



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 10:49 AM BST

PDB ID : 6KXV
Title : Crystal structure of a nucleosome containing Leishmania histone H3
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Deposited on : 2019-09-13
Resolution : 3.63 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

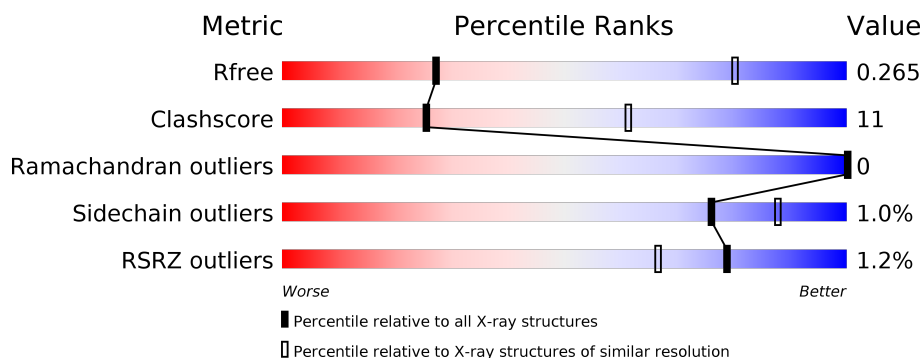
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.63 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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 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	133	<div> <div>58%</div> <div>13%</div> <div>29%</div> </div>
1	E	133	<div> <div>55%</div> <div>17%</div> <div>29%</div> </div>
2	B	106	<div> <div>63%</div> <div>10%</div> <div>26%</div> </div>
2	F	106	<div> <div>4%</div> <div>61%</div> <div>18%</div> <div>21%</div> </div>
3	C	133	<div> <div>3%</div> <div>67%</div> <div>14%</div> <div>19%</div> </div>
3	G	133	<div> <div>68%</div> <div>11%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	129	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>60%</div><div>13%</div><div>26%</div></div></div>
4	H	129	<div><div><div></div><div></div><div></div></div><div><div>60%</div><div>11%</div><div>29%</div></div></div>
5	I	146	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>38%</div><div>62%</div></div></div>
5	J	146	<div><div><div></div><div></div><div></div></div><div><div>45%</div><div>55%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11876 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 Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			745	467	141	132	5			
1	E	95	Total	C	N	O	S	0	0	0
			756	473	145	133	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q4QHB5
A	-2	SER	-	expression tag	UNP Q4QHB5
A	-1	HIS	-	expression tag	UNP Q4QHB5
E	-3	GLY	-	expression tag	UNP Q4QHB5
E	-2	SER	-	expression tag	UNP Q4QHB5
E	-1	HIS	-	expression tag	UNP Q4QHB5

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	91	Total	C	N	O	S	0	0	0
			708	447	125	134	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

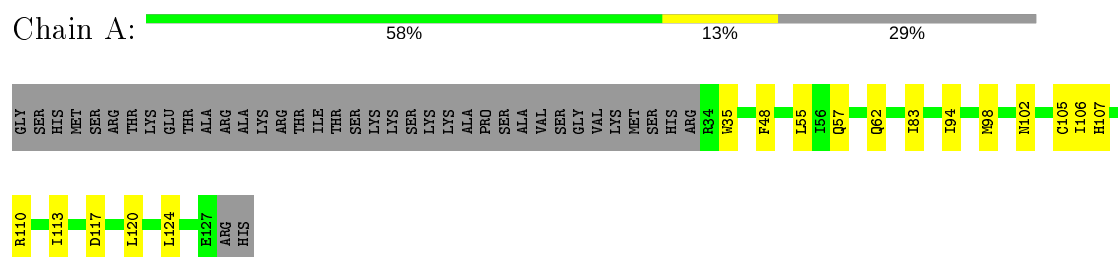
- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

