



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:50 PM GMT

PDB ID : 5DQU
Title : Crystal Structure of Cas-DNA-10 complex
Authors : Wang, J.; Li, J.; Zhao, H.; Sheng, G.; Wang, M.; Yin, M.; Wang, Y.
Deposited on : 2015-09-15
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

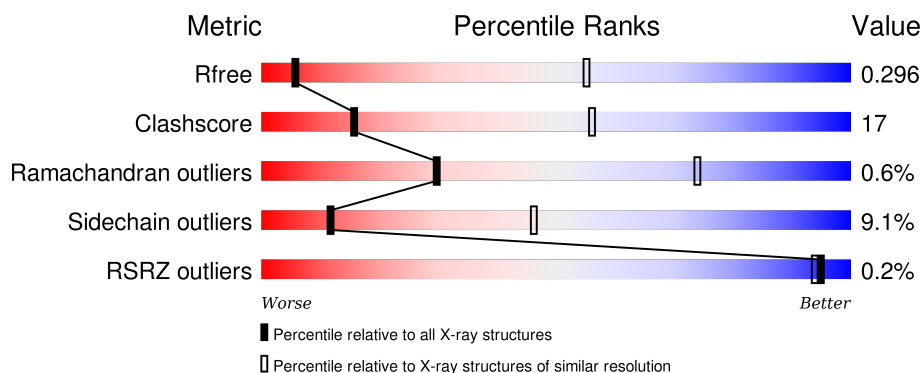
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.







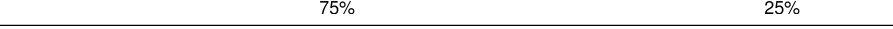
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	
1	C	305	
1	D	305	
2	E	94	

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Mol	Chain	Length	Quality of chain
2	F	94	 80% 14% . . .
3	H	15	 47% 53%
3	I	15	 53% 47%
4	G	12	 67% 33%
4	J	12	 75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10672 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 CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1270	351	359	7			
1	D	258	Total	C	N	O	S	0	0	0
			1967	1257	349	354	7			
1	C	274	Total	C	N	O	S	0	0	0
			2100	1344	373	376	7			
1	B	270	Total	C	N	O	S	0	0	0
			2068	1323	366	372	7			

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	93	Total	C	N	O	S	0	0	0
			732	470	127	131	4			
2	F	92	Total	C	N	O	S	0	0	0
			724	465	126	130	3			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*GP*TP*CP*GP*AP*TP*GP*CP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	15	Total	C	N	O	P	0	0	0
			305	148	50	93	14			
3	I	15	Total	C	N	O	P	0	0	0
			305	148	50	93	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*TP*GP*CP*AP*TP*CP*GP*AP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	12	Total	C	N	O	P	0	0	0
			242	116	40	74	12			

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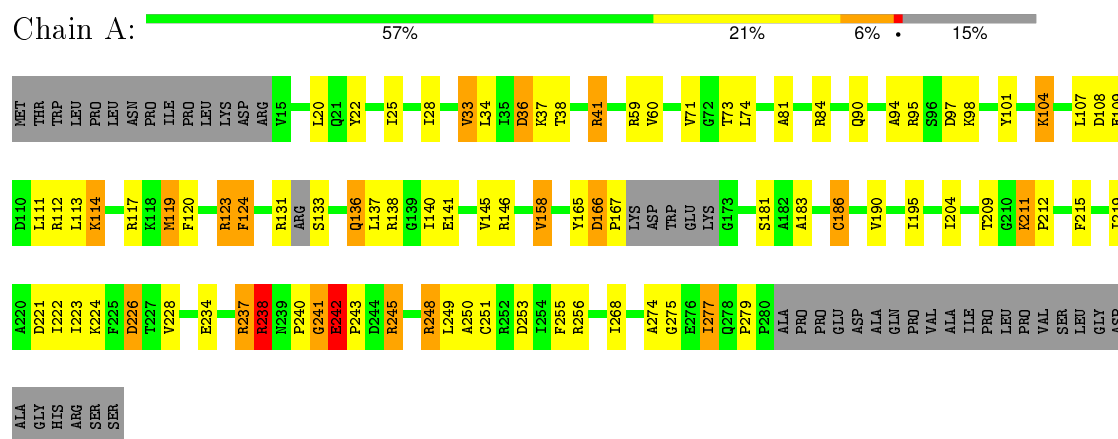
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	12	Total	C	N	O	P	0	0	0
			242	116	40	74	12			

