

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 04:54 AM EDT

PDB ID	:	3CLZ
Title	:	The set and ring associated (SRA) domain of UHRF1 bound to methylated
		DNA
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		S.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-03-20
Resolution	:	2.20 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.20 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.



Motria	Whole archive	Similar resolution		
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	4898 (2.20-2.20)		
Clashscore	141614	5594 (2.20-2.20)		
Ramachandran outliers	138981	5503 (2.20-2.20)		
Sidechain outliers	138945	5504 (2.20-2.20)		
RSRZ outliers	127900	4800 (2.20-2.20)		

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 >=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 <=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	А	212	86%	9%	·
1	В	212	90%	8%	·
1	С	212	88%	8%	•
1	D	212	88%	9%	••



Mol	Chain	Length	(Quality of chain	
2	Е	12	33%	58%	8%
2	G	12	33%	67%	
2	Ι	12	17%	67%	17%
2	K	12	42%	58%	
3	F	12	759	%	25%
3	Н	12	33%	58%	8%
3	J	12	33%	50%	17%
3	L	12	42%	33%	25%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9090 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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	204	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	A	204	1609	1007	299	299	4	0	1	0
1	В	210	Total	С	Ν	0	S	0	1	0
	D	210	1646	1028	307	307	4	0	1	0
1	C	204	Total	С	Ν	0	S	0	1	0
	C	204	1597	1000	294	299	4	0		0
1	1 D	000	Total	С	Ν	0	S	0	0	0
	209	1638	1025	306	303	4	0	0	0	

• Molecule 1 is a protein called E3 ubiquitin-protein ligase UHRF1.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	413	MET	-	initiating methionine	UNP Q96T88
А	618	ALA	-	expression tag	UNP Q96T88
А	619	HIS	-	expression tag	UNP Q96T88
А	620	HIS	-	expression tag	UNP Q96T88
А	621	HIS	-	expression tag	UNP Q96T88
А	622	HIS	-	expression tag	UNP Q96T88
А	623	HIS	-	expression tag	UNP Q96T88
А	624	HIS	-	expression tag	UNP Q96T88
В	413	MET	-	initiating methionine	UNP Q96T88
В	618	ALA	-	expression tag	UNP Q96T88
В	619	HIS	-	expression tag	UNP Q96T88
В	620	HIS	-	expression tag	UNP Q96T88
В	621	HIS	-	expression tag	UNP Q96T88
В	622	HIS	-	expression tag	UNP Q96T88
В	623	HIS	-	expression tag	UNP Q96T88
В	624	HIS	-	expression tag	UNP Q96T88
С	413	MET	-	initiating methionine	UNP Q96T88
С	618	ALA	-	expression tag	UNP Q96T88
С	619	HIS	-	expression tag	UNP Q96T88
С	620	HIS	-	expression tag	UNP Q96T88
С	621	HIS	-	expression tag	UNP Q96T88



Chain	Residue	Modelled	Actual	Comment	Reference
С	622	HIS	-	expression tag	UNP Q96T88
С	623	HIS	-	expression tag	UNP Q96T88
С	624	HIS	-	expression tag	UNP Q96T88
D	413	MET	-	initiating methionine	UNP Q96T88
D	618	ALA	-	expression tag	UNP Q96T88
D	619	HIS	-	expression tag	UNP Q96T88
D	620	HIS	-	expression tag	UNP Q96T88
D	621	HIS	-	expression tag	UNP Q96T88
D	622	HIS	-	expression tag	UNP Q96T88
D	623	HIS	-	expression tag	UNP Q96T88
D	624	HIS	-	expression tag	UNP Q96T88

• Molecule 2 is a DNA chain called 5'-D(*DGP*DGP*DGP*DCP*(5CM)P*DGP*DCP *DAP*DGP*DGP*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	F	19	Total	С	Ν	Ο	Р	0	0	0
		12	249	117	52	69	11	0	0	0
0	C	19	Total	С	Ν	Ο	Р	0	0	0
	G	12	249	117	52	69	11	0	0	0
0	т	12	Total	С	Ν	0	Р	0	0	0
	1		249	117	52	69	11			0
0		V 19	Total	С	Ν	Ο	Р	0	0	0
	12	249	117	52	69	11	0	0	U	

