



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:10 PM GMT

PDB ID : 3WA9  
Title : The nucleosome containing human H2A.Z.1  
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 : 3.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
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

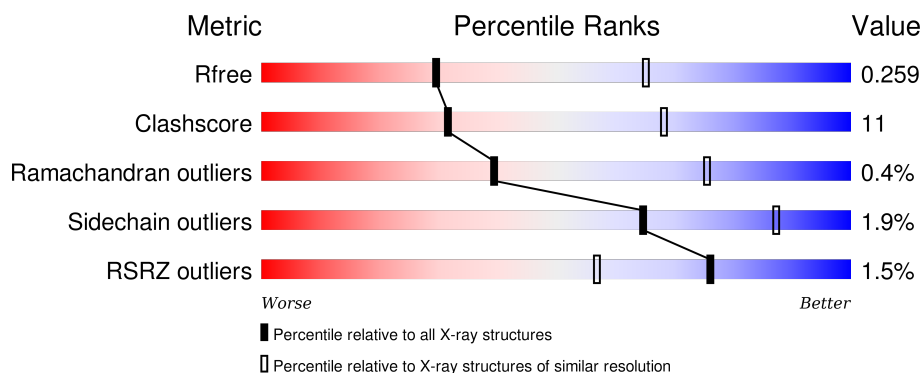
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	139	
1	E	139	
2	B	106	
2	F	106	
3	C	131	

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Mol	Chain	Length	Quality of chain
3	G	131	<div><div></div><div>57%21%21%</div></div>
4	D	129	<div><div>%</div><div>55%16%28%</div></div>
4	H	129	<div><div></div><div>59%12%28%</div></div>
5	I	146	<div><div>5%</div><div>36%55%10%</div></div>
5	J	146	<div><div>3%</div><div>34%52%14%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11925 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	98	Total	C	N	O	S	0	0	0
			810	511	157	138	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.Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	106	Total	C	N	O	0	0	0
			803	504	157	142			
3	G	104	Total	C	N	O	0	0	0
			789	495	154	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	EXPRESSION TAG	UNP P0C0S5
C	-2	SER	-	EXPRESSION TAG	UNP P0C0S5
C	-1	HIS	-	EXPRESSION TAG	UNP P0C0S5
G	-3	GLY	-	EXPRESSION TAG	UNP P0C0S5
G	-2	SER	-	EXPRESSION TAG	UNP P0C0S5
G	-1	HIS	-	EXPRESSION TAG	UNP P0C0S5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	93	Total	C	N	O	S	0	0	0
			725	456	130	137	2			
4	H	93	Total	C	N	O	S	0	0	0
			725	456	130	137	2			

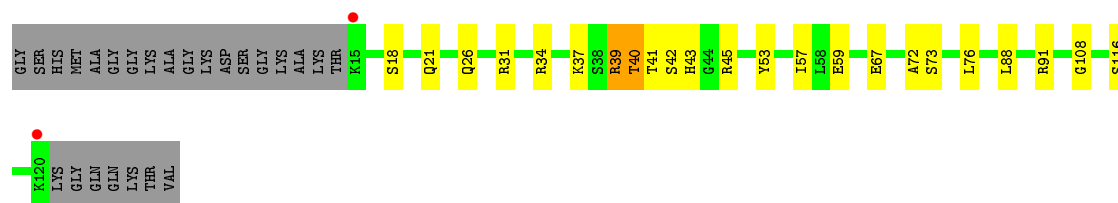
There are 6 discrepancies between the modelled and reference sequences:

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

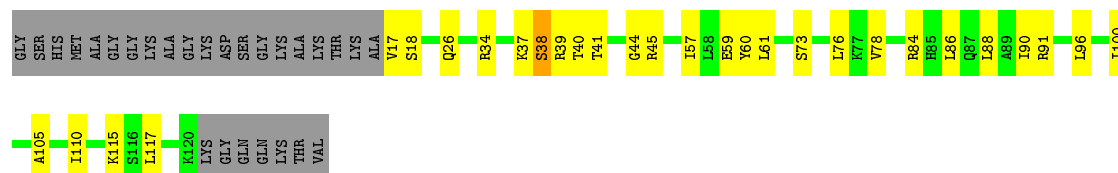
- Molecule 5 is a DNA chain called DNA (146-MER).

