



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:53 pm BST

PDB ID : 1HQ3  
Title : CRYSTAL STRUCTURE OF THE HISTONE-CORE-OCTAMER IN KCL/PHOSPHATE  
Authors : Chantalat, L.; Nicholson, J.M.; Lambert, S.J.; Reid, A.J.; Donovan, M.J.; Reynolds, C.D.; Wood, C.M.; Baldwin, J.P.  
Deposited on : 2000-12-14  
Resolution : 2.15 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

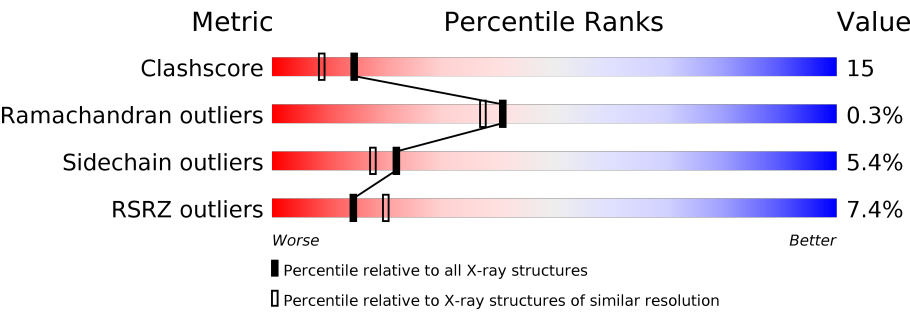
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	129	<div><div>5%</div><div><div></div><div>60%</div><div>19%</div><div>•</div><div>18%</div></div></div>
1	E	129	<div><div>5%</div><div><div></div><div>58%</div><div>20%</div><div>•</div><div>19%</div></div></div>
2	B	126	<div><div>5%</div><div><div></div><div>54%</div><div>17%</div><div>•</div><div>27%</div></div></div>
2	F	126	<div><div>6%</div><div><div></div><div>63%</div><div>10%</div><div>•</div><div>26%</div></div></div>
3	C	136	<div><div>4%</div><div><div></div><div>49%</div><div>19%</div><div>•</div><div>30%</div></div></div>
3	G	136	<div><div>7%</div><div><div></div><div>47%</div><div>23%</div><div>••</div><div>28%</div></div></div>
4	D	103	<div><div>8%</div><div><div></div><div>63%</div><div>14%</div><div>•</div><div>19%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	H	103	

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
5	PO4	C	505	-	-	-	X
5	PO4	E	504	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6466 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 H2A-IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	4	0	0
			815	516	158	141			
1	E	104	Total	C	N	O	0	0	0
			797	504	154	139			

- Molecule 2 is a protein called HISTONE H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	6	0	0
			720	453	129	136	2			
2	F	93	Total	C	N	O	S	5	0	0
			729	459	131	137	2			

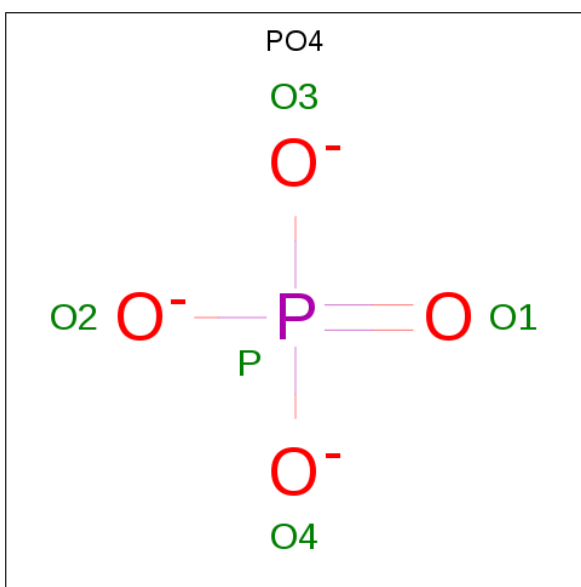
- Molecule 3 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	20	0	0
			779	491	148	137	3			
3	G	98	Total	C	N	O	S	7	0	0
			807	508	156	140	3			

- Molecule 4 is a protein called HISTONE H4-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	83	Total	C	N	O	S	5	0	0
			662	418	129	114	1			
4	H	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	4	Total	Cl	0	0
			4	4		
6	D	3	Total	Cl	0	0
			3	3		
6	E	2	Total	Cl	0	0
			2	2		
6	H	3	Total	Cl	0	0
			3	3		
6	B	1	Total	Cl	0	0
			1	1		
6	C	3	Total	Cl	0	0
			3	3		
6	A	5	Total	Cl	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

