



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:40 pm BST

PDB ID : 1XE0  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

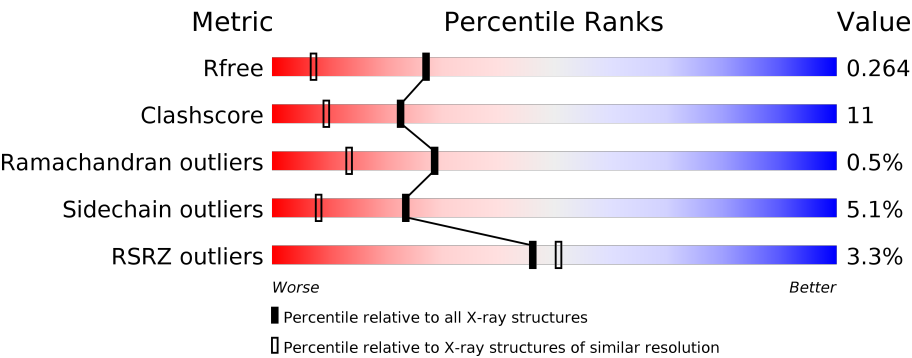
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	114	<div><div>4%</div><div><div></div><div>75%</div><div>14%</div><div>5%</div><div>5%</div></div></div>
1	B	114	<div><div>2%</div><div><div></div><div>70%</div><div>21%</div><div>6%</div></div></div>
1	C	114	<div><div>4%</div><div><div></div><div>66%</div><div>19%</div><div>11%</div></div></div>
1	D	114	<div><div>7%</div><div><div></div><div>68%</div><div>21%</div><div>8%</div></div></div>
1	E	114	<div><div>%</div><div><div></div><div>65%</div><div>25%</div><div>9%</div></div></div>
1	F	114	<div><div>%</div><div><div></div><div>77%</div><div>14%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain				
1	G	114	<div><div></div><div></div><div></div><div></div></div>	7%	68%	23%	• 9%
1	H	114	<div><div></div><div></div><div></div><div></div></div>	2%	71%	18%	•• 9%
1	I	114	<div><div></div><div></div><div></div><div></div></div>	2%	69%	18%	• • 8%
1	J	114	<div><div></div><div></div><div></div><div></div></div>	2%	72%	18%	• 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

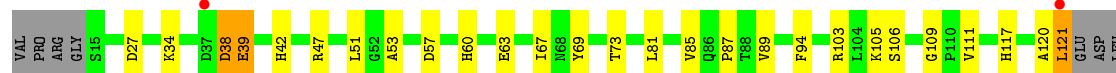
### 3 Residue-property plots [i](#)

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: Nucleophosmin



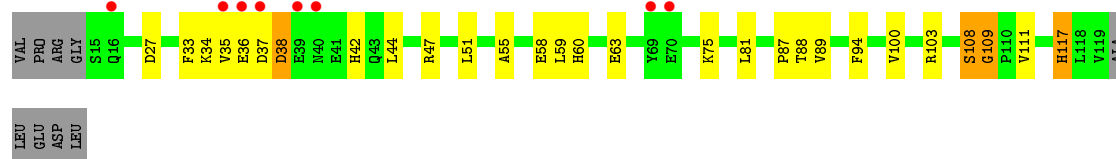
#### • Molecule 1: Nucleophosmin



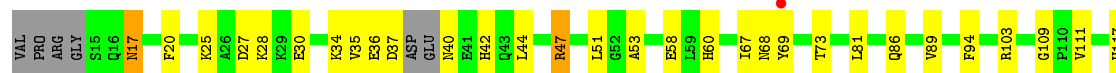
#### • Molecule 1: Nucleophosmin



#### • Molecule 1: Nucleophosmin

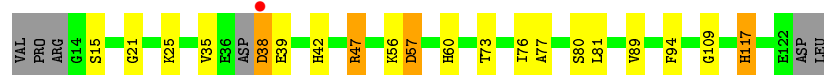
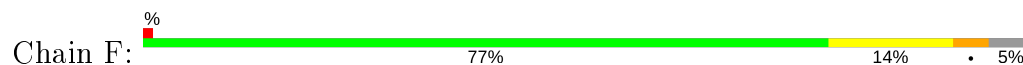


