



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:22 AM EDT

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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

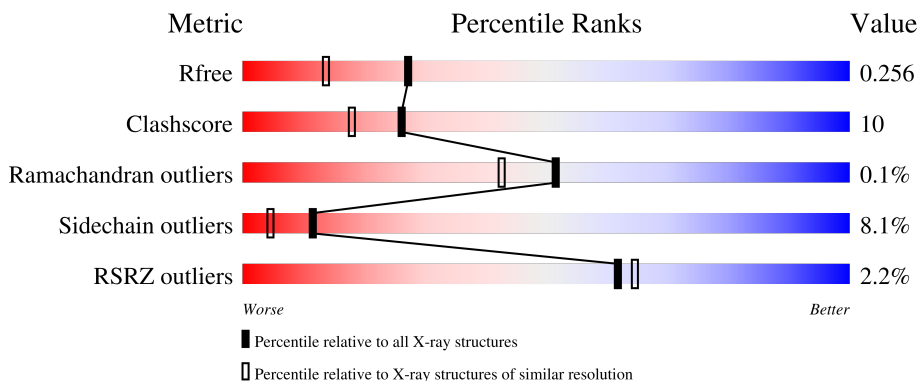
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 68% 23% • 5%</p>
1	B	114	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 76% 15% • 6%</p>
1	C	114	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 67% 18% 5% • 9%</p>
1	D	114	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">5% 54% 30% 5% • 9%</p>
1	E	114	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 63% 27% • • 7%</p>

Continued on next page...

Continued from previous page...

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

2 Entry composition

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
			Total	C	N	O	S			
1	A	108	Total 824	C 524	N 136	O 163	S 1	0	0	0
1	B	107	Total 811	C 517	N 135	O 158	S 1	0	0	0
1	C	104	Total 789	C 504	N 131	O 153	S 1	0	0	0
1	D	104	Total 793	C 504	N 131	O 157	S 1	0	0	0
1	E	106	Total 807	C 513	N 134	O 159	S 1	0	0	0
1	F	105	Total 795	C 507	N 132	O 155	S 1	0	0	0
1	G	105	Total 794	C 508	N 133	O 152	S 1	0	0	0
1	H	107	Total 805	C 515	N 134	O 155	S 1	0	0	0
1	I	107	Total 812	C 516	N 135	O 160	S 1	0	0	0
1	J	106	Total 802	C 512	N 134	O 155	S 1	0	0	0

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

Continued on next page...

Continued from previous page...

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, 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.

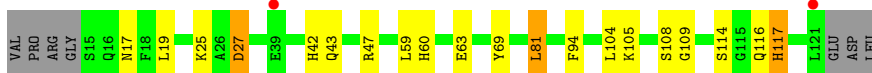
- Molecule 1: Nucleophosmin

Chain A: 



- Molecule 1: Nucleophosmin

Chain B: 



- Molecule 1: Nucleophosmin

Chain C: 



- Molecule 1: Nucleophosmin

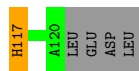
Chain D: 



- Molecule 1: Nucleophosmin

Chain E: 

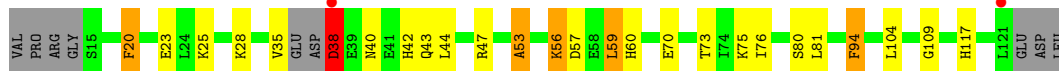




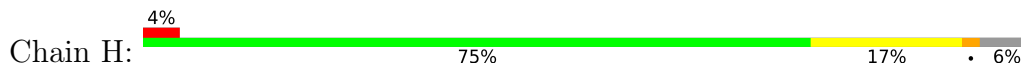
- Molecule 1: Nucleophosmin



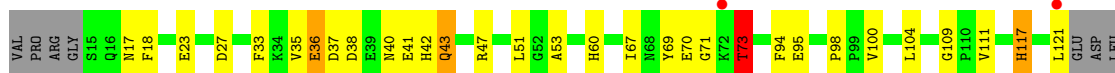
- Molecule 1: Nucleophosmin



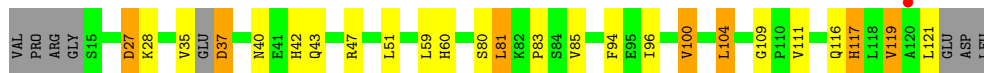
- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



