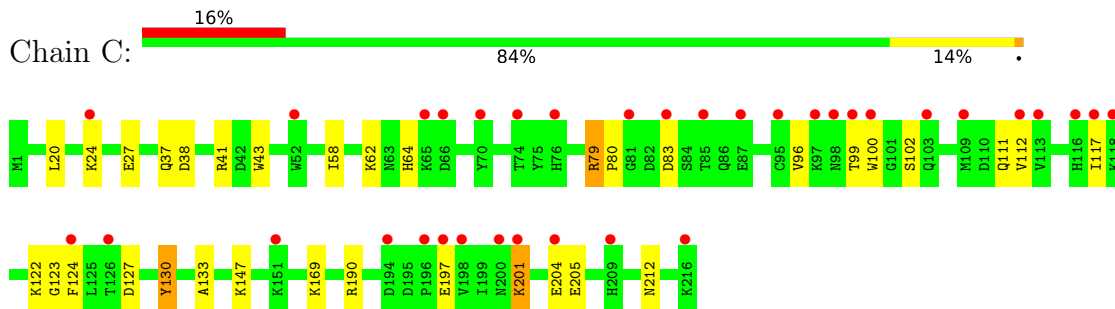
- Molecule 1: Nicotinamidase



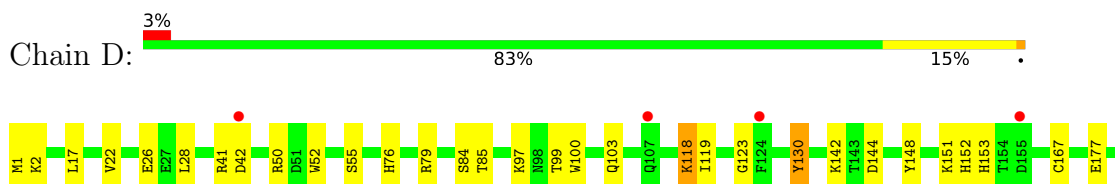
- Molecule 1: Nicotinamidase

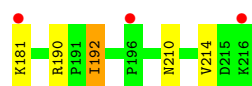


- Molecule 1: Nicotinamidase



- Molecule 1: Nicotinamidase

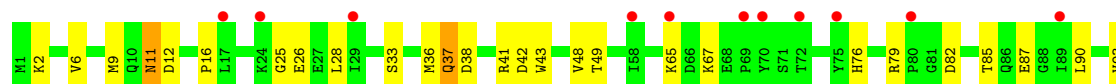
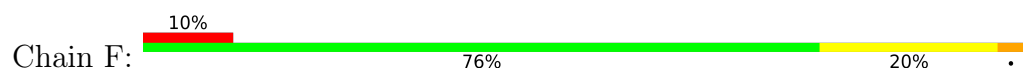




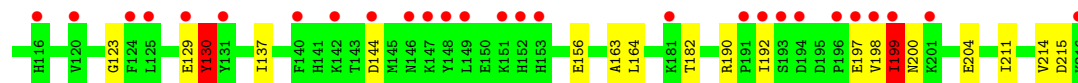
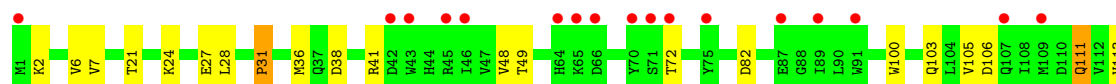
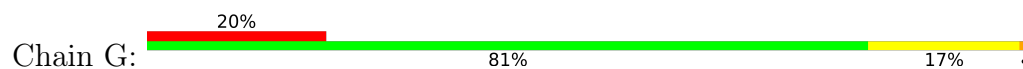
● Molecule 1: Nicotinamidase



