



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XB9
Title : The structure and function of Xenopus NO38-core, a histone chaperone in the nucleolus
Authors : Namboodiri, V.M.; Akey, I.V.; Schmidt-Zachmann, M.S.; Head, J.F.; Akey, C.W.
Deposited on : 2004-08-30
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

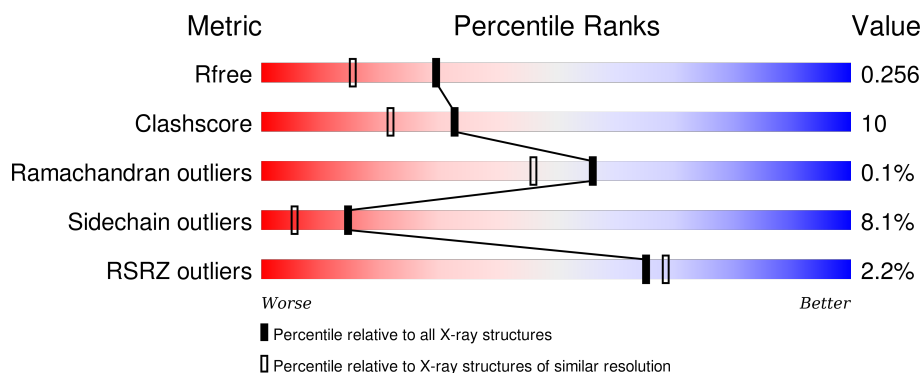
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 ≥ 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	114	<div> <div>2%</div> <div>68% 23% 5%</div> </div>
1	B	114	<div> <div>2%</div> <div>76% 15% 6%</div> </div>
1	C	114	<div> <div>2%</div> <div>67% 18% 5% 9%</div> </div>
1	D	114	<div> <div>5%</div> <div>54% 30% 5% 9%</div> </div>
1	E	114	<div> <div>%</div> <div>63% 27% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	114	<div> <div> <div></div> <div>68%</div> <div>21%</div> <div>8%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	G	114	<div> <div> <div></div> <div>69%</div> <div>18%</div> <div>8%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	H	114	<div> <div> <div></div> <div>75%</div> <div>17%</div> <div>6%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	I	114	<div> <div> <div></div> <div>67%</div> <div>24%</div> <div>6%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	J	114	<div> <div> <div></div> <div>71%</div> <div>16%</div> <div>6%</div> <div>7%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8337 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
			824	524	136	163	1			
1	B	107	Total	C	N	O	S	0	0	0
			811	517	135	158	1			
1	C	104	Total	C	N	O	S	0	0	0
			789	504	131	153	1			
1	D	104	Total	C	N	O	S	0	0	0
			793	504	131	157	1			
1	E	106	Total	C	N	O	S	0	0	0
			807	513	134	159	1			
1	F	105	Total	C	N	O	S	0	0	0
			795	507	132	155	1			
1	G	105	Total	C	N	O	S	0	0	0
			794	508	133	152	1			
1	H	107	Total	C	N	O	S	0	0	0
			805	515	134	155	1			
1	I	107	Total	C	N	O	S	0	0	0
			812	516	135	160	1			
1	J	106	Total	C	N	O	S	0	0	0
			802	512	134	155	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

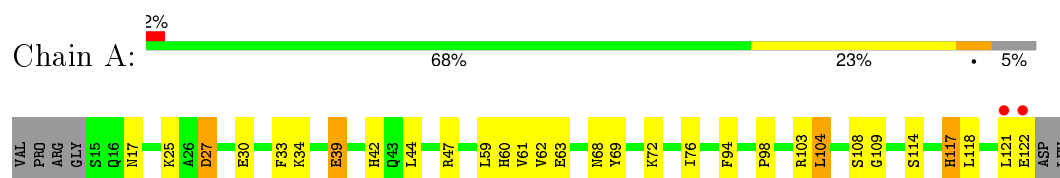
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total 41	O 41	0	0
2	B	37	Total 37	O 37	0	0
2	C	21	Total 21	O 21	0	0
2	D	21	Total 21	O 21	0	0
2	E	28	Total 28	O 28	0	0
2	F	31	Total 31	O 31	0	0
2	G	29	Total 29	O 29	0	0
2	H	27	Total 27	O 27	0	0
2	I	36	Total 36	O 36	0	0
2	J	34	Total 34	O 34	0	0

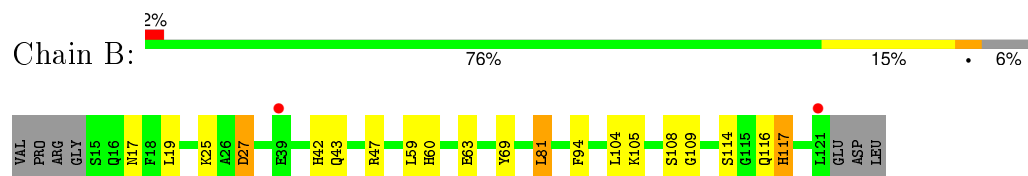
3 Residue-property plots [i](#)