#### • Molecule 1: Nucleophosmin

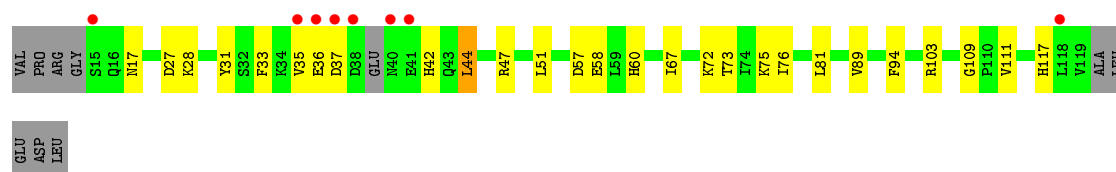




## ● Molecule 1: Nucleophosmin



## ● 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, $\alpha$ , $\beta$ , $\gamma$	59.00 Å 59.00 Å 87.20 Å 77.00° 88.30° 60.90°	Depositor
Resolution (Å)	84.52 – 1.70 84.59 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (84.52-1.70) 76.3 (84.59-1.50)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.50 Å)	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 <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 ⓘ

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	1.42	3/829 (0.4%)	1.35	7/1119 (0.6%)
1	B	1.40	4/824 (0.5%)	1.42	7/1114 (0.6%)
1	C	1.36	4/777 (0.5%)	1.22	4/1048 (0.4%)
1	D	1.34	2/815 (0.2%)	1.37	5/1101 (0.5%)
1	E	1.43	6/803 (0.7%)	1.22	3/1083 (0.3%)
1	F	1.36	3/829 (0.4%)	1.34	5/1118 (0.4%)
1	G	1.34	3/805 (0.4%)	1.24	7/1086 (0.6%)
1	H	1.35	4/800 (0.5%)	1.27	3/1078 (0.3%)
1	I	1.41	6/810 (0.7%)	1.37	8/1093 (0.7%)
1	J	1.36	1/803 (0.1%)	1.38	5/1083 (0.5%)
All	All	1.38	36/8095 (0.4%)	1.32	54/10923 (0.5%)

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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	47	ARG	CD-NE	-9.47	1.30	1.46
1	A	47	ARG	CD-NE	-9.12	1.30	1.46
1	D	109	GLY	N-CA	8.07	1.58	1.46
1	A	108	SER	CB-OG	7.64	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	GLY	CA-C	-7.52	1.39	1.51
1	F	47	ARG	CD-NE	-6.86	1.34	1.46
1	E	47	ARG	CD-NE	-6.73	1.35	1.46
1	I	108	SER	CB-OG	6.67	1.50	1.42
1	I	47	ARG	CD-NE	-6.50	1.35	1.46
1	B	47	ARG	CD-NE	-6.34	1.35	1.46
1	F	77	ALA	CA-CB	-6.32	1.39	1.52
1	H	47	ARG	CB-CG	-6.24	1.35	1.52
1	G	28	LYS	CE-NZ	6.23	1.64	1.49
1	B	67	ILE	CB-CG2	-6.18	1.33	1.52
1	C	28	LYS	CE-NZ	5.96	1.64	1.49
1	H	47	ARG	CD-NE	-5.87	1.36	1.46
1	G	31	TYR	CD1-CE1	-5.81	1.30	1.39
1	E	47	ARG	CZ-NH2	-5.79	1.25	1.33
1	E	17	ASN	CB-CG	-5.70	1.38	1.51
1	B	85	VAL	CB-CG1	-5.62	1.41	1.52
1	A	47	ARG	NE-CZ	-5.59	1.25	1.33
1	G	58	GLU	CD-OE2	5.58	1.31	1.25
1	C	27	ASP	CB-CG	-5.53	1.40	1.51
1	I	63	GLU	CG-CD	5.50	1.60	1.51
1	C	47	ARG	CD-NE	-5.46	1.37	1.46
1	E	47	ARG	NE-CZ	-5.45	1.25	1.33
1	I	17	ASN	CB-CG	-5.41	1.38	1.51
1	E	28	LYS	CB-CG	5.31	1.66	1.52
1	C	80	SER	CB-OG	-5.30	1.35	1.42
1	F	47	ARG	CG-CD	5.24	1.65	1.51
1	B	121	LEU	CG-CD1	5.22	1.71	1.51
1	I	56	LYS	CB-CG	5.19	1.66	1.52
1	H	31	TYR	CD2-CE2	5.12	1.47	1.39
1	H	25	LYS	CB-CG	-5.08	1.38	1.52
1	E	30	GLU	CD-OE1	-5.04	1.20	1.25
1	I	34	LYS	CD-CE	5.02	1.63	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH2	-21.39	109.60	120.30
1	I	47	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	F	47	ARG	NE-CZ-NH2	-18.27	111.16	120.30
1	A	47	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	J	47	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	D	47	ARG	NE-CZ-NH2	-12.31	114.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	H	47	ARG	NE-CZ-NH2	-11.07	114.77	120.30
1	G	47	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	D	109	GLY	N-CA-C	-10.41	87.08	113.10
1	J	47	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	A	38	ASP	CB-CG-OD2	8.84	126.26	118.30
1	C	103	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	47	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	F	47	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	47	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	I	27	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	57	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	47	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	G	27	ASP	CB-CG-OD2	7.13	124.72	118.30
1	J	27	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	27	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	38	ASP	CB-CG-OD2	6.75	124.38	118.30
1	F	38	ASP	CB-CG-OD2	6.63	124.27	118.30
1	G	37	ASP	CB-CG-OD2	6.56	124.20	118.30
1	C	103	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	47	ARG	NH1-CZ-NH2	6.18	126.20	119.40
1	G	103	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	I	47	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	B	121	LEU	CB-CG-CD2	6.09	121.35	111.00
1	D	109	GLY	CA-C-O	-6.04	109.73	120.60
1	A	17	ASN	N-CA-CB	5.90	121.22	110.60
1	H	47	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	J	94	PHE	CB-CG-CD2	5.79	124.86	120.80
1	G	57	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	38	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	I	37	ASP	CB-CG-OD2	5.63	123.37	118.30
1	F	39	GLU	CA-C-N	-5.62	104.85	117.20
1	B	121	LEU	CA-CB-CG	5.51	127.96	115.30
1	D	27	ASP	CB-CG-OD2	5.48	123.23	118.30
1	G	28	LYS	CD-CE-NZ	5.45	124.24	111.70
1	I	17	ASN	N-CA-CB	-5.40	100.89	110.60
1	E	47	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	27	ASP	N-CA-CB	-5.37	100.94	110.60
1	H	57	ASP	CB-CG-OD2	5.35	123.11	118.30
1	E	34	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	F	57	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	37	ASP	CB-CG-OD2	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	47	ARG	CD-NE-CZ	5.16	130.83	123.60
1	I	38	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	121	LEU	N-CA-C	-5.15	97.11	111.00
1	I	47	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	I	34	LYS	CD-CE-NZ	5.14	123.52	111.70
1	G	44	LEU	CA-CB-CG	5.11	127.06	115.30