● Molecule 1: Nicotinamidase



● Molecule 1: Nicotinamidase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	302.04Å 302.04Å 112.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.90) 99.9 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.220 0.190 , 0.219	Depositor DCC
R_{free} test set	4226 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12348	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.86	0/1809	1.06	9/2459 (0.4%)
1	B	0.66	0/1809	0.98	5/2459 (0.2%)
1	C	0.63	0/1809	0.92	0/2459
1	D	0.56	0/1809	0.88	0/2459
1	E	0.79	5/1809 (0.3%)	0.93	2/2459 (0.1%)
1	F	0.85	9/1809 (0.5%)	0.94	3/2459 (0.1%)
1	G	0.72	5/1809 (0.3%)	0.89	2/2459 (0.1%)
All	All	0.73	19/12663 (0.2%)	0.94	21/17213 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	103	GLN	C-N	14.44	1.53	1.33
1	E	106	ASP	C-O	13.57	1.41	1.24
1	G	106	ASP	C-O	12.05	1.39	1.24
1	E	106	ASP	C-N	11.20	1.49	1.33
1	E	105	VAL	C-O	8.83	1.34	1.24
1	G	41	ARG	CZ-NH1	7.58	1.43	1.32
1	F	102	SER	C-O	7.41	1.33	1.24
1	F	105	VAL	CB-CG1	7.15	1.76	1.52
1	G	31	PRO	N-CD	6.37	1.56	1.47
1	F	9	MET	C-O	6.33	1.32	1.23
1	F	105	VAL	CB-CG2	6.05	1.72	1.52
1	G	41	ARG	CZ-NH2	5.84	1.41	1.33
1	F	28	LEU	C-O	5.84	1.31	1.24
1	F	9	MET	C-N	5.66	1.41	1.33
1	G	105	VAL	C-O	5.57	1.29	1.24
1	E	105	VAL	C-N	5.32	1.41	1.33
1	F	102	SER	C-N	5.19	1.40	1.33
1	E	118	LYS	C-O	5.09	1.29	1.23
1	F	102	SER	CB-OG	5.08	1.52	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	TYR	CB-CA-C	-8.37	96.75	110.14
1	E	106	ASP	CA-C-N	-8.14	108.73	120.29
1	E	106	ASP	C-N-CA	-8.14	108.73	120.29
1	F	11	ASN	OD1-CG-ND2	7.63	130.24	122.60
1	F	103	GLN	CA-C-N	-7.58	110.58	121.42
1	F	103	GLN	C-N-CA	-7.58	110.58	121.42
1	A	144	ASP	N-CA-CB	-6.74	99.83	110.28
1	G	41	ARG	NE-CZ-NH2	-6.66	113.21	119.20
1	A	211	ILE	CA-C-N	-6.18	114.47	123.00
1	A	211	ILE	C-N-CA	-6.18	114.47	123.00
1	B	144	ASP	N-CA-CB	-5.79	100.77	110.39
1	A	195	ASP	CA-C-N	5.66	126.92	119.84
1	A	195	ASP	C-N-CA	5.66	126.92	119.84
1	A	124	PHE	N-CA-C	5.62	117.40	111.28
1	B	51	ASP	N-CA-C	-5.32	102.18	110.10
1	B	14	ILE	N-CA-C	5.20	116.29	111.81
1	A	143	THR	CA-C-N	5.20	128.22	120.31
1	A	143	THR	C-N-CA	5.20	128.22	120.31
1	B	68	GLU	CA-C-N	-5.05	114.57	119.78
1	B	68	GLU	C-N-CA	-5.05	114.57	119.78
1	G	130	TYR	CB-CA-C	-5.04	101.79	110.16