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

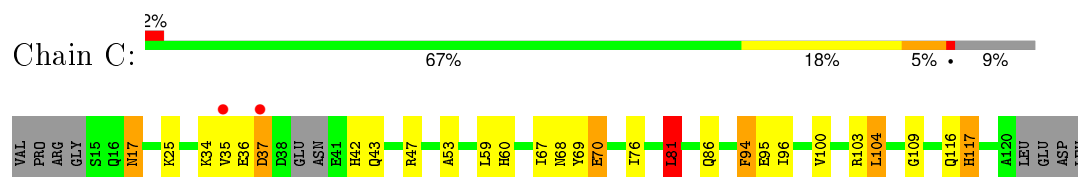
• Molecule 1: Nucleophosmin



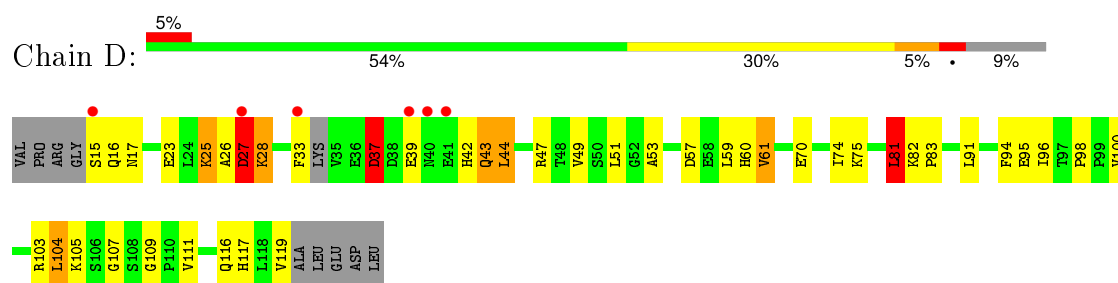
• Molecule 1: Nucleophosmin



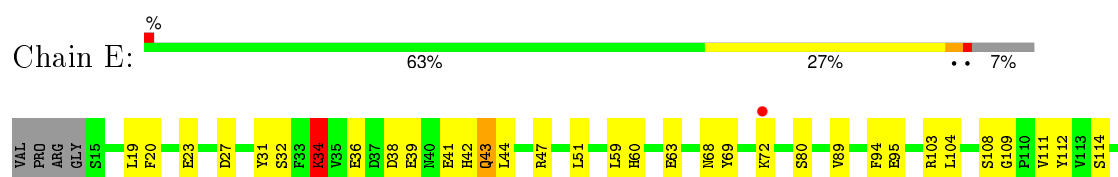
• Molecule 1: Nucleophosmin

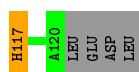


• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin

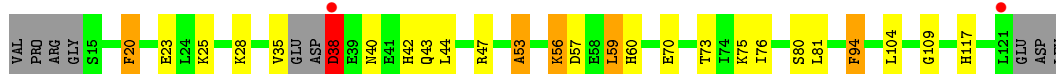




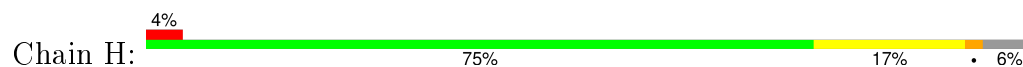
- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.91Å 64.55Å 97.46Å 90.00° 113.72° 90.00°	Depositor
Resolution (Å)	91.29 – 1.90 60.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.1 (91.29-1.90) 91.0 (60.84-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.255 0.209 , 0.256	Depositor DCC
R_{free} test set	6598 reflections (8.82%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 84025 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8337	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.55 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.5058e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.56	7/838 (0.8%)	1.28	4/1132 (0.4%)
1	B	1.65	7/825 (0.8%)	1.37	3/1115 (0.3%)
1	C	1.60	5/802 (0.6%)	1.41	9/1082 (0.8%)
1	D	1.59	5/806 (0.6%)	1.47	13/1088 (1.2%)
1	E	1.68	15/821 (1.8%)	1.43	5/1109 (0.5%)
1	F	1.54	7/808 (0.9%)	1.28	3/1090 (0.3%)
1	G	1.50	8/807 (1.0%)	1.36	6/1089 (0.6%)
1	H	1.53	4/818 (0.5%)	1.26	1/1104 (0.1%)
1	I	1.62	7/826 (0.8%)	1.34	7/1116 (0.6%)
1	J	1.61	6/815 (0.7%)	1.33	5/1100 (0.5%)
All	All	1.59	71/8166 (0.9%)	1.35	56/11025 (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	D	1	1
1	F	0	1
All	All	1	2

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	108	SER	CB-OG	11.07	1.56	1.42
1	J	100	VAL	CB-CG2	-10.55	1.30	1.52
1	B	47	ARG	CD-NE	-9.12	1.30	1.46
1	C	17	ASN	CB-CG	-8.31	1.31	1.51
1	F	50	SER	CB-OG	-8.28	1.31	1.42