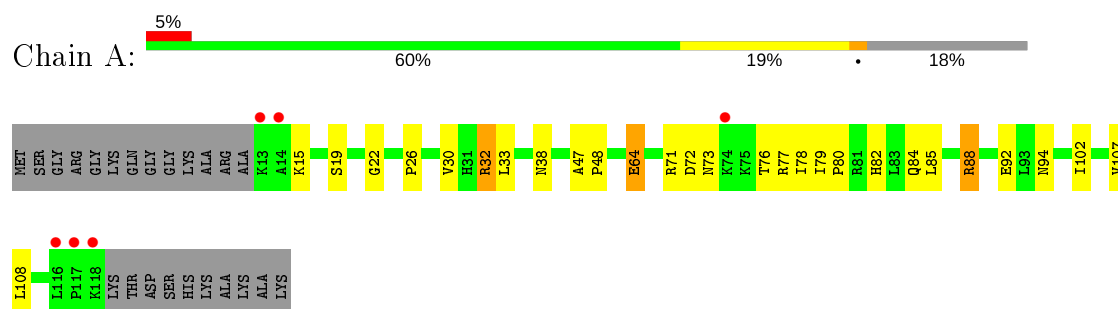
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	73	Total O 73 73	0	0
7	B	51	Total O 51 51	0	0
7	C	42	Total O 42 42	0	0
7	D	53	Total O 53 53	0	0
7	E	71	Total O 71 71	0	0
7	F	51	Total O 51 51	0	0
7	G	52	Total O 52 52	0	0
7	H	44	Total O 44 44	0	0

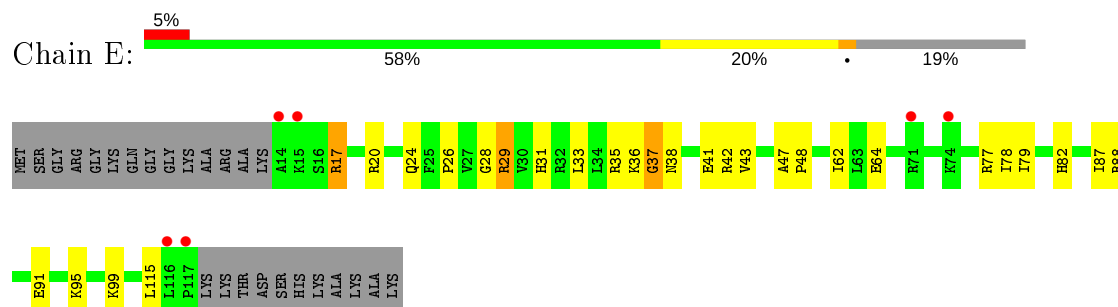
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