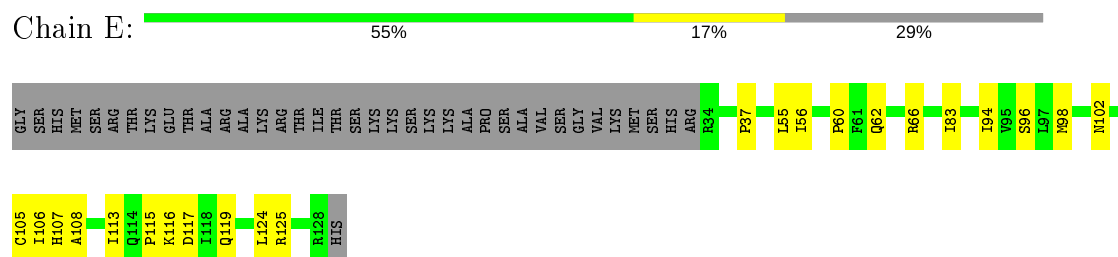
3 Residue-property plots [i](#)

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.

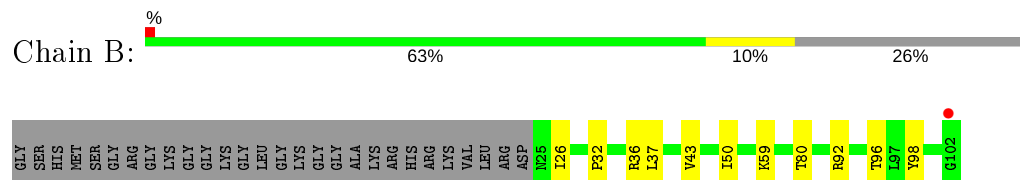
- Molecule 1: Histone H3



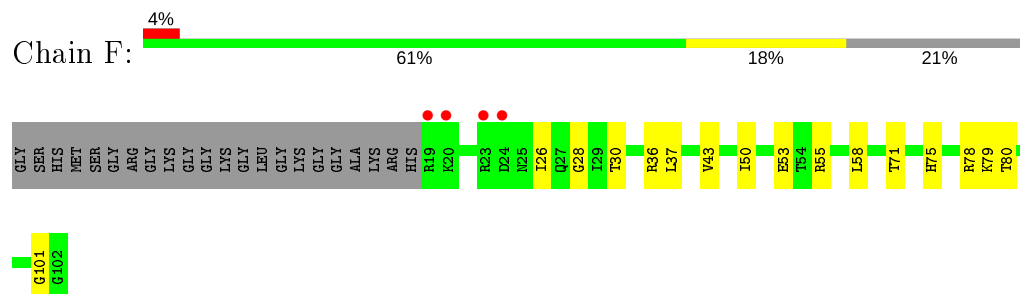
- Molecule 1: Histone H3



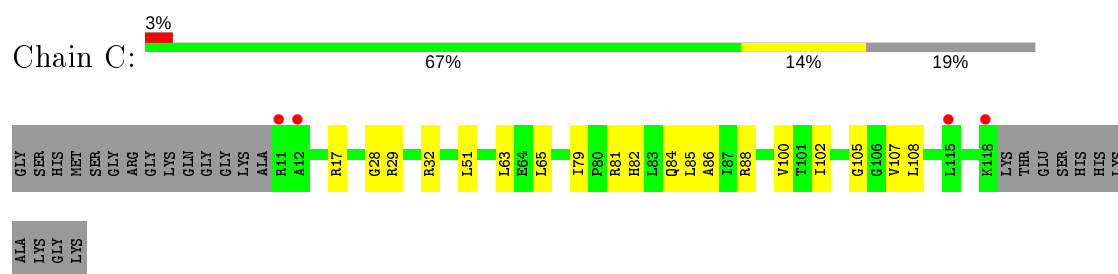
- Molecule 2: Histone H4



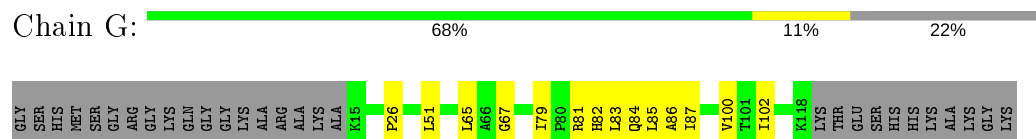
- Molecule 2: Histone H4



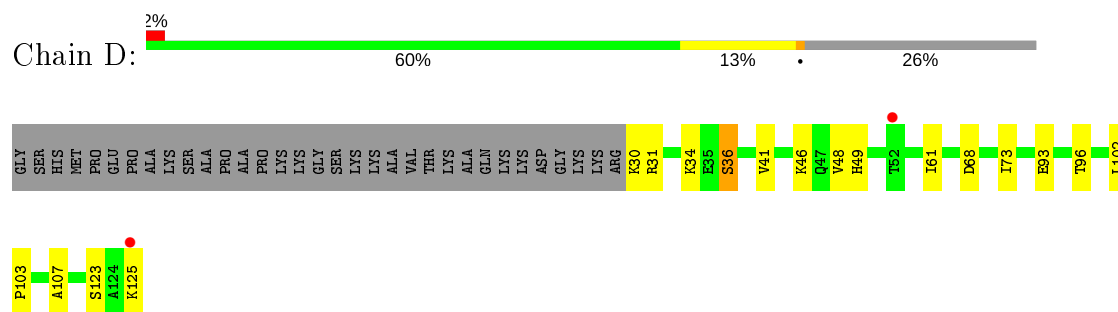
- Molecule 3: Histone H2A type 1-B/E



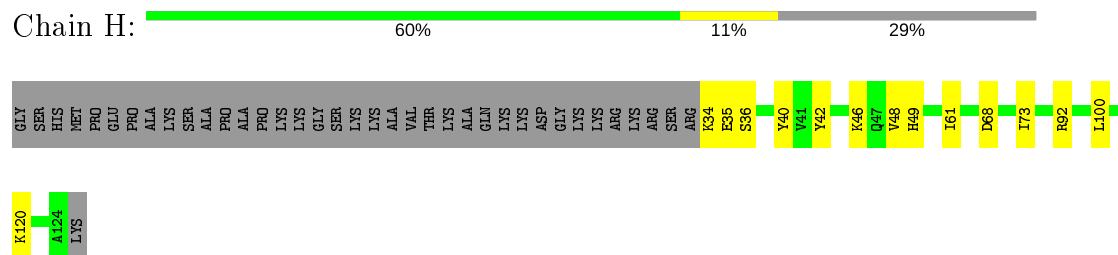
- Molecule 3: Histone H2A type 1-B/E