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			

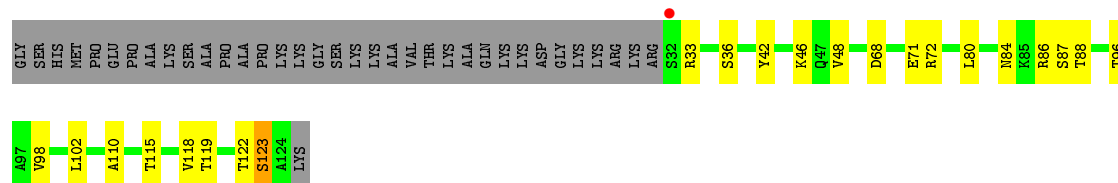




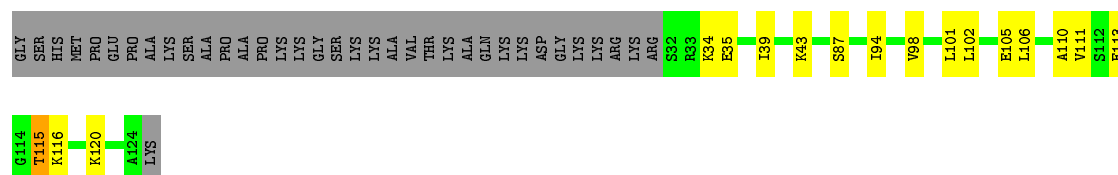
- Molecule 3: Histone H2A.Z



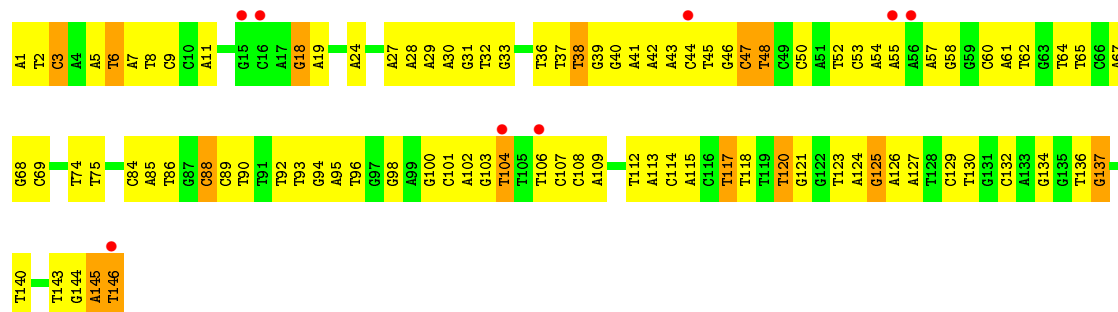
- Molecule 4: Histone H2B type 1-J



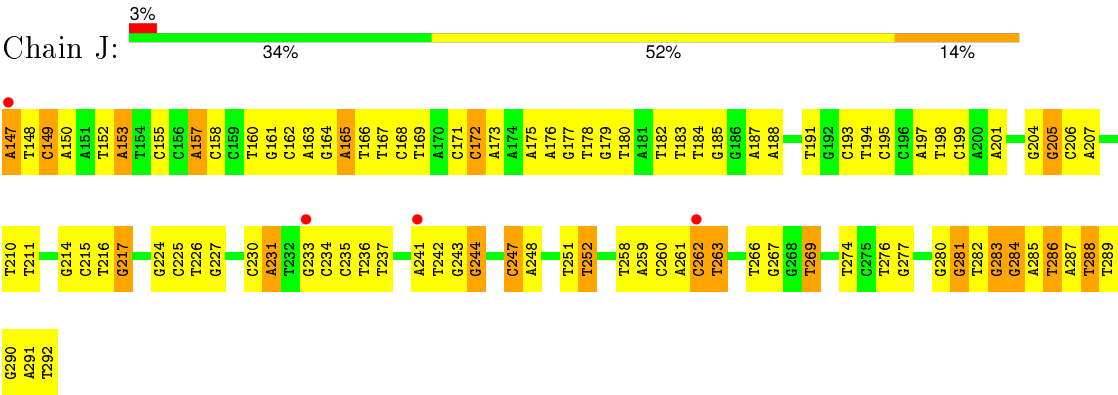
- Molecule 4: Histone H2B type 1-J



- Molecule 5: DNA (146-MER)



● Molecule 5: DNA (146-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.90Å 109.39Å 181.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.96 – 3.07 38.96 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.96-3.07) 96.4 (38.96-3.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.222 , 0.271 0.215 , 0.259	Depositor DCC
$R_{free}$ test set	1940 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 51.8	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 40448 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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	0.50	1/813 (0.1%)	0.65	0/1090
1	E	0.57	1/822 (0.1%)	0.82	2/1102 (0.2%)
2	B	0.48	0/626	0.65	0/837
2	F	0.53	0/680	0.67	0/908
3	C	0.47	0/814	0.81	3/1095 (0.3%)
3	G	0.45	0/800	0.57	0/1077
4	D	0.50	0/736	0.65	0/990
4	H	0.44	0/736	0.58	0/990
5	I	0.69	0/3354	1.46	57/5175 (1.1%)
5	J	0.66	0/3354	1.50	55/5175 (1.1%)
All	All	0.60	2/12735 (0.0%)	1.20	117/18439 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	CYS	CB-SG	-6.24	1.71	1.82
1	E	77	ASP	CB-CG	5.19	1.62	1.51

