



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3UTB  
Title : Crystal Structure of Nucleosome Core Particle Assembled with the 146b Alpha-Satellite Sequence (NCP146b)  
Authors : Chua, E.Y.D.; Vasudevan, D.; Davey, G.E.; Wu, B.; Davey, C.A.  
Deposited on : 2011-11-25  
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](mailto: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.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

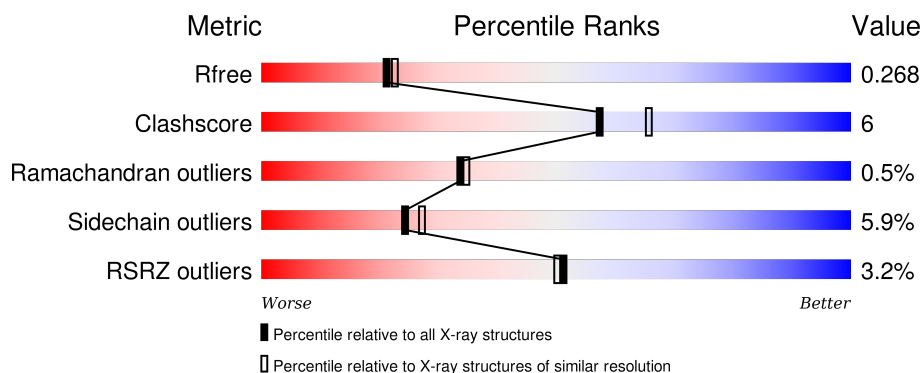
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	135	<div> <div>4%</div> <div>64% 8% 27%</div> </div>
1	E	135	<div> <div>66% 5% 28%</div> </div>
2	B	102	<div> <div>71% 10% 19%</div> </div>
2	F	102	<div> <div>4%</div> <div>67% 9% 24%</div> </div>
3	C	129	<div> <div>4%</div> <div>64% 14% 20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	129	
4	D	125	
4	H	125	
5	I	146	
5	J	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	C	1102	-	-	-	X
7	SO4	D	1101	-	-	-	X
7	SO4	G	1103	-	-	X	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12430 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 H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
1	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O		0	0	0
			795	501	155	139				
3	G	105	Total	C	N	O		0	0	0
			809	510	158	141				

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called 146-mer DNA.

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	9	Total	Mn	0	0
			9	9		
6	A	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		
6	J	9	Total	Mn	0	0
			9	9		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total	O	0	0
			62	62		
8	B	41	Total	O	0	0
			41	41		
8	C	31	Total	O	0	0
			31	31		
8	D	16	Total	O	0	0
			16	16		
8	E	37	Total	O	0	0
			37	37		
8	F	28	Total	O	0	0
			28	28		
8	G	52	Total	O	0	0
			52	52		
8	H	35	Total	O	0	0
			35	35		
8	I	50	Total	O	0	0
			50	50		

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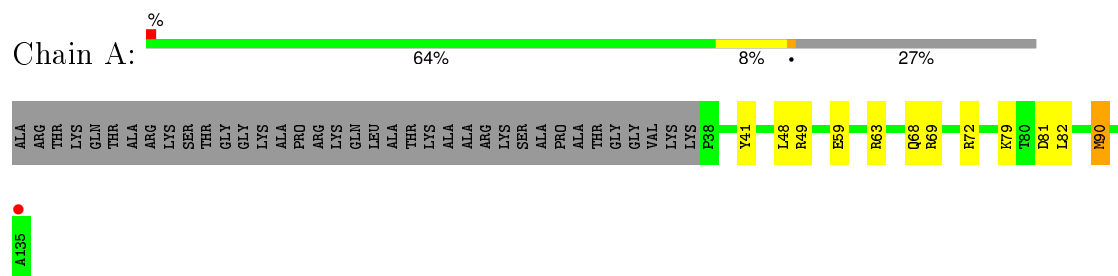
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	47	Total	O	0	0
			47	47		

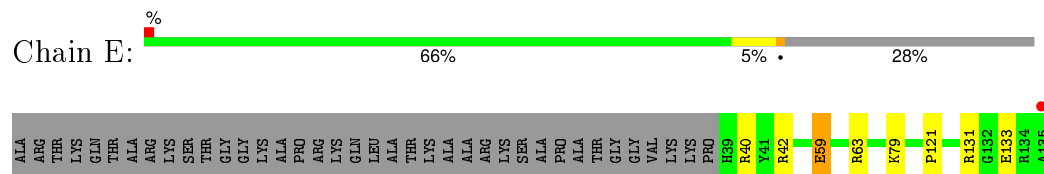
### 3 Residue-property plots [i](#)

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.

