



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2024 – 12:40 PM JST

PDB ID : 8YJM  
Title : Structure of human SPT16 MD-CTD and MCM2 HBD chaperoning a histone H3-H4 tetramer and a single chain H2B-H2A chimera  
Authors : Gan, S.L.; Yang, W.S.; Xu, R.M.  
Deposited on : 2024-03-02  
Resolution : 4.15 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

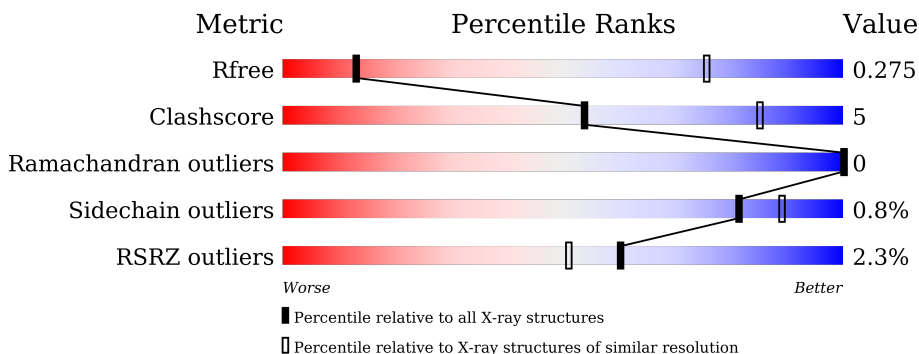
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.15 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.



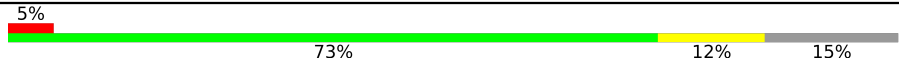
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	350	<p>75% 14% 11%</p>
2	B	93	<p>47% 15% 38%</p>
3	C	81	<p>85% 12%</p>
3	E	81	<p>86% 12%</p>
4	D	103	<p>60% 8% 31%</p>
4	F	103	<p>63% 8% 28%</p>

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Mol	Chain	Length	Quality of chain
5	G	213	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '5%', a large green segment labeled '73%', a yellow segment labeled '12%', and a grey segment at the end labeled '15%'.</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6879 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 FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2549	1622	422	493	12	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	GLY	-	expression tag	UNP Q9Y5B9
A	640	PRO	-	expression tag	UNP Q9Y5B9
A	641	LEU	-	expression tag	UNP Q9Y5B9
A	642	GLY	-	expression tag	UNP Q9Y5B9
A	643	SER	-	expression tag	UNP Q9Y5B9

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	58	455	268	81	104	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	SER	-	expression tag	UNP P49736

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	79	641	405	119	113	4	0	0	0
3	E	80	646	408	120	114	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	55	MET	-	initiating methionine	UNP P68431
E	55	MET	-	initiating methionine	UNP P68431

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	71	Total	C	N	O	S	0	0	0
			572	359	113	99	1			
4	F	74	Total	C	N	O	S	0	0	0
			591	374	115	101	1			

- Molecule 5 is a protein called Histone H2B 1/2/3/4/6,Histone H2A type 1-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	182	Total	C	N	O	S	0	2	0
			1425	898	264	261	2			

