



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:26 AM EDT

PDB ID : 1XE0 / pdb_00001xe0
Title : The structure and function of Xenopus NO38-core, a histone binding chaperone in the nucleolus
Authors : Namboodiri, V.M.; Akey, I.V.; Schmidt-Zachmann, M.S.; Head, J.F.; Akey, C.W.
Deposited on : 2004-09-08
Resolution : 1.70 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

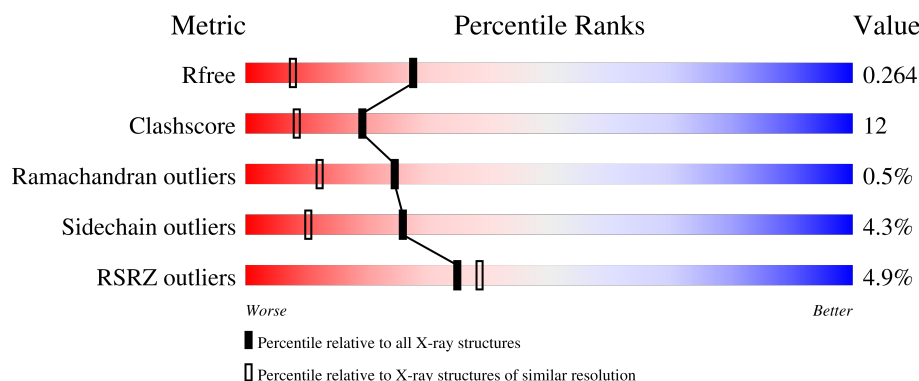
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	114	
1	B	114	
1	C	114	
1	D	114	
1	E	114	

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Mol	Chain	Length	Quality of chain
1	F	114	4% 72% 20% 5%
1	G	114	7% 73% 18% 9%
1	H	114	4% 70% 18% 9%
1	I	114	6% 69% 19% 8%
1	J	114	3% 61% 29% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8328 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 Nucleophosmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			815	517	136	161	1			
1	B	107	Total	C	N	O	S	0	0	0
			810	517	135	157	1			
1	C	101	Total	C	N	O	S	0	0	0
			764	491	128	144	1			
1	D	105	Total	C	N	O	S	0	0	0
			801	510	133	157	1			
1	E	104	Total	C	N	O	S	0	0	0
			790	504	132	153	1			
1	F	108	Total	C	N	O	S	0	0	0
			816	520	136	159	1			
1	G	104	Total	C	N	O	S	0	0	0
			792	505	132	154	1			
1	H	104	Total	C	N	O	S	0	0	0
			788	503	132	152	1			
1	I	105	Total	C	N	O	S	0	0	0
			797	508	133	155	1			
1	J	104	Total	C	N	O	S	0	0	0
			790	505	132	152	1			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	-	cloning artifact	UNP P07222
A	12	PRO	-	cloning artifact	UNP P07222
A	13	ARG	-	cloning artifact	UNP P07222
A	14	GLY	-	cloning artifact	UNP P07222
A	15	SER	-	cloning artifact	UNP P07222
B	11	VAL	-	cloning artifact	UNP P07222
B	12	PRO	-	cloning artifact	UNP P07222
B	13	ARG	-	cloning artifact	UNP P07222
B	14	GLY	-	cloning artifact	UNP P07222

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	SER	-	cloning artifact	UNP P07222
C	11	VAL	-	cloning artifact	UNP P07222
C	12	PRO	-	cloning artifact	UNP P07222
C	13	ARG	-	cloning artifact	UNP P07222
C	14	GLY	-	cloning artifact	UNP P07222
C	15	SER	-	cloning artifact	UNP P07222
D	11	VAL	-	cloning artifact	UNP P07222
D	12	PRO	-	cloning artifact	UNP P07222
D	13	ARG	-	cloning artifact	UNP P07222
D	14	GLY	-	cloning artifact	UNP P07222
D	15	SER	-	cloning artifact	UNP P07222
E	11	VAL	-	cloning artifact	UNP P07222
E	12	PRO	-	cloning artifact	UNP P07222
E	13	ARG	-	cloning artifact	UNP P07222
E	14	GLY	-	cloning artifact	UNP P07222
E	15	SER	-	cloning artifact	UNP P07222
F	11	VAL	-	cloning artifact	UNP P07222
F	12	PRO	-	cloning artifact	UNP P07222
F	13	ARG	-	cloning artifact	UNP P07222
F	14	GLY	-	cloning artifact	UNP P07222
F	15	SER	-	cloning artifact	UNP P07222
G	11	VAL	-	cloning artifact	UNP P07222
G	12	PRO	-	cloning artifact	UNP P07222
G	13	ARG	-	cloning artifact	UNP P07222
G	14	GLY	-	cloning artifact	UNP P07222
G	15	SER	-	cloning artifact	UNP P07222
H	11	VAL	-	cloning artifact	UNP P07222
H	12	PRO	-	cloning artifact	UNP P07222
H	13	ARG	-	cloning artifact	UNP P07222
H	14	GLY	-	cloning artifact	UNP P07222
H	15	SER	-	cloning artifact	UNP P07222
I	11	VAL	-	cloning artifact	UNP P07222
I	12	PRO	-	cloning artifact	UNP P07222
I	13	ARG	-	cloning artifact	UNP P07222
I	14	GLY	-	cloning artifact	UNP P07222
I	15	SER	-	cloning artifact	UNP P07222
J	11	VAL	-	cloning artifact	UNP P07222
J	12	PRO	-	cloning artifact	UNP P07222
J	13	ARG	-	cloning artifact	UNP P07222
J	14	GLY	-	cloning artifact	UNP P07222
J	15	SER	-	cloning artifact	UNP P07222

