



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:25 PM GMT

PDB ID : 3A6N
Title : The nucleosome containing a testis-specific histone variant, human H3T
Authors : Tachiwana, H.; Kagawa, W.; Osakabe, A.; Koichiro, K.; Shiga, T.; Kimura, H.; Kurumizaka, H.
Deposited on : 2009-09-04
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

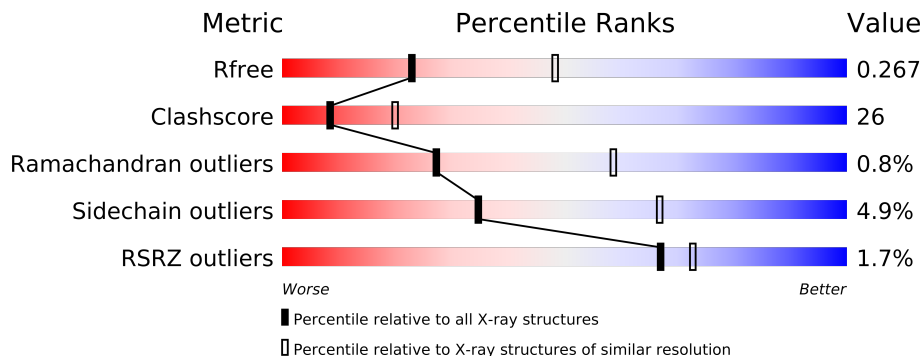
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	139	
1	E	139	
2	B	106	
2	F	106	
3	C	133	
3	G	133	
4	D	129	
4	H	129	
5	I	146	
5	J	146	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	MN	D	201	-	X
7	MN	I	203	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12062 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H3.1t.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			805	507	155	138	5			
1	E	98	Total	C	N	O	S	0	0	0
			811	510	156	140	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q16695
A	-2	SER	-	EXPRESSION TAG	UNP Q16695
A	-1	HIS	-	EXPRESSION TAG	UNP Q16695
E	-3	GLY	-	EXPRESSION TAG	UNP Q16695
E	-2	SER	-	EXPRESSION TAG	UNP Q16695
E	-1	HIS	-	EXPRESSION TAG	UNP Q16695

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			646	407	126	112	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	105	Total	C	N	O	0	0	0
			810	511	158	141			
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	94	Total	C	N	O	S	0	0	0
			736	462	134	138	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 146-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	P	0	0	0
			2970	1421	538	867	144			
5	J	145	Total	C	N	O	P	0	0	0
			2969	1421	535	869	144			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Cl 1	0	0
6	A	1	Total 1	Cl 1	0	0
6	C	1	Total 1	Cl 1	0	0
6	E	1	Total 1	Cl 1	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	4	Total 4	Mn 4	0	0
7	I	3	Total 3	Mn 3	0	0
7	D	1	Total 1	Mn 1	0	0

- Molecule 8 is water.

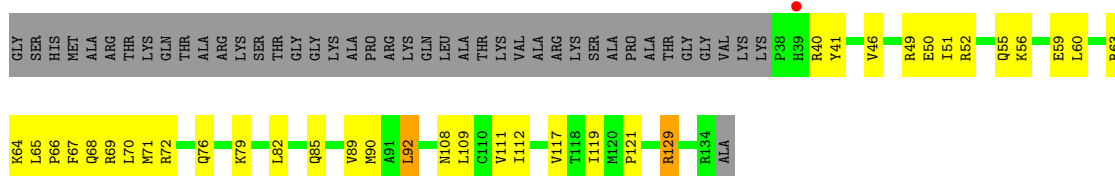
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total 8	O 8	0	0
8	B	9	Total 9	O 9	0	0
8	C	11	Total 11	O 11	0	0
8	D	9	Total 9	O 9	0	0
8	E	18	Total 18	O 18	0	0
8	F	13	Total 13	O 13	0	0
8	G	6	Total 6	O 6	0	0
8	H	7	Total 7	O 7	0	0
8	I	5	Total 5	O 5	0	0
8	J	14	Total 14	O 14	0	0

