



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 11:45 PM GMT

PDB ID : 3B6F
Title : Nucleosome core particle treated with cisplatin
Authors : Wu, B.; Davey, C.A.
Deposited on : 2007-10-29
Resolution : 3.45 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>

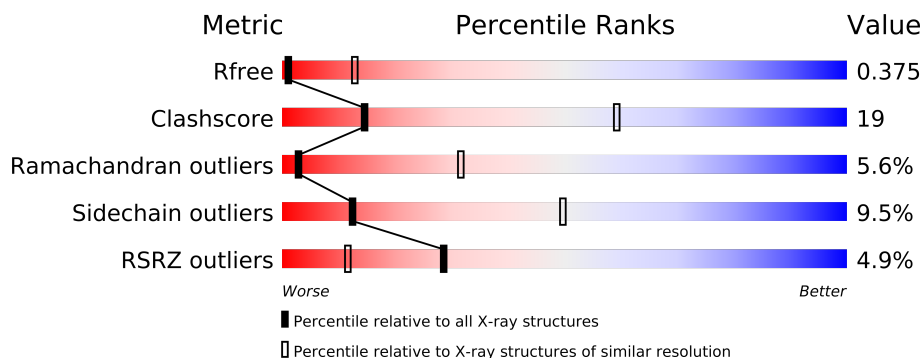
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.45 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)

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	I	147	
2	J	147	
3	A	135	
3	E	135	
4	B	102	
4	F	102	
5	C	128	
5	G	128	
6	D	125	
6	H	125	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12291 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 DNA chain called 147-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	147	Total	C	N	O	P	0	0	0
			3011	1440	546	879	146			

- Molecule 2 is a DNA chain called 147-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	147	Total	C	N	O	P	0	0	0
			3010	1440	543	881	146			

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	103	Total	C	N	O	S	0	0	0
			841	530	163	145	3			
3	E	105	Total	C	N	O	S	0	0	0
			853	537	165	148	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	CONFLICT	UNP P84233
E	102	ALA	GLY	CONFLICT	UNP P84233

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
4	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	106	Total	C	N	O	0	0	0
			820	517	160	143			
5	G	109	Total	C	N	O	0	0	0
			843	531	164	148			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	DELETION	UNP Q6AZJ8
G	?	-	ALA	DELETION	UNP Q6AZJ8

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	101	Total	C	N	O	S	0	0	0
			797	499	148	148	2			
6	H	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	CONFLICT	UNP P02281
H	29	THR	SER	CONFLICT	UNP P02281

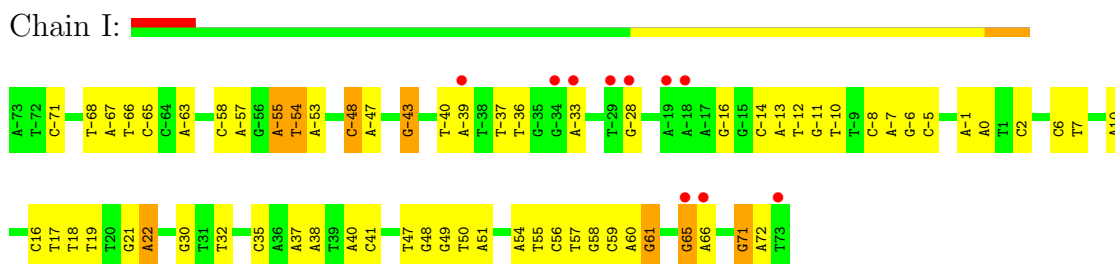
- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Mn	0	0
			1	1		

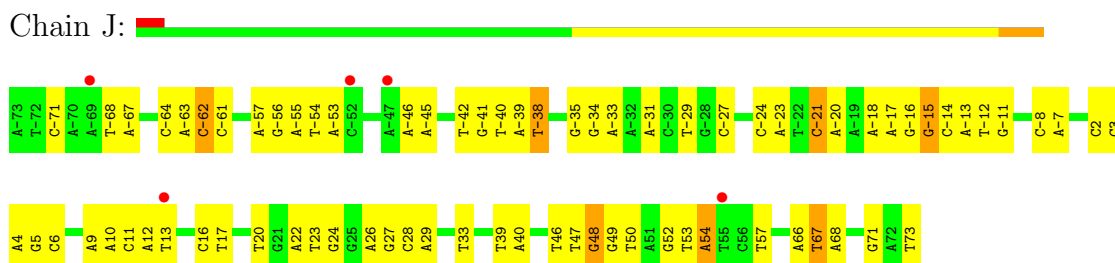
3 Residue-property plots

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.