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	ASP	CB-CG-OD1	11.49	128.64	118.30
5	J	241	DA	O4'-C1'-N9	10.08	115.05	108.00
3	C	39	ARG	CB-CA-C	9.42	129.23	110.40
3	C	40	THR	N-CA-CB	-9.02	93.15	110.30
5	I	143	DT	O4'-C1'-N1	8.63	114.05	108.00
5	J	291	DA	O4'-C1'-N9	8.46	113.92	108.00
5	I	18	DG	O4'-C1'-N9	8.45	113.91	108.00
5	J	231	DA	O4'-C1'-N9	8.33	113.83	108.00
5	J	280	DG	O4'-C1'-N9	8.19	113.73	108.00
5	J	236	DT	O4'-C1'-N1	8.07	113.65	108.00
5	I	124	DA	O4'-C1'-N9	8.03	113.62	108.00
5	I	94	DG	O4'-C1'-N9	7.88	113.52	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	241	DA	C4'-C3'-C2'	-7.83	96.05	103.10
5	I	146	DT	C5-C4-O4	-7.78	119.45	124.90
5	I	28	DA	O4'-C1'-N9	7.67	113.37	108.00
5	I	85	DA	O4'-C1'-N9	7.62	113.33	108.00
5	I	53	DC	O4'-C4'-C3'	-7.55	101.47	106.00
5	I	145	DA	O4'-C1'-N9	7.41	113.18	108.00
5	J	241	DA	C3'-C2'-C1'	-7.33	93.70	102.50
5	J	165	DA	O4'-C1'-N9	7.23	113.06	108.00
5	I	95	DA	O4'-C1'-N9	7.20	113.04	108.00
5	I	47	DC	O4'-C4'-C3'	-7.15	101.64	104.50
5	I	84	DC	O4'-C1'-N1	7.15	113.00	108.00
5	I	101	DC	P-O5'-C5'	-7.13	109.49	120.90
5	J	199	DC	O4'-C1'-N1	7.11	112.98	108.00
5	J	171	DC	O4'-C4'-C3'	-6.85	101.76	104.50
1	E	77	ASP	CB-CG-OD2	-6.71	112.26	118.30
5	I	38	DT	O4'-C1'-N1	6.60	112.62	108.00
5	I	54	DA	O4'-C1'-N9	6.53	112.57	108.00
5	J	160	DT	N3-C4-O4	6.51	123.81	119.90
5	I	75	DT	N3-C4-O4	6.50	123.80	119.90
5	J	241	DA	O4'-C1'-C2'	-6.46	100.73	105.90
5	J	286	DT	O4'-C1'-N1	6.31	112.42	108.00
5	I	6	DT	P-O5'-C5'	-6.21	110.97	120.90
5	J	201	DA	O4'-C1'-N9	6.17	112.32	108.00
5	J	198	DT	C5-C4-O4	-6.17	120.58	124.90
5	J	292	DT	C6-C5-C7	-6.15	119.21	122.90
5	I	92	DT	N3-C4-O4	6.14	123.59	119.90
5	I	123	DT	N3-C4-O4	6.08	123.55	119.90
5	I	48	DT	C3'-C2'-C1'	-6.04	95.26	102.50
5	I	74	DT	N3-C4-O4	6.00	123.50	119.90
5	I	102	DA	C3'-C2'-C1'	-5.92	95.39	102.50
5	I	88	DC	O4'-C1'-N1	-5.92	103.85	108.00
5	J	242	DT	C4'-C3'-C2'	-5.89	97.80	103.10
5	I	75	DT	C5-C4-O4	-5.87	120.79	124.90
5	J	224	DG	O4'-C1'-N9	-5.87	103.89	108.00
5	J	182	DT	N3-C4-O4	5.87	123.42	119.90
5	J	292	DT	C4-C5-C7	5.86	122.51	119.00
5	J	262	DC	C4'-C3'-C2'	-5.85	97.83	103.10
5	J	281	DG	O4'-C1'-N9	5.83	112.08	108.00
5	I	86	DT	N3-C2-O2	-5.82	118.81	122.30
5	I	134	DG	O4'-C1'-N9	5.80	112.06	108.00
5	J	183	DT	N3-C4-O4	5.80	123.38	119.90
5	I	93	DT	O4'-C1'-N1	5.78	112.05	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	180	DT	O4'-C1'-N1	5.78	112.04	108.00
5	J	233	DG	O4'-C1'-N9	5.77	112.04	108.00
5	J	157	DA	P-O5'-C5'	-5.68	111.82	120.90
5	J	225	DC	C3'-C2'-C1'	-5.66	95.71	102.50