• Molecule 3 is a DNA chain called 5'-D(*DCP*DCP*DCP*DTP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Б	19	Total	С	Ν	Ο	Р	0	0	0
J	Г	12	238	113	43	71	11	0	0	0
2	ц	19	Total	С	Ν	Ο	Р	0	0	0
J	11	12	238	113	43	71	11	0	0	0
2	т	J 12	Total	С	Ν	Ο	Р	0	0	0
J	1		238	113	43	71	11			0
2	о I	L 12	Total	С	Ν	Ο	Р	0	0	0
J L			238	113	43	71	11		U	U

• Molecule 4 is water.



201	7
201	

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	126	Total O 127 127	0	1
4	В	104	Total O 110 110	0	6
4	С	90	Total O 90 90	0	0
4	D	109	Total O 110 110	0	1
4	Е	36	Total O 37 37	0	1
4	F	19	Total O 19 19	0	0
4	G	29	TotalO2929	0	0
4	Н	20	TotalO2020	0	0
4	Ι	38	Total O 40 40	0	2
4	J	19	Total O 19 19	0	0
4	K	25	TotalO2626	0	1
4	L	25	TotalO2525	0	0



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.

- Chain A: 86% Q% • Molecule 1: E3 ubiquitin-protein ligase UHRF1 Chain B: 90% 8% • Molecule 1: E3 ubiquitin-protein ligase UHRF1 Chain C: 88% 8% • Molecule 1: E3 ubiquitin-protein ligase UHRF1 Chain D: 88% ۹% • Molecule 2: 5'-D(*DGP*DGP*DGP*DCP*DCP*(5CM)P*DGP*DCP*DAP*DGP*DGP*DGP-3' Chain E: 33% 58% 8%
- Molecule 1: E3 ubiquitin-protein ligase UHRF1

• Molecule 2: 5'-D(*DGP*DGP*DGP*DCP*(5CM)P*DGP*DCP*DAP*DGP*DGP*DGP*DG)-3'



Chain G:	33%	67%		
6 6 6 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	N H 5			
• Molecule 2: 5 3'	'-D(*DGP*DGF	P*DGP*DCP*DCP*(5Cl	M)P*DGP*DCP*D	AP*DGP*DGP*DG)-
Chain I: 17%	0	67%	17%	
6 6 6 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	7 11			
• Molecule 2: 5 3'	'-D(*DGP*DGF	P*DGP*DCP*DCP*(5C)	M)P*DGP*DCP*D	AP*DGP*DGP*DG)-
Chain K:	42%	58	8%	
<mark>61 63 64 61 61 61 61 61 61 61 61 61 61 61 61 61 </mark>				
• Molecule 3: 5	·-D(*DCP*DCI	P*DCP*DTP*DGP*DC	CP*DGP*DGP*DG	GP*DCP*DCP*DC)-3
Chain F:		75%	25%	
5 <mark>8 2 8 5</mark>				
• Molecule 3: 5	o'-D(*DCP*DC	P*DCP*DTP*DGP*DC	CP*DGP*DGP*DG	P*DCP*DCP*DC)-3
Chain H:	33%	58%	8%	
62 63 63 63 63 63 63 63 63 63 63 63 63 63				
• Molecule 3: 5	o'-D(*DCP*DCI	P*DCP*DTP*DGP*DC	CP*DGP*DGP*DG	P*DCP*DCP*DC)-3
Chain J:	33%	50%	17%	
22 28 88 88 88 88 88 88 88 88 88 88 88 8				
• Molecule 3: 5	-D(*DCP*DC	P*DCP*DTP*DGP*DC	CP*DGP*DGP*DG	P*DCP*DCP*DC)-3
Chain L:	42%	33%	25%	







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	76.20Å 111.36Å 97.40Å	Deperitor
a, b, c, α , β , γ	90.00° 90.53° 90.00°	Depositor
$\mathbf{P}_{\text{accolution}}\left(\overset{}{\boldsymbol{\lambda}}\right)$	38.63 - 2.20	Depositor
Resolution (A)	38.10 - 2.20	EDS
% Data completeness	99.0 (38.63-2.20)	Depositor
(in resolution range)	96.7 (38.10-2.20)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.17	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.189 , 0.231	Depositor
n, n_{free}	0.191 , 0.231	DCC
R_{free} test set	4085 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 32.2	EDS
L-test for twinning ²	$< L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9090	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 48.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1282e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: $5\mathrm{CM}$

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).