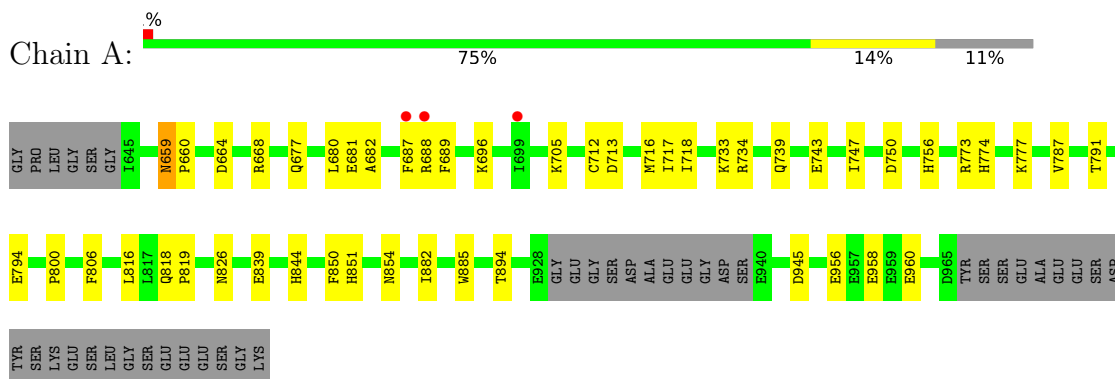
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	12	MET	-	initiating methionine	UNP P0C1H3
G	13	GLY	-	expression tag	UNP P0C1H3
G	14	SER	-	expression tag	UNP P0C1H3
G	15	SER	-	expression tag	UNP P0C1H3
G	16	HIS	-	expression tag	UNP P0C1H3
G	17	HIS	-	expression tag	UNP P0C1H3
G	18	HIS	-	expression tag	UNP P0C1H3
G	19	HIS	-	expression tag	UNP P0C1H3
G	20	HIS	-	expression tag	UNP P0C1H3
G	21	HIS	-	expression tag	UNP P0C1H3
G	22	SER	-	expression tag	UNP P0C1H3
G	23	SER	-	expression tag	UNP P0C1H3
G	24	GLY	-	expression tag	UNP P0C1H3
G	25	LEU	-	expression tag	UNP P0C1H3
G	26	VAL	-	expression tag	UNP P0C1H3
G	27	PRO	-	expression tag	UNP P0C1H3
G	28	ARG	-	expression tag	UNP P0C1H3
G	29	GLY	-	expression tag	UNP P0C1H3
G	30	SER	-	expression tag	UNP P0C1H3
G	31	HIS	-	expression tag	UNP P0C1H3
G	32	MET	-	expression tag	UNP P0C1H3

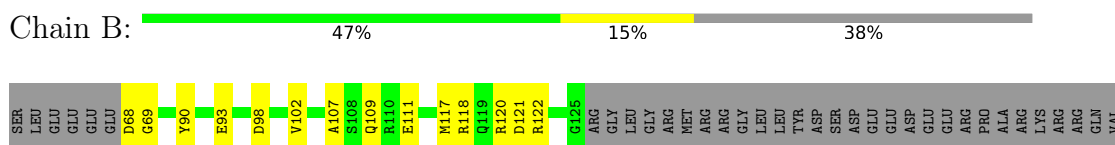
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

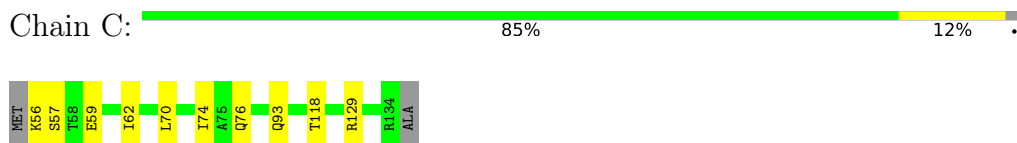
- Molecule 1: FACT complex subunit SPT16



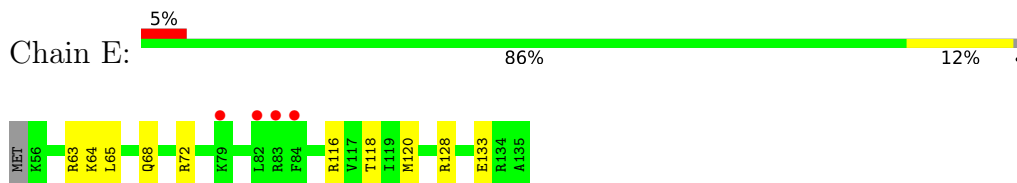
- Molecule 2: DNA replication licensing factor MCM2