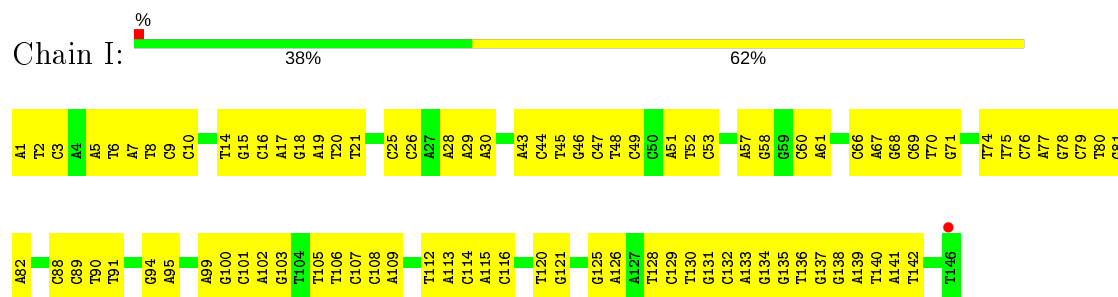
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



- Molecule 5: DNA (146-MER)



- Molecule 5: DNA (146-MER)



A147	T148	C149	G155	A157	C158	T159	G161	G164	A165	T166	C172	A173	G174	A175	T176	T180	A181	T182	A189	C190	T191	G192	C193	T194	C195	C196	A197	T198	A203	G204	A207	A213	C214	C215	T216	G217	T220	T221	C225	T226	G227	A228	A229	C230	C234	C235
T236	T237	T238	T239	G240	A241	G246	C247	A248	G249	T250	T251	T252	C253	C254	A255	A259	C260	A261	T265	T266	G267	G268	T269	A270	G271	A272	G273	T274	C275	C278	A279	G280	T286	A287	T288	T289	G290	A291	T292							