Mal	Chain	Bo	Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.62	1/1651~(0.1%)	0.66	1/2233~(0.0%)		
1	В	0.59	0/1691	0.64	0/2290		
1	С	0.62	0/1639	0.68	1/2220~(0.0%)		
1	D	0.60	0/1685	0.66	0/2284		
2	Ε	1.15	0/257	1.88	11/394~(2.8%)		
2	G	1.14	0/257	2.08	13/394~(3.3%)		
2	Ι	1.28	0/257	2.19	16/394~(4.1%)		
2	Κ	1.13	0/257	1.83	9/394~(2.3%)		
3	F	0.99	0/265	1.87	4/406~(1.0%)		
3	Н	1.01	0/265	1.88	10/406~(2.5%)		
3	J	1.07	0/265	1.98	10/406~(2.5%)		
3	L	1.12	1/265 (0.4%)	1.82	9/406 (2.2%)		
All	All	0.76	2/8754~(0.0%)	1.14	84/12227~(0.7%)		

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	619	HIS	C-O	5.81	1.34	1.23
3	L	8	DG	C3'-O3'	-5.01	1.37	1.44

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	G	4	DC	O4'-C1'-N1	-12.57	99.20	108.00
2	Е	7	DG	O4'-C1'-N9	-10.33	100.77	108.00
2	K	11	DG	O4'-C1'-N9	9.99	114.99	108.00
2	G	7	DG	O4'-C1'-N9	-9.86	101.10	108.00
2	G	8	DC	OP1-P-O3'	-9.64	83.98	105.20
2	Ι	11	DG	O4'-C1'-N9	9.62	114.73	108.00
3	F	3	DC	O4'-C1'-N1	-9.23	101.54	108.00



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	Н	3	DC	O4'-C1'-N1	-9.20	101.56	108.00
2	Ι	8	DC	OP1-P-O3'	-9.15	85.07	105.20
3	L	9	DG	O4'-C1'-N9	-8.81	101.83	108.00
3	F	4	DT	O4'-C1'-N1	-8.64	101.95	108.00
3	Н	12	DC	O4'-C1'-N1	8.59	114.01	108.00
3	J	3	DC	O4'-C1'-N1	-8.57	102.00	108.00
2	G	8	DC	O3'-P-O5'	-8.24	88.35	104.00
2	G	9	DA	OP1-P-OP2	8.18	131.88	119.60
2	Ι	8	DC	O3'-P-O5'	-8.11	88.59	104.00
3	Н	4	DT	O4'-C1'-N1	-8.10	102.33	108.00
2	G	11	DG	O4'-C1'-N9	7.92	113.55	108.00
3	J	4	DT	O4'-C1'-N1	-7.92	102.46	108.00
2	G	8	DC	OP2-P-O3'	-7.90	87.82	105.20
2	Ι	7	DG	O4'-C1'-N9	-7.89	102.48	108.00
3	F	9	DG	O4'-C1'-N9	-7.65	102.64	108.00
2	Ι	5	DC	O4'-C1'-N1	7.65	113.35	108.00
2	Ι	12	DG	O4'-C4'-C3'	-7.52	101.49	106.00
3	L	12	DC	O4'-C1'-N1	7.51	113.26	108.00
2	Е	4	DC	O4'-C1'-N1	-7.51	102.74	108.00
3	L	4	DT	O4'-C1'-N1	-7.49	102.76	108.00
2	Ι	8	DC	OP2-P-O3'	-7.46	88.78	105.20
2	Ι	3	DG	O4'-C1'-N9	-7.33	102.87	108.00
2	Ι	9	DA	OP1-P-OP2	7.27	130.51	119.60
2	Κ	7	DG	O4'-C1'-N9	-7.27	102.91	108.00
2	G	3	DG	O4'-C1'-N9	-7.12	103.02	108.00
2	Κ	4	DC	O4'-C1'-N1	-7.09	103.03	108.00
3	Н	9	DG	O4'-C1'-N9	-6.78	103.25	108.00
3	J	7	DG	C8-N9-C4	-6.69	103.72	106.40
3	J	5	DG	O4'-C1'-N9	6.49	112.54	108.00
2	Ε	11	DG	O4'-C1'-N9	6.33	112.43	108.00
2	Κ	3	DG	O4'-C1'-N9	-6.28	103.60	108.00
3	J	7	DG	O4'-C1'-N9	6.26	112.39	108.00
3	L	8	DG	P-O5'-C5'	-6.25	110.89	120.90
2	Е	10	DG	O4'-C1'-N9	-6.21	103.65	108.00
3	J	7	DG	N9-C4-C5	6.19	107.88	105.40
2	Ε	9	DA	O4'-C1'-N9	6.15	112.31	108.00
2	Κ	12	DG	O4'-C4'-C3'	-6.07	102.07	104.50
3	J	2	DC	N1-C2-O2	6.01	122.51	118.90
3	Н	10	DC	P-O3'-C3'	5.92	126.81	119.70
2	Ι	10	DG	O4'-C1'-N9	-5.91	103.86	108.00
2	G	4	DC	P-O3'-C3'	5.84	126.71	119.70
3	J	12	DC	O4'-C1'-N1	5.83	112.08	108.00