5	J	205	DG	N3-C4-C5	-5.64	125.78	128.60
5	I	28	DA	C3'-C2'-C1'	-5.62	95.75	102.50
5	I	62	DT	C1'-O4'-C4'	-5.58	104.52	110.10
5	J	194	DT	N3-C4-O4	5.58	123.25	119.90
5	J	198	DT	N3-C4-O4	5.57	123.24	119.90
5	I	11	DA	O4'-C1'-N9	5.56	111.89	108.00
5	I	112	DT	C5-C4-O4	-5.55	121.01	124.90
5	J	149	DC	C3'-C2'-C1'	-5.51	95.89	102.50
5	J	191	DT	O4'-C1'-N1	5.48	111.83	108.00
5	I	67	DA	O4'-C1'-N9	-5.48	104.17	108.00
5	J	247	DC	O4'-C1'-N1	5.47	111.83	108.00
5	J	217	DG	O4'-C1'-N9	-5.45	104.18	108.00
5	I	146	DT	N3-C4-O4	5.45	123.17	119.90
5	J	165	DA	C1'-O4'-C4'	-5.45	104.65	110.10
5	I	3	DC	O4'-C1'-C2'	-5.45	101.54	105.90
5	I	120	DT	C5-C4-O4	-5.45	121.09	124.90
5	I	64	DT	N3-C4-O4	5.43	123.16	119.90
5	I	92	DT	C5-C4-O4	-5.42	121.10	124.90
5	I	146	DT	C4-C5-C7	5.42	122.25	119.00
5	I	96	DT	O4'-C1'-N1	5.40	111.78	108.00
5	I	117	DT	O4'-C1'-N1	5.38	111.76	108.00
5	I	125	DG	O4'-C4'-C3'	-5.38	102.35	104.50
5	J	263	DT	N3-C4-O4	5.35	123.11	119.90
5	I	48	DT	C4'-C3'-C2'	-5.27	98.36	103.10
5	J	197	DA	O4'-C1'-N9	-5.27	104.31	108.00
3	C	40	THR	N-CA-C	5.25	125.17	111.00
5	J	288	DT	C3'-C2'-C1'	-5.23	96.22	102.50
5	J	147	DA	C5-C6-N6	-5.21	119.53	123.70
5	J	263	DT	C5-C4-O4	-5.21	121.25	124.90
5	I	113	DA	O4'-C1'-N9	5.21	111.64	108.00
5	J	193	DC	O4'-C1'-N1	5.21	111.64	108.00
5	J	241	DA	C1'-O4'-C4'	-5.21	104.89	110.10
5	J	160	DT	C5-C4-O4	-5.20	121.26	124.90
5	J	283	DG	O4'-C1'-N9	5.19	111.63	108.00
5	I	52	DT	C4'-C3'-C2'	-5.18	98.44	103.10
5	I	112	DT	N3-C4-O4	5.17	123.00	119.90
5	J	269	DT	N3-C4-O4	5.17	123.00	119.90
5	I	48	DT	N3-C4-O4	5.16	122.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	45	DT	N3-C4-O4	5.15	122.99	119.90
5	I	137	DG	O4'-C1'-N9	5.15	111.60	108.00
5	I	140	DT	N3-C2-O2	-5.14	119.22	122.30
5	J	284	DG	O4'-C1'-N9	5.14	111.60	108.00
5	J	244	DG	O4'-C1'-N9	5.11	111.58	108.00
5	I	64	DT	O4'-C4'-C3'	-5.11	102.46	104.50
5	J	205	DG	C8-N9-C4	-5.10	104.36	106.40
5	I	69	DC	P-O5'-C5'	-5.09	112.76	120.90
5	J	263	DT	O4'-C1'-N1	5.08	111.56	108.00
5	I	65	DT	N3-C4-O4	5.08	122.95	119.90
5	I	145	DA	C3'-C2'-C1'	-5.08	96.41	102.50
5	J	214	DG	O4'-C1'-N9	-5.05	104.47	108.00
5	J	172	DC	C4'-C3'-C2'	-5.04	98.56	103.10
5	J	157	DA	N1-C6-N6	5.03	121.62	118.60
5	I	53	DC	C4'-C3'-C2'	-5.03	98.58	103.10
5	J	153	DA	C6-N1-C2	5.02	121.61	118.60
5	I	48	DT	C5-C4-O4	-5.02	121.39	124.90
5	I	123	DT	C5-C4-O4	-5.01	121.39	124.90
5	I	104	DT	N3-C4-O4	5.00	122.90	119.90
5	J	252	DT	C5-C4-O4	-5.00	121.40	124.90
5	J	274	DT	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