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	1763	0	1723	14	0
1	B	1763	0	1723	17	0
1	C	1763	0	1723	20	0
1	D	1763	0	1723	16	0
1	E	1763	0	1723	29	0
1	F	1763	0	1723	25	0
1	G	1763	0	1723	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	130	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 (130) 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:CG1	1:F:105:VAL:CB	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:CG1	1:F:105:VAL:CA	2.62	0.76
1:F:25:GLY:HA2	1:F:190:ARG:HG3	1.68	0.76
1:G:36:MET:HE2	1:G:111:GLN:HG2	1.66	0.75
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:F:36:MET:HE2	1:F:111:GLN:HG2	1.71	0.72
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:B:118:LYS:NZ	1:B:144:ASP:OD2	2.31	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:G:198:VAL:C	1:G:200:ASN:H	2.20	0.50
1:G:36:MET:CE	1:G:111:GLN:HG2	2.38	0.50
1:E:182:THR:HB	1:E:211:ILE:HG12	1.93	0.49
1:A:99:THR:O	1:A:100:TRP:C	2.55	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:HA	1:B:147:LYS:HD3	1.70	0.47
1:A:164:LEU:HA	1:A:168:VAL:HB	1.97	0.47
1:A:1:MET:HE2	1:A:44:HIS:ND1	2.30	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:NZ	1:D:144:ASP:OD2	2.30	0.46
1:C:83:ASP:OD1	1:C:83:ASP:N	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: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: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:D:99:THR:O	1:D:100:TRP:C	2.58	0.45
1:E:36:MET:HE3	1:E:46:ILE:HG21	1.99	0.45
1:B:50:ARG:HH21	1:B:121:ASP:CG	2.26	0.44
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:F:67:LYS:HE3	1:F:90:LEU:HD11	2.00	0.44
1:A:113:VAL:HG11	1:C:127:ASP:CG	2.43	0.44
1:C:99:THR:O	1:C:100:TRP:C	2.61	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
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:G:28:LEU:C	1:G:31:PRO:HD2	2.43	0.43
1:B:28:LEU:C	1:B:31:PRO:HD2	2.43	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:CD1	1:E:130:TYR:N	2.87	0.43
1:C:62:LYS:O	1:C:62:LYS:HG2	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:CD1	1:C:130:TYR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:GLU:HA	1:F:87:GLU:OE1	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:CD1	1:D:130:TYR:N	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:79:ARG:HB3	1:B:82:ASP:HB3	2.02	0.41
1:B:191:PRO:HG3	1:B:199:ILE:HD11	2.01	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:HE21	1:F:37:GLN:H	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: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:16:PRO:HD3	1:F:26:GLU:OE1	2.21	0.41
1:F:105:VAL:HG23	1:F:108:ILE:HG13	2.02	0.41
1:A:106:ASP:HB3	1:C:124:PHE:CD2	2.56	0.40
1:G:163:ALA:O	1:G:164:LEU:C	2.64	0.40
1:E:61:ALA:HB2	1:E:90:LEU:HB3	2.03	0.40
1:F:43:TRP:CE3	1:F:43:TRP:HA	2.57	0.40

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	214/216 (99%)	203 (95%)	10 (5%)	1 (0%)	24	54
1	E	214/216 (99%)	195 (91%)	17 (8%)	2 (1%)	14	41
1	F	214/216 (99%)	195 (91%)	18 (8%)	1 (0%)	24	54
1	G	214/216 (99%)	195 (91%)	16 (8%)	3 (1%)	9	30
All	All	1498/1512 (99%)	1391 (93%)	100 (7%)	7 (0%)	24	54

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 [i](#)

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%)	32	66
1	B	199/199 (100%)	185 (93%)	14 (7%)	14	40
1	C	199/199 (100%)	190 (96%)	9 (4%)	24	58
1	D	199/199 (100%)	185 (93%)	14 (7%)	14	40
1	E	199/199 (100%)	186 (94%)	13 (6%)	15	44
1	F	199/199 (100%)	178 (89%)	21 (11%)	6	22
1	G	199/199 (100%)	186 (94%)	13 (6%)	15	44
All	All	1393/1393 (100%)	1302 (94%)	91 (6%)	15	44

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	72	THR
1	A	79	ARG
1	A	167	CYS
1	A	190	ARG
1	A	192	ILE
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	192	ILE
1	B	204	GLU
1	B	210	ASN
1	C	20	LEU
1	C	24	LYS
1	C	37	GLN
1	C	79	ARG
1	C	111	GLN
1	C	130	TYR
1	C	201	LYS
1	C	204	GLU
1	C	212	ASN
1	D	26	GLU
1	D	42	ASP
1	D	55	SER
1	D	79	ARG
1	D	97	LYS
1	D	118	LYS
1	D	130	TYR
1	D	142	LYS
1	D	167	CYS
1	D	177	GLU
1	D	181	LYS
1	D	192	ILE
1	D	210	ASN

