



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LTL
Title : THE DODECAMER STRUCTURE OF MCM FROM ARCHAEAL M. THERMOAUTOTROPHICUM
Authors : Fletcher, R.J.; Bishop, B.E.; Leon, R.P.; Sclafani, R.A.; Ogata, C.M.; Chen, X.S.
Deposited on : 2002-05-20
Resolution : 3.00 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

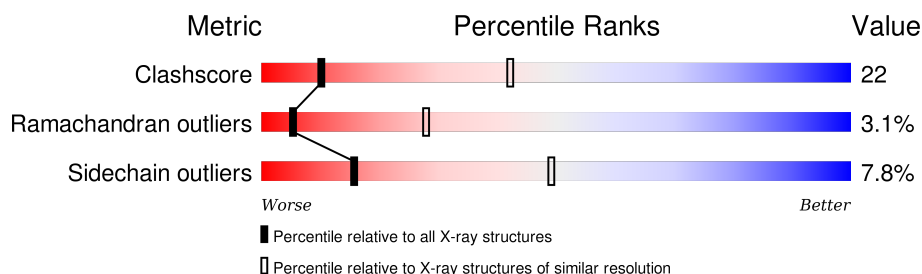
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	
1	B	279	
1	C	279	
1	D	279	
1	E	279	
1	F	279	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11633 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 DNA replication initiator (Cdc21/Cdc54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1941	1222	341	371	7			
1	B	239	Total	C	N	O	S	0	0	0
			1941	1222	341	371	7			
1	C	239	Total	C	N	O	S	0	0	0
			1926	1209	341	369	7			
1	D	239	Total	C	N	O	S	0	0	0
			1924	1211	341	365	7			
1	E	242	Total	C	N	O	S	0	0	0
			1956	1231	344	374	7			
1	F	239	Total	C	N	O	S	0	0	0
			1939	1220	341	371	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP O27798
A	-3	SER	-	CLONING ARTIFACT	UNP O27798
A	-2	GLY	-	CLONING ARTIFACT	UNP O27798
A	-1	SER	-	CLONING ARTIFACT	UNP O27798
A	0	ARG	-	CLONING ARTIFACT	UNP O27798
B	-4	GLY	-	CLONING ARTIFACT	UNP O27798
B	-3	SER	-	CLONING ARTIFACT	UNP O27798
B	-2	GLY	-	CLONING ARTIFACT	UNP O27798
B	-1	SER	-	CLONING ARTIFACT	UNP O27798
B	0	ARG	-	CLONING ARTIFACT	UNP O27798
C	-4	GLY	-	CLONING ARTIFACT	UNP O27798
C	-3	SER	-	CLONING ARTIFACT	UNP O27798
C	-2	GLY	-	CLONING ARTIFACT	UNP O27798
C	-1	SER	-	CLONING ARTIFACT	UNP O27798
C	0	ARG	-	CLONING ARTIFACT	UNP O27798
D	-4	GLY	-	CLONING ARTIFACT	UNP O27798
D	-3	SER	-	CLONING ARTIFACT	UNP O27798

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	CLONING ARTIFACT	UNP O27798
D	-1	SER	-	CLONING ARTIFACT	UNP O27798
D	0	ARG	-	CLONING ARTIFACT	UNP O27798
E	-4	GLY	-	CLONING ARTIFACT	UNP O27798
E	-3	SER	-	CLONING ARTIFACT	UNP O27798
E	-2	GLY	-	CLONING ARTIFACT	UNP O27798
E	-1	SER	-	CLONING ARTIFACT	UNP O27798
E	0	ARG	-	CLONING ARTIFACT	UNP O27798
F	-4	GLY	-	CLONING ARTIFACT	UNP O27798
F	-3	SER	-	CLONING ARTIFACT	UNP O27798
F	-2	GLY	-	CLONING ARTIFACT	UNP O27798
F	-1	SER	-	CLONING ARTIFACT	UNP O27798
F	0	ARG	-	CLONING ARTIFACT	UNP O27798