- Molecule 1: Nucleophosmin



4 Data and refinement statistics i

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)	Xtrriage
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 (7.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

All (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
1	B	17	ASN	CB-CG	-8.06	1.32	1.51
1	B	108	SER	CB-OG	7.69	1.52	1.42
1	I	36	GLU	CD-OE1	7.49	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	43	GLN	CG-CD	7.21	1.67	1.51
1	E	47	ARG	CD-NE	-7.20	1.34	1.46
1	I	23	GLU	CD-OE2	-7.13	1.17	1.25
1	G	47	ARG	CB-CG	-6.87	1.34	1.52
1	H	103	ARG	CG-CD	6.83	1.69	1.51
1	C	70	GLU	CD-OE2	6.72	1.33	1.25
1	A	47	ARG	CD-NE	-6.62	1.35	1.46
1	I	36	GLU	CD-OE2	6.61	1.32	1.25
1	G	47	ARG	CD-NE	-6.59	1.35	1.46
1	D	23	GLU	CD-OE2	-6.58	1.18	1.25
1	E	69	TYR	CG-CD1	6.52	1.47	1.39
1	E	89	VAL	CB-CG1	-6.43	1.39	1.52
1	E	69	TYR	CD1-CE1	6.32	1.48	1.39
1	E	36	GLU	CD-OE1	6.31	1.32	1.25
1	C	86	GLN	CG-CD	6.25	1.65	1.51
1	H	108	SER	CA-CB	6.20	1.62	1.52
1	J	85	VAL	CB-CG1	6.12	1.65	1.52
1	A	108	SER	CB-OG	6.10	1.50	1.42
1	C	36	GLU	CD-OE2	6.10	1.32	1.25
1	E	43	GLN	CG-CD	6.09	1.65	1.51
1	J	37	ASP	CB-CG	6.09	1.64	1.51
1	F	103	ARG	CG-CD	6.08	1.67	1.51
1	E	112	TYR	CD2-CE2	6.03	1.48	1.39
1	G	70	GLU	CD-OE1	6.00	1.32	1.25
1	B	69	TYR	CD2-CE2	5.98	1.48	1.39
1	E	41	GLU	CD-OE2	5.86	1.32	1.25
1	I	18	PHE	CE1-CZ	5.80	1.48	1.37
1	F	26	ALA	CA-CB	5.72	1.64	1.52
1	E	31	TYR	CE1-CZ	5.71	1.46	1.38
1	E	23	GLU	CD-OE2	-5.68	1.19	1.25
1	C	69	TYR	CD1-CE1	-5.68	1.30	1.39
1	E	34	LYS	CD-CE	5.66	1.65	1.51
1	B	69	TYR	CG-CD2	5.63	1.46	1.39
1	A	30	GLU	CD-OE2	5.59	1.31	1.25
1	H	47	ARG	CD-NE	-5.56	1.36	1.46
1	D	75	LYS	CE-NZ	5.54	1.62	1.49
1	J	119	VAL	CA-CB	-5.54	1.43	1.54
1	G	53	ALA	CA-CB	5.53	1.64	1.52
1	B	105	LYS	CD-CE	5.52	1.65	1.51
1	A	61	VAL	CB-CG2	-5.45	1.41	1.52
1	D	116	GLN	CB-CG	5.44	1.67	1.52
1	G	20	PHE	CB-CG	-5.41	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	23	GLU	CD-OE1	-5.39	1.19	1.25
1	D	61	VAL	CB-CG2	5.33	1.64	1.52
1	I	100	VAL	CB-CG2	-5.33	1.41	1.52
1	F	114	SER	CB-OG	5.30	1.49	1.42
1	J	100	VAL	CA-CB	5.30	1.65	1.54
1	G	56	LYS	CD-CE	5.29	1.64	1.51
1	E	108	SER	CB-OG	5.26	1.49	1.42
1	F	111	VAL	CB-CG2	-5.24	1.41	1.52
1	G	75	LYS	CE-NZ	5.22	1.62	1.49
1	D	82	LYS	CD-CE	5.20	1.64	1.51
1	E	114	SER	CB-OG	5.20	1.49	1.42
1	A	104	LEU	CG-CD2	-5.19	1.32	1.51
1	A	114	SER	CB-OG	5.19	1.49	1.42
1	B	63	GLU	CD-OE2	-5.18	1.20	1.25
1	F	63	GLU	CG-CD	5.15	1.59	1.51
1	I	18	PHE	CD2-CE2	5.09	1.49	1.39
1	E	39	GLU	CD-OE1	5.08	1.31	1.25
1	J	27	ASP	CB-CG	5.08	1.62	1.51
1	A	62	VAL	CB-CG2	-5.04	1.42	1.52
1	F	65	GLU	CD-OE1	-5.03	1.20	1.25
1	G	23	GLU	CD-OE1	-5.02	1.20	1.25