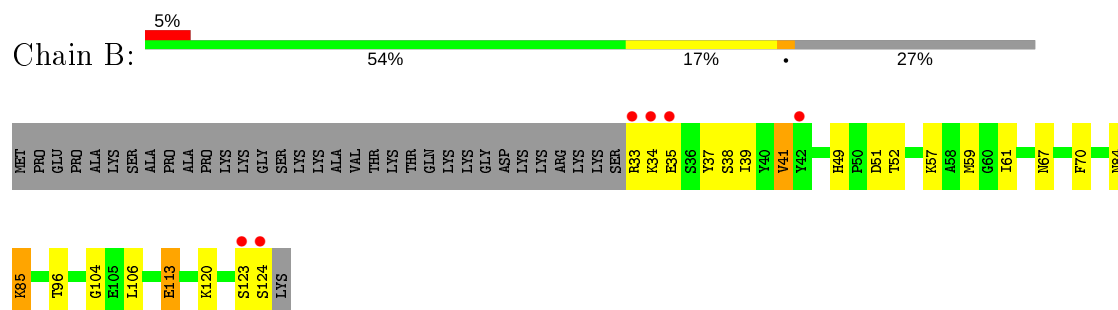
#### • Molecule 1: HISTONE H2A-IV



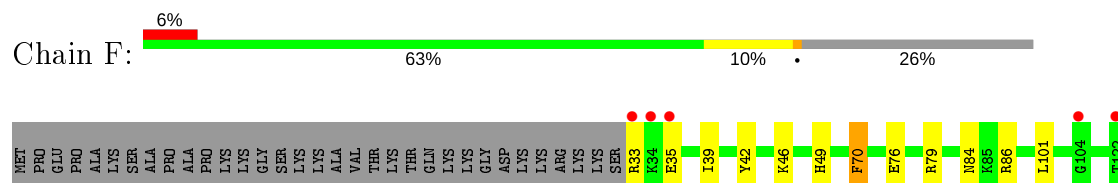
#### • Molecule 1: HISTONE H2A-IV



#### • Molecule 2: HISTONE H2B

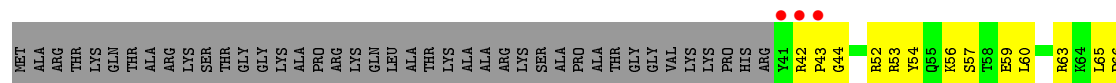


#### • Molecule 2: HISTONE H2B

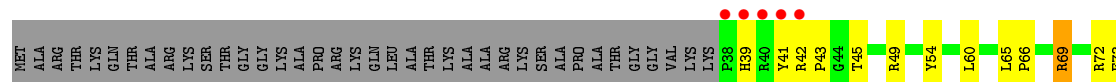




● Molecule 3: HISTONE H3



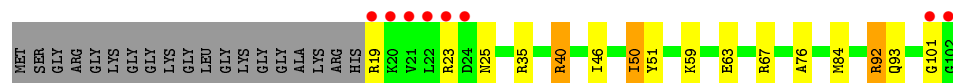
● Molecule 3: HISTONE H3



● Molecule 4: HISTONE H4-VI



● Molecule 4: HISTONE H4-VI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.56Å 158.56Å 102.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.15 137.32 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.15) 100.0 (137.32-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.253 0.216 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 16.3	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.209 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL

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	0.49	0/825	0.66	0/1112
1	E	0.46	0/807	0.67	1/1090 (0.1%)
2	B	0.54	0/731	0.70	1/983 (0.1%)
2	F	0.51	0/740	0.64	0/993
3	C	0.50	0/789	0.73	1/1057 (0.1%)
3	G	0.54	0/819	0.73	0/1097
4	D	0.51	0/669	0.73	0/894
4	H	0.53	0/680	0.74	0/908
All	All	0.51	0/6060	0.70	3/8134 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	116	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	37	GLY	N-CA-C	5.97	128.03	113.10
2	B	106	LEU	CA-CB-CG	5.38	127.68	115.30

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	815	0	877	30	0
1	E	797	0	851	25	0
2	B	720	0	740	28	0
2	F	729	0	750	15	0
3	C	779	0	816	35	0
3	G	807	0	844	34	0
4	D	662	0	709	30	0
4	H	673	0	722	21	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	E	10	0	0	2	0
6	A	5	0	0	0	0
6	B	1	0	0	1	0
6	C	3	0	0	0	0
6	D	3	0	0	1	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	4	0	0	0	0
6	H	3	0	0	0	0
7	A	73	0	0	5	0
7	B	51	0	0	3	0
7	C	42	0	0	5	0
7	D	53	0	0	5	0
7	E	71	0	0	1	0
7	F	51	0	0	1	0
7	G	52	0	0	4	0
7	H	44	0	0	4	0
All	All	6466	0	6309	188	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 15.