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total 59	O 59	0	0
2	B	30	Total 30	O 30	0	0
2	C	32	Total 32	O 32	0	0
2	D	44	Total 44	O 44	0	0
2	E	31	Total 31	O 31	0	0
2	F	37	Total 37	O 37	0	0
2	G	34	Total 34	O 34	0	0
2	H	29	Total 29	O 29	0	0
2	I	31	Total 31	O 31	0	0
2	J	38	Total 38	O 38	0	0

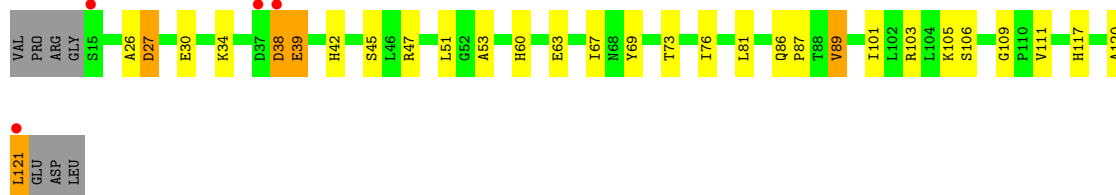
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

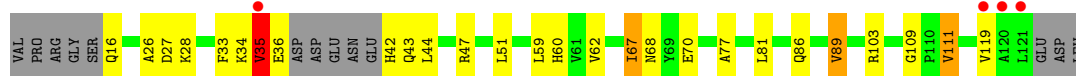
• Molecule 1: Nucleophosmin



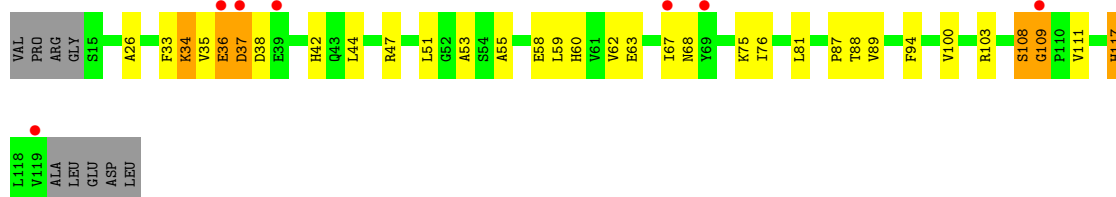
• Molecule 1: Nucleophosmin



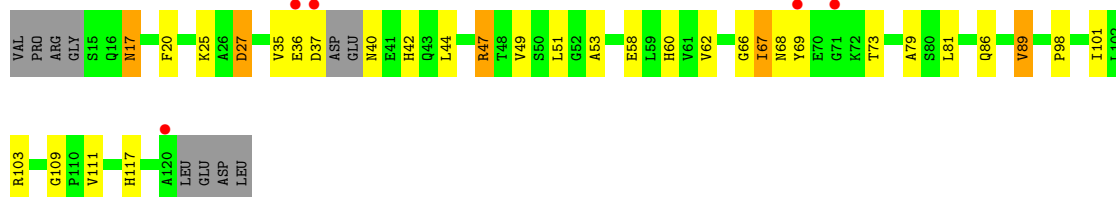
• Molecule 1: Nucleophosmin



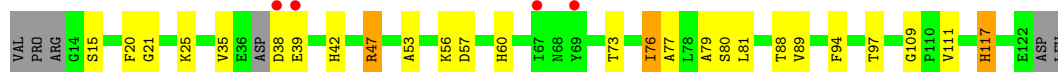
• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



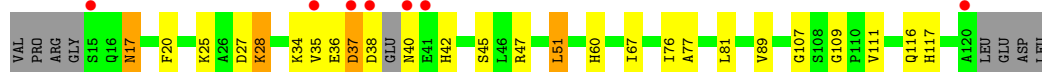
• Molecule 1: Nucleophosmin



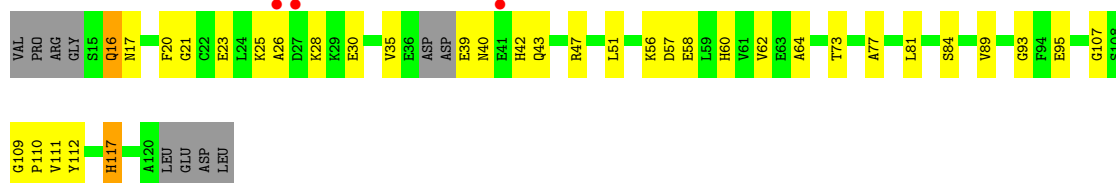
• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.00Å 59.00Å 87.20Å 77.00° 88.30° 60.90°	Depositor
Resolution (Å)	84.52 – 1.70 84.52 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.8 (84.52-1.70) 89.8 (84.52-1.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.259 0.217 , 0.264	Depositor DCC
R_{free} test set	7879 reflections (6.17%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8328	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 ⓘ

