



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P3K
Title : Crystallographic Studies of Nucleosome Core Particles containing Histone 'Sin' Mutants
Authors : Muthurajan, U.M.; Bao, Y.; Forsberg, L.J.; Edayathumangalam, R.S.; Dyer, P.N.; White, C.L.; Luger, K.
Deposited on : 2003-04-17
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

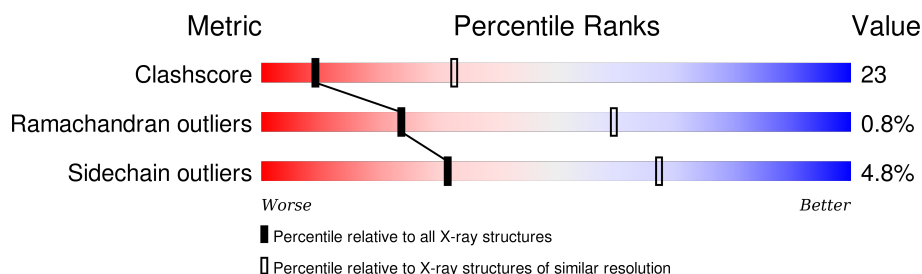
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)




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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	

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Mol	Chain	Length	Quality of chain
4	G	129	 53% 24% • • 18%
5	D	125	 61% 12% • 26%
5	H	125	 47% 26% • • 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12120 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 DNA chain called Palindromic 146bp Human Alpha-Satellite DNA fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	97	Total	C	N	O	S	0	0	0
			799	503	155	138	3			
2	E	99	Total	C	N	O	S	0	0	0
			815	514	158	140	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLU	GLY	CONFLICT	UNP Q7ZT64
A	435	SER	VAL	CONFLICT	UNP Q7ZT64
A	502	ALA	GLY	CONFLICT	UNP Q7ZT64
A	518	ALA	THR	CONFLICT	UNP Q7ZT64
E	634	GLU	GLY	CONFLICT	UNP Q7ZT64
E	635	SER	VAL	CONFLICT	UNP Q7ZT64
E	702	ALA	GLY	CONFLICT	UNP Q7ZT64
E	718	ALA	THR	CONFLICT	UNP Q7ZT64

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
3	F	81	Total	C	N	O	S	0	0	0
			646	407	126	112	1			

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	106	Total	C	N	O	0	0	0
			820	517	160	143			
4	G	106	Total	C	N	O	0	0	0
			818	516	160	142			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	814	ALA	SER	CONFLICT	UNP Q7ZT66
C	867	GLY	TRP	CONFLICT	UNP Q7ZT66
C	868	ASN	GLU	CONFLICT	UNP Q7ZT66
C	869	ALA	ARG	CONFLICT	UNP Q7ZT66
C	870	ALA	LEU	CONFLICT	UNP Q7ZT66
C	871	ARG	PRO	CONFLICT	UNP Q7ZT66
C	872	ASP	GLU	CONFLICT	UNP Q7ZT66
C	873	ASN	ILE	CONFLICT	UNP Q7ZT66
C	874	LYS	TRP	CONFLICT	UNP Q7ZT66
C	876	THR	ARG	CONFLICT	UNP Q7ZT66
C	877	ARG	PRO	CONFLICT	UNP Q7ZT66
C	878	ILE	VAL	CONFLICT	UNP Q7ZT66
C	879	ILE	LEU	CONFLICT	UNP Q7ZT66
C	880	PRO	SER	CONFLICT	UNP Q7ZT66
C	881	ARG	PRO	CONFLICT	UNP Q7ZT66
C	882	HIS	GLY	CONFLICT	UNP Q7ZT66
C	883	LEU	TRP	CONFLICT	UNP Q7ZT66
C	884	GLN	CYS	CONFLICT	UNP Q7ZT66
C	885	LEU	ASN	CONFLICT	UNP Q7ZT66
C	886	ALA	SER	CONFLICT	UNP Q7ZT66
C	887	VAL	LEU	CONFLICT	UNP Q7ZT66
C	888	ARG	CYS	CONFLICT	UNP Q7ZT66
C	923	ALA	SER	CONFLICT	UNP Q7ZT66
C	926	ALA	THR	CONFLICT	UNP Q7ZT66
G	1014	ALA	SER	CONFLICT	UNP Q7ZT66
G	1067	GLY	TRP	CONFLICT	UNP Q7ZT66
G	1068	ASN	GLU	CONFLICT	UNP Q7ZT66
G	1069	ALA	ARG	CONFLICT	UNP Q7ZT66
G	1070	ALA	LEU	CONFLICT	UNP Q7ZT66
G	1071	ARG	PRO	CONFLICT	UNP Q7ZT66
G	1072	ASP	GLU	CONFLICT	UNP Q7ZT66
G	1073	ASN	ILE	CONFLICT	UNP Q7ZT66
G	1074	LYS	TRP	CONFLICT	UNP Q7ZT66
G	1076	THR	ARG	CONFLICT	UNP Q7ZT66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1077	ARG	PRO	CONFLICT	UNP Q7ZT66
G	1078	ILE	VAL	CONFLICT	UNP Q7ZT66
G	1079	ILE	LEU	CONFLICT	UNP Q7ZT66
G	1080	PRO	SER	CONFLICT	UNP Q7ZT66
G	1081	ARG	PRO	CONFLICT	UNP Q7ZT66
G	1082	HIS	GLY	CONFLICT	UNP Q7ZT66
G	1083	LEU	TRP	CONFLICT	UNP Q7ZT66
G	1084	GLN	CYS	CONFLICT	UNP Q7ZT66
G	1085	LEU	ASN	CONFLICT	UNP Q7ZT66
G	1086	ALA	SER	CONFLICT	UNP Q7ZT66
G	1087	VAL	LEU	CONFLICT	UNP Q7ZT66
G	1088	ARG	CYS	CONFLICT	UNP Q7ZT66
G	1123	ALA	SER	CONFLICT	UNP Q7ZT66
G	1126	ALA	THR	CONFLICT	UNP Q7ZT66