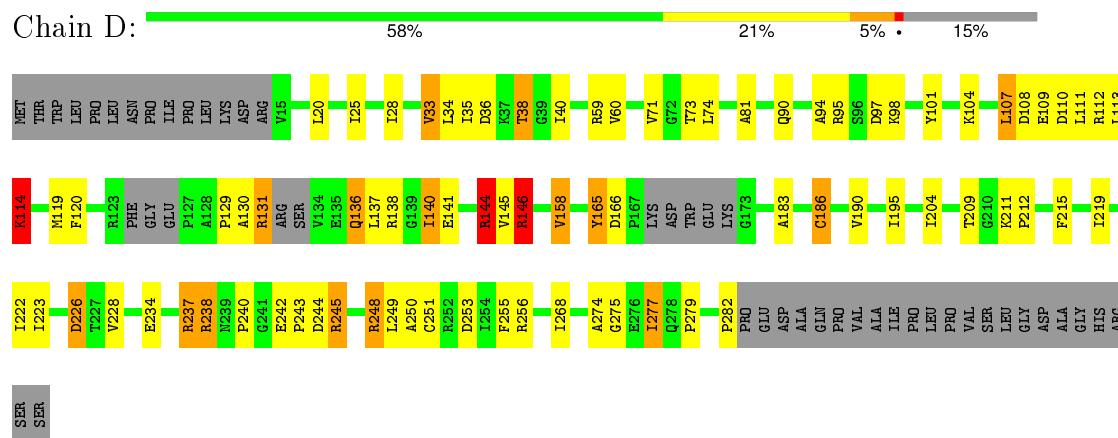
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

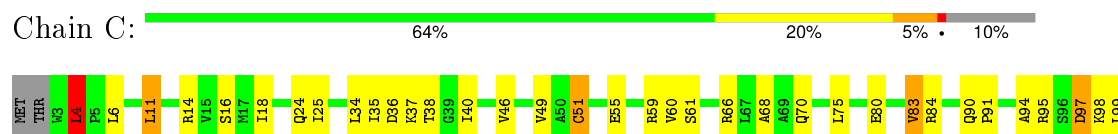
• Molecule 1: CRISPR-associated endonuclease Cas1

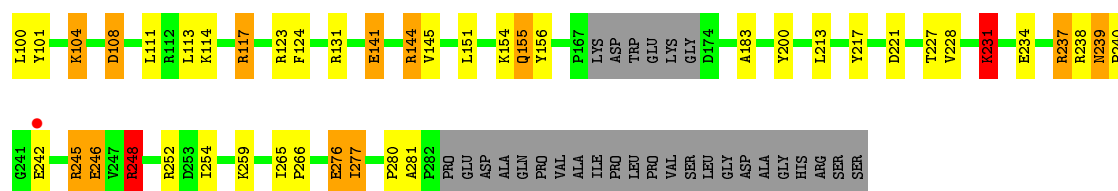


• Molecule 1: CRISPR-associated endonuclease Cas1



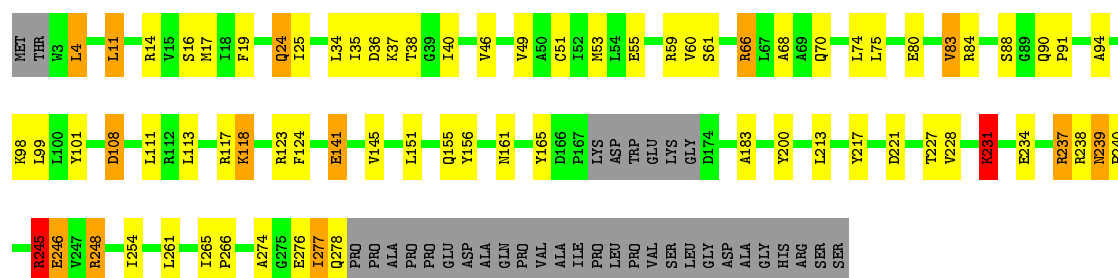
• Molecule 1: CRISPR-associated endonuclease Cas1





- Molecule 1: CRISPR-associated endonuclease Cas1

Chain B: 64% 20% 11%



- Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain E: 77% 19%



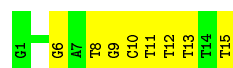
- Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F: 80% 14%



- Molecule 3: DNA (5'-D(*GP*AP*GP*TP*CP*GP*AP*TP*GP*CP*TP*TP*TP*TP*T)-3')

Chain H: 47% 53%



- Molecule 3: DNA (5'-D(*GP*AP*GP*TP*CP*GP*AP*TP*GP*CP*TP*TP*TP*TP*T)-3')

Chain I: 53% 47%



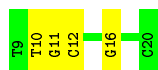
- Molecule 4: DNA (5'-D(P*TP*TP*GP*CP*AP*TP*CP*GP*AP*CP*TP*C)-3')

Chain J:  75% 25%



- Molecule 4: DNA (5'-D(P*TP*TP*GP*CP*AP*TP*CP*GP*AP*CP*TP*C)-3')