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 101.10Å 175.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.63 48.93 – 3.63	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93-3.63) 99.6 (48.93-3.63)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.220 , 0.264 0.220 , 0.265	Depositor DCC
R_{free} test set	1080 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	135.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11876	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [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	0.25	0/754	0.39	0/1013
1	E	0.25	0/765	0.40	0/1027
2	B	0.25	0/626	0.42	0/837
2	F	0.25	0/680	0.43	0/908
3	C	0.24	0/845	0.42	0/1139
3	G	0.23	0/815	0.41	0/1100
4	D	0.27	0/766	0.40	0/1026
4	H	0.29	0/719	0.40	0/968
5	I	0.52	0/3354	0.96	0/5175
5	J	0.51	0/3354	0.94	0/5175
All	All	0.41	0/12678	0.76	0/18368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	745	0	783	17	0
1	E	756	0	796	23	0
2	B	619	0	659	10	0
2	F	673	0	722	20	0
3	C	835	0	897	15	0
3	G	805	0	861	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	755	0	784	14	0
4	H	708	0	727	11	0
5	I	2990	0	1652	81	0
5	J	2990	0	1652	70	0
All	All	11876	0	9533	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 227 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)
5:J:259:DA:H2"	5:J:260:DC:H5"	1.66	0.76
5:I:101:DC:H2"	5:I:102:DA:H5"	1.67	0.75
5:I:108:DC:H2"	5:I:109:DA:N7	2.04	0.72
5:I:14:DT:O4	5:J:278:DC:N4	2.24	0.71
5:I:120:DT:H2"	5:I:121:DG:N7	2.06	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/133 (69%)	90 (98%)	2 (2%)	0	100	100
1	E	93/133 (70%)	90 (97%)	3 (3%)	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	82/106 (77%)	78 (95%)	4 (5%)	0	100	100
3	C	106/133 (80%)	104 (98%)	2 (2%)	0	100	100
3	G	102/133 (77%)	101 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	94/129 (73%)	91 (97%)	3 (3%)	0	100	100
4	H	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	734/1002 (73%)	715 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	80/113 (71%)	80 (100%)	0	100	100
1	E	81/113 (72%)	81 (100%)	0	100	100
2	B	63/81 (78%)	62 (98%)	1 (2%)	62	82
2	F	69/81 (85%)	68 (99%)	1 (1%)	67	84
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	83/102 (81%)	82 (99%)	1 (1%)	71	86
4	D	82/107 (77%)	81 (99%)	1 (1%)	71	86
4	H	77/107 (72%)	75 (97%)	2 (3%)	46	73
All	All	620/806 (77%)	614 (99%)	6 (1%)	76	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	92	ARG
4	H	42	TYR
3	G	84	GLN
4	D	36	SER
4	H	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	94/133 (70%)	-0.24	0 100 100	78, 98, 121, 131	0
1	E	95/133 (71%)	-0.15	0 100 100	80, 100, 124, 144	0
2	B	78/106 (73%)	-0.11	1 (1%) 77 64	79, 96, 115, 137	0
2	F	84/106 (79%)	0.00	4 (4%) 30 20	76, 94, 151, 163	0
3	C	108/133 (81%)	0.01	4 (3%) 41 27	73, 100, 131, 169	0
3	G	104/133 (78%)	-0.11	0 100 100	77, 99, 129, 140	0
4	D	96/129 (74%)	-0.08	2 (2%) 63 48	72, 96, 134, 164	0
4	H	91/129 (70%)	-0.18	0 100 100	72, 96, 116, 123	0
5	I	146/146 (100%)	-0.51	1 (0%) 87 79	105, 150, 185, 210	0
5	J	146/146 (100%)	-0.50	0 100 100	109, 148, 193, 199	0
All	All	1042/1294 (80%)	-0.22	12 (1%) 79 66	72, 104, 173, 210	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	12	ALA	5.1
2	F	19	ARG	4.1
3	C	11	ARG	3.7
2	F	23	ARG	3.3
2	F	24	ASP	3.2

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.