All (188) 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:H:92:ARG:HH11	4:H:92:ARG:HG3	0.99	1.11
4:D:44:LYS:HE2	7:D:645:HOH:O	1.59	1.02
3:G:128:ARG:HE	3:G:134:ARG:NH2	1.64	0.96
1:A:71:ARG:HH21	2:B:52:THR:HG22	1.32	0.93
4:H:92:ARG:NH1	4:H:92:ARG:HG3	1.74	0.92
4:D:30:THR:HG22	4:D:33:ALA:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:92:ARG:HH11	4:H:92:ARG:CG	1.87	0.85
4:D:30:THR:HB	6:D:612:CL:CL	2.16	0.83
3:C:52:ARG:O	3:C:56:LYS:HG2	1.81	0.79
3:C:42:ARG:HD3	3:C:44:GLY:H	1.47	0.79
3:G:125:GLN:HA	3:G:134:ARG:NH1	1.97	0.78
3:G:79:LYS:HD3	3:G:82:LEU:HD13	1.66	0.76
3:C:76:GLN:HE21	3:C:80:THR:HG22	1.50	0.76
3:G:72:ARG:HD2	7:G:663:HOH:O	1.85	0.76
3:C:42:ARG:HG2	3:C:43:PRO:HD2	1.68	0.76
3:G:85:GLN:OE1	7:G:631:HOH:O	2.05	0.75
2:B:85:LYS:HE2	2:F:33:ARG:NH1	2.03	0.74
4:D:92:ARG:HB3	4:D:92:ARG:NH1	2.04	0.73
1:E:17:ARG:HG3	1:E:17:ARG:HH21	1.53	0.72
4:D:35:ARG:NH2	7:D:660:HOH:O	2.13	0.71
1:A:32:ARG:HD3	5:A:501:PO4:O2	1.91	0.69
1:A:38:ASN:HA	7:A:646:HOH:O	1.91	0.69
3:G:69:ARG:NH1	7:G:658:HOH:O	2.26	0.69
4:H:19:ARG:HD3	4:H:19:ARG:C	2.13	0.68
3:C:57:SER:OG	3:C:59:GLU:HG2	1.93	0.68
4:D:30:THR:HG23	4:D:32:PRO:CD	2.23	0.68
4:H:67:ARG:NH2	7:H:658:HOH:O	2.24	0.68
2:F:101:LEU:HD23	4:H:92:ARG:NH2	2.08	0.68
3:G:41:TYR:HB3	7:G:643:HOH:O	1.93	0.68
3:C:42:ARG:HG2	3:C:43:PRO:CD	2.23	0.68
3:G:121:PRO:O	3:G:125:GLN:HG3	1.94	0.68
3:G:125:GLN:HG2	3:G:134:ARG:HH12	1.58	0.68
2:F:39:ILE:HG12	7:F:639:HOH:O	1.94	0.67
1:E:33:LEU:HD11	2:F:35:GLU:HG3	1.75	0.67
3:C:125:GLN:HB3	3:C:134:ARG:HH21	1.60	0.67
3:C:42:ARG:HD3	3:C:44:GLY:N	2.08	0.66
3:G:41:TYR:CE2	3:G:49:ARG:NH2	2.65	0.65
3:C:125:GLN:HB3	3:C:134:ARG:NH2	2.11	0.65
2:B:33:ARG:N	7:B:656:HOH:O	2.29	0.64
2:B:51:ASP:HA	7:B:662:HOH:O	1.98	0.64
3:C:65:LEU:HD23	7:C:625:HOH:O	1.97	0.64
1:E:77:ARG:HH12	5:E:504:PO4:P	2.19	0.64
4:H:19:ARG:O	4:H:19:ARG:HD3	1.98	0.64
3:C:79:LYS:HB3	3:C:82:LEU:CD1	2.29	0.63
1:E:17:ARG:HG3	1:E:17:ARG:NH2	2.14	0.63
1:A:38:ASN:HB3	7:E:662:HOH:O	1.97	0.63
3:G:42:ARG:HG2	3:G:43:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:125:GLN:HG2	3:G:134:ARG:NH1	2.14	0.62
1:A:88:ARG:HE	1:A:94:ASN:HD22	1.47	0.61
3:C:116:ARG:NH2	3:C:123:ASP:OD2	2.32	0.60
4:D:30:THR:HG23	4:D:32:PRO:HD2	1.83	0.60