All (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
1	J	27	ASP	CB-CG-OD2	9.75	127.08	118.30
1	C	47	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	I	47	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	G	47	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	F	38	ASP	CB-CG-OD2	8.80	126.22	118.30
1	J	47	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	A	47	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	G	38	ASP	CB-CG-OD2	8.56	126.00	118.30
1	J	37	ASP	CB-CG-OD2	8.32	125.79	118.30
1	F	57	ASP	CB-CG-OD2	8.16	125.65	118.30
1	E	27	ASP	CB-CG-OD2	8.00	125.50	118.30
1	D	37	ASP	CB-CA-C	7.92	126.24	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	ASP	CB-CG-OD2	7.87	125.38	118.30
1	D	103	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	103	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	37	ASP	CB-CG-OD2	6.92	124.53	118.30
1	D	103	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	37	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	E	103	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	27	ASP	CB-CG-OD2	6.58	124.22	118.30
1	E	47	ARG	NH1-CZ-NH2	6.51	126.56	119.40
1	G	57	ASP	CB-CG-OD2	6.38	124.05	118.30
1	D	37	ASP	CB-CG-OD1	6.37	124.04	118.30
1	I	27	ASP	CB-CG-OD2	6.37	124.04	118.30
1	A	104	LEU	CA-CB-CG	6.24	129.65	115.30
1	J	100	VAL	CB-CA-C	-6.22	99.58	111.40
1	G	25	LYS	CD-CE-NZ	6.21	125.99	111.70
1	I	37	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	103	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	59	LEU	CB-CG-CD2	5.99	121.18	111.00
1	I	38	ASP	OD1-CG-OD2	-5.93	112.02	123.30
1	G	73	THR	OG1-CB-CG2	-5.75	96.76	110.00
1	C	47	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	104	LEU	CB-CG-CD2	5.69	120.67	111.00
1	I	73	THR	OG1-CB-CG2	-5.64	97.03	110.00
1	C	94	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	E	38	ASP	CB-CG-OD1	5.53	123.28	118.30
1	I	43	GLN	CA-CB-CG	5.49	125.47	113.40
1	D	27	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	81	LEU	CA-CB-CG	5.36	127.64	115.30
1	J	104	LEU	CA-CB-CG	5.35	127.61	115.30
1	D	28	LYS	N-CA-CB	-5.31	101.05	110.60
1	D	43	GLN	CA-CB-CG	5.26	124.98	113.40
1	A	27	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	47	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	17	ASN	N-CA-CB	-5.24	101.17	110.60
1	C	94	PHE	CB-CG-CD2	5.22	124.46	120.80
1	B	47	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	C	81	LEU	CA-CB-CG	5.18	127.21	115.30
1	D	91	LEU	CB-CG-CD1	5.03	119.55	111.00
1	D	82	LYS	CD-CE-NZ	-5.02	100.14	111.70

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 [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	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
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.