3 Residue-property plots

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

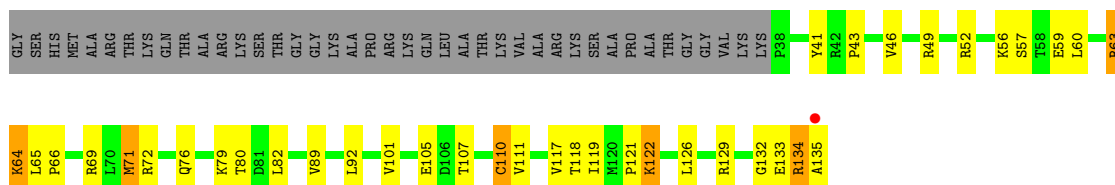
- Molecule 1: Histone H3.1t

Chain A: 



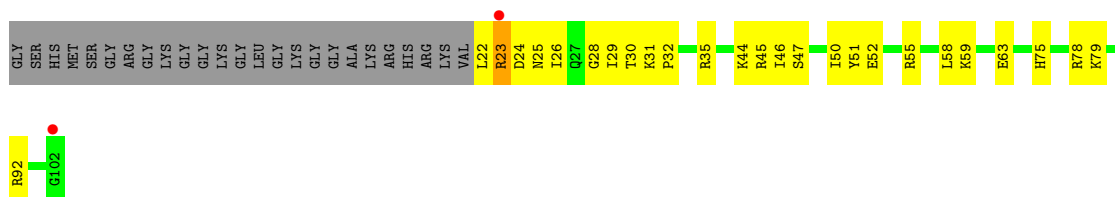
- Molecule 1: Histone H3.1t

Chain E: 



- Molecule 2: Histone H4

Chain B: 



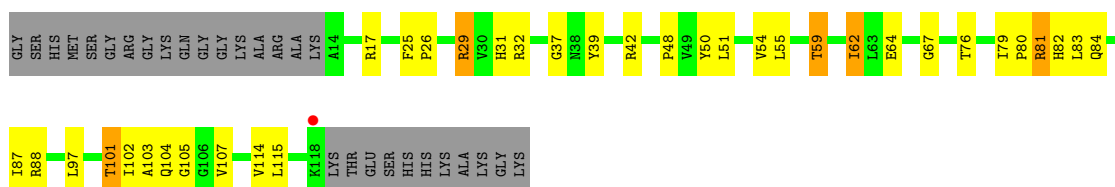
- Molecule 2: Histone H4

Chain F: 



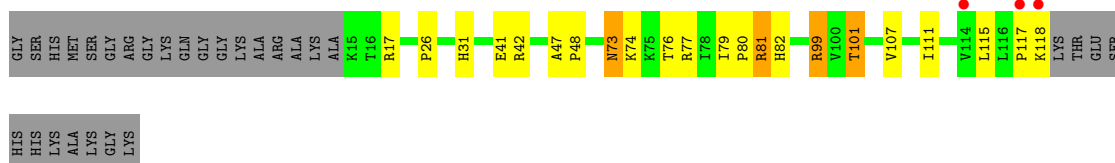
- Molecule 3: Histone H2A type 1-B/E

Chain C: 



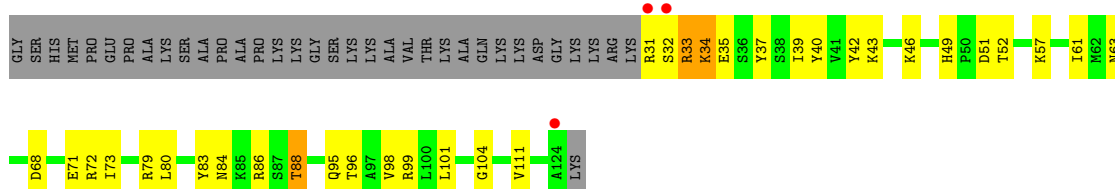
• Molecule 3: Histone H2A type 1-B/E

Chain G:



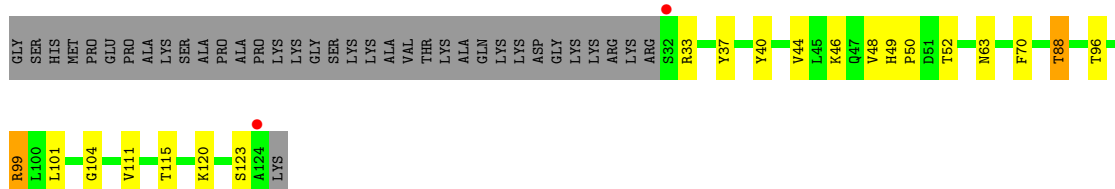
• Molecule 4: Histone H2B type 1-J

Chain D:



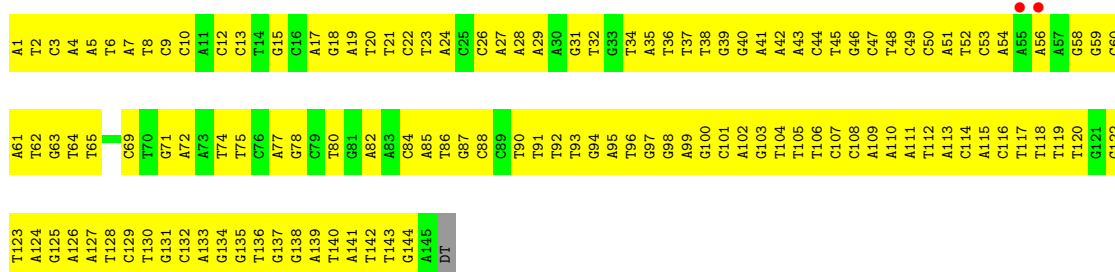
• Molecule 4: Histone H2B type 1-J

Chain H:



• Molecule 5: 146-MER DNA

Chain I:



• Molecule 5: 146-MER DNA

Chain J:

T269										DA									
A270										T148									
G271										C149									
A272										A150									
A273										A151									
T274										T152									
C275										A153									
T276										T154									
G277										C155									
C278										C156									
A279										A157									
G280										C158									
G281										C159									
T282										T160									
G283										G161									
G284										C162									
A285										A163									
T286										G164									
A287										T227									
T288										T228									
G289										A229									
A291										C230									
T292										A231									
										T232									
										G233									
										C234									
										C235									
										T236									
										T237									
										T238									
										T239									
										G241									
										A241									
										T242									
										G243									
										G244									
										A245									
										G246									
										C247									
										A248									
										G249									
										T250									
										T251									
										T252									
										C253									
										C254									
										A255									
										A256									
										A257									
										T258									
										A259									
										C260									
										A261									
										C262									
										T263									
										T264									
										T265									
										T266									
										G267									
										T268									
										G205									
										C206									
										A207									
										T208									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.48Å 109.52Å 181.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 38.88 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 98.5 (38.88-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.56 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.264 0.230 , 0.267	Depositor DCC
R_{free} test set	2921 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.4	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59477 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12062	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CL

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	0.42	0/817	0.64	0/1094
1	E	0.54	1/823 (0.1%)	0.67	0/1101
2	B	0.42	0/653	0.66	0/873
2	F	0.49	0/680	0.70	0/908
3	C	0.43	0/820	0.64	0/1107
3	G	0.38	0/815	0.61	0/1100
4	D	0.44	0/747	0.61	0/1004
4	H	0.41	0/736	0.59	0/990
5	I	0.40	0/3332	0.79	0/5141
5	J	0.39	0/3330	0.80	0/5138
All	All	0.42	1/12753 (0.0%)	0.73	0/18456

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
5	J	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	110	CYS	CB-SG	-5.49	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	214	DG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	805	0	843	44	0
1	E	811	0	848	45	0
2	B	646	0	687	28	0
2	F	673	0	722	34	0
3	C	810	0	866	38	0
3	G	805	0	861	25	0
4	D	736	0	758	41	0
4	H	725	0	745	20	0
5	I	2970	0	1640	174	0
5	J	2969	0	1641	190	0
6	A	1	0	0	1	0
6	C	1	0	0	0	0
6	E	1	0	0	1	0
6	G	1	0	0	0	0
7	D	1	0	0	0	0
7	I	3	0	0	0	0
7	J	4	0	0	0	0
8	A	8	0	0	0	0
8	B	9	0	0	1	0
8	C	11	0	0	0	0
8	D	9	0	0	4	0
8	E	18	0	0	1	0
8	F	13	0	0	1	0
8	G	6	0	0	1	0
8	H	7	0	0	0	0
8	I	5	0	0	1	0
8	J	14	0	0	1	0
All	All	12062	0	9611	560	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