1:A:79:ILE:H	1:A:82:HIS:CD2	2.19	0.60
3:C:77:ASP:CG	4:D:23:ARG:HH12	2.05	0.60
1:E:77:ARG:NH1	5:E:504:PO4:O3	2.32	0.59
4:H:46:ILE:CG2	4:H:50:ILE:HG12	2.32	0.59
2:B:37:TYR:O	2:B:41:VAL:HG12	2.03	0.58
1:A:33:LEU:HD11	2:B:35:GLU:HG3	1.85	0.58
4:D:30:THR:CG2	4:D:32:PRO:HG2	2.34	0.58
3:G:132:GLY:HA2	3:G:135:ALA:HB2	1.84	0.58
2:B:35:GLU:HB2	2:B:67:ASN:HD21	1.68	0.58
2:F:42:TYR:OH	2:F:46:LYS:HE3	2.04	0.58
3:G:125:GLN:HA	3:G:134:ARG:HH11	1.66	0.57
4:H:84:MET:HE1	4:H:101:GLY:HA2	1.86	0.57
1:E:79:ILE:H	1:E:82:HIS:CD2	2.22	0.57
7:A:658:HOH:O	2:B:113:GLU:HG2	2.05	0.57
3:C:53:ARG:NH2	5:C:505:PO4:O3	2.37	0.56
3:G:83:ARG:HG2	3:G:84:PHE:N	2.20	0.56
4:D:46:ILE:HG23	4:D:50:ILE:HG12	1.85	0.56
1:A:71:ARG:NH2	1:A:76:THR:HG22	2.21	0.56
1:E:62:ILE:HD11	1:E:87:ILE:HD11	1.88	0.54
3:G:65:LEU:HB3	3:G:66:PRO:HD3	1.90	0.54
4:H:23:ARG:NH1	7:H:644:HOH:O	2.40	0.54
2:B:96:THR:OG1	4:D:75:HIS:HD2	1.90	0.53
7:D:658:HOH:O	1:E:99:LYS:HD2	2.06	0.53
4:D:92:ARG:HB3	4:D:92:ARG:HH11	1.70	0.53
1:E:64:GLU:O	2:F:49:HIS:HE1	1.92	0.53
4:D:66:ILE:O	4:D:70:VAL:HG13	2.09	0.53
3:C:79:LYS:HB3	3:C:82:LEU:HD12	1.91	0.52
4:H:93:GLN:HG2	7:H:649:HOH:O	2.08	0.52
4:D:30:THR:CG2	4:D:33:ALA:H	2.15	0.52
3:C:63:ARG:NE	3:C:66:PRO:HG2	2.24	0.52
3:C:116:ARG:HD3	7:C:654:HOH:O	2.09	0.52
1:E:17:ARG:NH1	1:E:28:GLY:HA2	2.24	0.51
3:G:128:ARG:HE	3:G:134:ARG:CZ	2.23	0.51
1:A:88:ARG:HE	1:A:94:ASN:ND2	2.08	0.51
2:F:84:ASN:HD21	4:H:76:ALA:HB2	1.75	0.51
3:G:45:THR:O	3:G:49:ARG:HG3	2.11	0.51
1:A:33:LEU:CD1	2:B:35:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:THR:HG23	4:D:32:PRO:HG2	1.93	0.51
1:E:78:ILE:HA	1:E:82:HIS:HD2	1.75	0.51
3:C:77:ASP:OD1	4:D:23:ARG:NH1	2.43	0.51
4:D:35:ARG:NE	7:D:660:HOH:O	2.38	0.51
1:E:33:LEU:CD1	2:F:35:GLU:HG3	2.41	0.50
1:A:79:ILE:H	1:A:82:HIS:HD2	1.60	0.50
1:E:20:ARG:HD3	2:F:124:SER:O	2.11	0.50
3:C:42:ARG:HD3	3:C:44:GLY:CA	2.41	0.50
3:C:79:LYS:HB3	3:C:82:LEU:HD11	1.92	0.50
1:E:42:ARG:HG2	1:E:43:VAL:N	2.27	0.50
4:H:35:ARG:CD	7:H:629:HOH:O	2.59	0.50
2:B:41:VAL:HG11	2:B:59:MET:SD	2.52	0.50
3:G:131:ARG:HD3	3:G:133:GLU:OE2	2.12	0.50
4:D:50:ILE:O	4:D:50:ILE:HD12	2.12	0.50
2:B:39:ILE:HG12	7:B:640:HOH:O	2.11	0.50
3:G:54:TYR:O	4:H:40:ARG:HD3	2.11	0.50
4:H:59:LYS:HE2	4:H:63:GLU:OE1	2.12	0.50