All (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
1:F:17:ASN:HD22	1:G:43:GLN:HE22	1.24	0.85
1:A:17:ASN:HD22	1:B:43:GLN:HE22	1.25	0.85
1:H:34:LYS:HG3	1:H:35:VAL:H	1.44	0.82
1:A:33:PHE:CZ	1:A:44:LEU:HD13	2.13	0.81
1:D:17:ASN:HD22	1:E:43:GLN:NE2	1.82	0.77
1:C:60:HIS:HE1	1:C:109:GLY:H	1.32	0.75
1:I:60:HIS:CE1	1:I:109:GLY:H	2.03	0.75
1:I:60:HIS:HE1	1:I:109:GLY:H	1.35	0.73
1:I:42:HIS:ND1	1:I:117:HIS:HE1	1.85	0.73
1:E:60:HIS:CE1	1:E:109:GLY:H	2.06	0.73
1:A:60:HIS:CE1	1:A:109:GLY:H	2.07	0.73
1:I:53:ALA:HA	1:J:59:LEU:CD2	2.19	0.72
1:C:96:ILE:HG21	1:C:100:VAL:HG11	1.70	0.72
1:J:42:HIS:ND1	1:J:117:HIS:HE1	1.88	0.72
1:I:40:ASN:ND2	1:I:121:LEU:HA	2.03	0.72
1:H:34:LYS:HD3	1:H:99:PRO:HG3	1.73	0.71
1:D:25:LYS:HE3	1:D:28:LYS:HB3	1.73	0.70
1:E:42:HIS:ND1	1:E:117:HIS:HE1	1.88	0.70
1:C:42:HIS:ND1	1:C:117:HIS:HE1	1.90	0.70
1:H:42:HIS:HD2	1:H:117:HIS:CE1	2.10	0.69
1:C:60:HIS:CE1	1:C:109:GLY:H	2.10	0.69
1:J:35:VAL:HG11	1:J:42:HIS:CD2	2.28	0.69
1:H:42:HIS:CD2	1:H:117:HIS:HE1	2.11	0.69
1:C:96:ILE:CG2	1:C:100:VAL:HG11	2.22	0.68
1:D:25:LYS:N	1:D:25:LYS:HD3	2.09	0.68
1:D:17:ASN:HD22	1:E:43:GLN:HE22	1.40	0.68
1:D:26:ALA:O	1:D:27:ASP:O	2.11	0.67
1:E:60:HIS:HE1	1:E:109:GLY:H	1.41	0.67
1:F:19:LEU:HD22	1:G:76:ILE:CD1	2.25	0.67
1:G:60:HIS:CE1	1:G:109:GLY:H	2.13	0.67
1:D:26:ALA:C	1:D:27:ASP:O	2.33	0.66
1:H:34:LYS:HG3	1:H:35:VAL:N	2.06	0.66
1:B:60:HIS:HE1	1:B:109:GLY:N	1.90	0.66
1:C:53:ALA:N	2:C:142:HOH:O	2.30	0.64
1:J:40:ASN:ND2	1:J:121:LEU:HA	2.12	0.64
1:H:42:HIS:HD2	1:H:117:HIS:HE1	1.45	0.64
1:D:61:VAL:HG11	1:D:105:LYS:HE2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:HE1	1:A:109:GLY:H	1.47	0.62
1:J:60:HIS:CE1	1:J:109:GLY:H	2.16	0.62
1:B:116:GLN:NE2	2:B:153:HOH:O	2.32	0.61
1:F:60:HIS:CE1	1:F:109:GLY:H	2.18	0.61
1:F:42:HIS:ND1	1:F:117:HIS:HE1	1.99	0.60
1:C:35:VAL:HG11	1:C:42:HIS:CE1	2.37	0.60