The worst 5 of 560 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:J:242:DT:H2''	5:J:243:DG:H5''	1.31	1.09
5:J:152:DT:H2''	5:J:153:DA:H5''	1.30	1.08
5:I:36:DT:H2''	5:I:37:DT:H5''	1.32	1.06
5:I:101:DC:H2''	5:I:102:DA:H5'	1.36	1.04
5:I:47:DC:H2''	5:I:48:DT:H5''	1.41	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	96/139 (69%)	92 (96%)	3 (3%)	1 (1%)	22	51
2	B	79/106 (74%)	77 (98%)	1 (1%)	1 (1%)	18	43
2	F	82/106 (77%)	79 (96%)	3 (4%)	0	100	100
3	C	103/133 (77%)	100 (97%)	3 (3%)	0	100	100
3	G	102/133 (77%)	97 (95%)	4 (4%)	1 (1%)	22	51
4	D	92/129 (71%)	87 (95%)	4 (4%)	1 (1%)	21	49
4	H	91/129 (70%)	85 (93%)	4 (4%)	2 (2%)	10	25
All	All	740/1014 (73%)	710 (96%)	24 (3%)	6 (1%)	27	58

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	23	ARG
4	D	104	GLY
4	H	104	GLY
4	H	123	SER
3	G	117	PRO

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	87/116 (75%)	83 (95%)	4 (5%)	37	70
1	E	87/116 (75%)	82 (94%)	5 (6%)	29	58
2	B	66/81 (82%)	63 (96%)	3 (4%)	38	70
2	F	69/81 (85%)	68 (99%)	1 (1%)	78	95
3	C	83/102 (81%)	77 (93%)	6 (7%)	21	45
3	G	83/102 (81%)	77 (93%)	6 (7%)	21	45
4	D	80/107 (75%)	76 (95%)	4 (5%)	34	66
4	H	79/107 (74%)	77 (98%)	2 (2%)	60	89
All	All	634/812 (78%)	603 (95%)	31 (5%)	35	67

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	34	LYS
1	E	56	LYS
3	G	118	LYS
4	D	71	GLU
1	E	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	112	GLN
4	D	49	HIS
2	F	75	HIS
3	C	84	GLN
3	G	31	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	97/139 (69%)	0.16	1 (1%) 79 83	28, 43, 61, 87	0
1	E	98/139 (70%)	-0.05	1 (1%) 79 83	24, 36, 54, 73	0
2	B	81/106 (76%)	0.04	2 (2%) 54 61	30, 40, 63, 87	0
2	F	84/106 (79%)	-0.13	1 (1%) 75 81	20, 33, 50, 64	0
3	C	105/133 (78%)	-0.10	1 (0%) 79 83	20, 39, 61, 80	0
3	G	104/133 (78%)	0.04	3 (2%) 49 55	30, 45, 74, 103	0
4	D	94/129 (72%)	0.08	3 (3%) 45 50	25, 39, 65, 102	0
4	H	93/129 (72%)	0.12	2 (2%) 59 65	28, 43, 75, 94	0
5	I	145/146 (99%)	0.19	2 (1%) 72 77	45, 95, 133, 156	0
5	J	145/146 (99%)	0.22	2 (1%) 72 77	49, 97, 135, 147	0
All	All	1046/1306 (80%)	0.07	18 (1%) 67 73	20, 46, 124, 156	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	32	SER	8.5
3	G	118	LYS	5.0
4	D	31	ARG	4.3
3	C	118	LYS	3.8
1	A	39	HIS	3.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MN	D	201	1/1	0.25	7.27	35,35,35,35	0
7	MN	I	203	1/1	0.25	4.97	85,85,85,85	0
6	CL	G	201	1/1	0.14	-0.46	45,45,45,45	0
7	MN	J	1004	1/1	0.17	-0.46	72,72,72,72	0
7	MN	I	201	1/1	0.12	-1.32	127,127,127,127	0
7	MN	J	1002	1/1	0.07	-2.52	85,85,85,85	0
7	MN	I	202	1/1	0.09	-2.90	121,121,121,121	0
6	CL	A	201	1/1	0.08	-2.91	64,64,64,64	0
7	MN	J	1001	1/1	0.09	-3.16	112,112,112,112	0
6	CL	C	2001	1/1	0.09	-3.31	48,48,48,48	0
6	CL	E	201	1/1	0.06	-4.96	57,57,57,57	0
7	MN	J	1003	1/1	0.07	-7.78	85,85,85,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.