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	1.65	6/829 (0.7%)	1.44	8/1119 (0.7%)
1	B	1.65	10/824 (1.2%)	1.49	14/1114 (1.3%)
1	C	1.59	7/777 (0.9%)	1.37	5/1048 (0.5%)
1	D	1.62	6/815 (0.7%)	1.51	10/1101 (0.9%)
1	E	1.67	11/803 (1.4%)	1.38	5/1083 (0.5%)
1	F	1.62	7/829 (0.8%)	1.41	5/1118 (0.4%)
1	G	1.57	2/805 (0.2%)	1.26	1/1086 (0.1%)
1	H	1.57	5/800 (0.6%)	1.34	1/1078 (0.1%)
1	I	1.68	7/810 (0.9%)	1.45	6/1093 (0.5%)
1	J	1.63	7/803 (0.9%)	1.51	10/1083 (0.9%)
All	All	1.63	68/8095 (0.8%)	1.42	65/10923 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
All	All	0	6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	47	ARG	CD-NE	-11.36	1.30	1.46
1	A	47	ARG	CD-NE	-10.93	1.30	1.46
1	F	77	ALA	CA-CB	-10.13	1.39	1.53
1	D	109	GLY	N-CA	9.82	1.58	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	67	ILE	CA-CB	9.28	1.64	1.54
1	D	67	ILE	CA-CB	8.79	1.65	1.54
1	D	109	GLY	CA-C	-8.46	1.39	1.51
1	A	67	ILE	CA-CB	8.34	1.64	1.54
1	F	47	ARG	CD-NE	-8.18	1.34	1.46
1	E	47	ARG	CD-NE	-8.03	1.35	1.46
1	I	47	ARG	CD-NE	-7.75	1.35	1.46
1	F	76	ILE	C-O	-7.71	1.16	1.24
1	B	47	ARG	CD-NE	-7.56	1.35	1.46
1	H	47	ARG	CD-NE	-6.98	1.36	1.46
1	C	67	ILE	CA-CB	6.94	1.62	1.54
1	J	57	ASP	C-O	-6.89	1.15	1.23
1	C	62	VAL	CA-CB	6.70	1.62	1.54
1	A	47	ARG	NE-CZ	-6.60	1.25	1.33
1	E	62	VAL	CA-CB	6.57	1.62	1.54
1	C	47	ARG	CD-NE	-6.49	1.37	1.46
1	E	47	ARG	NE-CZ	-6.44	1.25	1.33
1	E	89	VAL	CA-CB	6.44	1.62	1.54
1	D	76	ILE	C-O	-6.43	1.17	1.24
1	I	76	ILE	C-O	-6.28	1.17	1.24
1	F	53	ALA	C-O	6.22	1.31	1.24
1	B	76	ILE	C-O	-6.18	1.18	1.24
1	B	101	ILE	CA-CB	6.16	1.61	1.54
1	E	47	ARG	CZ-NH2	-6.10	1.25	1.33
1	D	62	VAL	CA-CB	5.80	1.61	1.54
1	B	101	ILE	CA-C	-5.77	1.45	1.52
1	B	67	ILE	CB-CG2	-5.71	1.33	1.52
1	E	101	ILE	C-O	-5.71	1.17	1.24
1	C	89	VAL	C-O	-5.65	1.18	1.24
1	E	17	ASN	CB-CG	-5.64	1.38	1.52
1	B	121	LEU	CG-CD1	5.64	1.71	1.52
1	I	51	LEU	C-O	-5.61	1.17	1.24
1	H	47	ARG	CB-CG	-5.58	1.35	1.52
1	G	26	ALA	CA-CB	5.58	1.61	1.53
1	F	111	VAL	CA-CB	-5.57	1.47	1.54
1	A	78	LEU	C-O	-5.52	1.17	1.24
1	I	47	ARG	NE-CZ	-5.50	1.26	1.33
1	J	64	ALA	CA-CB	-5.48	1.44	1.53
1	C	26	ALA	CA-CB	5.47	1.61	1.53
1	J	77	ALA	CA-CB	-5.47	1.45	1.53
1	E	66	GLY	C-O	5.47	1.30	1.23
1	D	47	ARG	CD-NE	-5.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	96	ILE	CA-CB	-5.42	1.47	1.54
1	B	26	ALA	CA-C	5.39	1.60	1.52
1	I	17	ASN	CB-CG	-5.37	1.38	1.52
1	E	17	ASN	N-CA	-5.36	1.39	1.46
1	B	89	VAL	N-CA	-5.35	1.40	1.46
1	H	89	VAL	C-O	-5.33	1.18	1.24
1	H	49	VAL	C-O	-5.32	1.18	1.24
1	J	93	GLY	C-O	-5.26	1.16	1.23
1	F	88	THR	C-O	5.26	1.30	1.23
1	I	77	ALA	CA-CB	-5.25	1.45	1.53
1	F	79	ALA	CA-C	-5.23	1.45	1.52
1	J	62	VAL	C-O	-5.22	1.18	1.24
1	J	25	LYS	C-O	-5.18	1.18	1.24
1	E	49	VAL	N-CA	-5.16	1.40	1.46
1	B	67	ILE	CA-CB	5.14	1.60	1.54
1	B	45	SER	N-CA	-5.12	1.39	1.46
1	G	28	LYS	CE-NZ	5.09	1.64	1.49
1	C	77	ALA	CA-CB	-5.08	1.46	1.53
1	A	103	ARG	C-O	5.08	1.29	1.23
1	E	79	ALA	CA-CB	5.05	1.62	1.53
1	A	108	SER	CB-OG	5.02	1.52	1.42
1	C	111	VAL	CA-CB	-5.00	1.47	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	GLY	N-CA-C	-12.38	87.08	112.34
1	B	47	ARG	NE-CZ-NH2	-10.66	109.60	119.20
1	C	26	ALA	CA-C-N	9.58	133.12	120.28
1	C	26	ALA	C-N-CA	9.58	133.12	120.28
1	I	47	ARG	NE-CZ-NH2	-9.25	110.87	119.20
1	F	47	ARG	NE-CZ-NH2	-8.93	111.16	119.20
1	B	67	ILE	N-CA-CB	-8.73	101.21	110.72
1	F	39	GLU	N-CA-C	8.44	122.81	109.39
1	D	109	GLY	CA-C-O	-8.25	109.73	121.52
1	A	47	ARG	NE-CZ-NH2	-7.83	112.16	119.20
1	A	14	GLY	CA-C-N	7.39	133.41	121.74
1	A	14	GLY	C-N-CA	7.39	133.41	121.74
1	C	27	ASP	N-CA-C	7.11	119.03	111.28
1	D	109	GLY	O-C-N	7.10	128.87	121.77
1	J	26	ALA	N-CA-C	7.05	119.57	111.11
1	J	107	GLY	N-CA-C	6.93	121.41	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	LEU	CA-C-O	-6.56	109.65	120.80
1	J	47	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	D	53	ALA	N-CA-C	6.33	118.98	111.71
1	D	36	GLU	N-CA-C	6.26	118.07	108.42
1	C	27	ASP	N-CA-CB	-6.25	100.94	110.12
1	A	38	ASP	CA-C-N	-6.22	114.14	122.72
1	A	38	ASP	C-N-CA	-6.22	114.14	122.72
1	F	53	ALA	N-CA-C	6.07	117.89	111.28
1	A	17	ASN	N-CA-CB	6.02	121.22	110.80
1	D	37	ASP	N-CA-C	-5.94	104.06	111.90
1	H	119	VAL	CB-CA-C	-5.83	102.54	110.42
1	B	121	LEU	CD1-CG-CD2	-5.81	98.02	110.80
1	I	17	ASN	N-CA-CB	-5.73	100.89	110.80
1	B	30	GLU	N-CA-C	5.73	118.74	109.40
1	J	39	GLU	CA-C-N	5.68	132.40	121.54
1	J	39	GLU	C-N-CA	5.68	132.40	121.54
1	E	98	PRO	CB-CA-C	-5.63	104.05	110.92
1	D	47	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	F	39	GLU	CA-C-O	5.56	129.59	122.64
1	J	17	ASN	N-CA-CB	-5.51	102.46	110.84
1	F	97	THR	N-CA-C	-5.50	103.14	110.07
1	B	38	ASP	CA-C-N	-5.50	111.04	121.54
1	B	38	ASP	C-N-CA	-5.50	111.04	121.54
1	B	27	ASP	N-CA-C	5.42	117.94	111.71
1	G	27	ASP	CA-C-O	5.41	125.61	119.18
1	B	26	ALA	CA-C-N	5.38	128.02	120.28
1	B	26	ALA	C-N-CA	5.38	128.02	120.28
1	I	37	ASP	N-CA-C	5.37	119.31	112.87
1	D	26	ALA	N-CA-C	5.36	117.12	111.28
1	A	38	ASP	N-CA-C	-5.34	101.32	109.65
1	D	34	LYS	CA-C-N	-5.33	115.53	122.51
1	D	34	LYS	C-N-CA	-5.33	115.53	122.51
1	B	47	ARG	NH1-CZ-NH2	5.31	126.20	119.30
1	J	30	GLU	N-CA-C	5.31	118.21	109.72
1	J	84	SER	N-CA-C	5.29	119.60	113.20
1	E	17	ASN	N-CA-CB	-5.27	102.50	110.77
1	I	47	ARG	NH1-CZ-NH2	5.24	126.11	119.30
1	B	121	LEU	N-CA-CB	5.17	119.29	110.50
1	A	67	ILE	N-CA-CB	-5.13	104.94	110.53
1	E	67	ILE	N-CA-C	5.11	116.63	108.87
1	B	86	GLN	CA-C-N	5.10	124.71	119.56
1	B	86	GLN	C-N-CA	5.10	124.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	I	107	GLY	CA-C-N	5.06	129.24	120.58
1	I	107	GLY	C-N-CA	5.06	129.24	120.58
1	E	27	ASP	N-CA-C	5.06	119.16	112.89
1	J	16	GLN	CB-CA-C	-5.05	100.58	109.62
1	J	73	THR	OG1-CB-CG2	-5.04	99.22	109.30
1	C	27	ASP	CA-C-O	5.01	125.86	120.55