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	92	Total	C	N	O	S	0	0	0
			718	453	127	136	2			
5	H	94	Total	C	N	O	S	0	0	0
			735	462	132	139	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1219	GLN	PRO	CONFLICT	UNP P02281
D	1242	LEU	MET	CONFLICT	UNP P02281
D	1257	SER	GLY	CONFLICT	UNP P02281
D	1266	VAL	ILE	CONFLICT	UNP P02281
H	1419	GLN	PRO	CONFLICT	UNP P02281
H	1442	LEU	MET	CONFLICT	UNP P02281
H	1457	SER	GLY	CONFLICT	UNP P02281
H	1466	VAL	ILE	CONFLICT	UNP P02281

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	9	Total	O	0	0
			9	9		

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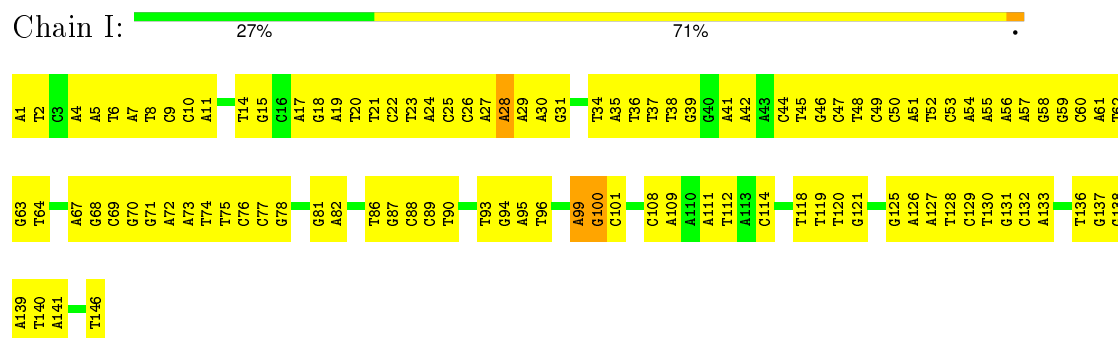
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	19	Total 19	O 19	0	0
6	D	9	Total 9	O 9	0	0
6	E	16	Total 16	O 16	0	0
6	F	17	Total 17	O 17	0	0
6	G	11	Total 11	O 11	0	0
6	H	10	Total 10	O 10	0	0
6	I	38	Total 38	O 38	0	0
6	J	22	Total 22	O 22	0	0