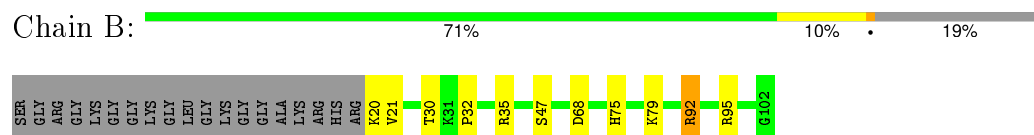
- Molecule 1: Histone H3.2



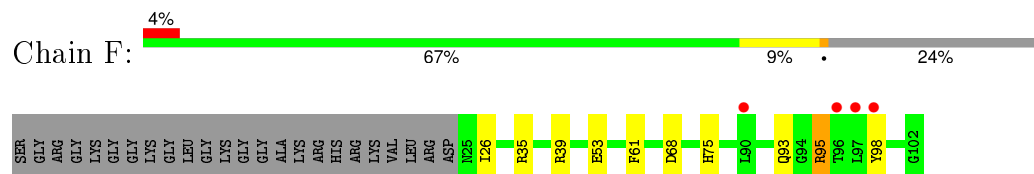
- Molecule 1: Histone H3.2



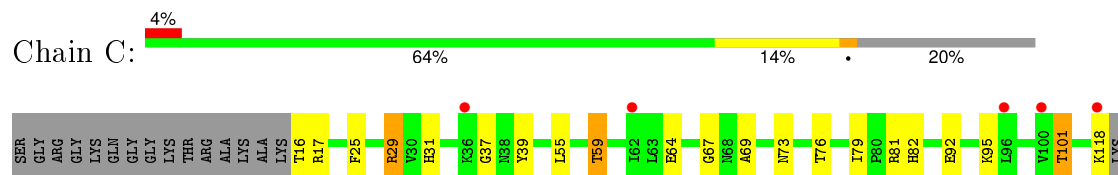
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A





THR  
GLU  
SER  
SER  
LYS  
LYS  
SER  
ALA  
LYS  
SER  
LYS

• Molecule 3: Histone H2A



SER  
GLY  
GLY  
SER  
GLY  
LYS  
GLN  
GLY  
GLY  
LYS  
THR  
ARG  
LYS  
LYS  
ALA  
LYS  
K14  
R17  
F25  
R31  
R38  
R42  
V43  
V44  
V45  
V54  
L55  
T59  
I62  
L63  
E64  
R71  
D72  
N73  
T76  
R77  
T78  
F79  
F80  
R81  
R82  
L83  
Q84  
R88  
I102  
K118  
LYS  
THR  
GLU

SER  
SER  
LYS  
LYS  
SER  
ALA  
LYS  
LYS  
SER  
LYS

• Molecule 4: Histone H2B 1.1



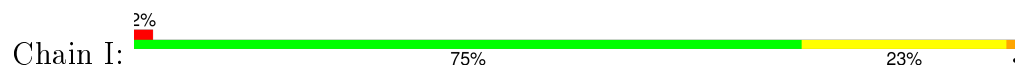
PRO  
GLU  
PRO  
ALA  
LYS  
SER  
SER  
ALA  
PRO  
ALA  
PRO  
LYS  
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LYS  
GLY  
SER  
VAL  
THR  
THR  
THR  
LYS  
LYS  
LYS  
ASP  
GLY  
K24  
K25  
R26  
R27  
K28  
T29  
R30  
K31  
E32  
S33  
Y34  
A35  
Y39  
K43  
H46  
M56  
S61  
F67  
E73  
L77  
A78  
H79  
T87  
S88  
R89  
T93  
R96  
L97  
L98  
L99  
P100  
E101  
E102  
L103  
A104  
S109  
V115  
T119  
A120  
A121  
K122