There are no planarity outliers.

## 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	801	0	839	22	0
1	E	810	0	851	23	0
2	B	619	0	659	7	0
2	F	673	0	722	12	0
3	C	803	0	853	27	0
3	G	789	0	835	24	0
4	D	725	0	745	22	0
4	H	725	0	745	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2990	0	1652	60	0
5	J	2990	0	1652	70	0
All	All	11925	0	9553	213	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.

All (213) 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:144:DG:H1	5:J:149:DC:H42	1.18	0.92
5:I:43:DA:H2"	5:I:44:DC:H5"	1.64	0.80
5:I:41:DA:N6	5:J:251:DT:O4	2.16	0.79
3:C:39:ARG:O	3:G:41:THR:HG22	1.84	0.76
3:C:34:ARG:NH1	5:I:29:DA:OP1	2.25	0.70
5:I:136:DT:H2'	5:I:137:DG:C8	2.26	0.70
5:J:205:DG:H2"	5:J:206:DC:H5"	1.72	0.70
5:I:46:DG:N2	5:J:247:DC:O2	2.21	0.69
5:I:33:DG:N2	5:J:260:DC:N3	2.40	0.69
3:G:18:SER:HA	5:J:177:DG:H5"	1.74	0.68
3:C:41:THR:H	3:C:42:SER:HA	1.58	0.68
2:F:26:ILE:HD13	2:F:59:LYS:HG3	1.76	0.67
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.27	0.67
5:I:132:DC:H42	5:J:161:DG:H1	1.41	0.67
3:C:43:HIS:ND1	3:C:43:HIS:O	2.27	0.67
1:A:87:SER:HB2	2:B:83:ALA:HB2	1.77	0.66
5:J:281:DG:H2"	5:J:282:DT:H5"	1.78	0.66
5:I:3:DC:H42	5:J:290:DG:H1	1.44	0.66
3:G:61:LEU:HD11	4:H:102:LEU:HD21	1.78	0.66
3:G:38:SER:O	3:G:39:ARG:NH1	2.30	0.65
5:I:144:DG:H1	5:J:149:DC:N4	1.92	0.65
5:I:55:DA:N6	5:J:237:DT:O4	2.31	0.64
1:A:69:ARG:NH2	5:J:237:DT:OP2	2.31	0.63
5:J:283:DG:H2"	5:J:284:DG:C8	2.33	0.63
5:J:206:DC:H2"	5:J:207:DA:C8	2.34	0.62
5:J:152:DT:H2"	5:J:153:DA:H5"	1.81	0.62
5:I:5:DA:H2"	5:I:6:DT:H5"	1.81	0.62
5:J:251:DT:H2"	5:J:252:DT:H5'	1.82	0.61
5:I:33:DG:H1	5:J:260:DC:H42	1.49	0.61
5:I:117:DT:H2"	5:I:118:DT:H5"	1.82	0.61
5:I:89:DC:H2"	5:I:90:DT:H71	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ARG:HH21	4:D:71:GLU:HG2	1.65	0.60
5:J:234:DC:H2"	5:J:235:DC:C5	2.35	0.60
5:J:230:DC:H2"	5:J:231:DA:C8	2.37	0.59
3:G:90:ILE:HD12	3:G:100:ILE:HD12	1.83	0.59
5:J:175:DA:H2"	5:J:176:DA:C8	2.38	0.59
1:A:117:VAL:HG22	3:G:117:LEU:HD23	1.84	0.59
5:J:157:DA:C8	5:J:157:DA:H5'	2.38	0.59
3:C:39:ARG:HH11	3:C:39:ARG:HG3	1.67	0.59
3:C:39:ARG:HB3	3:C:40:THR:HA	1.84	0.58
5:I:98:DG:H1	5:J:195:DC:H42	1.48	0.58
5:J:226:DT:H2"	5:J:227:DG:C8	2.38	0.58
5:J:215:DC:H2"	5:J:216:DT:H72	1.85	0.58
5:J:166:DT:H2'	5:J:167:DT:C6	2.39	0.57
1:A:69:ARG:HH22	5:J:237:DT:P	2.27	0.57
3:G:40:THR:O	3:G:44:GLY:HA3	2.05	0.56
3:C:57:ILE:HD12	4:D:110:ALA:HB1	1.87	0.56
5:I:31:DG:H2"	5:I:32:DT:H5"	1.87	0.56
5:J:266:DT:H2"	5:J:267:DG:C8	2.40	0.56
3:C:41:THR:HG21	4:D:87:SER:O	2.06	0.56
1:A:43:PRO:HG2	5:I:68:DG:H5'	1.88	0.56
5:I:36:DT:H2"	5:I:37:DT:H5"	1.88	0.56
5:I:103:DG:H2"	5:I:104:DT:H5"	1.89	0.55
5:J:247:DC:H2"	5:J:248:DA:N7	2.20	0.55
5:I:6:DT:H2"	5:I:7:DA:C8	2.41	0.55
4:D:115:THR:O	4:D:119:THR:HG23	2.07	0.55
5:I:37:DT:H2"	5:I:38:DT:C6	2.42	0.55
5:I:120:DT:H2"	5:I:121:DG:C8	2.42	0.55
3:C:108:GLY:HA3	1:E:58:THR:HG22	1.89	0.55
1:A:68:GLN:HG2	1:A:72:ARG:HE	1.72	0.54
5:I:24:DA:H5'	5:I:24:DA:H8	1.73	0.54
4:D:88:THR:HG22	5:I:39:DG:OP1	2.07	0.54
5:I:8:DT:H2"	5:I:9:DC:H5"	1.90	0.54
5:J:284:DG:H2"	5:J:285:DA:C8	2.42	0.53
3:G:57:ILE:HD12	4:H:110:ALA:HB1	1.89	0.53
5:I:125:DG:N2	5:J:169:DT:O2	2.42	0.53
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.42	0.53
5:J:243:DG:H2'	5:J:244:DG:C8	2.44	0.53
5:I:129:DC:H2"	5:I:130:DT:C5	2.44	0.53