- Molecule 3: Histone H3.1

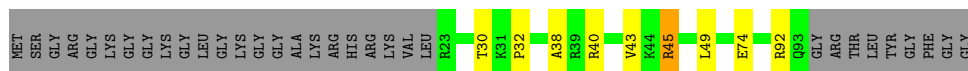


- Molecule 3: Histone H3.1

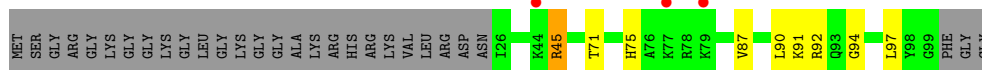


- Molecule 4: Histone H4

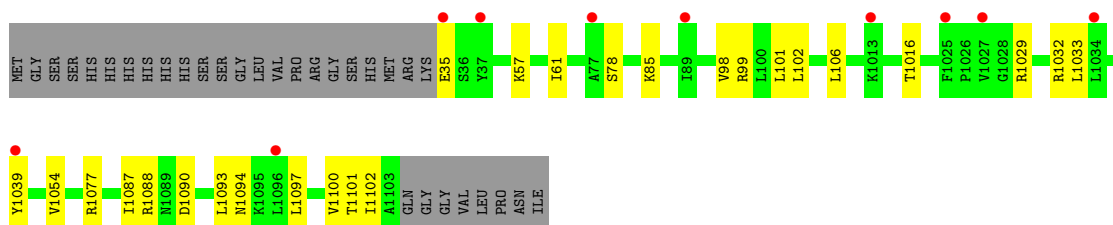
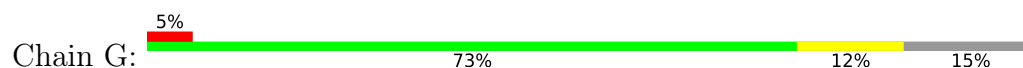




- Molecule 4: Histone H4



- Molecule 5: Histone H2B 1/2/3/4/6, Histone H2A type 1-D



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.34Å 191.34Å 80.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	165.70 – 4.15 165.70 – 4.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (165.70-4.15) 99.8 (165.70-4.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	497.77 (at 4.15Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.263 , 0.286 0.245 , 0.275	Depositor DCC
$R_{free}$ test set	1269 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	154.0	Xtrriage
Anisotropy	0.155	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 137.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	200.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.25	0/2607	0.47	0/3522
2	B	0.24	0/457	0.58	0/612
3	C	0.25	0/648	0.51	0/868
3	E	0.25	0/653	0.52	0/875
4	D	0.23	0/577	0.54	0/773
4	F	0.24	0/597	0.54	0/800
5	G	0.24	0/1451	0.48	0/1954
All	All	0.25	0/6990	0.50	0/9404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2549	0	2463	32	0
2	B	455	0	411	12	0
3	C	641	0	674	8	0
3	E	646	0	679	7	0
4	D	572	0	615	9	0
4	F	591	0	638	10	0
5	G	1425	0	1497	19	0
All	All	6879	0	6977	74	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 5.

