Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:07 am BST

PDB ID	:	3WAA
Title	:	The nucleosome containing human H2A.Z.2
Authors	:	Horikoshi, N.; Sato, K.; Shimada, K.; Arimura, Y.; Osakabe, A.; Tachiwana, H.; Iwasaki, W.; Kagawa, W.; Harata, M.; Kimura, H.; Kurumizaka, H.
Deposited on	:	2013-04-30
Resolution	:	3.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

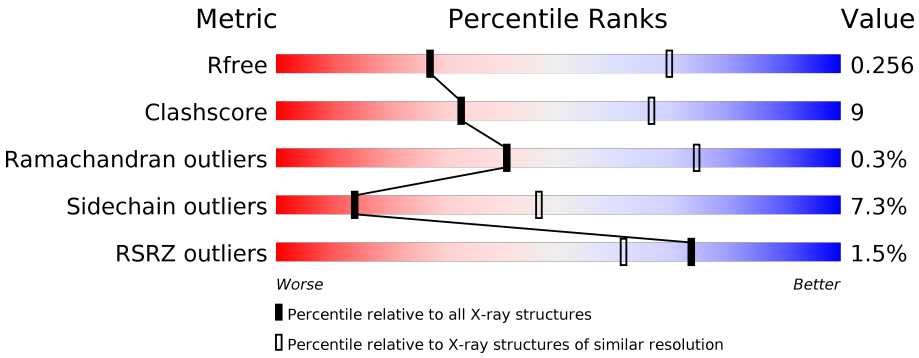
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	139	58% 10% 30%
1	E	139	3% 57% 13% 29%
2	B	106	63% 10% 26%
2	F	106	2% 64% 12% 21%
3	C	131	64% 15% 18%
3	G	131	64% 14% 21%

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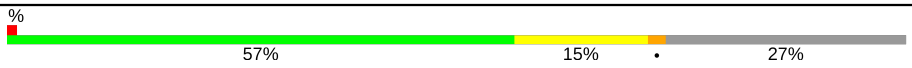
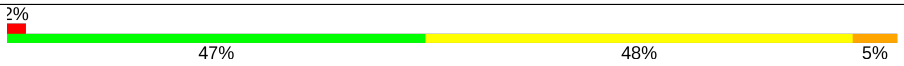
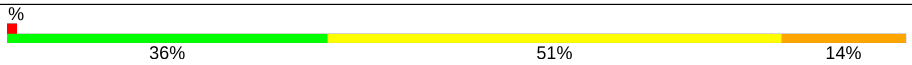
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11943 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 H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P68431
A	-2	SER	-	EXPRESSION TAG	UNP P68431
A	-1	HIS	-	EXPRESSION TAG	UNP P68431
E	-3	GLY	-	EXPRESSION TAG	UNP P68431
E	-2	SER	-	EXPRESSION TAG	UNP P68431
E	-1	HIS	-	EXPRESSION TAG	UNP P68431

- 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.V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	0	0	0
			809	508	158	143			
3	G	104	Total	C	N	O	0	0	0
			790	496	154	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	EXPRESSION TAG	UNP Q71UI9
C	-2	SER	-	EXPRESSION TAG	UNP Q71UI9
C	-1	HIS	-	EXPRESSION TAG	UNP Q71UI9
G	-3	GLY	-	EXPRESSION TAG	UNP Q71UI9
G	-2	SER	-	EXPRESSION TAG	UNP Q71UI9
G	-1	HIS	-	EXPRESSION TAG	UNP Q71UI9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	94	Total	C	N	O	S	0	0	0
			736	462	134	138	2			
4	H	92	Total	C	N	O	S	0	0	0
			719	453	129	135	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).

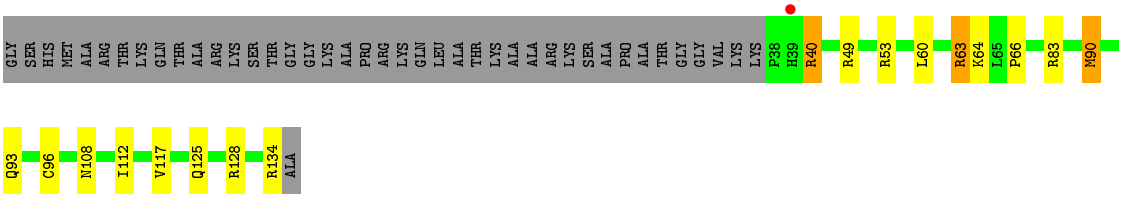
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

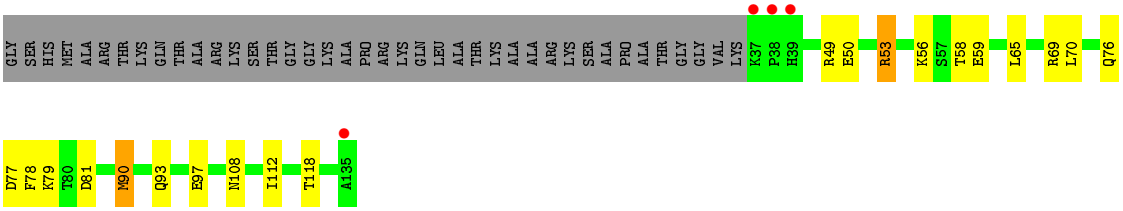
- Molecule 1: Histone H3.1

Chain A:



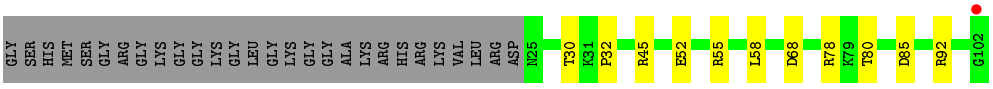
- Molecule 1: Histone H3.1

Chain E:



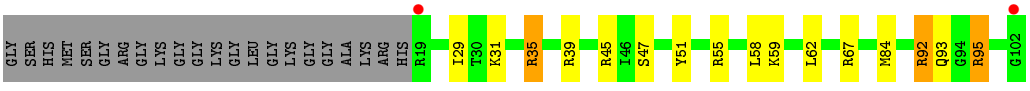
- Molecule 2: Histone H4

Chain B:



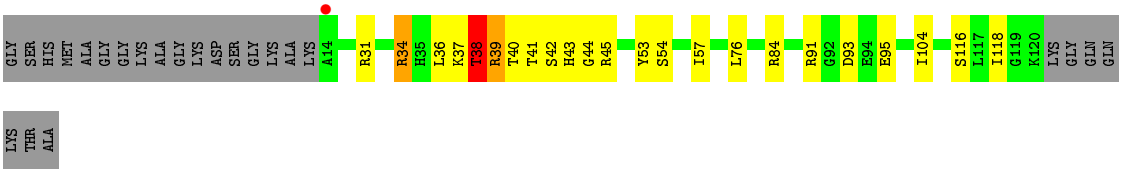
- Molecule 2: Histone H4

Chain F:

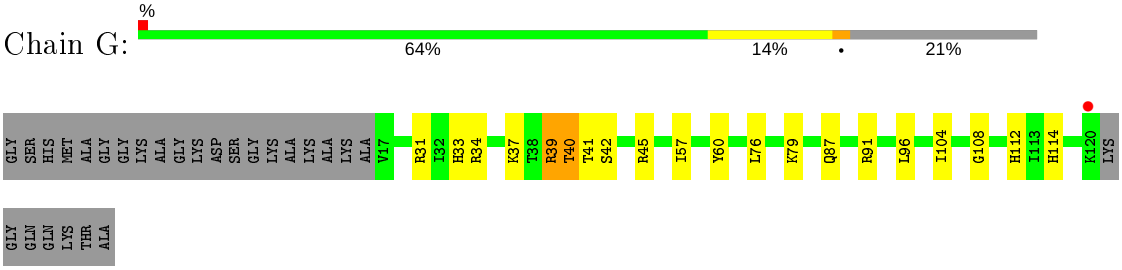


- Molecule 3: Histone H2A.V

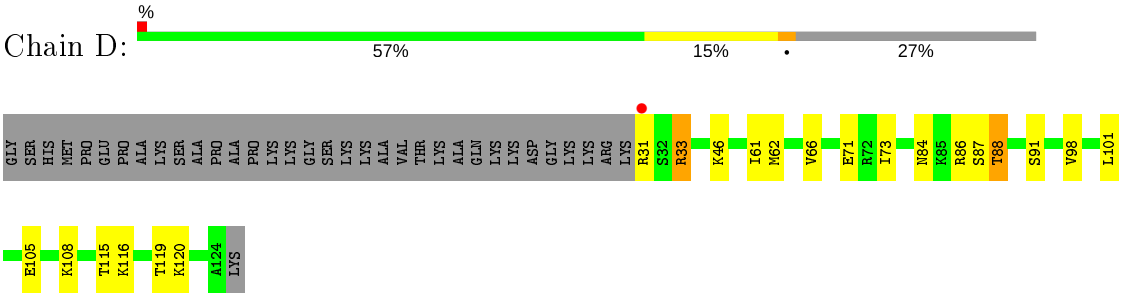
Chain C:



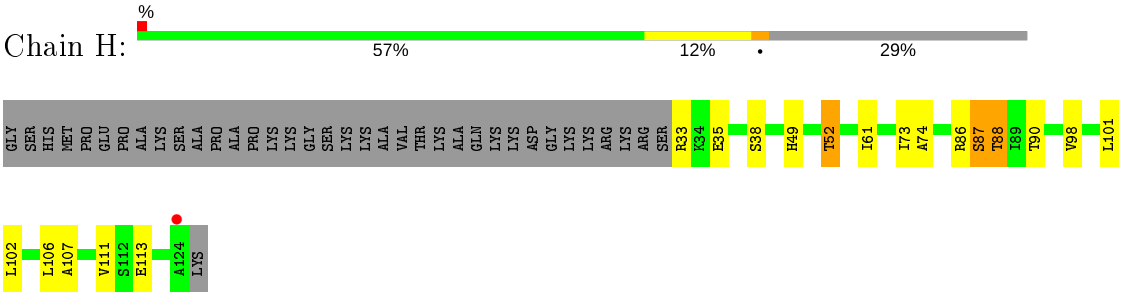
• Molecule 3: Histone H2A.V



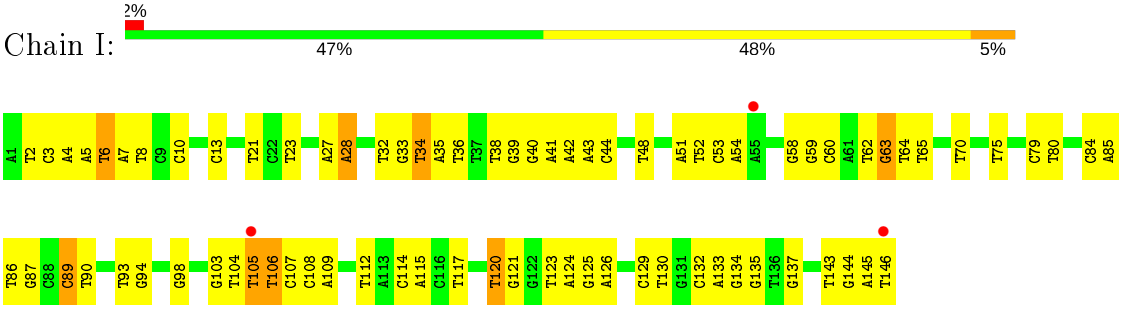
• Molecule 4: Histone H2B type 1-J



• Molecule 4: Histone H2B type 1-J

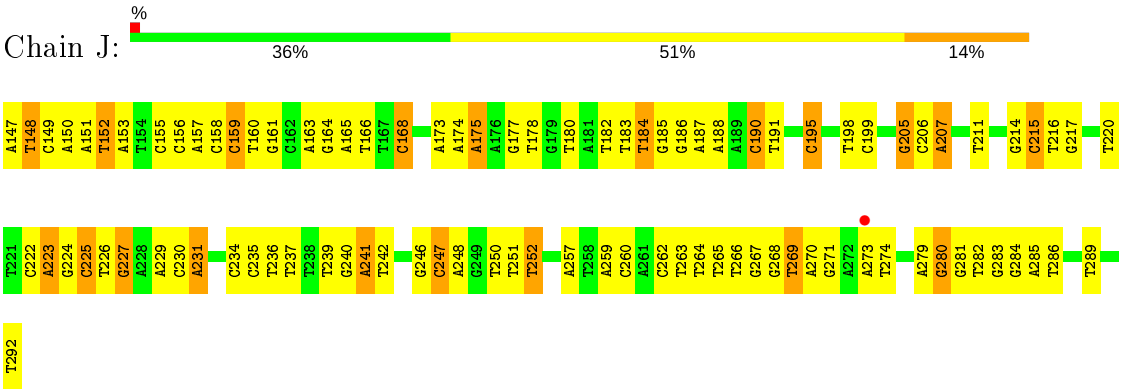


• Molecule 5: DNA (146-MER)



• Molecule 5: DNA (146-MER)

Chain J:


%
36%
51%
14%
A147 T148 C149 A150 A151 T152 A153 T154 C155 C156 A157 C158 C159 T160 G161 C162 A163 G164 A165 T166 T167 C168 A173 A174 A175 A176 G177 T178 G179 T180 A181 T182 T183 T184 G185 G186 A187 A188 A189 C190 T191 C195 T198 C199 G205 C206 A207 T211 G214 C215 T216 G217 T220
T221 C222 A223 G224 C225 T226 G227 A228 A229 C230 A231 C234 C235 T236 T237 T238 T239 G240 A241 T242 G246 C247 A248 G249 T250 T251 T252 A257 T258 A259 C260 A261 C262 T263 T264 T265 T266 G267 G268 T269 A270 G271 A272 A273 T274 A279 G280 G281 T282 G283 G284 A285 T286 T289
T292

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.36Å 109.84Å 182.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.20 – 3.20 47.50 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.20-3.20) 95.0 (47.50-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.217 , 0.271 0.204 , 0.256	Depositor DCC
R_{free} test set	1763 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11943	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.55	1/813 (0.1%)	0.65	0/1090
1	E	0.67	1/828 (0.1%)	0.86	2/1109 (0.2%)
2	B	0.52	0/626	0.64	0/837
2	F	0.62	0/680	0.69	1/908 (0.1%)
3	C	0.52	0/820	0.69	0/1104
3	G	0.46	0/801	0.62	0/1079
4	D	0.54	0/747	0.61	0/1004
4	H	0.52	0/730	0.63	0/982
5	I	0.73	1/3354 (0.0%)	1.46	41/5175 (0.8%)
5	J	0.74	0/3354	1.55	62/5175 (1.2%)
All	All	0.66	3/12753 (0.0%)	1.21	106/18463 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	ASP	CB-CG	8.01	1.68	1.51
1	A	96	CYS	CB-SG	-5.59	1.72	1.81
5	I	48	DT	C3'-O3'	-5.15	1.37	1.44