• Molecule 4: Histone H2B 1.1



PRO  
GLU  
PRO  
ALA  
LYS  
SER  
SER  
ALA  
PRO  
ALA  
PRO  
LYS  
LYS  
LYS  
GLY  
SER  
VAL  
THR  
THR  
THR  
LYS  
LYS  
LYS  
ASP  
GLY  
LYS  
LYS  
ARG  
ARG  
LYS  
T29  
R30  
Y34  
A35  
V38  
V45  
H46  
M56  
S57  
I58  
M59  
N60  
S61  
F62  
E68  
N81  
K82  
R83  
S84  
T85  
T93  
A94  
V95  
L98  
G101  
A104  
V108  
S120  
A121  
K122

• Molecule 5: 146-mer DNA

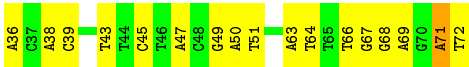


A-72  
C-67  
A-66  
A-62  
A-51  
A-46  
A-43  
G-35  
C-29  
T-28  
G-27  
T-23  
A-22  
T-21  
C-20  
A-19  
A-18  
G-14  
A-13  
A-12  
G-2  
T1  
T2  
C3  
A4  
A10  
G11  
C17  
A22  
T23  
A24  
G25  
G30  
T33  
G34  
C38  
A39  
C40  
C46  
T47  
C53  
C54  
G55  
C56  
A57  
G71  
A72  
T73

• Molecule 5: 146-mer DNA



A-73  
T-70  
C-60  
T-57  
G-56  
C-55  
G-54  
G-53  
C-50  
G-49  
C-34  
C-30  
T-29  
G-28  
C-25  
T-24  
C-21  
A-20  
A-19  
A-18  
G-17  
G-16  
G-15  
C-11  
T-10  
A-6  
C-5  
T-4  
G4  
T5  
T6  
G7  
A8  
T17  
G20  
A21  
A22  
A23  
G24  
C25  
G29  
T30  
T31  
T32  
G33



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.46Å 109.28Å 175.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.46 – 2.20 57.46 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (57.46-2.20) 98.1 (57.46-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.232 , 0.275 0.227 , 0.268	Depositor DCC
$R_{free}$ test set	2034 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.6	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 101641 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, SO4