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
2	Κ	8	DC	O4'-C1'-N1	-5.83	103.92	108.00
2	Ι	4	DC	P-O3'-C3'	5.78	126.63	119.70
2	G	8	DC	P-O3'-C3'	5.74	126.59	119.70
3	L	7	DG	C8-N9-C4	-5.74	104.10	106.40
2	G	10	DG	O4'-C1'-N9	-5.73	103.99	108.00
3	J	4	DT	N3-C2-O2	-5.69	118.88	122.30
2	Ι	4	DC	O4'-C1'-N1	-5.66	104.04	108.00
2	Ε	7	DG	N1-C6-O6	5.65	123.29	119.90
3	Н	5	DG	C5-C6-N1	5.64	114.32	111.50
2	Κ	11	DG	C2-N3-C4	5.54	114.67	111.90
2	Е	11	DG	C5-C6-O6	-5.53	125.28	128.60
1	С	433	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	Е	4	DC	P-O3'-C3'	5.38	126.16	119.70
2	Ι	8	DC	P-O3'-C3'	5.33	126.10	119.70
3	Н	3	DC	P-O3'-C3'	5.32	126.08	119.70
3	Н	9	DG	P-O3'-C3'	5.30	126.06	119.70
3	Н	6	DC	O4'-C1'-N1	-5.29	104.30	108.00
2	Ι	9	DA	N1-C6-N6	5.29	121.77	118.60
2	G	11	DG	P-O3'-C3'	5.26	126.01	119.70
3	Н	5	DG	C5-C6-O6	-5.24	125.45	128.60
2	Е	12	DG	O4'-C4'-C3'	-5.23	102.41	104.50
2	G	9	DA	O4'-C1'-N9	5.22	111.66	108.00
3	L	5	DG	C3'-C2'-C1'	-5.21	96.24	102.50
2	Ι	11	DG	P-O3'-C3'	5.17	125.90	119.70
2	Е	3	DG	O4'-C1'-N9	-5.17	104.38	108.00
3	F	9	DG	C6-N1-C2	-5.16	122.01	125.10
1	А	433	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	Κ	11	DG	P-O3'-C3'	5.14	125.87	119.70
2	Е	11	DG	O4'-C1'-C2'	-5.13	101.80	105.90
3	L	9	DG	P-O3'-C3'	5.12	125.85	119.70
3	J	8	DG	P-O5'-C5'	-5.07	112.78	120.90
3	L	3	DC	N1-C1'-C2'	5.05	122.20	112.60
2	Ι	8	DC	O4'-C1'-N1	-5.04	104.47	108.00
3	L	8	DG	C5'-C4'-C3'	-5.03	105.05	114.10
2	Κ	11	DG	C5-C6-N1	5.00	114.00	111.50