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ASP	CB-CG-OD1	14.64	131.48	118.30
5	I	145	DA	O4'-C1'-N9	11.51	116.06	108.00
5	I	143	DT	O4'-C1'-N1	11.37	115.96	108.00
5	J	214	DG	O4'-C1'-N9	-9.30	101.49	108.00
5	J	246	DG	O4'-C1'-N9	-8.99	101.71	108.00
5	I	84	DC	O4'-C1'-N1	8.89	114.22	108.00
5	I	86	DT	N3-C2-O2	-8.73	117.06	122.30
5	J	280	DG	O4'-C1'-N9	8.59	114.01	108.00
5	I	2	DT	O4'-C1'-N1	8.08	113.66	108.00
5	J	217	DG	N3-C4-N9	-7.67	121.40	126.00
5	I	133	DA	O4'-C1'-N9	7.54	113.28	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	252	DT	O4'-C1'-N1	7.47	113.23	108.00
5	I	85	DA	O4'-C1'-N9	7.47	113.23	108.00
5	J	217	DG	N3-C4-C5	7.40	132.30	128.60
5	J	157	DA	P-O5'-C5'	-7.39	109.08	120.90
5	I	79	DC	O4'-C1'-N1	-7.31	102.88	108.00
5	J	279	DA	O4'-C1'-N9	-7.31	102.88	108.00
5	J	175	DA	O4'-C4'-C3'	-7.22	101.61	104.50
5	I	65	DT	N3-C4-O4	7.21	124.22	119.90
5	J	225	DC	O4'-C1'-N1	7.14	113.00	108.00
1	E	77	ASP	CB-CG-OD2	-7.12	111.89	118.30
5	J	280	DG	N1-C6-O6	7.04	124.13	119.90
5	I	145	DA	O4'-C1'-C2'	-7.01	100.29	105.90
5	J	180	DT	O4'-C1'-N1	7.00	112.90	108.00
5	I	134	DG	O4'-C1'-N9	6.98	112.88	108.00
5	J	220	DT	O4'-C1'-N1	6.89	112.82	108.00
5	J	231	DA	C3'-C2'-C1'	-6.87	94.25	102.50
5	J	175	DA	C4'-C3'-C2'	-6.73	97.04	103.10
5	J	223	DA	N1-C6-N6	6.70	122.62	118.60
5	J	289	DT	P-O5'-C5'	-6.55	110.43	120.90
5	J	247	DC	O4'-C1'-N1	6.53	112.57	108.00
5	I	34	DT	O4'-C1'-N1	6.48	112.54	108.00
5	J	231	DA	O4'-C1'-N9	6.37	112.46	108.00
5	I	64	DT	N3-C4-O4	6.35	123.71	119.90
5	J	166	DT	C1'-O4'-C4'	-6.25	103.84	110.10
5	J	286	DT	O4'-C1'-N1	6.22	112.36	108.00
5	J	262	DC	O4'-C1'-N1	6.10	112.27	108.00
5	J	280	DG	C5-C6-N1	-6.07	108.47	111.50
5	J	148	DT	O4'-C4'-C3'	-6.05	102.08	104.50
5	I	6	DT	P-O5'-C5'	-6.04	111.23	120.90
5	I	2	DT	N3-C4-O4	6.03	123.52	119.90
5	I	106	DT	O4'-C1'-N1	5.93	112.16	108.00
5	J	257	DA	O4'-C1'-N9	5.93	112.15	108.00
5	J	165	DA	O4'-C1'-N9	5.93	112.15	108.00
5	I	137	DG	C3'-C2'-C1'	-5.92	95.40	102.50
5	J	224	DG	O4'-C1'-N9	-5.91	103.86	108.00
5	I	117	DT	O4'-C1'-N1	5.90	112.13	108.00
5	I	21	DT	O4'-C1'-N1	5.85	112.10	108.00
5	J	157	DA	O4'-C1'-N9	5.82	112.07	108.00
5	I	28	DA	O4'-C1'-N9	5.80	112.06	108.00
5	I	6	DT	O4'-C1'-N1	5.78	112.04	108.00
5	J	160	DT	N3-C4-O4	5.77	123.36	119.90
5	I	120	DT	C4-C5-C7	5.76	122.45	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	190	DC	O4'-C1'-N1	5.76	112.03	108.00
5	J	292	DT	C4-C5-C7	5.74	122.44	119.00
5	J	247	DC	O4'-C1'-C2'	-5.70	101.34	105.90
5	J	217	DG	C5-N7-C8	-5.70	101.45	104.30
5	J	237	DT	O4'-C1'-N1	-5.67	104.03	108.00
5	J	269	DT	N3-C4-O4	5.64	123.29	119.90
5	J	159	DC	P-O5'-C5'	-5.62	111.91	120.90
5	I	64	DT	C5-C4-O4	-5.58	120.99	124.90
5	J	217	DG	C8-N9-C1'	5.58	134.25	127.00
5	I	65	DT	C5-C4-O4	-5.57	121.00	124.90
5	J	220	DT	O4'-C1'-C2'	-5.56	101.45	105.90
5	I	70	DT	C5-C4-O4	-5.56	121.01	124.90
5	J	152	DT	O4'-C1'-N1	5.55	111.88	108.00
5	J	214	DG	N9-C1'-C2'	5.53	123.11	112.60
5	J	198	DT	N3-C4-O4	5.52	123.21	119.90
5	J	241	DA	O4'-C1'-N9	5.51	111.86	108.00
5	I	93	DT	O4'-C1'-N1	5.50	111.85	108.00
5	I	143	DT	C5-C4-O4	-5.46	121.08	124.90
5	I	63	DG	O4'-C1'-N9	5.42	111.80	108.00
5	J	205	DG	N1-C6-O6	-5.42	116.65	119.90
5	J	227	DG	N3-C4-C5	5.40	131.30	128.60
5	J	207	DA	N1-C6-N6	5.39	121.83	118.60
5	J	183	DT	N3-C4-O4	5.39	123.13	119.90
5	J	152	DT	N3-C2-O2	-5.37	119.08	122.30
5	J	263	DT	N3-C4-O4	5.36	123.12	119.90
2	F	95	ARG	NE-CZ-NH1	-5.36	117.62	120.30
5	I	80	DT	N3-C4-O4	5.34	123.10	119.90
5	I	23	DT	N3-C4-O4	5.33	123.10	119.90
5	J	195	DC	O4'-C1'-N1	5.32	111.72	108.00
5	I	2	DT	C5-C4-O4	-5.31	121.18	124.90
5	J	240	DG	O4'-C1'-N9	5.30	111.71	108.00
5	I	105	DT	O4'-C1'-N1	5.29	111.70	108.00
5	J	289	DT	C5-C4-O4	-5.29	121.20	124.90
5	I	146	DT	C4-C5-C7	5.29	122.17	119.00
5	J	182	DT	N3-C4-O4	5.26	123.06	119.90
5	J	207	DA	O4'-C1'-N9	-5.25	104.33	108.00
5	J	168	DC	O4'-C1'-N1	5.24	111.67	108.00
5	I	34	DT	N3-C4-O4	5.22	123.03	119.90
5	I	34	DT	C5-C4-O4	-5.21	121.25	124.90
5	I	86	DT	N1-C2-O2	5.21	127.27	123.10
5	J	215	DC	O4'-C1'-C2'	-5.18	101.75	105.90
5	I	75	DT	C5-C4-O4	-5.17	121.28	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	191	DT	C5-C4-O4	-5.17	121.28	124.90
5	I	36	DT	N3-C4-O4	5.17	123.00	119.90
5	I	79	DC	O4'-C4'-C3'	-5.16	102.43	104.50
5	J	252	DT	O4'-C1'-C2'	-5.16	101.78	105.90
5	I	106	DT	N3-C4-O4	5.13	122.97	119.90
5	J	239	DT	N3-C4-O4	5.12	122.97	119.90
5	J	211	DT	N3-C4-O4	5.07	122.94	119.90
5	J	269	DT	C5-C4-O4	-5.05	121.36	124.90
5	I	89	DC	C3'-C2'-C1'	-5.04	96.45	102.50
5	J	184	DT	O4'-C1'-N1	5.03	111.52	108.00
5	J	236	DT	N3-C4-O4	5.00	122.90	119.90

