WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:18 pm GMT

PDB ID	:	4YM5
Title	:	Crystal structure of the human nucleosome containing 6-4PP (inside)
Authors	:	Osakabe, A.; Tachiwana, H.; Kagawa, W.; Horikoshi, N.; Matsumoto, S.; Hasegawa, M.; Matsumoto, N.; Toga, T.; Yamamoto, J.; Hanaoka, F.; Thoma, N.H.; Sugasawa, K.; Iwai, S.; Kurumizaka, H.
Deposited on	:	2015-03-06
Resolution	:	4.00 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
http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 4.00 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.
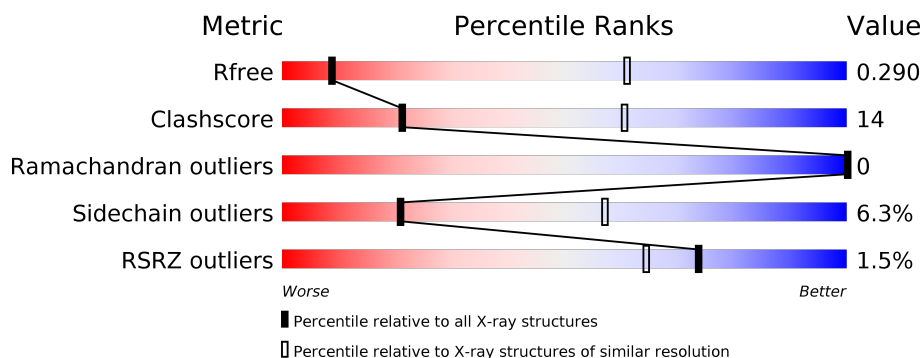
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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. 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	47% 23% • 29%
1	E	139	44% 24% • 30%
2	B	106	42% 31% • 25%
2	F	106	42% 40% • 18%
3	C	133	49% 29% • 21%
3	G	133	50% 25% • 23%

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Mol	Chain	Length	Quality of chain
4	D	129	39% · · · 30% · 28%
4	H	129	2% 42% 31% · 25%
5	I	144	3% 58% 42%
6	J	144	3% 51% 47% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 11974 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	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	E	97	Total	C	N	O	S	0	0	0
			801	505	155	137	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	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total 810	C 511	N 158	O 141	0	0	0
3	G	103	Total 796	C 502	N 155	O 139	0	0	0

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	93	Total 725	C 456	N 130	O 137	S 2	0	0	0
4	H	97	Total 766	C 480	N 142	O 142	S 2	0	0	0

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 144 mer-DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	144	Total 2969	C 1420	N 539	O 866	P 144	0	0	0