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	А	1609	0	1536	12	0
1	В	1646	0	1534	9	0
1	С	1597	0	1507	8	0
1	D	1638	0	1527	10	0
2	Е	249	0	136	1	0
2	G	249	0	136	0	0
2	Ι	249	0	136	2	0
2	Κ	249	0	136	0	0
3	F	238	0	135	0	0
3	Н	238	0	135	1	0
3	J	238	0	135	4	0
3	L	238	0	135	2	0
4	А	127	0	0	0	0
4	В	110	0	0	0	0
4	С	90	0	0	0	0
4	D	110	0	0	1	0
4	Е	37	0	0	1	0
4	F	19	0	0	0	0
4	G	29	0	0	0	0
4	Н	20	0	0	0	0
4	Ι	40	0	0	2	0
4	J	19	0	0	0	0
4	К	26	0	0	1	0
4	L	25	0	0	0	0
All	All	9090	0	7188	48	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 3.

All (48) 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)
3:L:7:DG:H2"	3:L:8:DG:H5"	1.31	1.11
3:J:7:DG:H2"	3:J:8:DG:H5"	1.52	0.92
1:A:416:ASN:HD22	1:A:416:ASN:N	1.73	0.86



	A h O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:589:PRO:HB3	1:D:598:ILE:HD11	1.71	0.72
1:B:429:MET:O	1:B:606:GLN:HG2	1.93	0.69
3:J:7:DG:C2'	3:J:8:DG:H5"	2.22	0.69
1:A:416:ASN:N	1:A:416:ASN:ND2	2.39	0.66
3:J:7:DG:H2"	3:J:8:DG:C5'	2.24	0.66
2:I:12:DG:N7	4:I:374:HOH:O	2.29	0.65
3:L:8:DG:H2"	3:L:9:DG:C8	2.34	0.62
1:A:589:PRO:HB3	1:A:598:ILE:HD11	1.84	0.60
1:A:537:ARG:HD2	1:A:556:ASP:OD2	2.04	0.57
1:B:589:PRO:HB3	1:B:598:ILE:HD11	1.88	0.55
1:D:537:ARG:HD2	1:D:556:ASP:OD2	2.09	0.53
1:A:460:LEU:HD12	1:A:460:LEU:C	2.30	0.52
1:C:460:LEU:C	1:C:460:LEU:HD12	2.31	0.51
1:C:448:GLY:O	1:C:460:LEU:HA	2.12	0.50
1:B:434:VAL:HG23	1:B:445:HIS:CE1	2.48	0.48
1:A:598:ILE:HG23	1:A:603:LEU:HB2	1.96	0.48
1:A:615:LEU:C	1:A:617:ASN:H	2.17	0.47
1:C:444:PRO:CD	1:C:450:HIS:HB2	2.44	0.47
1:D:460:LEU:C	1:D:460:LEU:HD12	2.35	0.47
1:D:555:TYR:CZ	1:D:557:GLY:HA2	2.50	0.47
3:J:8:DG:H2"	3:J:9:DG:C8	2.50	0.47
3:H:2:DC:H1'	3:H:3:DC:H5'	1.97	0.47
1:D:598:ILE:HG23	1:D:603:LEU:HB2	1.98	0.46
1:B:622:HIS:C	1:B:624:HIS:H	2.20	0.46
1:D:619:HIS:O	1:D:622:HIS:HB2	2.16	0.46
1:A:418:TYR:CZ	1:A:531:LYS:HD3	2.52	0.45
1:B:460:LEU:HD12	1:B:460:LEU:C	2.37	0.45
1:C:589:PRO:HB3	1:C:598:ILE:HD11	1.98	0.45
1:A:546:LYS:HD2	1:C:488:GLY:HA2	1.98	0.44
1:D:482:GLY:HA2	4:K:14:HOH:O	2.17	0.44
1:D:620:HIS:C	1:D:622:HIS:H	2.22	0.43
1:A:448:GLY:O	1:A:460:LEU:HA	2.20	0.42
1:C:429:MET:HA	1:C:553:ASN:O	2.19	0.42
1:B:588:GLY:HA2	1:B:589:PRO:HD3	1.91	0.42
1:C:598:ILE:HG23	1:C:603:LEU:HB2	2.02	0.42
1:B:537:ARG:HD2	1:B:556:ASP:OD2	2.20	0.42
1:B:448:GLY:O	1:B:460:LEU:HA	2.20	0.42
1:C:418:TYR:CZ	1:C:531:LYS:HD3	2.55	0.41
2:E:11:DG:N3	4:E:195:HOH:O	2.37	0.41
1:D:564:TYR:HA	1:D:577:ARG:O	2.21	0.41
2:I:9:DA:N3	4:I:57:HOH:O	2.37	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:SER:O	1:A:506[A]:ARG:NH1	2.42	0.41
1:D:504:THR:HG22	4:D:689:HOH:O	2.21	0.41
1:A:568:LYS:HB3	1:A:568:LYS:HE3	1.81	0.40
1:B:589:PRO:HD2	1:B:590:TRP:CE3	2.57	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	А	203/212 (96%)	195~(96%)	8 (4%)	0	100 100
1	В	209/212~(99%)	201 (96%)	7 (3%)	1 (0%)	29 31
1	С	203/212~(96%)	193~(95%)	10~(5%)	0	100 100
1	D	207/212 (98%)	197 (95%)	9 (4%)	1 (0%)	29 31
All	All	822/848~(97%)	786 (96%)	34 (4%)	2(0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	621	HIS
1	В	623	HIS