Chain G:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.09Å 195.78Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 49.53 – 4.44	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-4.50) 96.3 (49.53-4.44)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 4.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.265 , 0.287 0.279 , 0.296	Depositor DCC
R_{free} test set	838 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 2.0	EDS
Estimated twinning fraction	0.329 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17007 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	10672	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.58	1/2023 (0.0%)	0.92	11/2742 (0.4%)
1	B	0.50	0/2106	0.85	5/2857 (0.2%)
1	C	0.52	0/2141	0.90	5/2907 (0.2%)
1	D	0.56	0/2001	0.98	14/2711 (0.5%)
2	E	0.54	0/746	0.82	4/1014 (0.4%)
2	F	0.49	0/738	0.86	4/1004 (0.4%)
3	H	0.44	0/340	0.70	0/524
3	I	0.46	0/340	0.72	0/524
4	G	0.35	0/269	0.74	0/412
4	J	0.36	0/269	0.75	0/412
All	All	0.52	1/10973 (0.0%)	0.88	43/15107 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	PHE	CB-CG	-5.52	1.42	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	LEU	CA-CB-CG	9.22	136.51	115.30
1	A	124	PHE	CB-CG-CD1	-8.29	115.00	120.80
1	D	238	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	119	MET	CB-CG-SD	-8.12	88.04	112.40
1	D	144	ARG	CB-CA-C	-8.07	94.25	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	GLY	Peptide
1	A	242	GLU	Peptide

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	1987	0	2040	103	1
1	B	2068	0	2129	52	1
1	C	2100	0	2166	66	0
1	D	1967	0	2023	111	0
2	E	732	0	747	20	0
2	F	724	0	735	17	0
3	H	305	0	174	12	0
3	I	305	0	174	9	0
4	G	242	0	137	11	0
4	J	242	0	137	2	0
All	All	10672	0	10462	361	1

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 17.

The worst 5 of 361 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:D:120:PHE:HE2	1:D:140:ILE:HD11	1.07	1.18
1:D:242:GLU:CB	1:D:245:ARG:HD3	1.76	1.14
1:A:242:GLU:HG2	1:A:243:PRO:HD2	1.32	1.08
1:A:241:GLY:O	1:A:242:GLU:HB3	1.53	1.07
1:D:237:ARG:HA	1:D:237:ARG:CZ	1.86	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:NH1	1:B:161:ASN:ND2[1_455]	2.06	0.14

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	254/305 (83%)	245 (96%)	9 (4%)	0	100	100
1	B	266/305 (87%)	253 (95%)	10 (4%)	3 (1%)	17	64
1	C	270/305 (88%)	258 (96%)	9 (3%)	3 (1%)	17	64
1	D	250/305 (82%)	240 (96%)	9 (4%)	1 (0%)	39	80
2	E	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	F	90/94 (96%)	84 (93%)	6 (7%)	0	100	100
All	All	1221/1408 (87%)	1166 (96%)	48 (4%)	7 (1%)	30	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	80	GLU
1	B	80	GLU
1	C	4	LEU
1	B	4	LEU
1	D	130	ALA

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	206/245 (84%)	184 (89%)	22 (11%)	8	38
1	B	215/245 (88%)	194 (90%)	21 (10%)	10	42
1	C	219/245 (89%)	193 (88%)	26 (12%)	6	34
1	D	203/245 (83%)	187 (92%)	16 (8%)	15	53
2	E	78/79 (99%)	75 (96%)	3 (4%)	40	74
2	F	77/79 (98%)	74 (96%)	3 (4%)	39	73
All	All	998/1138 (88%)	907 (91%)	91 (9%)	12	46

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	LEU
1	C	108	ASP
1	B	231	LYS
1	C	11	LEU
1	C	51	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	D	161	ASN
1	C	24	GLN
1	B	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	260/305 (85%)	-0.22	0 100 100	21, 65, 122, 139	0
1	B	270/305 (88%)	-0.32	0 100 100	18, 61, 104, 139	0
1	C	274/305 (89%)	-0.31	1 (0%) 93 90	18, 62, 112, 140	0
1	D	258/305 (84%)	-0.20	0 100 100	24, 71, 121, 146	0
2	E	93/94 (98%)	-0.12	1 (1%) 82 76	21, 40, 73, 89	0
2	F	92/94 (97%)	-0.36	0 100 100	20, 42, 66, 91	0
3	H	15/15 (100%)	0.21	0 100 100	35, 65, 102, 103	0
3	I	15/15 (100%)	0.27	0 100 100	45, 61, 101, 109	0
4	G	12/12 (100%)	-0.02	0 100 100	34, 50, 117, 130	0
4	J	12/12 (100%)	-0.12	0 100 100	32, 56, 106, 117	0
All	All	1301/1462 (88%)	-0.25	2 (0%) 95 94	18, 59, 115, 146	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	GLU	2.4
2	E	9	GLU	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 carbohydrates 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.