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ALA	Peptide
1	C	35	VAL	Peptide
1	D	108	SER	Peptide
1	E	35	VAL	Peptide
1	F	38	ASP	Peptide
1	H	37	ASP	Peptide

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	815	0	818	22	0
1	B	810	0	818	13	0
1	C	764	0	784	17	0
1	D	801	0	806	24	0
1	E	790	0	803	28	1
1	F	816	0	825	16	0
1	G	792	0	799	31	0
1	H	788	0	797	19	0
1	I	797	0	804	19	1
1	J	790	0	802	18	0
2	A	59	0	0	1	1
2	B	30	0	0	2	0
2	C	32	0	0	1	0
2	D	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	31	0	0	2	0
2	F	37	0	0	2	0
2	G	34	0	0	0	0
2	H	29	0	0	1	1
2	I	31	0	0	0	0
2	J	38	0	0	0	0
All	All	8328	0	8056	187	2

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 12.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASP:O	1:B:39:GLU:CB	1.87	1.23
1:A:39:GLU:O	1:A:40:ASN:CG	2.09	0.96
1:G:81:LEU:CD2	1:G:89:VAL:HG23	1.97	0.94
1:C:81:LEU:HD21	1:C:89:VAL:HG23	1.52	0.92
1:A:39:GLU:HA	1:A:39:GLU:OE1	1.69	0.90
1:E:37:ASP:OD2	1:E:42:HIS:NE2	2.05	0.90
1:G:60:HIS:HE1	1:G:109:GLY:H	1.21	0.89
1:G:81:LEU:HD21	1:G:89:VAL:HG23	1.54	0.88
1:G:81:LEU:HD21	1:G:89:VAL:CG2	2.05	0.86
1:I:25:LYS:HE2	1:I:27:ASP:OD2	1.77	0.85
1:A:39:GLU:O	1:A:40:ASN:ND2	2.10	0.84
1:D:87:PRO:HD2	1:E:86:GLN:HE21	1.42	0.84
1:G:60:HIS:CE1	1:G:109:GLY:H	1.96	0.82
1:F:81:LEU:HD21	1:F:89:VAL:HG23	1.60	0.82
1:A:38:ASP:OD1	1:B:69:TYR:OH	1.97	0.82
1:C:33:PHE:CE1	1:C:44:LEU:HD13	2.14	0.82
2:C:135:HOH:O	1:D:59:LEU:HD11	1.81	0.81
1:H:25:LYS:HE2	1:H:27:ASP:OD1	1.80	0.80
1:G:42:HIS:ND1	1:G:117:HIS:HE1	1.79	0.80
1:A:40:ASN:HB3	1:A:120:ALA:O	1.82	0.80
1:H:60:HIS:CE1	1:H:109:GLY:H	1.99	0.80
1:D:108:SER:OG	1:D:109:GLY:N	2.14	0.79
1:C:81:LEU:HD21	1:C:89:VAL:CG2	2.13	0.78
1:F:81:LEU:CD2	1:F:89:VAL:HG23	2.14	0.77
1:E:81:LEU:HD21	1:E:89:VAL:HG23	1.67	0.76
1:G:33:PHE:CE1	1:G:44:LEU:HD13	2.20	0.76
1:D:55:ALA:HA	1:D:109:GLY:HA3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:HIS:CE1	1:E:109:GLY:H	2.03	0.75
1:D:81:LEU:CD2	1:D:89:VAL:HG23	2.17	0.74
1:D:60:HIS:HE1	1:D:109:GLY:H	1.36	0.74
1:I:42:HIS:ND1	1:I:117:HIS:HE1	1.84	0.74
1:C:81:LEU:CD2	1:C:89:VAL:HG23	2.17	0.74
1:E:81:LEU:CD2	1:E:89:VAL:HG23	2.18	0.74
1:A:53:ALA:O	1:F:56:LYS:NZ	2.21	0.73
1:I:38:ASP:OD2	1:I:40:ASN:HA	1.89	0.73
1:G:17:ASN:HD22	1:H:43:GLN:NE2	1.86	0.73
1:G:81:LEU:CD2	1:G:89:VAL:CG2	2.66	0.72
1:J:42:HIS:ND1	1:J:117:HIS:HE1	1.87	0.71
1:B:42:HIS:ND1	1:B:117:HIS:HE1	1.88	0.71
1:C:60:HIS:CE1	1:C:109:GLY:H	2.09	0.69
1:B:81:LEU:HD21	1:B:89:VAL:HG23	1.75	0.69
1:D:35:VAL:HG23	2:D:157:HOH:O	1.90	0.69
1:J:81:LEU:HD21	1:J:89:VAL:HG23	1.73	0.69
1:D:87:PRO:HD2	1:E:86:GLN:NE2	2.07	0.69
1:F:81:LEU:HD21	1:F:89:VAL:CG2	2.22	0.68
1:D:33:PHE:HD2	1:D:100:VAL:HG12	1.59	0.67
1:E:81:LEU:HD21	1:E:89:VAL:CG2	2.24	0.67
1:J:81:LEU:CD2	1:J:89:VAL:HG23	2.25	0.67
1:A:47:ARG:HD3	2:B:136:HOH:O	1.94	0.67
1:E:69:TYR:OH	2:E:148:HOH:O	2.10	0.67
1:G:35:VAL:HG12	1:G:36:GLU:N	2.10	0.67