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

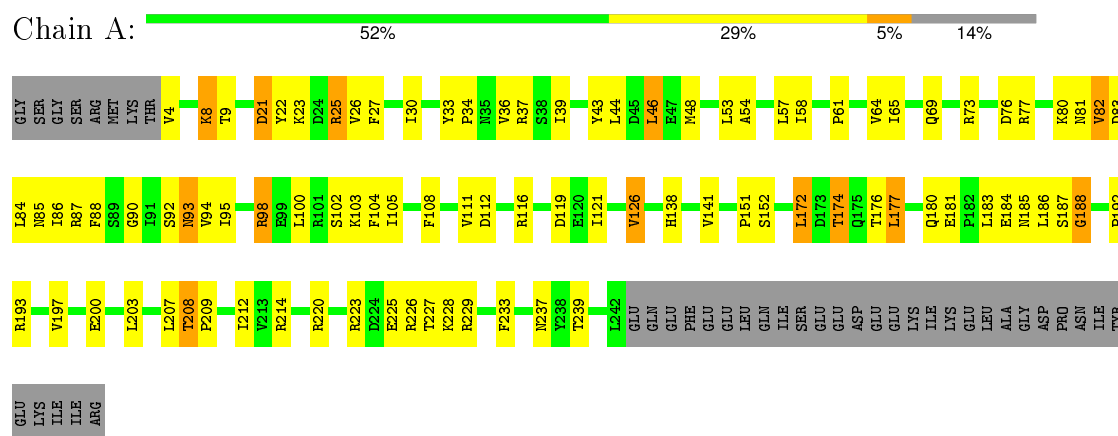
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

3 Residue-property plots

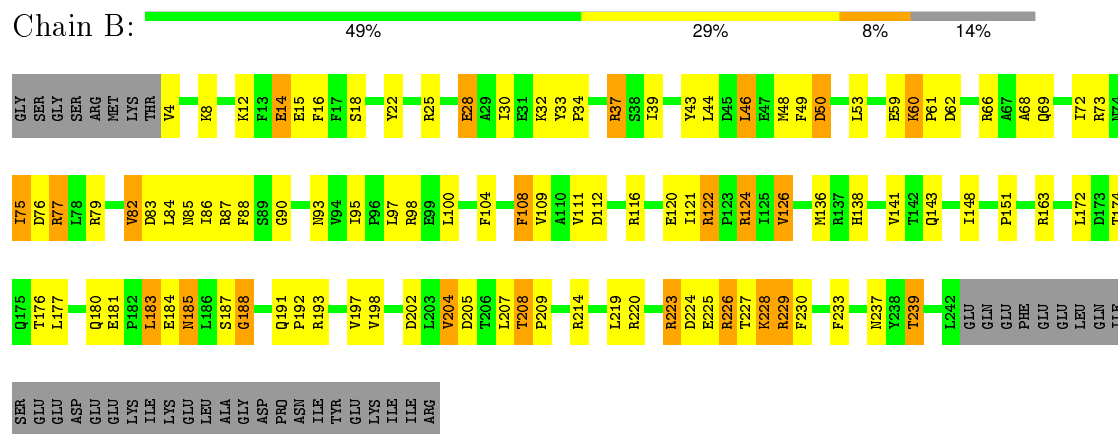
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

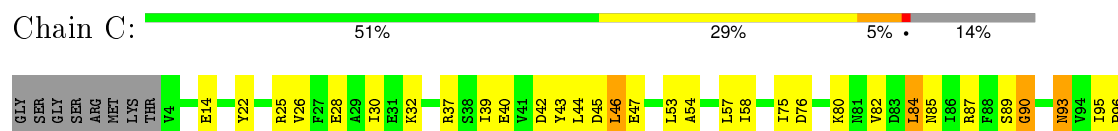
- Molecule 1: DNA replication initiator (Cdc21/Cdc54)

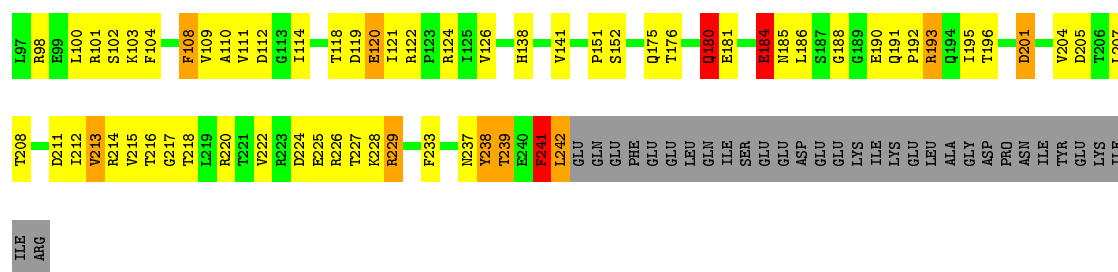


- Molecule 1: DNA replication initiator (Cdc21/Cdc54)