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	0.67	0/820	0.66	0/1099
1	E	0.54	0/812	0.65	0/1088
2	B	0.73	0/669	0.73	0/894
2	F	0.58	0/626	0.67	0/837
3	C	0.52	0/805	0.62	0/1088
3	G	0.62	0/819	0.71	0/1106
4	D	0.58	0/796	0.67	1/1065 (0.1%)
4	H	0.62	0/747	0.68	0/1004
5	I	0.73	0/3354	1.34	16/5175 (0.3%)
5	J	0.72	0/3354	1.37	25/5175 (0.5%)
All	All	0.67	0/12802	1.10	42/18531 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	-30	DC	O4'-C1'-N1	7.85	113.49	108.00
5	I	-14	DG	P-O3'-C3'	7.76	129.01	119.70
5	I	-35	DG	O4'-C1'-N9	-7.47	102.77	108.00
5	J	-19	DA	O4'-C1'-N9	7.44	113.21	108.00
5	J	23	DA	P-O3'-C3'	7.09	128.21	119.70
5	J	21	DA	P-O3'-C3'	6.98	128.07	119.70
5	J	45	DC	P-O3'-C3'	6.93	128.01	119.70
5	J	20	DG	P-O3'-C3'	6.72	127.76	119.70
5	J	-18	DA	P-O3'-C3'	6.68	127.72	119.70
5	I	53	DC	P-O3'-C3'	6.67	127.71	119.70
5	J	21	DA	O4'-C1'-N9	6.66	112.66	108.00
5	I	10	DA	O4'-C1'-N9	6.33	112.43	108.00
5	I	-51	DA	P-O3'-C3'	6.20	127.14	119.70
5	J	-17	DG	P-O3'-C3'	6.20	127.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	-29	DC	P-O3'-C3'	6.16	127.09	119.70
5	I	38	DC	O4'-C1'-N1	6.10	112.27	108.00
5	I	-12	DA	P-O3'-C3'	6.09	127.01	119.70
5	J	4	DG	P-O3'-C3'	6.08	127.00	119.70
5	J	30	DT	O4'-C1'-N1	6.03	112.22	108.00
5	J	-15	DG	O4'-C1'-N9	6.03	112.22	108.00
5	I	40	DC	P-O3'-C3'	6.01	126.92	119.70
5	J	-49	DG	P-O3'-C3'	5.96	126.85	119.70
5	I	25	DG	O4'-C1'-N9	5.86	112.10	108.00
5	I	57	DA	P-O3'-C3'	5.79	126.65	119.70
5	J	71	DA	P-O3'-C3'	5.64	126.47	119.70
5	J	32	DT	O4'-C1'-N1	5.62	111.93	108.00
5	J	-60	DC	P-O3'-C3'	5.60	126.42	119.70
5	I	1	DT	O4'-C1'-N1	5.50	111.85	108.00
5	J	29	DG	O4'-C1'-N9	5.49	111.84	108.00
5	I	-21	DT	O4'-C1'-N1	5.46	111.82	108.00
4	D	77	LEU	CA-CB-CG	5.37	127.64	115.30
5	J	-6	DA	O4'-C1'-N9	-5.30	104.29	108.00
5	J	25	DC	O4'-C1'-N1	5.30	111.71	108.00
5	I	-2	DG	O4'-C1'-N9	5.26	111.68	108.00
5	J	-20	DA	P-O3'-C3'	5.17	125.90	119.70
5	J	5	DT	O4'-C1'-N1	-5.13	104.41	108.00
5	I	-35	DG	P-O3'-C3'	5.10	125.83	119.70
5	I	-18	DA	P-O3'-C3'	5.09	125.81	119.70
5	J	64	DT	P-O3'-C3'	5.07	125.79	119.70
5	J	-11	DC	P-O3'-C3'	5.06	125.78	119.70
5	J	51	DT	P-O3'-C3'	5.03	125.73	119.70
5	J	43	DT	O4'-C1'-N1	5.00	111.50	108.00

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	808	0	846	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	801	0	838	4	0
2	B	662	0	709	10	0
2	F	619	0	659	9	0
3	C	795	0	846	16	0
3	G	809	0	864	28	0
4	D	785	0	825	24	0
4	H	736	0	760	25	0
5	I	2990	0	1651	21	0
5	J	2990	0	1651	32	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	I	9	0	0	0	0
6	J	9	0	0	0	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	G	5	0	0	3	0
8	A	62	0	0	2	0
8	B	41	0	0	1	0
8	C	31	0	0	0	0
8	D	16	0	0	3	0
8	E	37	0	0	0	0
8	F	28	0	0	2	0
8	G	52	0	0	4	0
8	H	35	0	0	0	0
8	I	50	0	0	0	0
8	J	47	0	0	1	0
All	All	12430	0	9649	130	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 6.