1:B:42:HIS:ND1	1:B:117:HIS:HE1	1.99	0.60
1:I:43:GLN:HG2	2:I:153:HOH:O	1.99	0.60
1:D:42:HIS:ND1	1:D:117:HIS:HE1	1.99	0.60
1:G:59:LEU:HD11	1:G:80:SER:HB3	1.82	0.59
1:I:17:ASN:HD22	1:J:43:GLN:HE22	1.48	0.59
1:J:59:LEU:HD11	1:J:80:SER:HB3	1.83	0.59
1:F:20:PHE:CD1	1:F:44:LEU:HD11	2.38	0.59
1:F:19:LEU:HD22	1:G:76:ILE:HD13	1.83	0.59
1:H:34:LYS:CG	1:H:35:VAL:N	2.66	0.59
1:E:59:LEU:HD11	1:E:80:SER:HB3	1.85	0.58
1:E:43:GLN:HG2	1:E:95:GLU:OE1	2.03	0.58
1:A:33:PHE:CE1	1:A:44:LEU:HD13	2.38	0.58
1:G:60:HIS:HE1	1:G:109:GLY:H	1.51	0.57
1:I:42:HIS:ND1	1:I:117:HIS:CE1	2.70	0.57
1:H:119:VAL:HG13	1:H:119:VAL:O	2.05	0.57
1:J:81:LEU:HD12	1:J:81:LEU:N	2.21	0.56
1:D:51:LEU:HD13	1:D:83:PRO:HD3	1.88	0.56
1:A:33:PHE:CE2	1:A:98:PRO:HB3	2.41	0.56
1:I:67:ILE:HD13	1:I:73:THR:OG1	2.06	0.55
1:J:96:ILE:HG21	1:J:100:VAL:HG21	1.88	0.55
1:D:25:LYS:HE3	1:D:28:LYS:CB	2.37	0.55
1:D:15:SER:HB2	1:D:119:VAL:O	2.06	0.54
1:J:35:VAL:HG11	1:J:42:HIS:NE2	2.22	0.54
1:A:42:HIS:ND1	1:A:117:HIS:HE1	2.05	0.54
1:G:59:LEU:HD13	1:G:60:HIS:N	2.22	0.54
1:D:33:PHE:CE2	1:D:44:LEU:HD13	2.43	0.54
1:D:33:PHE:CZ	1:D:98:PRO:HB3	2.44	0.53
1:D:33:PHE:CD1	1:D:44:LEU:HD22	2.43	0.53
1:H:34:LYS:HD3	1:H:99:PRO:CG	2.36	0.53
1:A:17:ASN:HD22	1:B:43:GLN:NE2	2.01	0.53
1:I:43:GLN:OE1	1:I:95:GLU:OE1	2.27	0.53
1:A:68:ASN:OD1	1:A:68:ASN:C	2.46	0.53
1:D:17:ASN:ND2	1:E:43:GLN:NE2	2.56	0.53
1:G:38:ASP:OD1	1:G:40:ASN:HB2	2.08	0.53
1:B:81:LEU:HD12	1:B:81:LEU:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:HOH:O	1:E:68:ASN:HB2	2.08	0.52
1:G:59:LEU:HD13	1:G:59:LEU:C	2.30	0.52
1:E:42:HIS:ND1	1:E:117:HIS:CE1	2.75	0.52
1:E:32:SER:OG	1:E:34:LYS:HE3	2.08	0.52
1:E:20:PHE:CD2	1:E:44:LEU:HD11	2.44	0.52
1:D:33:PHE:CG	1:D:44:LEU:HD22	2.46	0.51
1:A:33:PHE:CE1	1:A:44:LEU:CD1	2.93	0.51
1:E:60:HIS:HE1	1:E:109:GLY:N	2.07	0.51
1:J:119:VAL:HG12	1:J:119:VAL:O	2.08	0.51