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	801	0	839	12	0
1	E	816	0	856	14	0
2	B	619	0	659	9	0
2	F	673	0	722	13	0
3	C	809	0	860	18	0
3	G	790	0	837	19	0
4	D	736	0	758	17	0
4	H	719	0	740	14	0
5	I	2990	0	1652	51	0
5	J	2990	0	1652	61	0
All	All	11943	0	9575	178	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 9.

All (178) 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:I:41:DA:N6	5:J:251:DT:O4	2.13	0.82
5:I:144:DG:H1	5:J:149:DC:H42	1.30	0.80
5:I:103:DG:H1	5:J:190:DC:H42	1.30	0.80
3:C:45:ARG:HB2	4:D:88:THR:HB	1.64	0.79
5:J:270:DA:H2"	5:J:271:DG:H5"	1.68	0.76
3:G:57:ILE:HD13	4:H:98:VAL:HG21	1.69	0.74
5:I:132:DC:H42	5:J:161:DG:H1	1.37	0.73
5:I:103:DG:H2"	5:I:104:DT:H5"	1.70	0.72
4:D:86:ARG:NH1	5:I:40:DG:OP1	2.24	0.70
1:E:53:ARG:HG3	1:E:53:ARG:HH11	1.57	0.69
5:J:259:DA:H2"	5:J:260:DC:H5"	1.74	0.69
3:G:104:ILE:HG23	4:H:61:ILE:HD13	1.73	0.67
3:C:39:ARG:NH1	4:D:71:GLU:OE2	2.26	0.67
3:G:37:LYS:NZ	5:I:112:DT:OP1	2.27	0.67
5:I:87:DG:N2	5:J:206:DC:O2	2.18	0.66
5:I:51:DA:H2"	5:I:52:DT:H5"	1.77	0.65
5:J:230:DC:H2"	5:J:231:DA:C8	2.31	0.65
5:I:105:DT:O4	5:J:187:DA:N6	2.29	0.64
3:C:57:ILE:HD13	4:D:98:VAL:HG21	1.79	0.64
1:A:40:ARG:NH2	5:J:229:DA:N3	2.48	0.62
4:D:73:ILE:HD13	4:D:101:LEU:HD12	1.82	0.61
5:I:125:DG:H1	5:J:168:DC:H42	1.48	0.61
4:H:49:HIS:HB3	4:H:52:THR:OG1	2.01	0.61
5:I:40:DG:H2'	5:I:41:DA:C8	2.34	0.61
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.36	0.60
5:J:283:DG:H2"	5:J:284:DG:C8	2.36	0.60
1:E:108:ASN:O	1:E:112:ILE:HG12	2.02	0.60
1:A:60:LEU:HD13	1:A:93:GLN:HG2	1.84	0.59
3:C:104:ILE:HG23	4:D:61:ILE:HD13	1.84	0.59
5:I:42:DA:H2"	5:I:43:DA:H5'	1.84	0.59
1:E:50:GLU:OE1	2:F:35:ARG:NH1	2.36	0.58
1:A:49:ARG:HD2	5:J:155:DC:OP1	2.03	0.58
5:I:43:DA:H2"	5:I:44:DC:H5"	1.85	0.57
5:I:58:DG:H2'	5:I:59:DG:C8	2.39	0.57
1:A:63:ARG:HH11	5:I:60:DC:H5"	1.70	0.57
5:J:163:DA:H2"	5:J:164:DG:C8	2.40	0.56
3:G:33:HIS:HE1	3:G:37:LYS:HE2	1.71	0.56
5:J:151:DA:H2"	5:J:152:DT:H5"	1.88	0.56
5:I:53:DC:H2"	5:I:54:DA:H5'	1.88	0.55
5:I:6:DT:H2"	5:I:7:DA:C8	2.41	0.55
5:J:273:DA:H2"	5:J:274:DT:H5"	1.87	0.55
5:J:158:DC:H2"	5:J:159:DC:H5"	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:ARG:HD2	5:J:270:DA:H4'	1.89	0.54
3:G:87:GLN:NE2	3:G:108:GLY:O	2.32	0.54
3:C:42:SER:OG	3:C:43:HIS:N	2.40	0.54
2:B:92:ARG:HH21	4:D:101:LEU:HD23	1.73	0.53
4:D:62:MET:O	4:D:66:VAL:HG23	2.09	0.53
5:J:152:DT:H2'	5:J:153:DA:C8	2.42	0.53
5:J:173:DA:H2"	5:J:174:DA:N7	2.22	0.53
1:A:90:MET:HA	1:A:90:MET:HE3	1.90	0.53
1:E:53:ARG:HG3	1:E:53:ARG:NH1	2.24	0.53
5:I:3:DC:H2"	5:I:4:DA:C8	2.44	0.53
5:J:184:DT:H2"	5:J:185:DG:C8	2.44	0.53