All (74) 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:A:660:PRO:HG2	1:A:682:ALA:HB3	1.53	0.88
3:C:59:GLU:HB3	4:D:40:ARG:HH22	1.47	0.76
1:A:750:ASP:HB3	4:D:45:ARG:HG3	1.77	0.67
4:D:92:ARG:HH22	5:G:101:LEU:HD23	1.61	0.65
4:D:74:GLU:OE2	5:G:99:ARG:NH1	2.32	0.62
2:B:68:ASP:HB3	4:F:45:ARG:HH21	1.65	0.61
1:A:712:CYS:HB3	1:A:718:ILE:HB	1.83	0.61
5:G:1090:ASP:HB3	5:G:1093:LEU:HB2	1.82	0.61
3:C:62:ILE:O	3:C:93:GLN:NE2	2.35	0.60
1:A:717:ILE:HG22	1:A:743:GLU:HA	1.85	0.58
1:A:854:ASN:OD1	3:C:129:ARG:NH2	2.37	0.57
1:A:668:ARG:HB2	1:A:739:GLN:HG2	1.86	0.57
1:A:680:LEU:HD11	1:A:687:PHE:HB3	1.86	0.57
2:B:120:ARG:NH1	2:B:121:ASP:OD1	2.38	0.57
5:G:1087:ILE:HD13	5:G:1097:LEU:HD12	1.86	0.57
2:B:69:GLY:H	4:F:45:ARG:HH21	1.54	0.56
1:A:664:ASP:HA	1:A:677:GLN:HE21	1.70	0.55
5:G:1088:ARG:HA	5:G:1094:ASN:HB2	1.87	0.55
1:A:705:LYS:NZ	1:A:839:GLU:OE2	2.28	0.55
5:G:1029:ARG:HG2	5:G:1032:ARG:NH2	2.22	0.54
1:A:689:PHE:O	1:A:696:LYS:HA	2.08	0.53
4:D:30:THR:HB	4:D:32:PRO:HD2	1.90	0.53
5:G:102:LEU:HD23	5:G:106:LEU:HB3	1.90	0.53
1:A:659:ASN:ND2	1:A:681:GLU:OE2	2.42	0.53
1:A:713:ASP:HA	1:A:773:ARG:HH22	1.74	0.53
1:A:716:MET:HE3	1:A:747:ILE:HA	1.91	0.53
5:G:78:SER:HB2	5:G:1039:TYR:HB3	1.91	0.52
1:A:687:PHE:HZ	1:A:787:VAL:HG11	1.74	0.52
1:A:774:HIS:HA	1:A:777:LYS:HG2	1.92	0.50
2:B:107:ALA:O	2:B:111:GLU:HG3	2.12	0.50
1:A:688:ARG:HH11	1:A:696:LYS:HD2	1.76	0.50
1:A:716:MET:SD	4:D:49:LEU:HG	2.52	0.50
5:G:35:GLU:HG2	5:G:1033:LEU:HD11	1.93	0.49
1:A:960:GLU:OE2	5:G:1016:THR:HA	2.13	0.49
1:A:806:PHE:CG	1:A:882:ILE:HD11	2.49	0.48
2:B:109:GLN:HB3	4:F:75:HIS:HB3	1.94	0.48
5:G:1029:ARG:HG2	5:G:1032:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1097:LEU:O	5:G:1100:VAL:HG13	2.13	0.48
1:A:791:THR:HB	1:A:794:GLU:HB3	1.97	0.47
2:B:117:MET:HG3	4:F:71:THR:HG21	1.97	0.47
3:C:70:LEU:O	3:C:74:ILE:HG12	2.14	0.47
5:G:98:VAL:HG21	5:G:1054:VAL:HG21	1.96	0.47
3:C:118:THR:HA	4:D:45:ARG:HB3	1.96	0.47
3:E:63:ARG:HD3	3:E:63:ARG:HA	1.80	0.47
2:B:98:ASP:OD2	2:B:102:VAL:HG22	2.15	0.46
2:B:69:GLY:H	4:F:45:ARG:NH2	2.13	0.46
1:A:819:PRO:HB3	1:A:885:TRP:CZ2	2.51	0.46
1:A:816:LEU:O	1:A:826:ASN:ND2	2.36	0.46
1:A:750:ASP:OD1	1:A:750:ASP:N	2.47	0.45
2:B:93:GLU:HB3	3:E:72:ARG:HH12	1.81	0.45
3:C:59:GLU:H	4:D:40:ARG:HH12	1.64	0.45
4:F:97:LEU:O	5:G:1102:ILE:HD13	2.16	0.45
1:A:844:HIS:ND1	1:A:894:THR:OG1	2.44	0.45
1:A:733:LYS:HG2	1:A:734:ARG:H	1.81	0.45
5:G:57:LYS:O	5:G:61:ILE:HG13	2.18	0.44
4:F:87:VAL:O	4:F:91:LYS:HG2	2.17	0.44
2:B:118:ARG:O	2:B:122:ARG:HG2	2.17	0.44
4:D:38:ALA:HB1	4:D:43:VAL:HB	1.98	0.44
1:A:945:ASP:HB3	5:G:1077:ARG:HH22	1.81	0.44
3:E:118:THR:HA	4:F:45:ARG:HB3	1.99	0.43
1:A:851:HIS:NE2	5:G:1101:THR:HA	2.34	0.43
3:E:65:LEU:O	3:E:68:GLN:HG2	2.18	0.43
2:B:117:MET:HB3	4:F:92:ARG:HH12	1.84	0.43
3:C:76:GLN:HE21	3:C:76:GLN:HB2	1.67	0.42
1:A:713:ASP:HA	1:A:773:ARG:NH2	2.35	0.42
2:B:90:TYR:CE1	3:E:64:LYS:HB3	2.55	0.41
1:A:945:ASP:HB3	5:G:1077:ARG:NH2	2.35	0.41
3:C:56:LYS:HB3	3:C:57:SER:H	1.67	0.41
1:A:956:GLU:HB3	1:A:958:GLU:HG2	2.03	0.41
1:A:800:PRO:HB3	1:A:818:GLN:HB2	2.02	0.41
3:E:116:ARG:NH1	3:E:120:MET:HG3	2.36	0.40
4:F:90:LEU:O	4:F:94:GLY:N	2.52	0.40
1:A:851:HIS:CE1	5:G:1102:ILE:H	2.39	0.40
3:E:128:ARG:NH1	3:E:133:GLU:OE1	2.54	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	306/350 (87%)	295 (96%)	11 (4%)	0	100	100
2	B	56/93 (60%)	55 (98%)	1 (2%)	0	100	100
3	C	77/81 (95%)	77 (100%)	0	0	100	100
3	E	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	69/103 (67%)	69 (100%)	0	0	100	100
4	F	72/103 (70%)	69 (96%)	3 (4%)	0	100	100
5	G	182/213 (85%)	179 (98%)	3 (2%)	0	100	100
All	All	840/1024 (82%)	821 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	285/315 (90%)	282 (99%)	3 (1%)	73	84
2	B	44/75 (59%)	44 (100%)	0	100	100
3	C	69/70 (99%)	69 (100%)	0	100	100
3	E	69/70 (99%)	69 (100%)	0	100	100
4	D	60/79 (76%)	59 (98%)	1 (2%)	60	78
4	F	61/79 (77%)	60 (98%)	1 (2%)	62	79
5	G	152/176 (86%)	151 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	740/864 (86%)	734 (99%)	6 (1%)	81	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	659	ASN
1	A	756	HIS
1	A	850	PHE
4	D	45	ARG
4	F	45	ARG
5	G	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	677	GLN
3	C	76	GLN