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH2	-19.22	110.69	120.30
1	E	47	ARG	NE-CZ-NH2	-16.50	112.05	120.30
1	G	47	ARG	NE-CZ-NH2	-12.85	113.87	120.30
1	H	47	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	I	38	ASP	CB-CG-OD2	10.24	127.51	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	37	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	37	ASP	Peptide
1	F	39	GLU	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	824	0	831	19	0
1	B	811	0	821	12	0
1	C	789	0	798	17	0
1	D	793	0	795	31	0
1	E	807	0	814	20	0
1	F	795	0	803	14	0
1	G	794	0	810	18	0
1	H	805	0	814	20	1
1	I	812	0	816	20	0
1	J	802	0	814	20	0
2	A	41	0	0	1	0
2	B	37	0	0	1	0
2	C	21	0	0	3	1
2	D	21	0	0	1	0
2	E	28	0	0	0	1
2	F	31	0	0	0	1
2	G	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	27	0	0	0	0
2	I	36	0	0	1	0
2	J	34	0	0	0	0
All	All	8337	0	8116	168	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 10.

The worst 5 of 168 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:D:96:ILE:CG2	1:D:100:VAL:HG21	1.92	1.00
1:B:60:HIS:HE1	1:B:109:GLY:H	1.11	0.97
1:I:40:ASN:HD22	1:I:121:LEU:HA	1.29	0.96
1:D:96:ILE:HG21	1:D:100:VAL:HG21	1.53	0.89
1:B:60:HIS:CE1	1:B:109:GLY:H	1.91	0.89

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:E:131:HOH:O	2:F:153:HOH:O[4_547]	0.74	1.46
1:H:38:ASP:O	2:C:142:HOH:O[3_445]	1.28	0.92

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%)	104 (98%)	2 (2%)	0	100	100
1	B	105/114 (92%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	100/114 (88%)	97 (97%)	3 (3%)	0	100	100
1	D	100/114 (88%)	93 (93%)	6 (6%)	1 (1%)	19	7
1	E	104/114 (91%)	99 (95%)	5 (5%)	0	100	100
1	F	101/114 (89%)	96 (95%)	5 (5%)	0	100	100
1	G	101/114 (89%)	96 (95%)	5 (5%)	0	100	100
1	H	103/114 (90%)	101 (98%)	2 (2%)	0	100	100
1	I	105/114 (92%)	101 (96%)	4 (4%)	0	100	100
1	J	102/114 (90%)	101 (99%)	1 (1%)	0	100	100
All	All	1027/1140 (90%)	988 (96%)	38 (4%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	27	ASP

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	92/97 (95%)	83 (90%)	9 (10%)	10	3
1	B	90/97 (93%)	83 (92%)	7 (8%)	16	6
1	C	87/97 (90%)	78 (90%)	9 (10%)	9	3
1	D	89/97 (92%)	78 (88%)	11 (12%)	6	2
1	E	90/97 (93%)	84 (93%)	6 (7%)	20	9
1	F	88/97 (91%)	82 (93%)	6 (7%)	20	9
1	G	88/97 (91%)	82 (93%)	6 (7%)	20	9
1	H	88/97 (91%)	84 (96%)	4 (4%)	34	21
1	I	90/97 (93%)	83 (92%)	7 (8%)	16	6
1	J	89/97 (92%)	82 (92%)	7 (8%)	15	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	891/970 (92%)	819 (92%)	72 (8%)	15 5

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	ILE
1	E	104	LEU
1	J	28	LYS
1	D	81	LEU
1	E	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	116	GLN
1	F	117	HIS
1	J	60	HIS
1	E	117	HIS
1	F	60	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 [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, 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%)	-0.12	2 (1%) 70 73	18, 24, 39, 48	0
1	B	107/114 (93%)	-0.20	2 (1%) 70 73	18, 24, 35, 43	0
1	C	104/114 (91%)	-0.20	2 (1%) 70 73	20, 28, 38, 48	0
1	D	104/114 (91%)	0.05	6 (5%) 26 29	22, 29, 43, 47	0
1	E	106/114 (92%)	-0.22	1 (0%) 85 87	19, 25, 35, 43	0
1	F	105/114 (92%)	-0.15	1 (0%) 84 86	18, 25, 39, 49	0
1	G	105/114 (92%)	-0.16	2 (1%) 70 73	20, 27, 41, 51	0
1	H	107/114 (93%)	0.02	4 (3%) 45 49	19, 30, 42, 50	0
1	I	107/114 (93%)	-0.19	2 (1%) 70 73	19, 25, 37, 45	0
1	J	106/114 (92%)	-0.10	1 (0%) 85 87	19, 26, 39, 44	0
All	All	1059/1140 (92%)	-0.13	23 (2%) 65 68	18, 26, 40, 51	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	GLU	4.7
1	G	121	LEU	4.3
1	D	15	SER	4.2
1	D	33	PHE	4.2
1	A	121	LEU	3.4

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 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.