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	А	162/172~(94%)	158~(98%)	4 (2%)	47 60			
1	В	162/172~(94%)	157~(97%)	5(3%)	40 51			
1	С	159/172~(92%)	153~(96%)	6 (4%)	33 42			
1	D	162/172~(94%)	153~(94%)	9~(6%)	21 25			
All	All	645/688~(94%)	621 (96%)	24 (4%)	35 43			

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type		
1	А	416	ASN		
1	А	516	ILE		
1	А	560	LYS		
1	А	567	GLU		
1	В	470	VAL		
1	В	474	ASN		
1	В	516	ILE		
1	В	606	GLN		
1	В	620	HIS		
1	С	438[A]	GLU		
1	С	438[B]	GLU		
1	С	470	VAL		
1	С	474	ASN		
1	С	516	ILE		
1	С	560	LYS		
1	D	470	VAL		
1	D	474	ASN		
1	D	504	THR		
1	D	520	GLU		
1	D	560	LYS		
1	D	596	ASP		
1	D	615	LEU		
1	D	619	HIS		
1	D	620	HIS		

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such side chains are listed below:

Mol	Chain	Res	Type
1	А	445	HIS
1	А	544	ASN
1	В	445	HIS



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Mol	Chain	Res	Type
1	D	416	ASN
1	D	445	HIS
1	D	617	ASN
1	D	620	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)

4 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 T	Turne	Chain	Dec	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5CM	Е	6	2	17,21,22	1.09	1 (5%)	24,30,33	1.49	5 (20%)
2	5CM	Ι	6	2	17,21,22	1.10	1 (5%)	24,30,33	1.61	5 (20%)
2	5CM	K	6	2	17,21,22	0.99	2 (11%)	24,30,33	1.59	5 (20%)
2	5CM	G	6	2	17,21,22	1.16	1 (5%)	24,30,33	1.85	8 (33%)

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
2	5CM	Е	6	2	-	0/7/21/22	0/2/2/2
2	5CM	Ι	6	2	-	0/7/21/22	0/2/2/2
2	5CM	K	6	2	-	0/7/21/22	0/2/2/2
2	5CM	G	6	2	-	0/7/21/22	0/2/2/2