All (130) 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)
2:B:75:HIS:CD2	4:D:93:THR:HG21	1.80	1.17
2:F:75:HIS:CD2	4:H:93:THR:HG21	1.85	1.10
2:B:75:HIS:HD2	4:D:93:THR:HG21	1.18	0.98
2:B:95:ARG:HD2	8:B:502:HOH:O	1.69	0.92
2:F:75:HIS:HD2	4:H:93:THR:HG21	1.28	0.90
3:C:55:LEU:O	3:C:59:THR:HG23	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:55:LEU:O	3:G:59:THR:HG23	1.75	0.87
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.56	0.85
2:B:75:HIS:HD2	4:D:93:THR:CG2	1.92	0.83
2:B:75:HIS:CD2	4:D:93:THR:CG2	2.62	0.82
2:F:75:HIS:CD2	4:H:93:THR:CG2	2.62	0.82
4:D:30:ARG:HG3	5:J:49:DG:H4'	1.63	0.81
4:D:79:HIS:HE1	3:G:38:ASN:HD22	1.28	0.81
4:H:35:ALA:HA	4:H:56:MET:CE	2.11	0.80
4:D:98:LEU:HB2	8:D:503:HOH:O	1.82	0.79
3:G:44:GLY:HA3	7:G:1103:SO4:O3	1.84	0.78
4:H:35:ALA:HA	4:H:56:MET:HE1	1.67	0.77
3:G:46:GLY:N	7:G:1103:SO4:O1	2.17	0.74
4:H:34:TYR:H	4:H:60:ASN:ND2	1.87	0.73
3:C:29:ARG:NH2	4:D:33:SER:O	2.22	0.72
4:D:79:HIS:CE1	3:G:38:ASN:HD22	2.09	0.71
5:J:67:DG:H2''	5:J:68:DG:H5''	1.73	0.70
2:F:75:HIS:HD2	4:H:93:THR:CG2	1.99	0.70
4:H:85:THR:HG23	5:J:-34:DC:OP1	1.93	0.69
3:G:62:ILE:HD11	4:H:62:PHE:CZ	2.27	0.68
1:A:69:ARG:NH2	5:J:17:DT:OP2	2.28	0.67
5:J:68:DG:H2''	5:J:69:DA:C8	2.30	0.67
1:A:69:ARG:NH2	5:J:17:DT:P	2.70	0.65
3:C:17:ARG:HH12	3:C:31:HIS:CD2	2.16	0.64
4:D:35:ALA:HA	4:D:56:MET:HE1	1.82	0.62
4:H:34:TYR:H	4:H:60:ASN:HD21	1.49	0.61
1:A:90:MET:HE1	8:A:404:HOH:O	2.02	0.60
3:G:71:ARG:NH1	8:G:137:HOH:O	2.35	0.59
3:G:42:ARG:HB2	4:H:85:THR:HB	1.83	0.59
3:G:84:GLN:NE2	3:G:88:ARG:HD2	2.18	0.58
3:G:84:GLN:O	3:G:88:ARG:HG2	2.04	0.58
1:E:63:ARG:HE	5:I:17:DC:H5''	1.69	0.57
3:C:16:THR:HA	5:I:-43:DA:H5''	1.87	0.57
5:I:-46:DA:H2	5:J:47:DA:H2	1.54	0.55
2:B:20:LYS:HG3	2:B:21:VAL:N	2.20	0.54
3:G:64:GLU:O	4:H:46:HIS:HE1	1.90	0.54
5:J:-21:DC:H2''	5:J:-20:DA:O5'	2.07	0.54
3:G:44:GLY:CA	7:G:1103:SO4:O3	2.55	0.54
3:G:17:ARG:HH12	3:G:31:HIS:CD2	2.26	0.54
5:I:46:DC:H2''	5:I:47:DT:H71	1.90	0.53
1:A:69:ARG:HH22	5:J:17:DT:P	2.31	0.53
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:LEU:HD11	4:H:38:VAL:HG13	1.91	0.53
3:C:55:LEU:O	3:C:59:THR:CG2	2.53	0.53
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.40	0.53
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.91	0.52
8:G:545:HOH:O	4:H:68:GLU:HG3	2.09	0.52
4:D:96:ARG:NH1	8:D:470:HOH:O	2.39	0.51
5:J:-20:DA:H2"	5:J:-19:DA:OP2	2.10	0.51
5:J:66:DT:OP1	8:J:517:HOH:O	2.18	0.51
4:H:85:THR:CG2	5:J:-34:DC:OP1	2.58	0.51
1:A:63:ARG:HH12	2:B:30:THR:CG2	2.25	0.50
4:H:35:ALA:HA	4:H:56:MET:HE2	1.92	0.50
3:C:101:THR:CG2	8:F:105:HOH:O	2.59	0.50
5:I:-28:DT:H2"	5:I:-27:DG:C8	2.47	0.49
3:G:55:LEU:O	3:G:59:THR:CG2	2.55	0.49
3:G:84:GLN:HE21	3:G:84:GLN:HA	1.77	0.49
4:D:35:ALA:HA	4:D:56:MET:CE	2.43	0.49
5:J:-29:DT:H2"	5:J:-28:DG:C8	2.49	0.48
5:J:-5:DC:H2"	5:J:-4:DT:H72	1.96	0.47
4:D:39:TYR:CE2	4:D:43:LYS:HE2	2.49	0.47
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.49	0.47
5:J:-50:DC:H2"	5:J:-49:DG:C8	2.49	0.47
4:D:115:VAL:O	4:D:119:THR:HG23	2.15	0.46
5:I:33:DT:H2"	5:I:34:DG:C8	2.50	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.50	0.46