### 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 monosaccharides 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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	310/350 (88%)	-0.00	3 (0%) 82 74	116, 188, 262, 306	0
2	B	58/93 (62%)	-0.14	0 100 100	157, 251, 369, 409	0
3	C	79/81 (97%)	0.07	0 100 100	141, 177, 228, 247	0
3	E	80/81 (98%)	0.44	4 (5%) 28 24	125, 167, 234, 244	0
4	D	71/103 (68%)	0.22	0 100 100	153, 195, 226, 236	0
4	F	74/103 (71%)	0.36	3 (4%) 37 30	135, 187, 240, 262	0
5	G	182/213 (85%)	0.35	10 (5%) 25 21	166, 219, 258, 301	0
All	All	854/1024 (83%)	0.16	20 (2%) 60 51	116, 200, 272, 409	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	35	GLU	4.5
5	G	1013	LYS	3.5
3	E	82	LEU	3.3
1	A	687	PHE	3.0
3	E	84	PHE	2.9
5	G	1034	LEU	2.8
3	E	83	ARG	2.7
5	G	1039	TYR	2.5
4	F	77	LYS	2.4
4	F	79	LYS	2.4
5	G	77	ALA	2.4
5	G	1025	PHE	2.4
1	A	688	ARG	2.3
5	G	37	TYR	2.2
5	G	1096	LEU	2.1
4	F	44	LYS	2.1
5	G	1027	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	79	LYS	2.1
5	G	89	ILE	2.0
1	A	699	ILE	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 monosaccharides 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.