1:A:72:ASP:C	1:A:73:ASN:HD22	2.16	0.49
2:B:51:ASP:OD2	2:B:51:ASP:N	2.46	0.48
7:A:658:HOH:O	2:B:113:GLU:CG	2.62	0.48
3:G:128:ARG:NE	3:G:134:ARG:NH2	2.48	0.48
3:G:97:GLU:O	3:G:101:VAL:HG13	2.13	0.48
4:H:84:MET:CE	4:H:101:GLY:HA2	2.43	0.48
3:C:54:TYR:CZ	4:D:36:ARG:HG2	2.48	0.48
3:G:41:TYR:N	3:G:41:TYR:CD1	2.81	0.48
1:A:38:ASN:HB2	7:A:695:HOH:O	2.13	0.48
2:B:38:SER:HA	2:B:41:VAL:CG1	2.43	0.48
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.78	0.48
2:B:41:VAL:CG1	2:B:59:MET:SD	3.02	0.48
1:E:47:ALA:N	1:E:48:PRO:HD2	2.28	0.48
3:C:76:GLN:HB3	4:D:23:ARG:HH22	1.78	0.47
3:G:125:GLN:CA	3:G:134:ARG:NH1	2.74	0.47
2:B:84:ASN:HD21	4:D:76:ALA:HB2	1.80	0.47
3:C:65:LEU:H	3:C:65:LEU:HD22	1.80	0.47
1:E:91:GLU:O	1:E:95:LYS:HG3	2.15	0.47
3:G:134:ARG:O	3:G:135:ALA:OXT	2.33	0.47
2:B:96:THR:OG1	4:D:75:HIS:CD2	2.68	0.47
4:D:30:THR:HG23	4:D:32:PRO:CG	2.44	0.47
1:E:79:ILE:H	1:E:82:HIS:HD2	1.63	0.47
3:C:65:LEU:N	3:C:65:LEU:HD22	2.29	0.47
1:E:37:GLY:O	1:E:38:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:ILE:HG23	4:H:50:ILE:HG12	1.98	0.46
3:C:56:LYS:NZ	7:C:623:HOH:O	2.41	0.46
3:G:128:ARG:HE	3:G:134:ARG:HH21	1.55	0.46
1:A:102:ILE:CG2	2:B:61:ILE:HD13	2.45	0.46
3:G:79:LYS:HB3	3:G:82:LEU:HD22	1.96	0.46
1:A:102:ILE:HG23	2:B:61:ILE:HD13	1.98	0.46
3:C:101:VAL:CG2	7:C:659:HOH:O	2.64	0.46
3:C:65:LEU:HB2	3:C:66:PRO:HD3	1.97	0.46
2:B:34:LYS:HD2	6:B:614:CL:CL	2.54	0.45
1:E:62:ILE:CD1	1:E:87:ILE:HD11	2.46	0.45
1:A:78:ILE:HA	1:A:82:HIS:HD2	1.80	0.45
2:F:42:TYR:CZ	2:F:46:LYS:HE3	2.51	0.45
1:A:22:GLY:CA	2:B:120:LYS:HE2	2.47	0.45
1:E:91:GLU:HG2	1:E:95:LYS:HE3	1.99	0.45
4:D:35:ARG:CZ	7:D:660:HOH:O	2.59	0.45
3:C:76:GLN:NE2	3:C:80:THR:HA	2.32	0.45
3:C:63:ARG:CZ	3:C:66:PRO:HG2	2.47	0.44
1:A:22:GLY:HA3	2:B:120:LYS:HE2	1.99	0.44
2:F:101:LEU:CD2	4:H:92:ARG:NH2	2.77	0.44
3:C:42:ARG:HD3	3:C:44:GLY:HA3	1.99	0.44
1:A:71:ARG:NH2	2:B:52:THR:HG22	2.16	0.43
1:A:92:GLU:HG3	7:A:674:HOH:O	2.17	0.43
4:H:50:ILE:HG13	4:H:51:TYR:N	2.33	0.43
2:F:70:PHE:CD1	2:F:70:PHE:C	2.92	0.43
4:D:92:ARG:HB3	4:D:92:ARG:CZ	2.48	0.43
3:G:79:LYS:HG2	3:G:80:THR:O	2.18	0.43
3:G:60:LEU:HD12	3:G:90:MET:HE1	2.00	0.43
2:B:85:LYS:HE2	2:F:33:ARG:HH11	1.80	0.42
2:F:101:LEU:CD2	4:H:92:ARG:HH21	2.32	0.42
1:A:64:GLU:O	2:B:49:HIS:HE1	2.03	0.42