4:D:67:PHE:C	4:D:67:PHE:CD2	2.89	0.46
5:J:20:DG:H2"	5:J:21:DA:OP2	2.15	0.46
4:H:81:ASN:O	4:H:83:ARG:NH1	2.48	0.45
1:A:41:TYR:HA	5:I:71:DG:H5"	1.98	0.45
5:I:71:DG:N2	5:J:-70:DT:O2	2.50	0.45
5:I:-67:DC:H2'	5:I:-66:DA:C8	2.52	0.45
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.16	0.45
5:I:-29:DC:H2"	5:I:-28:DT:OP2	2.15	0.45
3:G:64:GLU:HB2	4:H:45:VAL:HG11	1.98	0.45
4:H:121:ALA:O	4:H:122:LYS:HB2	2.16	0.44
4:H:104:ALA:O	4:H:108:VAL:HG23	2.17	0.44
5:I:57:DA:H61	5:J:-57:DT:H3	1.64	0.44
3:G:62:ILE:HD11	4:H:62:PHE:CE1	2.52	0.44
3:C:69:ALA:O	3:C:73:ASN:ND2	2.50	0.44
5:J:49:DG:H2'	5:J:50:DA:C8	2.53	0.44
5:J:-25:DC:H2"	5:J:-24:DT:H72	1.99	0.44
5:I:-62:DA:C2	5:J:63:DA:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLY:HA3	4:D:46:HIS:CE1	2.53	0.44
3:C:64:GLU:O	4:D:46:HIS:HE1	2.00	0.44
4:D:29:THR:HB	5:I:30:DG:OP1	2.18	0.43
3:C:37:GLY:HA3	3:C:39:TYR:CE1	2.53	0.43
5:J:71:DA:H2"	5:J:72:DT:OP2	2.18	0.43
4:D:89:ARG:O	4:D:93:THR:HG22	2.19	0.43
5:J:7:DG:H2"	5:J:8:DA:OP2	2.18	0.43
3:C:17:ARG:HH22	3:C:31:HIS:HD2	1.67	0.43
2:B:35:ARG:HH22	5:J:8:DA:P	2.40	0.43
4:D:25:LYS:HA	4:D:25:LYS:HE3	2.00	0.43
1:A:72:ARG:HH22	5:I:-23:DT:P	2.42	0.42
5:I:-46:DA:H2	5:J:47:DA:C2	2.35	0.42
3:G:77:ARG:NE	5:J:-55:DC:H4'	2.35	0.42
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.67	0.42
5:I:3:DC:H2"	5:I:4:DA:N7	2.35	0.42
3:G:73:ASN:ND2	8:G:136:HOH:O	2.44	0.42
3:C:101:THR:HG22	8:F:105:HOH:O	2.19	0.42
1:A:49:ARG:NH2	8:A:137:HOH:O	2.48	0.42
5:I:11:DG:N2	5:J:-10:DT:C2	2.88	0.42
1:A:79:LYS:HB3	1:A:82:LEU:HD11	2.02	0.42
2:B:30:THR:HB	2:B:32:PRO:HD2	2.02	0.42
5:I:54:DC:H2"	5:I:55:DG:N7	2.35	0.42
5:I:-20:DC:H2"	5:I:-19:DA:C8	2.55	0.42
5:I:-35:DG:N2	5:J:36:DA:C2	2.88	0.41
7:C:1102:SO4:O3	4:D:87:THR:HB	2.20	0.41
1:E:59:GLU:HG3	1:E:59:GLU:H	1.41	0.41
3:C:95:LYS:HE3	3:C:95:LYS:HB2	1.85	0.41
3:G:77:ARG:CZ	5:J:-55:DC:H4'	2.50	0.41
3:C:92:GLU:HB3	4:D:103:LEU:HD22	2.01	0.41
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.53	0.41
2:F:61:PHE:HE1	2:F:95:ARG:HD2	1.85	0.41
3:G:25:PHE:CZ	3:G:59:THR:HG21	2.55	0.41
3:G:64:GLU:OE2	4:H:45:VAL:CG1	2.68	0.41
4:D:73:GLU:HG3	8:D:503:HOH:O	2.20	0.41
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.03	0.41
5:J:38:DA:H2"	5:J:39:DC:OP2	2.21	0.41
4:D:61:SER:HB3	2:F:98:TYR:CD1	2.56	0.41
3:G:62:ILE:HD11	4:H:62:PHE:CE2	2.56	0.41
3:G:81:ARG:HD3	8:G:145:HOH:O	2.22	0.40
5:I:-46:DA:C2	5:J:47:DA:H2	2.35	0.40
2:F:35:ARG:O	2:F:39:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:71:DA:H1'	5:J:72:DT:H5'	2.02	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	96/135 (71%)	96 (100%)	0	0	100	100
1	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	81/102 (79%)	81 (100%)	0	0	100	100
2	F	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	101/129 (78%)	98 (97%)	3 (3%)	0	100	100
3	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
4	D	97/125 (78%)	95 (98%)	0	2 (2%)	9	5
4	H	92/125 (74%)	90 (98%)	0	2 (2%)	8	4
All	All	741/982 (76%)	729 (98%)	8 (1%)	4 (0%)	34	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	H	120	SER
4	D	25	LYS