- Molecule 6 is a DNA chain called 144-mer DNA.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	J	144	2970	1421	535	870	144	0	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 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.
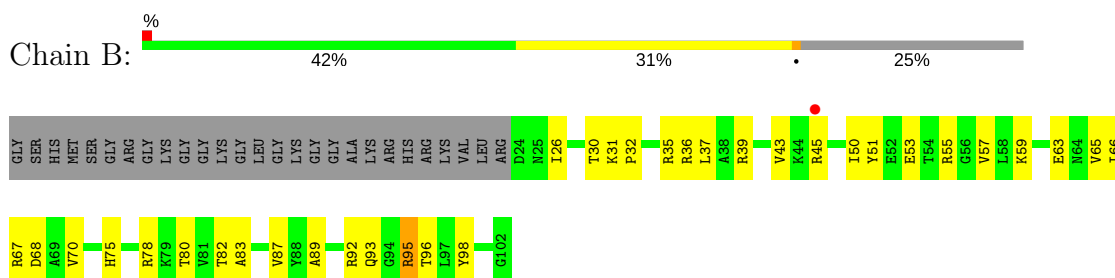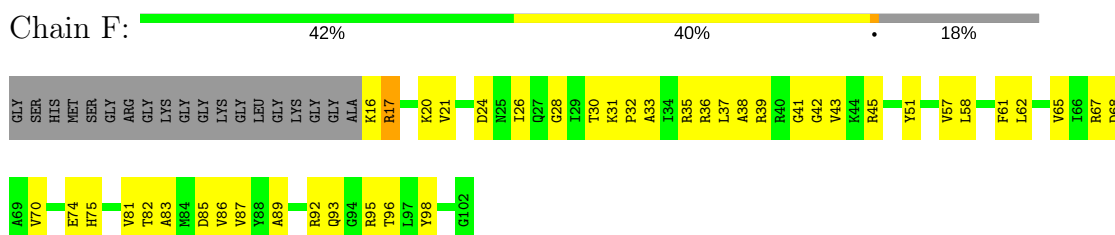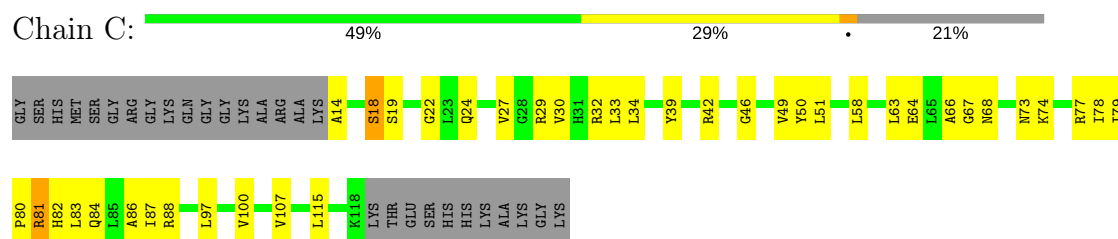
• Molecule 1: Histone H3.1
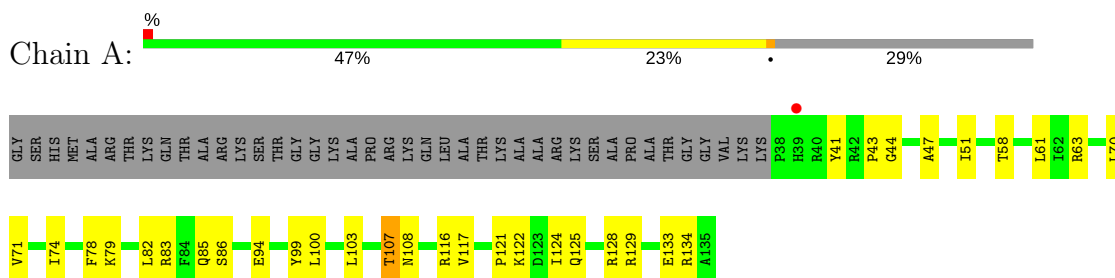
• Molecule 1: Histone H3.1
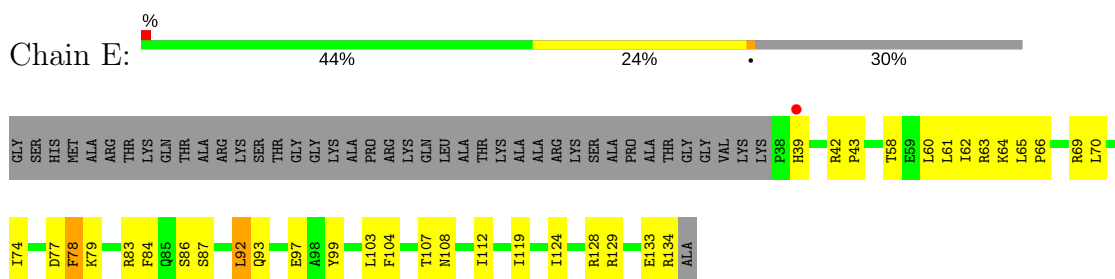
• Molecule 2: Histone H4
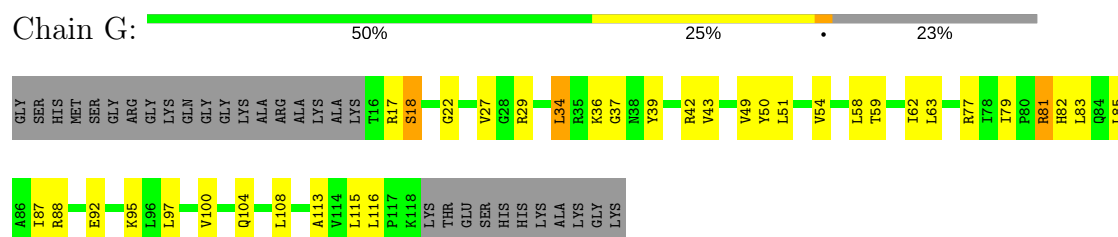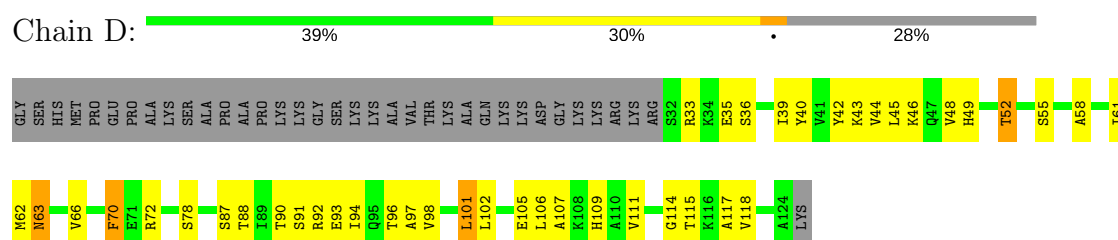