3:C:60:LEU:CD1	3:C:90:MET:HE1	2.50	0.42
1:E:26:PRO:HB2	1:E:29:ARG:HB2	2.00	0.42
1:A:47:ALA:N	1:A:48:PRO:HD2	2.33	0.42
2:B:123:SER:OG	2:B:124:SER:N	2.53	0.42
1:E:36:LYS:HG2	1:E:36:LYS:O	2.19	0.42
4:D:84:MET:HE1	4:D:101:GLY:HA2	2.01	0.42
3:C:117:VAL:HG22	1:E:115:LEU:HD22	2.00	0.41
1:A:84:GLN:OE1	1:A:88:ARG:HD3	2.19	0.41
4:D:30:THR:HG21	4:D:32:PRO:HG2	2.01	0.41
3:G:60:LEU:CD1	3:G:90:MET:HE1	2.49	0.41
1:A:15:LYS:HG2	1:A:19:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:GLN:NE2	7:C:634:HOH:O	2.53	0.41
3:C:54:TYR:O	4:D:40:ARG:HD3	2.20	0.41
1:A:79:ILE:HB	1:A:80:PRO:HD2	2.03	0.41
3:C:108:ASN:HD22	3:C:108:ASN:HA	1.69	0.41
1:A:85:LEU:HD23	1:A:108:LEU:HD23	2.02	0.41
2:B:70:PHE:CD1	2:B:70:PHE:C	2.94	0.41
1:E:17:ARG:CG	1:E:17:ARG:HH21	2.25	0.41
3:G:83:ARG:HG2	3:G:84:PHE:H	1.86	0.41
4:D:50:ILE:C	4:D:50:ILE:HD12	2.41	0.41
3:G:125:GLN:CB	3:G:134:ARG:HH11	2.34	0.41
2:F:76:GLU:HA	2:F:79:ARG:NH2	2.36	0.40
3:G:73:GLU:OE1	4:H:25:ASN:HB2	2.21	0.40
4:D:27:GLN:NE2	4:D:27:GLN:HA	2.36	0.40
1:A:26:PRO:O	1:A:30:VAL:HG23	2.22	0.40
3:G:125:GLN:CA	3:G:134:ARG:HH11	2.31	0.40
1:A:79:ILE:HG12	1:A:82:HIS:CD2	2.57	0.40
1:A:107:VAL:HG13	1:A:108:LEU:N	2.36	0.40
1:E:31:HIS:CE1	1:E:35:ARG:CZ	3.05	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	104/129 (81%)	98 (94%)	6 (6%)	0	100	100
1	E	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
2	B	90/126 (71%)	87 (97%)	2 (2%)	1 (1%)	14	8
2	F	91/126 (72%)	91 (100%)	0	0	100	100
3	C	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
3	G	96/136 (71%)	90 (94%)	5 (5%)	1 (1%)	15	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	81/103 (79%)	81 (100%)	0	0	100	100
4	H	82/103 (80%)	82 (100%)	0	0	100	100
All	All	739/988 (75%)	720 (97%)	17 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	104	GLY
3	G	134	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	
1	A	83/98 (85%)	80 (96%)	3 (4%)	35	33
1	E	81/98 (83%)	76 (94%)	5 (6%)	18	14
2	B	79/107 (74%)	75 (95%)	4 (5%)	24	20
2	F	79/107 (74%)	76 (96%)	3 (4%)	33	31
3	C	82/111 (74%)	78 (95%)	4 (5%)	25	21
3	G	85/111 (77%)	77 (91%)	8 (9%)	8	4
4	D	68/79 (86%)	64 (94%)	4 (6%)	19	15
4	H	69/79 (87%)	66 (96%)	3 (4%)	29	27
All	All	626/790 (79%)	592 (95%)	34 (5%)	22	18