### 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	85/110 (77%)	81 (95%)	4 (5%)	32	39
1	E	84/110 (76%)	80 (95%)	4 (5%)	31	37
2	B	68/78 (87%)	65 (96%)	3 (4%)	35	42
2	F	63/78 (81%)	61 (97%)	2 (3%)	46	57
3	C	82/101 (81%)	76 (93%)	6 (7%)	17	18
3	G	83/101 (82%)	77 (93%)	6 (7%)	18	18
4	D	85/105 (81%)	80 (94%)	5 (6%)	24	27
4	H	80/105 (76%)	73 (91%)	7 (9%)	12	12
All	All	630/788 (80%)	593 (94%)	37 (6%)	24	27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	59	GLU
1	A	81	ASP
1	A	90	MET
2	B	47	SER
2	B	79	LYS
2	B	92	ARG
3	C	29	ARG
3	C	59	THR
3	C	76	THR
3	C	81	ARG
3	C	101	THR
3	C	118	LYS
4	D	25	LYS
4	D	77	LEU
4	D	93	THR
4	D	103	LEU
4	D	109	SER
1	E	40	ARG

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Mol	Chain	Res	Type
1	E	42	ARG
1	E	59	GLU
1	E	79	LYS
2	F	26	ILE
2	F	95	ARG
3	G	42	ARG
3	G	59	THR
3	G	76	THR
3	G	81	ARG
3	G	84	GLN
3	G	88	ARG
4	H	30	ARG
4	H	68	GLU
4	H	82	LYS
4	H	83	ARG
4	H	85	THR
4	H	93	THR
4	H	120	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
2	B	75	HIS
3	C	31	HIS
4	D	46	HIS
4	D	79	HIS
2	F	75	HIS
3	G	31	HIS
3	G	84	GLN
4	H	46	HIS
4	H	60	ASN
4	H	92	GLN
4	H	106	HIS

### 5.3.3 RNA ⓘ

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](#)

Of 24 ligands modelled in this entry, 21 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
7	SO4	C	1102	-	4,4,4	0.52	0	6,6,6	0.33	0
7	SO4	D	1101	-	4,4,4	0.25	0	6,6,6	0.10	0
7	SO4	G	1103	-	4,4,4	0.74	0	6,6,6	0.35	0

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
7	SO4	C	1102	-	-	0/0/0/0	0/0/0/0
7	SO4	D	1101	-	-	0/0/0/0	0/0/0/0
7	SO4	G	1103	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1102	SO4	1	0
7	G	1103	SO4	3	0