• Molecule 2: Histone H4

• 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:
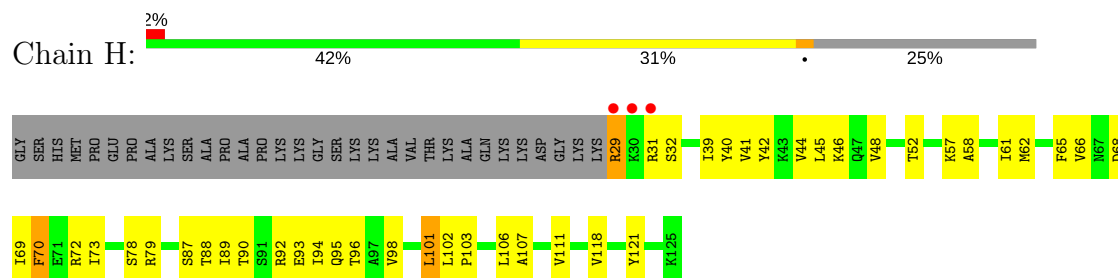
• Molecule 5: 144 mer-DNA

Chain I:
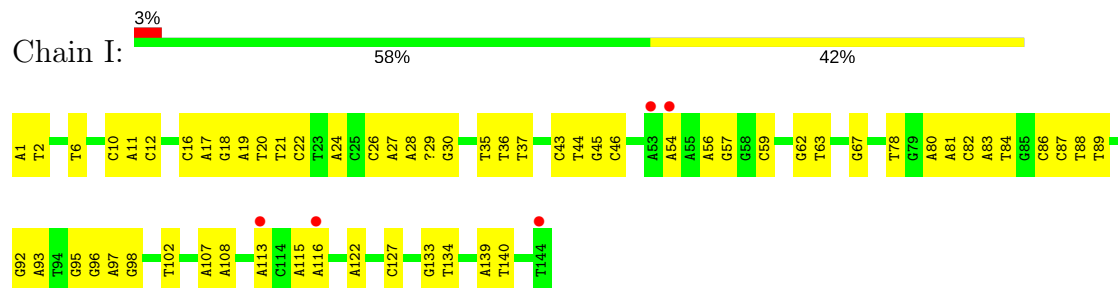
• Molecule 6: 144-mer DNA

Chain J:
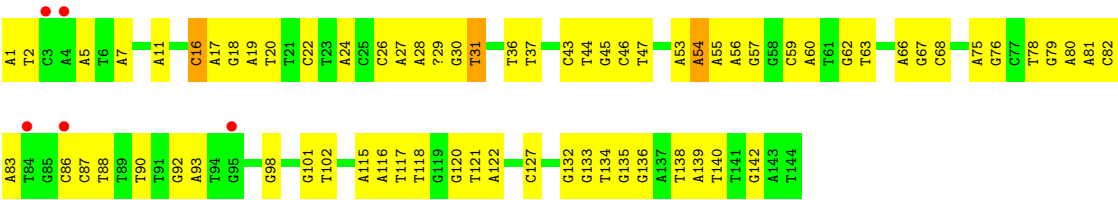
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.19Å 109.36Å 174.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.23 – 4.00 48.42 – 4.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.23-4.00) 95.1 (48.42-4.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.89 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.203 , 0.289 0.203 , 0.290	Depositor DCC
R_{free} test set	866 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	140.4	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 85.3	EDS
L-test for twinning[2]	$<|L|>$ = 0.46, $<L^2>$ = 0.29	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å^2)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T64

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	0.53	0/819	0.66	0/1097
1	E	0.72	1/813 (0.1%)	0.89	2/1090 (0.2%)
2	B	0.57	0/634	0.73	0/848
2	F	0.76	0/711	0.85	0/948
3	C	0.61	0/820	0.83	0/1107
3	G	0.52	0/806	0.75	0/1089
4	D	0.69	0/736	0.78	0/990
4	H	0.59	0/777	0.74	0/1040
5	I	0.89	1/3286 (0.0%)	1.10	6/5067 (0.1%)
6	J	0.88	2/3286 (0.1%)	1.10	6/5068 (0.1%)
All	All	0.77	4/12688 (0.0%)	0.97	14/18344 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	ASP	CB-CG	7.32	1.67	1.51
6	J	16	DC	C3'-O3'	-6.21	1.35	1.44
5	I	84	DT	C1'-N1	6.08	1.57	1.49
6	J	78	DT	C3'-O3'	-5.01	1.37	1.44

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ASP	CB-CG-OD1	8.80	126.22	118.30
5	I	35	DT	O4'-C1'-N1	6.04	112.23	108.00
6	J	24	DA	O4'-C1'-N9	5.93	112.15	108.00
5	I	20	DT	O4'-C1'-N1	5.92	112.15	108.00
1	E	92	LEU	CA-CB-CG	-5.92	101.69	115.30

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	807	0	844	31	0
1	E	801	0	839	36	0
2	B	627	0	663	29	0
2	F	703	0	755	39	0
3	C	810	0	866	36	0
3	G	796	0	848	35	0
4	D	725	0	745	36	0
4	H	766	0	797	34	0
5	I	2969	0	1639	58	0
6	J	2970	0	1641	65	0
All	All	11974	0	9637	290	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 14.