2:B:92:ARG:NH1	2:B:92:ARG:HB3	2.24	0.52
5:J:150:DA:H2'	5:J:151:DA:C8	2.44	0.52
5:I:104:DT:H2"	5:I:105:DT:H5"	1.91	0.52
1:A:63:ARG:HE	1:A:66:PRO:HG2	1.75	0.52
5:J:177:DG:H2"	5:J:178:DT:H5"	1.92	0.52
5:J:187:DA:H2'	5:J:188:DA:C8	2.45	0.52
3:G:39:ARG:HD2	4:H:74:ALA:HB1	1.92	0.52
4:D:105:GLU:OE2	4:D:108:LYS:HE2	2.10	0.51
5:I:38:DT:H2"	5:I:39:DG:O4'	2.10	0.51
5:J:205:DG:H2"	5:J:206:DC:H5"	1.93	0.51
3:G:57:ILE:CD1	4:H:98:VAL:HG21	2.40	0.51
5:J:234:DC:H2"	5:J:235:DC:C5	2.46	0.50
5:I:120:DT:H2"	5:I:121:DG:C8	2.46	0.50
1:E:90:MET:HE3	1:E:90:MET:HA	1.93	0.50
1:E:70:LEU:HD22	2:F:29:ILE:HD11	1.92	0.50
1:E:59:GLU:OE2	1:E:59:GLU:N	2.40	0.50
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.45	0.50
1:E:93:GLN:O	1:E:97:GLU:HG3	2.12	0.49
5:I:108:DC:H2"	5:I:109:DA:C8	2.48	0.49
4:H:87:SER:OG	5:J:186:DG:OP1	2.29	0.49
5:I:125:DG:H2"	5:I:126:DA:H5'	1.93	0.49
5:I:32:DT:H2'	5:I:33:DG:C8	2.48	0.48
3:G:40:THR:HA	3:G:41:THR:HA	1.63	0.48
3:G:79:LYS:O	4:H:52:THR:HG22	2.14	0.48
5:I:98:DG:H1	5:J:195:DC:H42	1.62	0.48
3:C:53:TYR:CE1	3:C:57:ILE:HD11	2.49	0.48
3:G:33:HIS:CE1	3:G:37:LYS:HE2	2.49	0.48
4:D:115:THR:O	4:D:119:THR:HG23	2.14	0.47
4:H:98:VAL:HG13	4:H:102:LEU:HD22	1.95	0.47
2:F:35:ARG:HB3	2:F:35:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ARG:HD2	5:I:8:DT:OP1	2.14	0.47
5:I:135:DG:H1	5:J:158:DC:H42	1.62	0.47
5:J:284:DG:H2"	5:J:285:DA:C8	2.50	0.47
3:C:53:TYR:CD1	3:C:57:ILE:HD11	2.50	0.46
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.46	0.46
5:J:152:DT:H2"	5:J:153:DA:O4'	2.15	0.46
5:J:173:DA:H2"	5:J:174:DA:C8	2.50	0.46
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.16	0.46
5:J:226:DT:H2"	5:J:227:DG:C8	2.51	0.46
5:I:5:DA:H2"	5:I:6:DT:H5"	1.96	0.45
5:J:175:DA:H5'	5:J:175:DA:H2'	1.75	0.45
4:D:116:LYS:HB3	4:D:116:LYS:HE2	1.80	0.45
5:I:6:DT:H2"	5:I:7:DA:H8	1.81	0.45
3:G:34:ARG:HB3	3:G:34:ARG:HE	1.66	0.45
5:I:144:DG:H1	5:J:149:DC:N4	2.06	0.45
5:J:250:DT:H2"	5:J:251:DT:H5"	1.99	0.45
2:B:45:ARG:CZ	5:J:227:DG:H4'	2.47	0.45
3:C:34:ARG:O	3:C:38:THR:HG23	2.16	0.45
1:A:63:ARG:NH1	5:I:60:DC:H5"	2.31	0.45
5:I:114:DC:H2"	5:I:115:DA:H5'	1.97	0.45
5:I:123:DT:H2'	5:I:124:DA:C8	2.51	0.45
5:I:32:DT:H2"	5:I:33:DG:H5'	1.99	0.45
3:C:91:ARG:HA	3:C:91:ARG:HD3	1.72	0.45
5:I:114:DC:H2'	5:I:115:DA:C8	2.52	0.45
5:I:27:DA:C6	5:I:28:DA:C6	3.05	0.45
5:J:147:DA:C6	5:J:148:DT:C2	3.04	0.44
2:F:31:LYS:HG3	2:F:51:TYR:CZ	2.52	0.44
5:J:266:DT:H2"	5:J:267:DG:C8	2.52	0.44
5:J:148:DT:C4	5:J:149:DC:C4	3.06	0.44
3:C:34:ARG:HE	3:C:34:ARG:HB3	1.42	0.44
2:F:29:ILE:HD13	2:F:58:LEU:HD23	1.98	0.44
3:C:42:SER:HA	3:G:41:THR:O	2.18	0.44
3:C:84:ARG:HD3	1:E:58:THR:HG21	2.00	0.43