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	64	GLU
1	A	88	ARG
2	B	41	VAL
2	B	57	LYS

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Mol	Chain	Res	Type
2	B	85	LYS
2	B	113	GLU
3	C	103	LEU
3	C	108	ASN
3	C	117	VAL
3	C	129	ARG
4	D	30	THR
4	D	40	ARG
4	D	50	ILE
4	D	92	ARG
1	E	17	ARG
1	E	24	GLN
1	E	29	ARG
1	E	41	GLU
1	E	88	ARG
2	F	70	PHE
2	F	86	ARG
2	F	125	LYS
3	G	39	HIS
3	G	69	ARG
3	G	77	ASP
3	G	101	VAL
3	G	116	ARG
3	G	117	VAL
3	G	129	ARG
3	G	134	ARG
4	H	40	ARG
4	H	50	ILE
4	H	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	73	ASN
1	A	82	HIS
1	A	89	ASN
1	A	94	ASN
2	B	49	HIS
2	B	67	ASN
2	B	84	ASN
2	B	95	GLN

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Mol	Chain	Res	Type
3	C	76	GLN
3	C	108	ASN
3	C	125	GLN
4	D	25	ASN
4	D	27	GLN
4	D	75	HIS
1	E	31	HIS
1	E	68	ASN
1	E	82	HIS
2	F	47	GLN
2	F	49	HIS
2	F	84	ASN
3	G	93	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 22 are monoatomic - leaving 5 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	$\# Z  > 2$
5	PO4	C	505	-	4,4,4	1.23	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	PO4	A	501	-	4,4,4	1.75	0	6,6,6	0.43	0
5	PO4	E	503	-	4,4,4	1.34	0	6,6,6	0.43	0
5	PO4	B	502	-	4,4,4	1.28	0	6,6,6	0.45	0
5	PO4	E	504	-	4,4,4	1.52	0	6,6,6	0.43	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	PO4	1	0
5	A	501	PO4	1	0
5	E	504	PO4	2	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	106/129 (82%)	-0.10	6 (5%)	23 32	24, 35, 79, 100	1 (0%)
1	E	104/129 (80%)	-0.16	6 (5%)	23 31	22, 37, 64, 94	2 (1%)
2	B	92/126 (73%)	-0.03	6 (6%)	18 25	22, 36, 69, 87	1 (1%)
2	F	93/126 (73%)	-0.05	8 (8%)	10 15	21, 34, 68, 97	2 (2%)
3	C	95/136 (69%)	0.15	5 (5%)	26 35	24, 36, 76, 92	4 (4%)
3	G	98/136 (72%)	0.16	9 (9%)	9 13	22, 34, 92, 100	3 (3%)
4	D	83/103 (80%)	-0.15	8 (9%)	8 11	23, 33, 56, 86	3 (3%)
4	H	84/103 (81%)	0.13	8 (9%)	8 12	20, 31, 61, 100	0
All	All	755/988 (76%)	-0.01	56 (7%)	14 20	20, 35, 75, 100	16 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	135	ALA	16.9
2	F	125	LYS	10.9
2	B	33	ARG	9.7
4	H	21	VAL	9.5
3	C	42	ARG	9.4
1	A	118	LYS	9.0
3	C	41	TYR	8.9
4	H	102	GLY	8.9
3	G	40	ARG	8.8
4	D	20	LYS	7.7
2	B	124	SER	7.6
1	A	117	PRO	7.5
3	G	42	ARG	7.3
3	C	134	ARG	7.3
3	G	135	ALA	7.2
1	E	14	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
3	G	39	HIS	7.0
3	G	134	ARG	7.0
1	E	116	LEU	6.7
4	H	22	LEU	6.7
4	H	19	ARG	6.4
1	E	74	LYS	6.2
2	F	33	ARG	6.1
2	F	124	SER	5.5
3	C	43	PRO	5.5
4	H	20	LYS	5.0
3	G	41	TYR	5.0
4	D	23	ARG	4.7
2	F	123	SER	4.6
2	F	34	LYS	4.6
2	B	34	LYS	4.6
4	D	21	VAL	4.5
3	G	38	PRO	4.0
1	A	74	LYS	3.9
1	A	116	LEU	3.9
4	H	24	ASP	3.8
1	A	13	LYS	3.8
1	E	117	PRO	3.7
1	A	14	ALA	3.7
1	E	71	ARG	3.4
4	H	101	GLY	3.3
2	F	35	GLU	3.3
4	D	102	GLY	3.1
2	B	35	GLU	3.0
3	G	78	PHE	2.7
2	B	123	SER	2.7
2	F	122	THR	2.7
4	D	79	LYS	2.6
4	D	22	LEU	2.5
4	H	23	ARG	2.5
1	E	15	LYS	2.5
4	D	67	ARG	2.5
2	F	104	GLY	2.4
3	G	83	ARG	2.3
4	D	92	ARG	2.2
2	B	42	TYR	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	C	505	5/5	0.79	0.67	70,70,70,70	0
6	CL	A	613	1/1	0.84	0.10	76,76,76,76	0
5	PO4	E	504	5/5	0.86	0.64	70,70,70,70	0
5	PO4	B	502	5/5	0.86	0.72	58,60,70,70	0
5	PO4	E	503	5/5	0.87	0.49	69,70,70,70	0
6	CL	G	608	1/1	0.91	0.07	48,48,48,48	0
6	CL	G	601	1/1	0.92	0.08	42,42,42,42	0
6	CL	H	610	1/1	0.95	0.08	47,47,47,47	0
6	CL	A	620	1/1	0.96	0.14	81,81,81,81	0
6	CL	D	612	1/1	0.96	0.07	44,44,44,44	0
6	CL	G	609	1/1	0.96	0.09	46,46,46,46	0
6	CL	B	614	1/1	0.97	0.08	39,39,39,39	0
6	CL	C	619	1/1	0.97	0.08	58,58,58,58	0
6	CL	E	621	1/1	0.97	0.11	70,70,70,70	0
6	CL	D	617	1/1	0.98	0.06	43,43,43,43	0
6	CL	A	622	1/1	0.98	0.08	48,48,48,48	0
6	CL	C	607	1/1	0.98	0.09	47,47,47,47	0
5	PO4	A	501	5/5	0.98	0.11	46,46,53,61	0
6	CL	A	606	1/1	0.98	0.08	38,38,38,38	0
6	CL	H	605	1/1	0.98	0.11	42,42,42,42	0
6	CL	H	618	1/1	0.99	0.09	54,54,54,54	0
6	CL	E	602	1/1	0.99	0.09	45,45,45,45	0
6	CL	G	611	1/1	0.99	0.10	47,47,47,47	0
6	CL	A	604	1/1	0.99	0.07	34,34,34,34	0
6	CL	D	603	1/1	0.99	0.07	45,45,45,45	0
6	CL	F	616	1/1	0.99	0.09	44,44,44,44	0
6	CL	C	615	1/1	0.99	0.06	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.