The worst 5 of 290 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PRO:HG2	6:J:67:DG:H5'	1.45	0.99
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.50	0.94
6:J:1:DA:H2"	6:J:2:DT:H5'	1.53	0.91
1:A:117:VAL:HG13	3:G:115:LEU:HD22	1.58	0.85
3:G:77:ARG:HE	6:J:19:DA:H4'	1.42	0.83

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	96/139 (69%)	95 (99%)	1 (1%)	0	100	100
1	E	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
2	B	77/106 (73%)	71 (92%)	6 (8%)	0	100	100
2	F	85/106 (80%)	79 (93%)	6 (7%)	0	100	100
3	C	103/133 (77%)	99 (96%)	4 (4%)	0	100	100
3	G	101/133 (76%)	97 (96%)	4 (4%)	0	100	100
4	D	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
4	H	95/129 (74%)	92 (97%)	3 (3%)	0	100	100
All	All	743/1014 (73%)	716 (96%)	27 (4%)	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	85/113 (75%)	83 (98%)	2 (2%)	54	79
1	E	85/113 (75%)	83 (98%)	2 (2%)	54	79
2	B	64/81 (79%)	58 (91%)	6 (9%)	10	41
2	F	72/81 (89%)	64 (89%)	8 (11%)	7	34
3	C	83/102 (81%)	80 (96%)	3 (4%)	40	72
3	G	82/102 (80%)	79 (96%)	3 (4%)	39	71
4	D	79/107 (74%)	72 (91%)	7 (9%)	11	44
4	H	83/107 (78%)	74 (89%)	9 (11%)	7	36
All	All	633/806 (78%)	593 (94%)	40 (6%)	21	57

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	78	PHE
2	F	24	ASP
4	H	87	SER
2	F	16	LYS
2	F	26	ILE

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

Mol	Chain	Res	Type
4	D	49	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	T64	I	29	5	35,44,45	1.33	2 (5%)	46,69,72	1.77	9 (19%)
6	T64	J	29	6	35,44,45	1.50	3 (8%)	46,69,72	1.86	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	T64	I	29	5	-	0/21/76/77	0/1/5/5
6	T64	J	29	6	-	0/21/76/77	0/1/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	29	T64	C2-N1	-4.39	1.27	1.36
5	I	29	T64	C2-N1	-4.16	1.28	1.36
6	J	29	T64	C5T-C4T	-3.33	1.36	1.40
6	J	29	T64	C1'-N1	4.77	1.51	1.45
5	I	29	T64	C1'-N1	5.00	1.52	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	29	T64	C6-C5-C4	-4.39	102.85	109.70
5	I	29	T64	C5T-C4T-N3T	-4.12	118.69	123.34
6	J	29	T64	C4T-C6-N1	-3.34	106.49	110.25
6	J	29	T64	C2'-C3R-C4R	-2.66	97.67	102.97
5	I	29	T64	C2R-C1R-N1T	-2.42	108.51	114.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	29	T64	5	0
6	J	29	T64	2	0

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, 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	98/139 (70%)	0.09	1 (1%)	82	74	117, 147, 194, 209	0
1	E	97/139 (69%)	-0.04	1 (1%)	82	74	92, 117, 155, 182	0
2	B	79/106 (74%)	-0.11	1 (1%)	77	68	111, 138, 160, 172	0
2	F	87/106 (82%)	0.01	0	100	100	89, 107, 141, 189	0
3	C	105/133 (78%)	-0.19	0	100	100	93, 117, 156, 174	0
3	G	103/133 (77%)	-0.15	0	100	100	111, 137, 172, 184	0
4	D	93/129 (72%)	-0.12	0	100	100	99, 121, 159, 191	0
4	H	97/129 (75%)	0.00	3 (3%)	49	39	104, 133, 202, 222	0
5	I	143/144 (99%)	0.14	5 (3%)	44	35	148, 215, 248, 257	0
6	J	143/144 (99%)	0.08	5 (3%)	44	35	148, 214, 250, 271	0
All	All	1045/1302 (80%)	-0.02	16 (1%)	74	64	89, 140, 235, 271	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	30	LYS	4.0
5	I	53	DA	3.8
5	I	116	DA	3.5
6	J	4	DA	3.3
1	E	39	HIS	3.0

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

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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
6	T64	J	29	40/41	0.77	0.31	-	186,220,233,235	0
5	T64	I	29	40/41	0.76	0.20	-	175,212,232,234	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.