1:E:60:HIS:HE1	1:E:109:GLY:H	1.43	0.66
1:A:39:GLU:O	1:A:40:ASN:CB	2.44	0.66
1:A:43:GLN:HE22	1:E:17:ASN:HD22	1.41	0.65
1:A:42:HIS:ND1	1:A:117:HIS:HE1	1.94	0.65
1:C:60:HIS:HE1	1:C:109:GLY:H	1.45	0.65
1:D:88:THR:H	1:E:86:GLN:HE22	1.45	0.65
1:G:17:ASN:HD22	1:H:43:GLN:HE22	1.44	0.65
1:H:25:LYS:CE	1:H:27:ASP:OD1	2.45	0.65
2:A:127:HOH:O	1:E:47:ARG:HD3	1.96	0.64
1:G:75:LYS:HB2	1:G:75:LYS:HZ3	1.63	0.64
1:I:17:ASN:HD22	1:J:43:GLN:HE22	1.45	0.63
1:D:81:LEU:HD21	1:D:89:VAL:HG23	1.81	0.62
1:F:60:HIS:CE1	1:F:109:GLY:H	2.17	0.62
1:J:60:HIS:CE1	1:J:109:GLY:H	2.17	0.62
1:F:42:HIS:ND1	1:F:117:HIS:HE1	1.98	0.62
1:H:60:HIS:HE1	1:H:109:GLY:H	1.44	0.61
1:G:35:VAL:CG1	1:G:36:GLU:N	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLN:N	1:C:119:VAL:O	2.33	0.61
1:A:47:ARG:CD	2:B:136:HOH:O	2.48	0.61
1:A:60:HIS:CE1	1:A:109:GLY:H	2.18	0.61
1:A:81:LEU:CD2	1:A:89:VAL:HG23	2.31	0.60
1:E:37:ASP:CG	1:E:42:HIS:HE2	2.09	0.60
1:I:25:LYS:CE	1:I:27:ASP:OD2	2.50	0.60
1:F:47:ARG:HD3	2:F:134:HOH:O	2.01	0.60
1:D:35:VAL:HG21	1:D:42:HIS:CD2	2.36	0.59
1:F:25:LYS:HB2	2:F:132:HOH:O	2.02	0.59
1:I:38:ASP:OD2	1:I:40:ASN:CA	2.51	0.59
1:B:53:ALA:HA	1:C:59:LEU:CD2	2.33	0.59
1:A:38:ASP:O	1:A:39:GLU:OE1	2.21	0.58
1:A:81:LEU:HD21	1:A:89:VAL:HG23	1.86	0.57
1:H:25:LYS:HE3	2:H:132:HOH:O	2.03	0.57
1:I:81:LEU:CD2	1:I:89:VAL:HG23	2.34	0.57
1:D:81:LEU:HD21	1:D:89:VAL:CG2	2.35	0.57
1:H:81:LEU:HD21	1:H:89:VAL:HG23	1.86	0.57
1:B:81:LEU:CD2	1:B:89:VAL:HG23	2.34	0.56
1:B:60:HIS:CE1	1:B:109:GLY:H	2.24	0.56
1:J:42:HIS:ND1	1:J:117:HIS:CE1	2.73	0.55
1:D:63:GLU:OE2	1:D:75:LYS:HE3	2.05	0.55
1:C:68:ASN:ND2	1:C:70:GLU:OE2	2.40	0.55
1:B:51:LEU:CD2	1:B:111:VAL:HG22	2.36	0.55
1:A:59:LEU:HD23	1:E:53:ALA:HA	1.88	0.55
1:A:15:SER:HB2	1:A:119:VAL:O	2.07	0.54
1:I:42:HIS:ND1	1:I:117:HIS:CE1	2.72	0.54
1:A:39:GLU:C	1:A:40:ASN:CG	2.75	0.54
1:D:81:LEU:HD22	1:D:89:VAL:HG23	1.88	0.54
1:D:81:LEU:CD2	1:D:89:VAL:CG2	2.86	0.54
1:G:42:HIS:ND1	1:G:117:HIS:CE1	2.70	0.53
1:B:81:LEU:HD21	1:B:89:VAL:CG2	2.38	0.53
1:H:42:HIS:ND1	1:H:117:HIS:HE1	2.06	0.52
1:D:108:SER:OG	1:D:109:GLY:CA	2.58	0.52
1:E:20:PHE:CD2	1:E:44:LEU:HD11	2.44	0.52
1:F:60:HIS:HE1	1:F:109:GLY:H	1.55	0.52
1:G:51:LEU:CD2	1:G:111:VAL:HG22	2.40	0.52
1:G:35:VAL:HG11	1:G:42:HIS:CD2	2.44	0.52
1:B:51:LEU:HD23	1:B:111:VAL:HG22	1.91	0.52
1:G:35:VAL:CG1	1:G:36:GLU:H	2.23	0.52
1:H:35:VAL:HG21	1:H:42:HIS:CD2	2.44	0.52
1:I:37:ASP:O	1:I:38:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:C	1:C:35:VAL:HG23	2.36	0.51
1:A:81:LEU:HD21	1:A:89:VAL:CG2	2.41	0.51
1:D:33:PHE:CD2	1:D:100:VAL:HG12	2.43	0.51
1:G:60:HIS:HE1	1:G:109:GLY:N	1.99	0.51
1:I:51:LEU:HD23	1:I:111:VAL:HG22	1.92	0.50
1:F:76:ILE:HG22	1:J:21:GLY:HA3	1.93	0.50
1:A:37:ASP:O	1:A:37:ASP:OD1	2.30	0.49
1:G:42:HIS:HE1	1:H:69:TYR:CE2	2.29	0.49
1:G:35:VAL:CG1	1:G:42:HIS:CD2	2.96	0.49
1:C:35:VAL:HG12	1:C:36:GLU:H	1.78	0.48
1:E:25:LYS:HE2	2:E:143:HOH:O	2.13	0.48
1:I:60:HIS:CE1	1:I:109:GLY:H	2.30	0.48