1:C:67:ILE:HG12	2:C:135:HOH:O	2.11	0.51
1:F:19:LEU:HD22	1:G:76:ILE:HD11	1.93	0.50
1:C:68:ASN:OD1	1:C:70:GLU:HG2	2.10	0.50
1:J:51:LEU:HD23	1:J:111:VAL:HG22	1.93	0.50
1:A:25:LYS:NZ	2:A:149:HOH:O	2.42	0.50
1:J:60:HIS:HE1	1:J:109:GLY:H	1.55	0.50
1:A:33:PHE:CD2	1:A:98:PRO:HB3	2.47	0.50
1:D:33:PHE:CE1	1:D:98:PRO:HB3	2.47	0.49
1:F:20:PHE:CG	1:F:44:LEU:HD11	2.47	0.49
1:F:42:HIS:ND1	1:F:117:HIS:CE1	2.78	0.49
1:E:51:LEU:CD2	1:E:111:VAL:HG22	2.43	0.49
1:B:114:SER:HB2	1:C:76:ILE:HD12	1.95	0.48
1:D:51:LEU:HD23	1:D:111:VAL:HG22	1.95	0.48
1:D:60:HIS:CE1	1:D:109:GLY:H	2.32	0.48
1:D:96:ILE:HG22	1:D:100:VAL:HG21	1.91	0.48
1:J:51:LEU:CD2	1:J:111:VAL:HG22	2.43	0.48
1:D:33:PHE:CZ	1:D:98:PRO:HD3	2.48	0.48
1:C:42:HIS:ND1	1:C:117:HIS:CE1	2.78	0.48
1:I:67:ILE:CG2	1:I:71:GLY:HA2	2.44	0.47
1:F:33:PHE:CD2	1:F:44:LEU:HD22	2.49	0.47
1:C:116:GLN:HG2	2:C:132:HOH:O	2.15	0.47
1:I:17:ASN:HD22	1:J:43:GLN:NE2	2.11	0.47
1:I:69:TYR:CE2	1:I:70:GLU:OE1	2.67	0.47
1:A:69:TYR:CZ	1:E:42:HIS:HE1	2.33	0.47
1:G:42:HIS:ND1	1:G:117:HIS:HE1	2.12	0.47
1:G:53:ALA:HA	1:H:59:LEU:HD12	1.96	0.47
1:D:17:ASN:ND2	1:E:43:GLN:HE22	2.12	0.47
1:H:37:ASP:OD1	1:H:38:ASP:N	2.48	0.46
1:H:34:LYS:CD	1:H:99:PRO:HG3	2.43	0.46
1:I:53:ALA:HA	1:J:59:LEU:HD23	1.94	0.46
1:C:81:LEU:HD12	1:C:81:LEU:N	2.31	0.46
1:I:60:HIS:HE1	1:I:109:GLY:N	2.11	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:CD1	1:E:19:LEU:HD22	2.47	0.45
1:F:60:HIS:HE1	1:F:109:GLY:H	1.60	0.45
1:H:42:HIS:CD2	1:H:117:HIS:CE1	2.91	0.45
1:H:59:LEU:HD21	1:H:80:SER:HB3	1.98	0.45
1:D:104:LEU:HD11	1:D:107:GLY:O	2.16	0.45
1:B:19:LEU:HD22	1:C:76:ILE:CD1	2.47	0.44
1:G:38:ASP:N	2:G:149:HOH:O	2.49	0.44
1:A:63:GLU:HB2	1:A:76:ILE:O	2.17	0.44
1:C:43:GLN:HG3	1:C:95:GLU:OE1	2.18	0.44
1:G:35:VAL:HG21	1:G:42:HIS:CE1	2.54	0.43
1:A:69:TYR:CE1	1:E:42:HIS:HE1	2.37	0.43