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Mol	Chain	Res	Type
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	197	GLU
1	E	198	VAL
1	E	201	LYS
1	E	212	ASN
1	F	37	GLN
1	F	42	ASP
1	F	49	THR
1	F	65	LYS
1	F	79	ARG
1	F	82	ASP
1	F	93	VAL
1	F	103	GLN
1	F	105	VAL
1	F	108	ILE
1	F	114	THR
1	F	119	ILE
1	F	130	TYR
1	F	142	LYS
1	F	165	GLU
1	F	167	CYS
1	F	182	THR
1	F	200	ASN
1	F	204	GLU
1	F	212	ASN
1	F	213	VAL
1	G	21	THR
1	G	24	LYS
1	G	72	THR
1	G	82	ASP
1	G	111	GLN
1	G	113	VAL
1	G	130	TYR

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Mol	Chain	Res	Type
1	G	144	ASP
1	G	192	ILE
1	G	197	GLU
1	G	199	ILE
1	G	204	GLU
1	G	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	HIS
1	C	44	HIS
1	C	64	HIS
1	C	111	GLN
1	D	111	GLN
1	D	146	ASN
1	D	153	HIS
1	D	209	HIS
1	E	37	GLN
1	E	139	ASN
1	E	209	HIS
1	F	11	ASN
1	F	37	GLN
1	F	111	GLN
1	F	209	HIS
1	G	37	GLN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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, 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	216/216 (100%)	0.22	2 (0%) 81 75	67, 75, 86, 95	0
1	B	216/216 (100%)	1.29	50 (23%) 2 2	66, 75, 90, 96	0
1	C	216/216 (100%)	1.04	35 (16%) 4 4	67, 76, 89, 93	0
1	D	216/216 (100%)	0.60	7 (3%) 50 41	66, 77, 84, 92	0
1	E	216/216 (100%)	0.86	19 (8%) 15 13	70, 77, 89, 92	0
1	F	216/216 (100%)	0.90	22 (10%) 12 10	70, 77, 90, 91	0
1	G	216/216 (100%)	1.21	44 (20%) 3 2	70, 77, 90, 92	0
All	All	1512/1512 (100%)	0.87	179 (11%) 9 7	66, 76, 89, 96	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	THR	4.4
1	G	153	HIS	4.4
1	C	116	HIS	4.4
1	E	198	VAL	4.2
1	E	213	VAL	3.9
1	G	198	VAL	3.6
1	B	123	GLY	3.5
1	B	61	ALA	3.5
1	B	216	LYS	3.3
1	B	93	VAL	3.2
1	B	96	VAL	3.2
1	B	194	ASP	3.2
1	B	125	LEU	3.2
1	F	214	VAL	3.2
1	F	194	ASP	3.2
1	F	196	PRO	3.2
1	F	213	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	147	LYS	3.1
1	A	66	ASP	3.1
1	G	193	SER	3.1
1	B	56	ARG	3.1
1	B	52	TRP	3.0
1	G	1	MET	3.0
1	B	103	GLN	3.0
1	E	196	PRO	3.0
1	F	199	ILE	3.0
1	B	210	ASN	3.0
1	B	54	PRO	3.0
1	G	87	GLU	3.0
1	B	62	LYS	2.9
1	B	204	GLU	2.9
1	B	65	LYS	2.9
1	B	124	PHE	2.9
1	F	65	LYS	2.9
1	F	104	LEU	2.9
1	B	98	ASN	2.9
1	G	116	HIS	2.9
1	G	201	LYS	2.9
1	C	194	ASP	2.9
1	B	95	CYS	2.9
1	B	42	ASP	2.8
1	E	163	ALA	2.8
1	B	55	SER	2.8
1	F	69	PRO	2.8
1	C	66	ASP	2.8
1	B	107	GLN	2.8
1	C	124	PHE	2.8
1	G	152	HIS	2.8
1	E	201	LYS	2.8
1	G	71	SER	2.8
1	B	100	TRP	2.7
1	E	158	TYR	2.7
1	G	151	LYS	2.7
1	G	197	GLU	2.7
1	D	216	LYS	2.7
1	B	40	ASP	2.7
1	D	107	GLN	2.7
1	G	89	ILE	2.7