1:I:20:PHE:CD2	1:I:20:PHE:C	2.91	0.48
1:I:38:ASP:OD2	1:I:40:ASN:N	2.46	0.48
1:H:60:HIS:HE1	1:H:109:GLY:N	2.10	0.48
1:G:35:VAL:HG21	1:G:42:HIS:CB	2.44	0.48
1:H:59:LEU:HD11	1:H:80:SER:HB3	1.95	0.47
1:B:87:PRO:HD2	1:C:86:GLN:OE1	2.14	0.47
1:E:51:LEU:CD2	1:E:111:VAL:HG22	2.44	0.47
1:J:60:HIS:HE1	1:J:109:GLY:H	1.61	0.47
1:G:42:HIS:HE1	1:H:69:TYR:CZ	2.32	0.47
1:H:81:LEU:CD2	1:H:89:VAL:HG23	2.44	0.47
1:I:35:VAL:HG11	1:I:42:HIS:CE1	2.49	0.47
1:J:35:VAL:HG21	1:J:42:HIS:CD2	2.50	0.47
1:J:58:GLU:O	1:J:60:HIS:CD2	2.67	0.47
1:G:81:LEU:HD22	1:G:89:VAL:HG23	1.89	0.47
1:I:38:ASP:CG	1:I:40:ASN:HA	2.40	0.46
1:D:58:GLU:O	1:D:60:HIS:HD2	1.99	0.46
1:J:23:GLU:OE2	1:J:110:PRO:HB3	2.16	0.46
1:G:75:LYS:HZ3	1:G:75:LYS:CB	2.24	0.46
1:D:87:PRO:CD	1:E:86:GLN:HE21	2.19	0.45
1:E:67:ILE:HG22	1:E:68:ASN:O	2.17	0.45
1:H:35:VAL:HG21	1:H:42:HIS:CG	2.52	0.45
1:J:20:PHE:CD2	1:J:20:PHE:C	2.95	0.45
1:E:51:LEU:HD23	1:E:111:VAL:HG22	1.99	0.45
1:H:17:ASN:HD22	1:H:17:ASN:N	2.15	0.44
1:J:110:PRO:HB2	1:J:112:TYR:CE1	2.52	0.44
1:I:51:LEU:CD2	1:I:111:VAL:HG22	2.47	0.44
1:J:43:GLN:HE21	1:J:95:GLU:HB3	1.82	0.44
1:D:117:HIS:HD2	1:E:69:TYR:CD2	2.35	0.44
1:J:51:LEU:CD2	1:J:111:VAL:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:PHE:CZ	1:G:44:LEU:HD13	2.52	0.44
1:D:51:LEU:CD2	1:D:111:VAL:HG22	2.48	0.44
1:F:81:LEU:CD2	1:F:89:VAL:CG2	2.89	0.44
1:G:33:PHE:CE1	1:G:44:LEU:CD1	2.96	0.43
1:I:81:LEU:HD21	1:I:89:VAL:HG23	1.99	0.43
1:A:15:SER:HB3	1:A:120:ALA:HB2	2.01	0.43
1:E:37:ASP:OD2	1:E:40:ASN:HB2	2.19	0.43
1:J:58:GLU:O	1:J:60:HIS:HD2	2.02	0.43
1:C:68:ASN:OD1	1:C:68:ASN:C	2.62	0.42
1:E:67:ILE:HD13	1:E:73:THR:HA	2.01	0.42
1:C:51:LEU:CD2	1:C:111:VAL:HG22	2.49	0.42
1:G:51:LEU:HD23	1:G:111:VAL:HG22	2.01	0.42
1:H:21:GLY:HA2	1:H:113:VAL:O	2.19	0.42
1:F:60:HIS:O	1:F:80:SER:HA	2.20	0.42
1:E:37:ASP:OD2	1:E:42:HIS:CE1	2.69	0.42
1:E:58:GLU:O	1:E:60:HIS:HD2	2.02	0.42
1:C:42:HIS:CD2	1:C:42:HIS:N	2.88	0.42
1:G:67:ILE:CD1	1:G:73:THR:OG1	2.68	0.42
1:E:81:LEU:CD2	1:E:89:VAL:CG2	2.90	0.42
1:H:58:GLU:O	1:H:60:HIS:HD2	2.03	0.42
1:G:35:VAL:HG11	1:G:42:HIS:CG	2.55	0.41
1:G:33:PHE:CD1	1:G:44:LEU:HD13	2.53	0.41
1:B:63:GLU:OE2	1:B:103:ARG:HD2	2.20	0.41
1:B:105:LYS:O	1:B:106:SER:HB3	2.20	0.41
1:J:56:LYS:HZ3	1:J:56:LYS:HG3	1.63	0.41
1:A:69:TYR:CD1	1:E:117:HIS:CE1	3.09	0.41
1:F:56:LYS:HD2	1:F:57:ASP:H	1.86	0.41
1:I:45:SER:HB3	1:I:116:GLN:HE21	1.85	0.41
1:C:33:PHE:CD1	1:C:44:LEU:HD13	2.54	0.41
1:D:68:ASN:OD1	1:D:68:ASN:C	2.63	0.41
1:D:117:HIS:CD2	1:E:69:TYR:CD2	3.08	0.41
1:F:20:PHE:CD2	1:F:20:PHE:C	2.99	0.41
1:J:81:LEU:HD21	1:J:89:VAL:CG2	2.48	0.41
1:F:21:GLY:HA3	1:G:76:ILE:HG22	2.02	0.41
1:I:35:VAL:HG12	1:I:36:GLU:O	2.22	0.40
1:C:33:PHE:CZ	1:C:44:LEU:HD13	2.56	0.40
1:F:35:VAL:O	1:F:35:VAL:HG13	2.22	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:HOH:O	2:H:151:HOH:O[1_545]	1.01	1.19
1:E:25:LYS:NZ	1:I:28:LYS:NZ[1_455]	1.99	0.21