1:A:83:ARG:O	2:B:80:THR:HA	2.19	0.43
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.53	0.43
5:J:206:DC:H2"	5:J:207:DA:C8	2.54	0.43
1:A:64:LYS:HB2	1:A:64:LYS:HE2	1.85	0.43
3:C:104:ILE:HG23	4:D:61:ILE:CD1	2.48	0.43
2:F:95:ARG:HB3	2:F:95:ARG:HE	1.66	0.43
5:I:89:DC:H1'	5:I:90:DT:C6	2.53	0.43
5:J:150:DA:H8	5:J:150:DA:H5"	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:125:DG:H2"	5:I:126:DA:C8	2.54	0.43
5:J:158:DC:C2'	5:J:159:DC:H5"	2.49	0.43
5:J:241:DA:H2"	5:J:242:DT:H5'	2.01	0.43
2:F:35:ARG:O	2:F:39:ARG:HG2	2.18	0.43
2:B:78:ARG:NH1	2:B:80:THR:O	2.52	0.43
3:G:60:TYR:HB2	4:H:113:GLU:HG3	2.00	0.43
5:I:62:DT:H2"	5:I:63:DG:C8	2.53	0.43
5:I:13:DC:H42	5:J:280:DG:H22	1.65	0.43
5:I:43:DA:C2'	5:I:44:DC:H5"	2.48	0.42
5:J:185:DG:H8	5:J:185:DG:OP2	2.02	0.42
5:J:247:DC:H2"	5:J:248:DA:N7	2.33	0.42
2:F:51:TYR:O	2:F:55:ARG:HG3	2.20	0.42
5:I:129:DC:H2"	5:I:130:DT:C7	2.49	0.42
2:F:92:ARG:HB3	2:F:92:ARG:CZ	2.50	0.42
5:J:186:DG:H1'	5:J:187:DA:C8	2.54	0.42
3:G:39:ARG:HB2	3:G:39:ARG:HE	1.53	0.42
5:J:222:DC:H2"	5:J:223:DA:C8	2.55	0.42
3:G:34:ARG:NH2	4:H:35:GLU:OE2	2.52	0.42
3:G:96:LEU:HD23	4:H:106:LEU:HD11	2.02	0.42
3:C:57:ILE:CD1	4:D:98:VAL:HG21	2.48	0.41
5:J:184:DT:H2"	5:J:185:DG:N7	2.34	0.41
3:G:91:ARG:HD3	3:G:91:ARG:HA	1.79	0.41
5:I:34:DT:H2"	5:I:35:DA:H8	1.86	0.41
1:E:118:THR:HA	2:F:45:ARG:HB3	2.01	0.41
3:C:37:LYS:O	3:G:42:SER:HB3	2.21	0.41
5:I:94:DG:H1	5:J:199:DC:H42	1.67	0.41
1:A:128:ARG:NH1	1:A:134:ARG:HD3	2.36	0.41
1:E:65:LEU:HG	1:E:69:ARG:NH2	2.35	0.41
4:H:107:ALA:O	4:H:111:VAL:HG23	2.20	0.41
5:I:129:DC:C4	5:J:163:DA:N6	2.89	0.41
5:I:34:DT:H2"	5:I:35:DA:C8	2.55	0.41
5:I:135:DG:N2	5:J:158:DC:N3	2.59	0.41
5:J:264:DT:H1'	5:J:265:DT:H5'	2.02	0.41
3:C:42:SER:C	3:C:44:GLY:H	2.23	0.41
5:I:106:DT:H1'	5:I:107:DC:H5"	2.02	0.41
4:D:33:ARG:HB3	5:J:269:DT:O3'	2.21	0.41
3:C:36:LEU:HD23	3:C:36:LEU:HA	1.78	0.41
1:E:70:LEU:CD2	2:F:29:ILE:HD11	2.51	0.41
1:A:125:GLN:HA	1:A:134:ARG:HH12	1.85	0.40
5:J:215:DC:H2"	5:J:216:DT:H71	2.04	0.40
5:J:251:DT:H2"	5:J:252:DT:H5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:O	1:A:112:ILE:HG12	2.22	0.40
4:D:46:LYS:HE2	4:D:46:LYS:HA	2.03	0.40
3:G:45:ARG:HB2	4:H:88:THR:HB	2.01	0.40
5:I:10:DC:H2'	5:I:10:DC:H6	1.71	0.40
5:J:156:DC:H6	5:J:156:DC:H2'	1.74	0.40
5:J:225:DC:H2"	5:J:226:DT:C7	2.52	0.40
5:I:125:DG:H2"	5:I:126:DA:H8	1.86	0.40
4:H:73:ILE:HD13	4:H:101:LEU:HD12	2.04	0.40
5:J:281:DG:H2"	5:J:282:DT:H5'	2.03	0.40
2:B:78:ARG:HH22	2:B:85:ASP:CG	2.25	0.40
3:C:93:ASP:OD2	3:C:95:GLU:HB2	2.22	0.40
4:D:84:ASN:O	4:D:86:ARG:HG2	2.22	0.40
5:J:267:DG:H1'	5:J:268:DG:H5"	2.02	0.40