1	G	125	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	100	TRP	2.7
1	E	62	LYS	2.7
1	G	216	LYS	2.7
1	B	197	GLU	2.7
1	B	181	LYS	2.7
1	E	65	LYS	2.7
1	B	193	SER	2.7
1	B	53	HIS	2.6
1	G	199	ILE	2.6
1	B	64	HIS	2.6
1	C	52	TRP	2.6
1	A	204	GLU	2.6
1	G	124	PHE	2.6
1	C	87	GLU	2.6
1	B	60	PHE	2.6
1	B	196	PRO	2.6
1	F	70	TYR	2.6
1	B	101	GLY	2.5
1	G	43	TRP	2.5
1	G	120	VAL	2.5
1	D	181	LYS	2.5
1	C	209	HIS	2.5
1	G	144	ASP	2.5
1	C	81	GLY	2.5
1	E	89	ILE	2.5
1	G	192	ILE	2.5
1	G	45	ARG	2.5
1	F	72	THR	2.5
1	B	57	HIS	2.5
1	G	64	HIS	2.5
1	B	66	ASP	2.4
1	G	129	GLU	2.4
1	B	130	TYR	2.4
1	C	103	GLN	2.4
1	C	98	ASN	2.4
1	C	200	ASN	2.4
1	D	42	ASP	2.4
1	C	201	LYS	2.4
1	C	74	THR	2.4
1	E	199	ILE	2.4
1	G	46	ILE	2.4
1	F	203	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	66	ASP	2.4
1	E	109	MET	2.4
1	G	131	TYR	2.4
1	C	76	HIS	2.4
1	B	24	LYS	2.3
1	C	95	CYS	2.3
1	C	216	LYS	2.3
1	C	109	MET	2.3
1	B	71	SER	2.3
1	E	71	SER	2.3
1	C	117	ILE	2.3
1	G	181	LYS	2.3
1	E	214	VAL	2.3
1	G	109	MET	2.3
1	B	97	LYS	2.3
1	B	199	ILE	2.3
1	F	89	ILE	2.3
1	F	118	LYS	2.3
1	G	142	LYS	2.3
1	B	72	THR	2.3
1	D	155	ASP	2.3
1	C	112	VAL	2.3
1	F	80	PRO	2.3
1	F	24	LYS	2.2
1	G	91	TRP	2.2
1	B	80	PRO	2.2
1	C	198	VAL	2.2
1	G	75	TYR	2.2
1	D	124	PHE	2.2
1	C	204	GLU	2.2
1	B	11	ASN	2.2
1	F	58	ILE	2.2
1	G	107	GLN	2.2
1	F	126	THR	2.2
1	G	196	PRO	2.2
1	F	75	TYR	2.2
1	F	29	ILE	2.2
1	C	83	ASP	2.2
1	G	194	ASP	2.2
1	C	113	VAL	2.2
1	G	70	TYR	2.2
1	F	124	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	65	LYS	2.2
1	G	146	ASN	2.2
1	D	196	PRO	2.2
1	G	72	THR	2.2
1	C	97	LYS	2.2
1	E	216	LYS	2.2
1	E	70	TYR	2.2
1	F	17	LEU	2.2
1	B	50	ARG	2.1
1	B	212	ASN	2.1
1	E	187	ASP	2.1
1	G	42	ASP	2.1
1	C	151	LYS	2.1
1	C	85	THR	2.1
1	E	126	THR	2.1
1	C	24	LYS	2.1
1	C	65	LYS	2.1
1	C	196	PRO	2.1
1	F	216	LYS	2.1
1	G	191	PRO	2.1
1	G	149	LEU	2.1
1	B	156	GLU	2.1
1	C	118	LYS	2.0
1	G	140	PHE	2.0
1	B	99	THR	2.0
1	B	12	ASP	2.0
1	C	70	TYR	2.0
1	B	59	SER	2.0
1	B	198	VAL	2.0
1	C	99	THR	2.0
1	C	126	THR	2.0
1	B	68	GLU	2.0
1	C	197	GLU	2.0
1	E	118	LYS	2.0
1	G	148	TYR	2.0
1	E	93	VAL	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 [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, 95th 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	301	1/1	0.97	0.06	84,84,84,84	0
2	ZN	C	301	1/1	0.97	0.08	90,90,90,90	0
2	ZN	D	301	1/1	0.97	0.12	87,87,87,87	0
2	ZN	B	301	1/1	0.98	0.06	87,87,87,87	0
2	ZN	E	301	1/1	0.98	0.18	97,97,97,97	0
2	ZN	F	301	1/1	0.98	0.21	92,92,92,92	0
2	ZN	G	301	1/1	0.98	0.14	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.