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	106/114 (93%)	99 (93%)	5 (5%)	2 (2%)	6	1
1	B	105/114 (92%)	99 (94%)	5 (5%)	1 (1%)	12	3
1	C	97/114 (85%)	90 (93%)	6 (6%)	1 (1%)	12	3
1	D	103/114 (90%)	95 (92%)	8 (8%)	0	100	100
1	E	100/114 (88%)	96 (96%)	4 (4%)	0	100	100
1	F	104/114 (91%)	101 (97%)	3 (3%)	0	100	100
1	G	100/114 (88%)	94 (94%)	6 (6%)	0	100	100
1	H	98/114 (86%)	95 (97%)	3 (3%)	0	100	100
1	I	101/114 (89%)	95 (94%)	6 (6%)	0	100	100
1	J	100/114 (88%)	97 (97%)	2 (2%)	1 (1%)	12	3
All	All	1014/1140 (89%)	961 (95%)	48 (5%)	5 (0%)	24	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	C	35	VAL
1	J	40	ASN
1	B	39	GLU
1	A	15	SER

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	90/97 (93%)	86 (96%)	4 (4%)	25	10
1	B	89/97 (92%)	85 (96%)	4 (4%)	24	9
1	C	84/97 (87%)	79 (94%)	5 (6%)	17	5
1	D	89/97 (92%)	81 (91%)	8 (9%)	9	2
1	E	88/97 (91%)	85 (97%)	3 (3%)	32	16
1	F	90/97 (93%)	86 (96%)	4 (4%)	25	10
1	G	88/97 (91%)	87 (99%)	1 (1%)	65	54
1	H	87/97 (90%)	83 (95%)	4 (5%)	24	9
1	I	88/97 (91%)	86 (98%)	2 (2%)	44	27
1	J	87/97 (90%)	84 (97%)	3 (3%)	32	16
All	All	880/970 (91%)	842 (96%)	38 (4%)	26	10