4:D:86:ARG:NH1	5:I:40:DG:OP1	2.43	0.52
1:E:108:ASN:O	1:E:112:ILE:HG12	2.09	0.52
5:I:145:DA:H61	5:J:147:DA:H62	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:VAL:O	4:D:122:THR:HG23	2.09	0.51
1:E:118:THR:HA	2:F:45:ARG:HB3	1.92	0.51
5:J:172:DC:H2"	5:J:173:DA:C8	2.45	0.51
3:G:96:LEU:HD23	4:H:106:LEU:HD11	1.93	0.51
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.43	0.51
3:G:91:ARG:HB2	3:G:110:ILE:HD11	1.92	0.51
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.92	0.51
3:G:26:GLN:N	3:G:59:GLU:OE1	2.42	0.51
3:G:86:LEU:O	3:G:90:ILE:HG12	2.11	0.50
5:I:47:DC:C6	5:I:47:DC:H5'	2.45	0.50
4:D:33:ARG:HB2	5:J:269:DT:H4'	1.93	0.50
3:C:45:ARG:HG3	4:D:88:THR:HB	1.93	0.50
1:E:37:LYS:HD3	1:E:39:HIS:HB2	1.93	0.50
5:J:260:DC:H2'	5:J:261:DA:C8	2.47	0.50
5:I:126:DA:H2"	5:I:127:DA:C8	2.46	0.50
1:E:59:GLU:OE2	1:E:59:GLU:N	2.43	0.50
4:D:46:LYS:HA	4:D:46:LYS:HE2	1.94	0.50
5:J:259:DA:H2"	5:J:260:DC:H5"	1.94	0.49
3:C:57:ILE:HG13	4:D:98:VAL:HG21	1.94	0.49
3:C:53:TYR:O	3:C:57:ILE:HG12	2.12	0.49
5:I:125:DG:O6	5:J:168:DC:N4	2.40	0.49
4:D:42:TYR:CE2	4:D:46:LYS:HD2	2.48	0.49
5:J:148:DT:H1'	5:J:149:DC:H5'	1.94	0.49
5:J:178:DT:H1'	5:J:179:DG:H5'	1.95	0.49
3:C:26:GLN:N	3:C:59:GLU:OE1	2.44	0.49
5:I:114:DC:H2'	5:I:115:DA:C8	2.47	0.49
5:I:7:DA:C2	5:J:287:DA:C2	3.01	0.49
1:A:108:ASN:O	1:A:112:ILE:HG12	2.13	0.49
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.47	0.49
1:E:69:ARG:HD2	2:F:25:ASN:OD1	2.13	0.48
2:B:30:THR:HB	2:B:32:PRO:HD2	1.95	0.48
3:C:37:LYS:O	3:C:40:THR:CG2	2.62	0.48
5:I:129:DC:H2"	5:I:130:DT:C6	2.49	0.48
4:D:123:SER:O	4:D:123:SER:OG	2.28	0.48
4:D:84:ASN:O	4:D:86:ARG:HG3	2.13	0.48
3:C:41:THR:N	3:C:42:SER:HA	2.25	0.48
1:E:85:GLN:NE2	2:F:82:THR:HG22	2.29	0.48
5:J:157:DA:H8	5:J:157:DA:H5'	1.78	0.48
1:A:126:LEU:O	1:A:130:ILE:HG12	2.14	0.48
2:B:84:MET:SD	2:B:101:GLY:HA3	2.54	0.47
1:A:49:ARG:HG2	5:J:155:DC:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:THR:HG22	3:C:41:THR:OG1	2.15	0.47
5:I:47:DC:H1'	5:I:48:DT:H5'	1.95	0.47
5:J:258:DT:H2''	5:J:259:DA:H8	1.79	0.47
5:I:57:DA:H2''	5:I:58:DG:C8	2.50	0.47
1:A:128:ARG:HH11	1:A:134:ARG:HH21	1.63	0.47
5:J:286:DT:H2''	5:J:287:DA:H8	1.79	0.47
1:A:64:LYS:HE2	1:A:64:LYS:HB2	1.72	0.47
4:D:33:ARG:HD3	5:I:27:DA:H4'	1.98	0.46
2:B:97:LEU:HD11	3:G:105:ALA:HB2	1.96	0.46
3:C:39:ARG:O	3:G:41:THR:CG2	2.57	0.46
4:H:111:VAL:O	4:H:115:THR:OG1	2.32	0.46
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.97	0.46
3:C:40:THR:H	3:G:41:THR:HA	1.80	0.46
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.48	0.46
3:C:40:THR:OG1	3:G:41:THR:HB	2.16	0.46
3:G:73:SER:HB2	3:G:78:VAL:HG23	1.97	0.46
1:A:117:VAL:HG22	3:G:117:LEU:CD2	2.44	0.46
5:I:42:DA:H2''	5:I:43:DA:H5'	1.98	0.46
1:E:83:ARG:HD2	5:I:100:DG:H5''	1.98	0.46
4:H:94:ILE:O	4:H:98:VAL:HG23	2.16	0.46
5:J:276:DT:H2''	5:J:277:DG:N7	2.31	0.45
5:J:262:DC:H1'	5:J:263:DT:H5''	1.98	0.45
5:I:6:DT:H2''	5:I:7:DA:H8	1.81	0.45
1:A:128:ARG:NH1	1:A:134:ARG:HE	2.15	0.45
2:F:83:ALA:O	2:F:87:VAL:HG23	2.17	0.45
1:E:134:ARG:HE	1:E:134:ARG:HB2	1.32	0.45
1:A:113:HIS:HB2	1:E:126:LEU:HD22	1.99	0.44
5:I:60:DC:H2''	5:I:61:DA:C8	2.51	0.44
2:F:59:LYS:HB3	2:F:59:LYS:HE2	1.84	0.44
3:C:91:ARG:HA	3:C:91:ARG:HD3	1.85	0.44
5:J:165:DA:H2''	5:J:166:DT:O4'	2.18	0.44
1:A:125:GLN:HG2	1:A:134:ARG:HH12	1.82	0.44
3:C:88:LEU:HA	3:C:88:LEU:HD23	1.82	0.44
3:G:34:ARG:HA	3:G:37:LYS:HE2	1.99	0.44