3 Residue-property plots

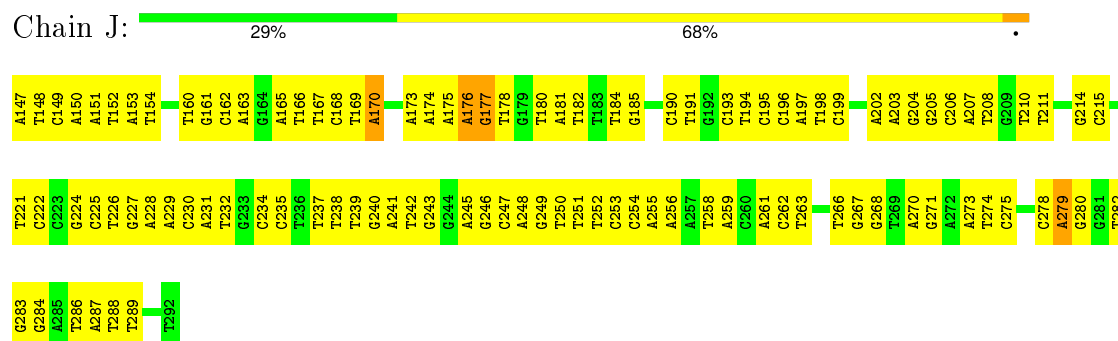
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

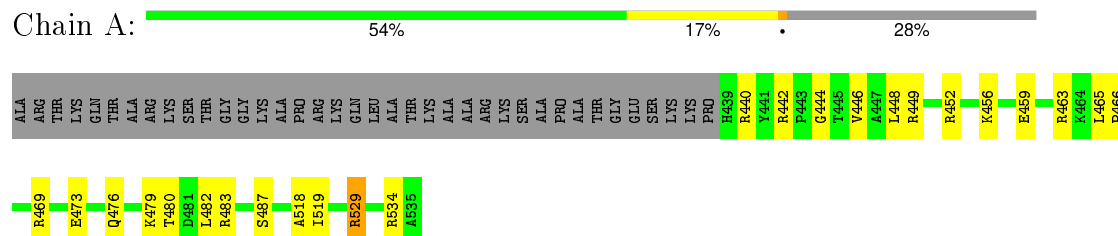
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment



- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment



- Molecule 2: Histone H3



- Molecule 2: Histone H3

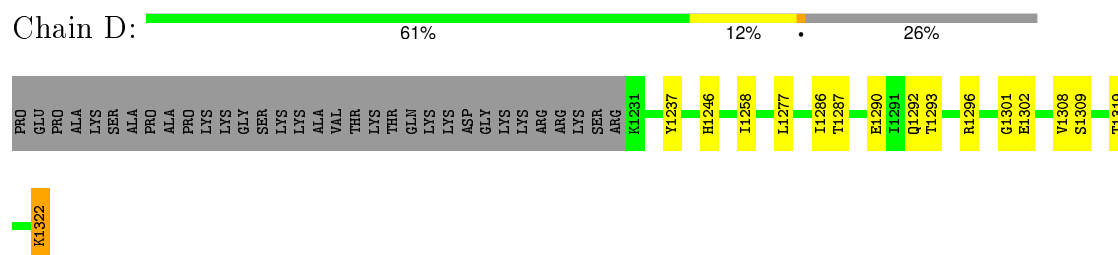
- Molecule 3: Histone H4

- Molecule 3: Histone H4

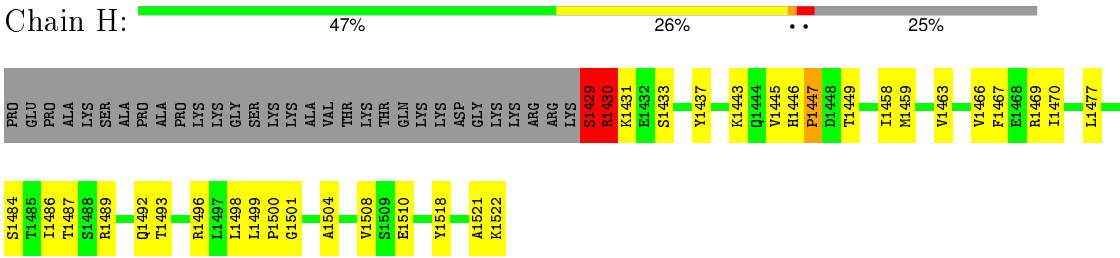
- Molecule 4: Histone H2A

- Molecule 4: Histone H2A

- Molecule 5: Histone H2B



● Molecule 5: Histone H2B



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.99Å 109.68Å 180.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.9 (50.00-2.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