1:H:33:PHE:CE1	1:H:44:LEU:HD13	2.54	0.43
1:I:33:PHE:CE2	1:I:98:PRO:HB3	2.53	0.43
1:F:81:LEU:HD12	1:F:81:LEU:N	2.34	0.43
1:D:53:ALA:HA	1:E:59:LEU:CD2	2.49	0.43
1:H:59:LEU:HD22	1:H:60:HIS:N	2.34	0.43
1:C:96:ILE:HG22	1:C:100:VAL:HG11	1.99	0.43
1:H:44:LEU:HD12	1:H:44:LEU:HA	1.88	0.42
1:I:33:PHE:CD2	1:I:98:PRO:HB3	2.53	0.42
1:E:20:PHE:CG	1:E:44:LEU:HD11	2.54	0.42
1:I:67:ILE:HG21	1:I:71:GLY:HA2	2.02	0.42
1:I:51:LEU:CD2	1:I:111:VAL:HG22	2.49	0.42
1:G:20:PHE:CD2	1:G:44:LEU:HD11	2.54	0.42
1:H:20:PHE:CD1	1:H:44:LEU:HD11	2.54	0.42
1:J:96:ILE:HG21	1:J:100:VAL:CG2	2.49	0.42
1:D:43:GLN:HE21	1:D:95:GLU:HB3	1.85	0.41
1:B:19:LEU:HD22	1:C:76:ILE:HD13	2.03	0.41
1:D:60:HIS:HE1	1:D:109:GLY:H	1.68	0.41
1:H:67:ILE:HG22	1:H:68:ASN:O	2.20	0.41
1:D:49:VAL:HG12	1:D:81:LEU:HD21	2.02	0.41
1:J:42:HIS:ND1	1:J:117:HIS:CE1	2.78	0.41
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.97	0.41
1:H:68:ASN:OD1	1:H:68:ASN:C	2.57	0.41
1:D:25:LYS:N	1:D:25:LYS:CD	2.79	0.41
1:G:81:LEU:HD12	1:G:81:LEU:N	2.35	0.41
1:A:60:HIS:HE1	1:A:109:GLY:N	2.15	0.41
1:F:25:LYS:HA	1:F:104:LEU:HD12	2.01	0.41
1:A:39:GLU:O	1:A:122:GLU:HB2	2.21	0.40
1:F:95:GLU:H	1:J:116:GLN:NE2	2.19	0.40
1:G:94:PHE:C	1:G:94:PHE:CD2	2.95	0.40
1:J:51:LEU:HD13	1:J:83:PRO:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:HIS:CE1	1:B:109:GLY:N	2.73	0.40
1:D:25:LYS:HD3	1:D:25:LYS:H	1.85	0.40
1:G:38:ASP:CB	1:G:42:HIS:HE2	2.34	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: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 [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%)	104 (98%)	2 (2%)	0	100	100
1	B	105/114 (92%)	100 (95%)	5 (5%)	0	100	100
1	C	100/114 (88%)	97 (97%)	3 (3%)	0	100	100
1	D	100/114 (88%)	93 (93%)	6 (6%)	1 (1%)	15	6
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%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	27	ASP