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	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	97/139 (70%)	94 (97%)	3 (3%)	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	82/106 (77%)	81 (99%)	1 (1%)	0	100	100
3	C	105/131 (80%)	94 (90%)	10 (10%)	1 (1%)	15	54
3	G	102/131 (78%)	92 (90%)	9 (9%)	1 (1%)	15	54
4	D	92/129 (71%)	91 (99%)	1 (1%)	0	100	100
4	H	90/129 (70%)	87 (97%)	3 (3%)	0	100	100
All	All	739/1010 (73%)	706 (96%)	31 (4%)	2 (0%)	41	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	THR
3	G	112	HIS

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	85/113 (75%)	80 (94%)	5 (6%)	19 54
1	E	86/113 (76%)	80 (93%)	6 (7%)	15 48
2	B	63/81 (78%)	62 (98%)	1 (2%)	62 84
2	F	69/81 (85%)	62 (90%)	7 (10%)	7 29
3	C	83/97 (86%)	73 (88%)	10 (12%)	5 22
3	G	82/97 (84%)	77 (94%)	5 (6%)	18 54
4	D	80/107 (75%)	75 (94%)	5 (6%)	18 52
4	H	78/107 (73%)	71 (91%)	7 (9%)	9 34
All	All	626/796 (79%)	580 (93%)	46 (7%)	14 46

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	53	ARG
1	A	63	ARG
1	A	90	MET
1	A	117	VAL
2	B	58	LEU
3	C	31	ARG
3	C	34	ARG
3	C	38	THR
3	C	39	ARG
3	C	40	THR
3	C	41	THR

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Mol	Chain	Res	Type
3	C	54	SER
3	C	76	LEU
3	C	116	SER
3	C	118	ILE
4	D	33	ARG
4	D	87	SER
4	D	88	THR
4	D	91	SER
4	D	120	LYS
1	E	53	ARG
1	E	56	LYS
1	E	76	GLN
1	E	79	LYS
1	E	81	ASP
1	E	90	MET
2	F	35	ARG
2	F	47	SER
2	F	59	LYS
2	F	62	LEU
2	F	84	MET
2	F	92	ARG
2	F	93	GLN
3	G	31	ARG
3	G	39	ARG
3	G	40	THR
3	G	76	LEU
3	G	114	HIS
4	H	33	ARG
4	H	38	SER
4	H	52	THR
4	H	86	ARG
4	H	87	SER
4	H	88	THR
4	H	90	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	33	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^{th} 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	97/139 (69%)	-0.10	1 (1%)	82	72	52, 68, 90, 127	0
1	E	99/139 (71%)	-0.03	4 (4%)	38	25	47, 61, 93, 123	0
2	B	78/106 (73%)	-0.14	1 (1%)	77	65	54, 65, 81, 83	0
2	F	84/106 (79%)	-0.06	2 (2%)	59	44	48, 58, 81, 107	0
3	C	107/131 (81%)	-0.12	1 (0%)	84	75	51, 68, 128, 140	0
3	G	104/131 (79%)	-0.07	1 (0%)	82	72	59, 78, 117, 139	0
4	D	94/129 (72%)	-0.03	1 (1%)	80	69	54, 69, 104, 152	0
4	H	92/129 (71%)	0.08	1 (1%)	80	69	59, 76, 100, 138	0
5	I	146/146 (100%)	-0.28	3 (2%)	63	49	63, 127, 162, 174	0
5	J	146/146 (100%)	-0.30	1 (0%)	87	81	72, 128, 162, 179	0
All	All	1047/1302 (80%)	-0.12	16 (1%)	73	61	47, 75, 151, 179	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	6.3
2	F	102	GLY	4.1
2	B	102	GLY	4.1
1	E	37	LYS	3.9
4	D	31	ARG	3.6
3	C	14	ALA	3.3
5	J	273	DA	2.8
1	A	39	HIS	2.5
1	E	38	PRO	2.5
1	E	39	HIS	2.4
1	E	135	ALA	2.3
4	H	124	ALA	2.2
2	F	19	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	120	LYS	2.1
5	I	55	DA	2.0
5	I	105	DT	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.