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	6	5CM	C6-C5	3.13	1.39	1.34
2	Е	6	5CM	C6-C5	2.90	1.39	1.34
2	Ι	6	5CM	C6-C5	2.66	1.39	1.34
2	Κ	6	5CM	C6-C5	2.37	1.38	1.34
2	Κ	6	5CM	C6-N1	-2.13	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	G	6	5CM	C2'-C1'-N1	4.28	123.64	113.77
2	Ι	6	5CM	C2'-C1'-N1	3.62	122.11	113.77
2	G	6	5CM	C5-C4-N3	-3.38	118.03	121.67
2	K	6	5CM	C2'-C1'-N1	3.35	121.49	113.77
2	К	6	5CM	C5A-C5-C6	-3.25	118.51	122.85
2	G	6	5CM	O3'-C3'-C4'	-3.17	97.96	110.10
2	Ι	6	5CM	C5A-C5-C6	-3.08	118.73	122.85
2	К	6	5CM	C5-C4-N3	-3.07	118.36	121.67
2	K	6	5CM	O3'-C3'-C4'	-3.06	98.41	110.10
2	Ι	6	5CM	O3'-C3'-C4'	-3.00	98.62	110.10
2	Ι	6	5CM	O4'-C1'-N1	-2.98	102.53	107.86
2	Е	6	5CM	O3'-C3'-C4'	-2.96	98.77	110.10
2	Е	6	5CM	O4'-C1'-N1	-2.86	102.75	107.86
2	Е	6	5CM	C2'-C1'-N1	2.82	120.26	113.77
2	G	6	5CM	C5A-C5-C6	-2.65	119.31	122.85
2	Е	6	5CM	O2-C2-N3	-2.61	118.08	122.33
2	Ι	6	5CM	C5-C4-N3	-2.57	118.90	121.67
2	G	6	5CM	O2-C2-N3	-2.55	118.19	122.33
2	G	6	5CM	O4'-C1'-N1	-2.55	103.31	107.86
2	G	6	5CM	C2'-C3'-C4'	2.50	107.98	102.76
2	Е	6	5CM	C2'-C3'-C4'	2.24	107.44	102.76
2	G	6	5CM	C5-C6-N1	-2.18	121.09	123.34
2	K	6	5CM	O4'-C1'-N1	-2.08	104.14	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

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^{th} 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 $>$	ŧ	#RSF	RZ>2	$OWAB(Å^2)$	Q<0.9
1	А	204/212 (96%)	-0.63	0	100	100	28, 41, 70, 163	0
1	В	210/212 (99%)	-0.62	0	100	100	28, 43, 71, 117	0
1	С	204/212 (96%)	-0.64	0	100	100	29, 41, 73, 144	0
1	D	209/212 (98%)	-0.60	0	100	100	28, 43, 72, 143	0
2	E	11/12~(91%)	-1.13	0	100	100	35, 45, 52, 53	0
2	G	11/12~(91%)	-1.14	0	100	100	34, 46, 51, 53	0
2	Ι	11/12~(91%)	-1.10	0	100	100	35, 44, 50, 54	0
2	K	11/12~(91%)	-1.12	0	100	100	35, 45, 51, 54	0
3	F	12/12~(100%)	-1.10	0	100	100	35, 44, 51, 53	0
3	Н	12/12~(100%)	-1.06	0	100	100	37, 46, 52, 52	0
3	J	12/12~(100%)	-1.14	0	100	100	36, 46, 51, 52	0
3	L	$12\overline{/12}\ (100\%)$	-1.05	0	100	100	34, 47, 53, 54	0
All	All	919/944~(97%)	-0.67	0	100	100	28, 43, 72, 163	0

There are no RSRZ outliers to report.

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

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	5CM	Е	6	20/21	0.98	0.09	$25,\!30,\!34,\!36$	0
2	5CM	Ι	6	20/21	0.98	0.10	$25,\!28,\!35,\!38$	0
2	5CM	G	6	20/21	0.99	0.09	27,30,33,36	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	5CM	Κ	6	20/21	0.99	0.11	29,34,35,36	0

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.