5:J:251:DT:H2'	5:J:252:DT:C6	2.53	0.44
1:E:37:LYS:HB2	1:E:38:PRO:O	2.17	0.44
1:E:49:ARG:HD2	5:I:8:DT:OP1	2.18	0.44
2:F:92:ARG:HH21	4:H:101:LEU:HD23	1.83	0.44
1:A:113:HIS:CE1	1:E:123:ASP:OD1	2.70	0.44
2:F:62:LEU:HA	2:F:62:LEU:HD23	1.75	0.44
4:D:80:LEU:CD1	4:D:96:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:145:DA:C2	5:I:146:DT:C4	3.06	0.44
1:E:37:LYS:HD2	5:I:5:DA:H4'	2.00	0.44
5:I:145:DA:H61	5:J:147:DA:N6	2.15	0.43
5:J:152:DT:C2'	5:J:153:DA:H5''	2.48	0.43
1:E:121:PRO:HB3	2:F:53:GLU:HG3	2.00	0.43
1:A:42:ARG:NE	5:I:68:DG:OP1	2.51	0.43
5:J:288:DT:H1'	5:J:289:DT:H5''	1.99	0.43
3:G:34:ARG:HH22	4:H:35:GLU:CD	2.22	0.43
1:E:56:LYS:HE3	1:E:56:LYS:HB2	1.78	0.43
3:C:72:ALA:O	3:C:76:LEU:HG	2.19	0.43
3:G:76:LEU:HD12	3:G:76:LEU:HA	1.83	0.43
3:C:39:ARG:N	3:C:40:THR:OG1	2.52	0.42
5:I:89:DC:H2''	5:I:90:DT:C7	2.47	0.42
5:J:163:DA:H2''	5:J:164:DG:C8	2.54	0.42
5:I:24:DA:H5'	5:I:24:DA:C8	2.52	0.42
4:H:39:ILE:HG22	4:H:43:LYS:HE3	2.01	0.42
5:J:287:DA:H2''	5:J:288:DT:H5'	2.01	0.42
5:J:243:DG:H2''	5:J:244:DG:H5'	2.01	0.42
3:G:60:TYR:HB2	4:H:113:GLU:HG3	2.01	0.42
5:J:147:DA:N1	5:J:148:DT:C2	2.87	0.42
3:G:45:ARG:HD2	5:J:185:DG:H4'	2.01	0.42
5:I:88:DC:N4	5:J:204:DG:C6	2.88	0.42
3:C:18:SER:HA	5:I:30:DA:H5''	2.01	0.42
5:J:184:DT:H2''	5:J:185:DG:N7	2.34	0.42
1:A:76:GLN:NE2	1:A:80:THR:HG22	2.33	0.42
1:A:96:CYS:SG	2:B:62:LEU:HD21	2.60	0.42
5:J:147:DA:C6	5:J:148:DT:C4	3.07	0.42
5:J:258:DT:H2''	5:J:259:DA:C8	2.53	0.42
1:E:37:LYS:N	1:E:38:PRO:HA	2.35	0.42
4:D:68:ASP:O	4:D:72:ARG:HG3	2.20	0.42
4:D:86:ARG:HB3	4:D:86:ARG:HE	1.67	0.42
2:F:92:ARG:HB3	2:F:92:ARG:NH1	2.35	0.42
5:I:145:DA:N6	5:J:147:DA:N6	2.68	0.41
1:E:118:THR:OG1	2:F:45:ARG:NH1	2.51	0.41
4:H:116:LYS:HE3	4:H:116:LYS:HB2	1.77	0.41
4:H:34:LYS:HE3	4:H:34:LYS:HB2	1.72	0.41
5:I:106:DT:H2''	5:I:107:DC:H5'	2.02	0.41
5:I:18:DG:H2''	5:I:19:DA:H5''	2.02	0.41
5:J:282:DT:H2'	5:J:283:DG:C8	2.55	0.41
5:J:187:DA:H2''	5:J:188:DA:C8	2.55	0.41
1:E:125:GLN:HB3	1:E:134:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLU:OE1	4:D:48:VAL:HB	2.21	0.41
5:I:29:DA:H2'	5:I:30:DA:C8	2.56	0.41
5:J:157:DA:H2''	5:J:158:DC:H5'	2.03	0.41
4:H:120:LYS:HB2	4:H:120:LYS:HE3	1.76	0.41
1:E:65:LEU:HB3	1:E:66:PRO:HD3	2.03	0.41
4:D:98:VAL:O	4:D:102:LEU:HB2	2.20	0.40
3:G:84:ARG:O	3:G:88:LEU:HG	2.21	0.40
5:J:162:DC:H2'	5:J:162:DC:H6	1.63	0.40
5:J:210:DT:H2'	5:J:211:DT:H71	2.02	0.40
5:J:147:DA:C2	5:J:148:DT:C2	3.09	0.40
5:J:216:DT:H2''	5:J:217:DG:C8	2.57	0.40
5:I:50:DC:H42	5:J:243:DG:H1	1.69	0.40
4:D:80:LEU:HD11	4:D:96:THR:HB	2.03	0.40
3:C:31:ARG:NH1	4:D:36:SER:O	2.54	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.91	0.40
5:I:1:DA:C2	5:I:2:DT:C2	3.09	0.40
5:I:108:DC:H2''	5:I:109:DA:C8	2.57	0.40
5:J:149:DC:N4	5:J:150:DA:C6	2.90	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%)	94 (99%)	1 (1%)	0	100	100
1	E	96/139 (69%)	94 (98%)	2 (2%)	0	100	100
2	B	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
2	F	82/106 (77%)	79 (96%)	3 (4%)	0	100	100
3	C	104/131 (79%)	97 (93%)	7 (7%)	0	100	100
3	G	102/131 (78%)	94 (92%)	7 (7%)	1 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	91/129 (70%)	87 (96%)	3 (3%)	1 (1%)	17	55
4	H	91/129 (70%)	87 (96%)	3 (3%)	1 (1%)	17	55
All	All	737/1010 (73%)	704 (96%)	30 (4%)	3 (0%)	39	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	123	SER
4	H	105	GLU
3	G	115	LYS