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	I	0.57	0/3354	0.80	4/5175 (0.1%)
1	J	0.60	0/3354	0.85	4/5175 (0.1%)
2	A	0.61	0/810	0.67	0/1085
2	E	0.94	4/827 (0.5%)	0.95	6/1108 (0.5%)
3	B	0.57	0/634	0.74	0/848
3	F	0.73	0/653	0.84	1/873 (0.1%)
4	C	0.59	0/830	0.78	1/1120 (0.1%)
4	G	1.76	12/828 (1.4%)	1.28	13/1117 (1.2%)
5	D	0.81	1/729 (0.1%)	0.89	2/980 (0.2%)
5	H	0.73	2/746 (0.3%)	0.80	0/1002
All	All	0.77	19/12765 (0.1%)	0.86	31/18483 (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
1	J	0	2
5	H	0	1
All	All	0	3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1015	LYS	N-CA	26.32	1.99	1.46
4	G	1015	LYS	CB-CG	15.47	1.94	1.52
4	G	1014	ALA	N-CA	15.43	1.77	1.46
4	G	1015	LYS	CA-CB	14.69	1.86	1.53
4	G	1014	ALA	C-O	-13.51	0.97	1.23

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	1016	THR	N-CA-CB	15.80	140.31	110.30
4	G	1015	LYS	CB-CG-CD	12.56	144.27	111.60
4	G	1016	THR	N-CA-C	-11.56	79.78	111.00
4	G	1014	ALA	C-N-CA	10.24	147.29	121.70
4	G	1014	ALA	O-C-N	-9.79	107.04	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	1429	SER	Mainchain
1	J	202	DA	Sidechain
1	J	279	DA	Sidechain

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	I	2990	0	1651	154	0
1	J	2990	0	1651	146	0
2	A	799	0	836	30	0
2	E	815	0	856	36	0
3	B	627	0	663	19	0
3	F	646	0	687	13	0
4	C	820	0	879	47	0
4	G	818	0	876	57	0
5	D	718	0	740	29	0
5	H	735	0	758	34	0
6	A	11	0	0	0	0
6	B	9	0	0	1	0
6	C	19	0	0	1	0
6	D	9	0	0	0	0
6	E	16	0	0	6	0
6	F	17	0	0	3	0
6	G	11	0	0	1	0
6	H	10	0	0	1	0
6	I	38	0	0	3	0
6	J	22	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12120	0	9597	483	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 23.

The worst 5 of 483 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)
4:G:1015:LYS:CD	4:G:1015:LYS:CE	1.82	1.55
4:G:1016:THR:CA	4:G:1016:THR:CB	1.86	1.52
2:E:677:ASP:CG	2:E:677:ASP:CB	1.75	1.51
4:G:1015:LYS:CB	4:G:1015:LYS:CA	1.86	1.50
4:G:1015:LYS:CD	4:G:1015:LYS:CG	1.92	1.47

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	
2	A	95/135 (70%)	93 (98%)	2 (2%)	0	100	100
2	E	97/135 (72%)	91 (94%)	5 (5%)	1 (1%)	19	54
3	B	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
3	F	79/102 (78%)	77 (98%)	2 (2%)	0	100	100
4	C	104/129 (81%)	99 (95%)	5 (5%)	0	100	100
4	G	104/129 (81%)	93 (89%)	9 (9%)	2 (2%)	10	35
5	D	90/125 (72%)	85 (94%)	4 (4%)	1 (1%)	17	51
5	H	92/125 (74%)	84 (91%)	6 (6%)	2 (2%)	8	31
All	All	738/982 (75%)	696 (94%)	36 (5%)	6 (1%)	24	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	1301	GLY
4	G	1015	LYS
4	G	1072	ASP
5	H	1501	GLY
5	H	1430	ARG

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	
2	A	83/110 (76%)	81 (98%)	2 (2%)	57	86
2	E	85/110 (77%)	81 (95%)	4 (5%)	32	68
3	B	64/78 (82%)	63 (98%)	1 (2%)	70	91
3	F	66/78 (85%)	64 (97%)	2 (3%)	48	83
4	C	85/100 (85%)	76 (89%)	9 (11%)	8	25
4	G	84/100 (84%)	80 (95%)	4 (5%)	31	67
5	D	78/105 (74%)	76 (97%)	2 (3%)	54	85
5	H	80/105 (76%)	74 (92%)	6 (8%)	17	44
All	All	625/786 (80%)	595 (95%)	30 (5%)	31	67

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1319	THR
2	E	721	PRO
5	H	1433	SER
2	E	659	GLU
2	E	722	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	1292	GLN
5	H	1506	HIS
2	E	668	GLN
4	C	831	HIS
4	G	1031	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.