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	38	ASP
1	A	39	GLU
1	A	106	SER
1	B	27	ASP
1	B	34	LYS
1	B	73	THR
1	B	121	LEU
1	C	28	LYS
1	C	35	VAL
1	C	43	GLN
1	C	67	ILE
1	C	103	ARG
1	D	34	LYS
1	D	36	GLU
1	D	37	ASP

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Mol	Chain	Res	Type
1	D	38	ASP
1	D	44	LEU
1	D	94	PHE
1	D	103	ARG
1	D	117	HIS
1	E	27	ASP
1	E	36	GLU
1	E	103	ARG
1	F	15	SER
1	F	73	THR
1	F	94	PHE
1	F	117	HIS
1	G	72	LYS
1	H	17	ASN
1	H	25	LYS
1	H	34	LYS
1	H	72	LYS
1	I	28	LYS
1	I	34	LYS
1	J	16	GLN
1	J	28	LYS
1	J	117	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	40	ASN
1	A	43	GLN
1	A	116	GLN
1	A	117	HIS
1	B	16	GLN
1	B	60	HIS
1	B	117	HIS
1	C	16	GLN
1	C	60	HIS
1	D	43	GLN
1	D	60	HIS
1	D	117	HIS
1	E	60	HIS
1	E	86	GLN
1	F	60	HIS

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Mol	Chain	Res	Type
1	F	116	GLN
1	F	117	HIS
1	G	16	GLN
1	G	60	HIS
1	G	117	HIS
1	H	17	ASN
1	H	43	GLN
1	H	60	HIS
1	H	117	HIS
1	I	43	GLN
1	I	116	GLN
1	I	117	HIS
1	J	40	ASN
1	J	43	GLN
1	J	60	HIS
1	J	116	GLN
1	J	117	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	108/114 (94%)	0.41	4 (3%)	45	49	16, 23, 37, 45	0
1	B	107/114 (93%)	0.49	4 (3%)	45	49	16, 23, 34, 39	0
1	C	101/114 (88%)	0.50	4 (3%)	42	46	17, 24, 35, 46	0
1	D	105/114 (92%)	0.59	7 (6%)	24	26	17, 24, 38, 48	0
1	E	104/114 (91%)	0.63	5 (4%)	35	39	18, 25, 35, 44	0
1	F	108/114 (94%)	0.40	4 (3%)	45	49	16, 23, 35, 43	0
1	G	104/114 (91%)	0.43	8 (7%)	19	21	16, 23, 37, 45	0
1	H	104/114 (91%)	0.52	5 (4%)	35	39	17, 25, 34, 44	0
1	I	105/114 (92%)	0.43	7 (6%)	24	26	17, 23, 33, 45	0
1	J	104/114 (91%)	0.58	3 (2%)	53	58	17, 25, 37, 45	0
All	All	1050/1140 (92%)	0.50	51 (4%)	35	38	16, 24, 37, 48	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	LEU	5.7
1	B	37	ASP	4.6
1	H	69	TYR	4.5
1	A	14	GLY	4.3
1	C	121	LEU	4.2
1	F	38	ASP	3.8
1	D	69	TYR	3.8
1	D	109	GLY	3.8
1	C	35	VAL	3.7
1	I	38	ASP	3.7
1	I	37	ASP	3.6
1	C	120	ALA	3.4
1	E	37	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	39	GLU	3.4
1	G	119	VAL	3.3
1	H	38	ASP	3.2
1	G	40	ASN	3.1
1	F	39	GLU	3.1
1	J	26	ALA	3.0
1	H	37	ASP	3.0
1	C	119	VAL	2.9
1	D	36	GLU	2.9
1	B	38	ASP	2.9
1	F	67	ILE	2.8
1	E	69	TYR	2.7
1	J	27	ASP	2.7
1	D	67	ILE	2.7
1	H	15	SER	2.7
1	I	15	SER	2.6
1	G	73	THR	2.6
1	A	39	GLU	2.6
1	G	38	ASP	2.6
1	G	41	GLU	2.6
1	A	37	ASP	2.5
1	E	71	GLY	2.5
1	J	41	GLU	2.5
1	A	38	ASP	2.5
1	D	37	ASP	2.5
1	H	35	VAL	2.5
1	E	36	GLU	2.5
1	I	41	GLU	2.5
1	I	35	VAL	2.5
1	I	40	ASN	2.4
1	D	119	VAL	2.4
1	I	120	ALA	2.3
1	G	118	LEU	2.3
1	B	15	SER	2.2
1	G	27	ASP	2.2
1	E	120	ALA	2.1
1	F	69	TYR	2.0
1	G	35	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.