## 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, 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	98/135 (72%)	0.28	1 (1%) 84 83	27, 40, 60, 69	0
1	E	97/135 (71%)	0.26	1 (1%) 84 83	36, 48, 62, 70	0
2	B	83/102 (81%)	0.32	0 100 100	27, 38, 47, 54	0
2	F	78/102 (76%)	0.47	4 (5%) 32 31	37, 44, 55, 59	0
3	C	103/129 (79%)	0.54	5 (4%) 33 33	36, 50, 64, 75	0
3	G	105/129 (81%)	0.46	2 (1%) 70 68	28, 43, 60, 73	0
4	D	99/125 (79%)	0.76	10 (10%) 9 8	39, 52, 87, 100	0
4	H	94/125 (75%)	0.65	3 (3%) 51 50	32, 44, 67, 79	0
5	I	146/146 (100%)	0.21	3 (2%) 67 65	48, 95, 144, 155	0
5	J	146/146 (100%)	0.14	5 (3%) 49 47	52, 93, 129, 142	0
All	All	1049/1274 (82%)	0.39	34 (3%) 51 50	27, 50, 118, 155	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	24	LYS	8.6
1	A	135	ALA	6.7
3	C	118	LYS	6.4
4	H	122	LYS	3.8
5	J	-18	DA	3.5
4	D	122	LYS	3.0
3	G	118	LYS	3.0
3	C	100	VAL	2.9
3	G	14	ALA	2.7
5	J	33	DG	2.7
5	I	22	DA	2.6
4	D	25	LYS	2.6
4	D	27	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	97	LEU	2.5
1	E	135	ALA	2.5
4	D	98	LEU	2.3
5	J	-53	DG	2.2
4	H	45	VAL	2.2
4	D	99	LEU	2.2
4	D	104	ALA	2.2
4	D	39	TYR	2.2
3	C	36	LYS	2.1
3	C	96	LEU	2.1
4	D	121	ALA	2.1
2	F	98	TYR	2.1
5	I	-19	DA	2.1
4	D	31	LYS	2.1
3	C	62	ILE	2.1
5	J	23	DA	2.1
5	J	-50	DC	2.1
2	F	96	THR	2.1
5	I	23	DT	2.0
4	H	98	LEU	2.0
2	F	90	LEU	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	SO4	G	1103	5/5	0.97	0.30	5.77	32,37,40,41	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	D	1101	5/5	0.79	0.40	4.40	148,148,148,148	0
7	SO4	C	1102	5/5	0.93	0.22	3.80	45,48,49,51	5
6	MN	A	1001	1/1	1.00	0.18	0.53	37,37,37,37	0
6	MN	J	1009	1/1	0.45	0.12	-	120,120,120,120	0
6	MN	I	1014	1/1	0.95	0.13	-	108,108,108,108	0
6	MN	J	1015	1/1	0.70	0.11	-	124,124,124,124	0
6	MN	I	1017	1/1	0.61	0.12	-	125,125,125,125	0
6	MN	I	1021	1/1	0.74	0.19	-	134,134,134,134	0
6	MN	J	1012	1/1	0.79	0.09	-	121,121,121,121	0
6	MN	E	1002	1/1	0.96	0.20	-	94,94,94,94	0
6	MN	I	1005	1/1	0.87	0.14	-	83,83,83,83	0
6	MN	D	1007	1/1	0.72	0.17	-	130,130,130,130	0
6	MN	J	1011	1/1	0.67	0.18	-	124,124,124,124	0
6	MN	J	1020	1/1	0.79	0.18	-	150,150,150,150	0
6	MN	J	1010	1/1	0.06	0.38	-	188,188,188,188	0
6	MN	I	1013	1/1	-0.58	0.19	-	176,176,176,176	0
6	MN	I	1003	1/1	0.95	0.22	-	77,77,77,77	0
6	MN	J	1016	1/1	0.87	0.19	-	102,102,102,102	0
6	MN	I	1006	1/1	0.92	0.12	-	83,83,83,83	0
6	MN	I	1019	1/1	0.95	0.23	-	118,118,118,118	0
6	MN	J	1018	1/1	0.53	0.15	-	115,115,115,115	0
6	MN	I	1004	1/1	0.80	0.13	-	127,127,127,127	0
6	MN	J	1008	1/1	0.98	0.05	-	147,147,147,147	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.