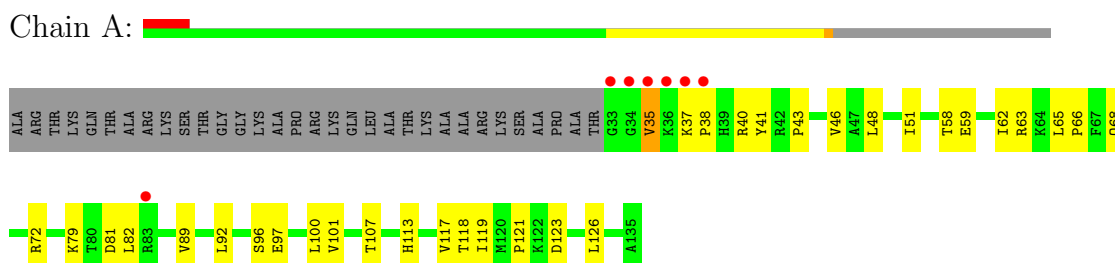
• Molecule 1: 147-MER DNA



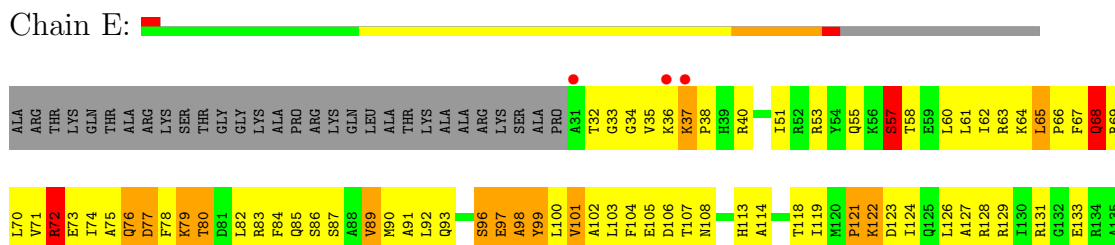
• Molecule 2: 147-MER DNA



• Molecule 3: Histone H3.2

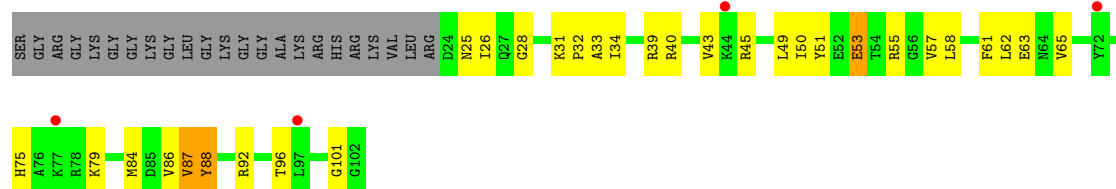


• Molecule 3: Histone H3.2



- Molecule 4: Histone H4

Chain B:



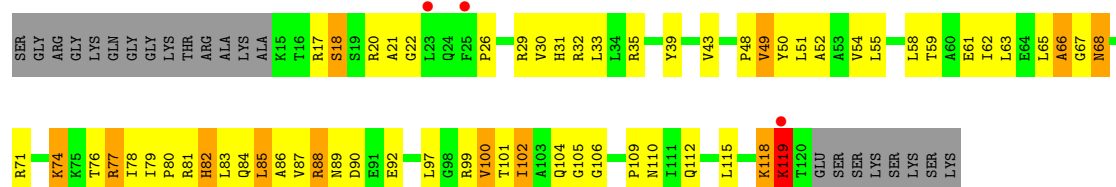
- Molecule 4: Histone H4

Chain F:



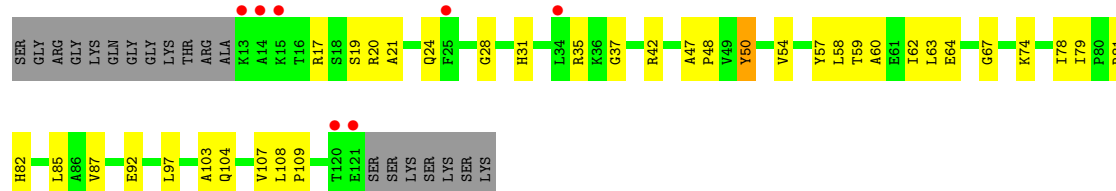
- Molecule 5: Histone H2A

Chain C:



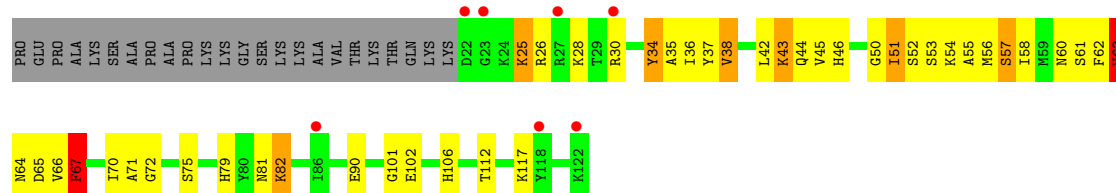
- Molecule 5: Histone H2A

Chain G:



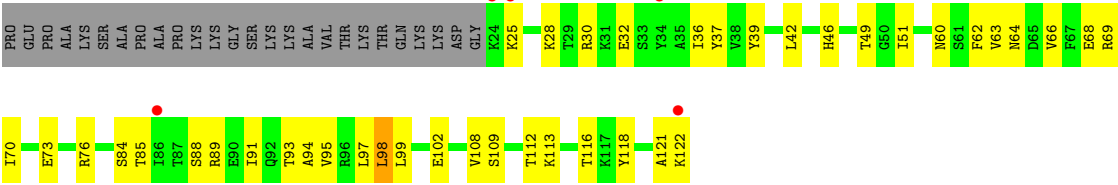
- Molecule 6: Histone H2B 1.1

Chain D:



- Molecule 6: Histone H2B 1.1

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.33Å 109.38Å 180.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.66 – 3.45 93.56 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.9 (93.66-3.45) 98.9 (93.56-3.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.330 , 0.402 0.315 , 0.375	Depositor DCC
R_{free} test set	588 reflections (2.14%)	DCC
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 113.3	EDS
Estimated twinning fraction	0.066 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 28107 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12291	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

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	I	0.65	0/3378	1.35	23/5212 (0.4%)
2	J	0.65	0/3376	1.32	21/5209 (0.4%)
3	A	0.34	0/853	0.51	0/1142
3	E	0.61	0/865	0.86	1/1159 (0.1%)
4	B	0.32	0/634	0.56	0/848
4	F	0.68	0/711	0.82	0/948
5	C	0.52	0/830	0.77	2/1120 (0.2%)
5	G	0.32	0/853	0.56	0/1150
6	D	0.58	0/808	0.70	0/1081
6	H	0.35	0/796	0.57	0/1065
All	All	0.58	0/13104	1.09	47/18934 (0.2%)

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
3	E	0	1

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	-10	DT	O4'-C4'-C3'	-8.43	100.94	106.00
1	I	-36	DT	O4'-C1'-N1	7.33	113.13	108.00
2	J	-56	DG	O4'-C1'-N9	7.19	113.03	108.00
1	I	32	DT	O4'-C1'-N1	6.87	112.81	108.00
1	I	35	DC	O4'-C1'-N1	6.83	112.78	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	57	SER	Peptide

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	I	3011	0	1662	51	0
2	J	3010	0	1663	56	0
3	A	841	0	886	32	0
3	E	853	0	898	94	0
4	B	627	0	663	24	0
4	F	703	0	755	84	0
5	C	820	0	879	79	0
5	G	843	0	903	26	0
6	D	797	0	832	53	0
6	H	785	0	825	30	0
7	E	1	0	0	0	0
All	All	12291	0	9966	423	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 19.