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

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	16	0
1	D	801	0	806	23	0
1	E	790	0	803	28	1
1	F	816	0	825	15	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
2	E	31	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	184	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 11.

All (184) 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: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:O	1:A:40:ASN:CG	2.09	0.91
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
1:E:60:HIS:CE1	1:E:109:GLY:H	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ3	1:G:75:LYS:HB2	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
1:C:16:GLN:N	1:C:119:VAL:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CE1	1:A:109:GLY:H	2.18	0.61
1:A:47:ARG:CD	2:B:136:HOH:O	2.48	0.61
1:A:81:LEU:CD2	1:A:89:VAL:HG23	2.31	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:E:37:ASP:CG	1:E:42:HIS:HE2	2.09	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:37:ASP:O	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: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:C:34:LYS:C	1:C:35:VAL:HG23	2.36	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:E:67:ILE:HG22	1:E:68:ASN:O	2.17	0.45
1:D:87:PRO:CD	1:E:86:GLN:HE21	2.19	0.45
1:H:35:VAL:HG21	1:H:42:HIS:CG	2.52	0.45
1:A:39:GLU:C	1:A:40:ASN:CG	2.75	0.45
1:E:51:LEU:HD23	1:E:111:VAL:HG22	1.99	0.45
1:H:17:ASN:N	1:H:17:ASN:HD22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:PHE:CD2	1:I:20:PHE:C	2.91	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: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:I:38:ASP:CG	1:I:40:ASN:HA	2.40	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:117:HIS:CD2	1:E:69:TYR:CD2	3.08	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:HG13	1:F:35:VAL:O	2.22	0.40
1:J:20:PHE:C	1:J:20:PHE:CD2	2.95	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

### 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	106/114 (93%)	99 (93%)	5 (5%)	2 (2%)	8	1
1	B	105/114 (92%)	99 (94%)	5 (5%)	1 (1%)	15	4
1	C	97/114 (85%)	90 (93%)	6 (6%)	1 (1%)	15	4
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%)	15	4
All	All	1014/1140 (89%)	961 (95%)	48 (5%)	5 (0%)	29	13