### 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	85/113 (75%)	83 (98%)	2 (2%)	57	84
1	E	86/113 (76%)	84 (98%)	2 (2%)	58	84
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	69/81 (85%)	68 (99%)	1 (1%)	74	91
3	C	83/99 (84%)	80 (96%)	3 (4%)	42	77
3	G	82/99 (83%)	80 (98%)	2 (2%)	57	84
4	D	79/107 (74%)	79 (100%)	0	100	100
4	H	79/107 (74%)	77 (98%)	2 (2%)	55	84
All	All	626/800 (78%)	614 (98%)	12 (2%)	65	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	87	SER
3	C	21	GLN
3	C	73	SER

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Mol	Chain	Res	Type
3	C	116	SER
1	E	37	LYS
1	E	117	VAL
2	F	47	SER
3	G	17	VAL
3	G	38	SER
4	H	87	SER
4	H	115	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	114	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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	97/139 (69%)	-0.37	0 100 100	26, 42, 64, 104	0
1	E	98/139 (70%)	-0.40	1 (1%) 84 68	21, 33, 60, 99	0
2	B	78/106 (73%)	-0.45	0 100 100	30, 39, 52, 61	0
2	F	84/106 (79%)	-0.45	0 100 100	23, 33, 52, 78	0
3	C	106/131 (80%)	-0.25	2 (1%) 70 47	25, 42, 87, 112	0
3	G	104/131 (79%)	-0.31	0 100 100	33, 52, 87, 111	0
4	D	93/129 (72%)	-0.28	1 (1%) 82 65	29, 43, 65, 102	0
4	H	93/129 (72%)	-0.37	0 100 100	32, 50, 74, 109	0
5	I	146/146 (100%)	0.24	8 (5%) 29 12	46, 103, 140, 147	0
5	J	146/146 (100%)	0.18	4 (2%) 58 33	51, 104, 140, 154	0
All	All	1045/1302 (80%)	-0.20	16 (1%) 76 57	21, 49, 127, 154	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	6.2
1	E	37	LYS	4.6
3	C	15	LYS	3.5
3	C	120	LYS	3.2
5	I	44	DC	3.1
5	J	147	DA	3.1
5	J	262	DC	3.0
5	I	55	DA	2.9
5	J	233	DG	2.5
5	I	15	DG	2.5
5	I	56	DA	2.4
5	I	104	DT	2.2
5	J	241	DA	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	32	SER	2.1
5	I	16	DC	2.0
5	I	106	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.