The worst 5 of 423 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:79:ILE:HA	6:D:55:ALA:HB2	1.29	1.06
2:J:9:DA:H5'	3:A:43:PRO:HA	1.38	1.05
5:C:39:TYR:HB3	6:D:75:SER:HB2	1.42	1.00
5:C:79:ILE:HG13	5:C:82:HIS:CE1	2.01	0.96
3:E:101:VAL:O	3:E:105:GLU:HG3	1.73	0.89

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	
3	A	101/135 (75%)	85 (84%)	12 (12%)	4 (4%)	5	43
3	E	103/135 (76%)	66 (64%)	25 (24%)	12 (12%)	1	10
4	B	77/102 (76%)	60 (78%)	14 (18%)	3 (4%)	5	44
4	F	85/102 (83%)	59 (69%)	21 (25%)	5 (6%)	2	30
5	C	104/128 (81%)	68 (65%)	31 (30%)	5 (5%)	4	36
5	G	107/128 (84%)	86 (80%)	18 (17%)	3 (3%)	8	54
6	D	99/125 (79%)	68 (69%)	21 (21%)	10 (10%)	1	13
6	H	97/125 (78%)	73 (75%)	23 (24%)	1 (1%)	22	78
All	All	773/980 (79%)	565 (73%)	165 (21%)	43 (6%)	3	31

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	32	THR
3	E	98	ALA
3	E	122	LYS
3	A	35	VAL
3	A	81	ASP

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	
3	A	88/110 (80%)	87 (99%)	1 (1%)	84	96
3	E	89/110 (81%)	76 (85%)	13 (15%)	5	26
4	B	64/78 (82%)	60 (94%)	4 (6%)	25	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	72/78 (92%)	57 (79%)	15 (21%)	2	9
5	C	85/101 (84%)	74 (87%)	11 (13%)	6	32
5	G	87/101 (86%)	84 (97%)	3 (3%)	49	88
6	D	86/105 (82%)	79 (92%)	7 (8%)	17	60
6	H	85/105 (81%)	77 (91%)	8 (9%)	13	50
All	All	656/788 (83%)	594 (90%)	62 (10%)	12	50

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	73	GLU
3	E	99	TYR
6	H	84	SER
3	E	80	THR
4	F	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	64	ASN
3	E	108	ASN
5	G	31	HIS
5	C	104	GLN
4	F	64	ASN

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 1 ligands modelled in this entry, 1 is 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	I	147/147 (100%)	-0.03	10 (6%) 17 8	147, 237, 259, 262	0
2	J	147/147 (100%)	-0.08	5 (3%) 43 18	140, 239, 262, 268	0
3	A	103/135 (76%)	0.68	7 (6%) 17 8	142, 169, 230, 234	0
3	E	105/135 (77%)	0.28	3 (2%) 49 22	64, 105, 199, 207	0
4	B	79/102 (77%)	0.43	4 (5%) 27 11	143, 158, 174, 175	0
4	F	87/102 (85%)	0.28	2 (2%) 57 26	60, 98, 120, 143	0
5	C	106/128 (82%)	0.46	3 (2%) 50 22	78, 107, 154, 157	0
5	G	109/128 (85%)	0.55	7 (6%) 19 8	136, 167, 198, 207	0
6	D	101/125 (80%)	0.65	7 (6%) 17 7	72, 131, 176, 190	0
6	H	99/125 (79%)	0.44	5 (5%) 27 11	126, 150, 208, 213	0
All	All	1083/1274 (85%)	0.33	53 (4%) 28 11	60, 157, 251, 268	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	34	GLY	18.2
3	A	33	GLY	8.6
3	A	36	LYS	6.4
6	D	22	ASP	6.2
3	A	38	PRO	5.8

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	E	3132	1/1	0.26	-0.58	83,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.