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%)	85 (94%)	5 (6%)	21	7
1	B	89/97 (92%)	83 (93%)	6 (7%)	16	4
1	C	84/97 (87%)	78 (93%)	6 (7%)	14	3
1	D	89/97 (92%)	81 (91%)	8 (9%)	9	2
1	E	88/97 (91%)	84 (96%)	4 (4%)	27	10
1	F	90/97 (93%)	86 (96%)	4 (4%)	28	11
1	G	88/97 (91%)	86 (98%)	2 (2%)	50	33
1	H	87/97 (90%)	83 (95%)	4 (5%)	27	10
1	I	88/97 (91%)	84 (96%)	4 (4%)	27	10
1	J	87/97 (90%)	85 (98%)	2 (2%)	50	33
All	All	880/970 (91%)	835 (95%)	45 (5%)	24	8

All (45) 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	94	PHE
1	A	106	SER
1	B	27	ASP
1	B	34	LYS
1	B	38	ASP
1	B	73	THR
1	B	94	PHE
1	B	121	LEU
1	C	27	ASP
1	C	28	LYS
1	C	43	GLN
1	C	67	ILE
1	C	94	PHE
1	C	103	ARG
1	D	34	LYS
1	D	36	GLU
1	D	37	ASP
1	D	38	ASP
1	D	44	LEU
1	D	94	PHE
1	D	103	ARG

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Mol	Chain	Res	Type
1	D	117	HIS
1	E	27	ASP
1	E	36	GLU
1	E	94	PHE
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	G	94	PHE
1	H	17	ASN
1	H	25	LYS
1	H	72	LYS
1	H	94	PHE
1	I	28	LYS
1	I	34	LYS
1	I	38	ASP
1	I	94	PHE
1	J	94	PHE
1	J	117	HIS

Some 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	60	HIS
1	D	60	HIS
1	D	117	HIS
1	E	60	HIS
1	E	86	GLN
1	E	116	GLN
1	F	16	GLN
1	F	60	HIS
1	F	116	GLN

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Mol	Chain	Res	Type
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 ⓘ

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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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	108/114 (94%)	-0.00	4 (3%) 41 46	16, 23, 37, 45	0
1	B	107/114 (93%)	-0.04	2 (1%) 66 70	16, 23, 34, 39	0
1	C	101/114 (88%)	0.13	5 (4%) 28 32	17, 24, 35, 46	0
1	D	105/114 (92%)	0.23	8 (7%) 13 16	17, 24, 38, 48	0
1	E	104/114 (91%)	-0.02	1 (0%) 82 85	18, 25, 35, 44	0
1	F	108/114 (94%)	-0.04	1 (0%) 84 87	16, 23, 35, 43	0
1	G	104/114 (91%)	0.13	8 (7%) 13 15	16, 23, 37, 45	0
1	H	104/114 (91%)	-0.04	2 (1%) 66 70	17, 25, 34, 44	0
1	I	105/114 (92%)	-0.10	2 (1%) 66 70	17, 23, 33, 45	0
1	J	104/114 (91%)	0.03	2 (1%) 66 70	17, 25, 37, 45	0
All	All	1050/1140 (92%)	0.03	35 (3%) 46 51	16, 24, 37, 48	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	VAL	6.4
1	D	39	GLU	6.3
1	C	121	LEU	6.2
1	C	120	ALA	5.1
1	H	69	TYR	4.7
1	A	39	GLU	4.3
1	B	37	ASP	4.1
1	D	36	GLU	4.0
1	D	37	ASP	3.7
1	A	14	GLY	3.7
1	G	38	ASP	3.6
1	F	38	ASP	3.4
1	G	36	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	3.3
1	G	37	ASP	3.3
1	I	38	ASP	3.3
1	D	69	TYR	3.3
1	J	39	GLU	3.2
1	G	40	ASN	3.2
1	G	41	GLU	3.1
1	C	36	GLU	3.1
1	D	35	VAL	3.0
1	I	37	ASP	2.8
1	G	35	VAL	2.8
1	J	40	ASN	2.6
1	H	37	ASP	2.6
1	D	16	GLN	2.5
1	G	15	SER	2.5
1	B	121	LEU	2.5
1	C	119	VAL	2.3
1	D	40	ASN	2.2
1	D	70	GLU	2.2
1	A	38	ASP	2.2
1	G	118	LEU	2.1
1	E	69	TYR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.