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	92/97 (95%)	83 (90%)	9 (10%)	8	3
1	B	90/97 (93%)	83 (92%)	7 (8%)	12	5
1	C	87/97 (90%)	78 (90%)	9 (10%)	7	2
1	D	89/97 (92%)	78 (88%)	11 (12%)	4	1
1	E	90/97 (93%)	84 (93%)	6 (7%)	16	7
1	F	88/97 (91%)	82 (93%)	6 (7%)	16	7
1	G	88/97 (91%)	82 (93%)	6 (7%)	16	7
1	H	88/97 (91%)	84 (96%)	4 (4%)	27	18
1	I	90/97 (93%)	83 (92%)	7 (8%)	12	5
1	J	89/97 (92%)	82 (92%)	7 (8%)	12	5
All	All	891/970 (92%)	819 (92%)	72 (8%)	11	4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	34	LYS
1	A	39	GLU
1	A	72	LYS
1	A	94	PHE
1	A	104	LEU
1	A	117	HIS
1	A	118	LEU
1	A	121	LEU
1	B	25	LYS
1	B	27	ASP
1	B	59	LEU
1	B	81	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	94	PHE
1	B	104	LEU
1	B	117	HIS
1	C	17	ASN
1	C	25	LYS
1	C	34	LYS
1	C	37	ASP
1	C	59	LEU
1	C	81	LEU
1	C	94	PHE
1	C	104	LEU
1	C	117	HIS
1	D	16	GLN
1	D	25	LYS
1	D	37	ASP
1	D	39	GLU
1	D	44	LEU
1	D	59	LEU
1	D	70	GLU
1	D	74	ILE
1	D	81	LEU
1	D	94	PHE
1	D	104	LEU
1	E	34	LYS
1	E	63	GLU
1	E	72	LYS
1	E	94	PHE
1	E	104	LEU
1	E	117	HIS
1	F	28	LYS
1	F	34	LYS
1	F	39	GLU
1	F	59	LEU
1	F	94	PHE
1	F	104	LEU
1	G	28	LYS
1	G	38	ASP
1	G	56	LYS
1	G	59	LEU
1	G	94	PHE
1	G	104	LEU
1	H	35	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	59	LEU
1	H	94	PHE
1	H	104	LEU
1	I	35	VAL
1	I	36	GLU
1	I	41	GLU
1	I	73	THR
1	I	94	PHE
1	I	104	LEU
1	I	117	HIS
1	J	27	ASP
1	J	28	LYS
1	J	37	ASP
1	J	81	LEU
1	J	94	PHE
1	J	104	LEU
1	J	117	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	117	HIS
1	B	43	GLN
1	B	60	HIS
1	B	116	GLN
1	B	117	HIS
1	C	60	HIS
1	C	116	GLN
1	C	117	HIS
1	D	43	GLN
1	D	60	HIS
1	D	116	GLN
1	D	117	HIS
1	E	43	GLN
1	E	60	HIS
1	E	116	GLN
1	E	117	HIS
1	F	60	HIS
1	F	116	GLN
1	F	117	HIS
1	G	43	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	60	HIS
1	G	117	HIS
1	H	42	HIS
1	H	43	GLN
1	H	60	HIS
1	H	117	HIS
1	I	40	ASN
1	I	60	HIS
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 monosaccharides 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 [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%)	-0.15	2 (1%) 66 69	18, 24, 39, 48	0
1	B	107/114 (93%)	-0.23	2 (1%) 66 69	18, 24, 35, 43	0
1	C	104/114 (91%)	-0.24	2 (1%) 66 69	20, 28, 38, 48	0
1	D	104/114 (91%)	0.02	6 (5%) 23 25	22, 29, 43, 47	0
1	E	106/114 (92%)	-0.25	1 (0%) 84 85	19, 25, 35, 43	0
1	F	105/114 (92%)	-0.18	1 (0%) 82 84	18, 25, 39, 49	0
1	G	105/114 (92%)	-0.19	2 (1%) 66 69	20, 27, 41, 51	0
1	H	107/114 (93%)	-0.02	4 (3%) 41 44	19, 30, 42, 50	0
1	I	107/114 (93%)	-0.23	2 (1%) 66 69	19, 25, 37, 45	0
1	J	106/114 (92%)	-0.14	1 (0%) 84 85	19, 26, 39, 44	0
All	All	1059/1140 (92%)	-0.16	23 (2%) 62 64	18, 26, 40, 51	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	GLU	4.6
1	G	121	LEU	4.2
1	D	15	SER	4.1
1	D	33	PHE	4.1
1	A	121	LEU	3.3
1	B	121	LEU	3.0
1	D	41	GLU	3.0
1	C	37	ASP	2.9
1	D	39	GLU	2.9
1	J	120	ALA	2.9
1	I	121	LEU	2.8
1	H	15	SER	2.7
1	D	27	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	121	LEU	2.6
1	D	40	ASN	2.5
1	F	36	GLU	2.4
1	E	72	LYS	2.2
1	H	37	ASP	2.2
1	G	38	ASP	2.2
1	I	72	LYS	2.2
1	A	122	GLU	2.1
1	H	73	THR	2.0
1	C	35	VAL	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 monosaccharides 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.