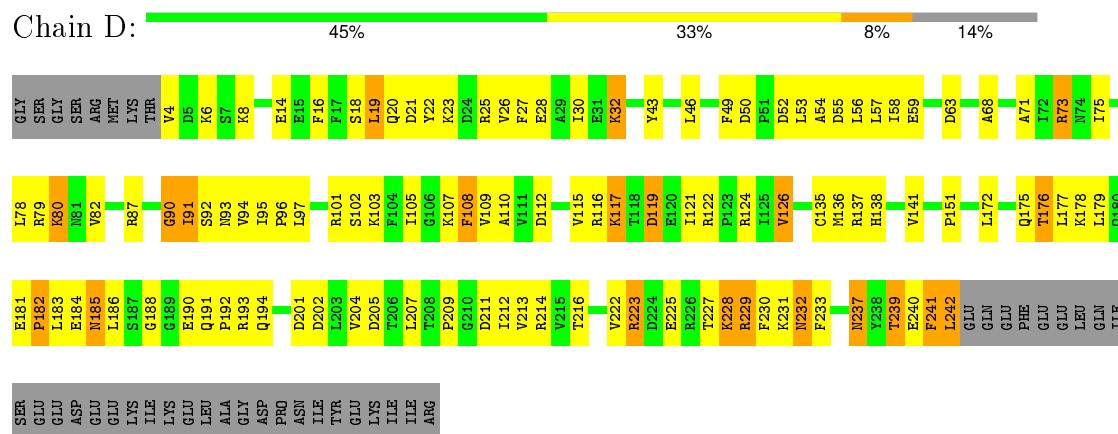


- Molecule 1: DNA replication initiator (Cdc21/Cdc54)

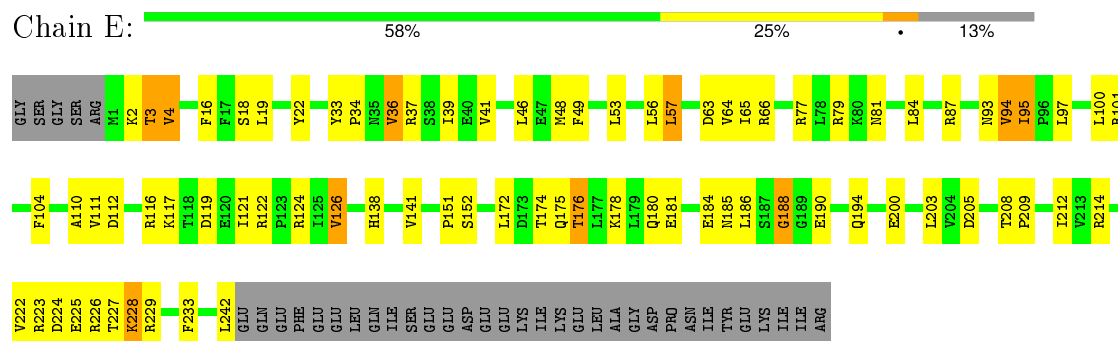




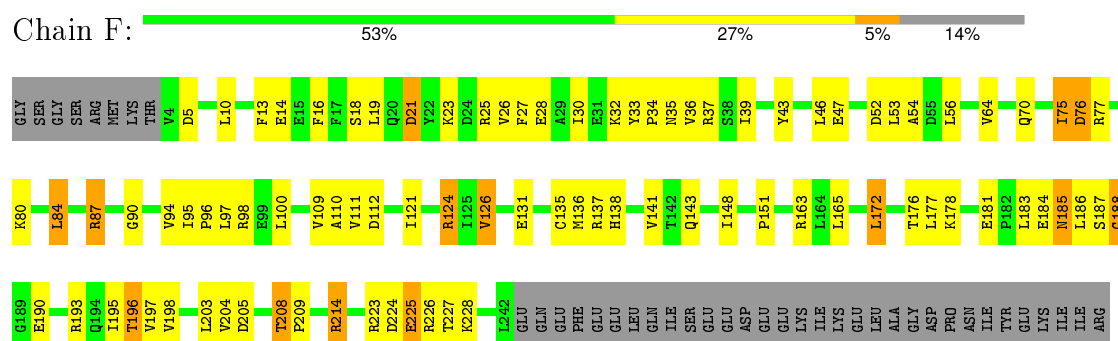
- Molecule 1: DNA replication initiator (Cdc21/Cdc54)



- Molecule 1: DNA replication initiator (Cdc21/Cdc54)



- Molecule 1: DNA replication initiator (Cdc21/Cdc54)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.32Å 192.32Å 365.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

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: ZN

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	0.51	0/1970	0.68	0/2656
1	B	0.57	0/1970	0.71	0/2656
1	C	0.68	3/1954 (0.2%)	1.53	11/2635 (0.4%)
1	D	1.14	6/1953 (0.3%)	1.01	14/2633 (0.5%)
1	E	0.52	0/1985	0.68	0/2677
1	F	0.50	0/1968	0.65	0/2653
All	All	0.69	9/11800 (0.1%)	0.93	25/15910 (0.2%)

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	C	0	3
1	D	0	1
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	ASN	C-N	-35.13	0.53	1.34
1	D	182	PRO	C-N	17.60	1.74	1.34
1	D	241	PHE	C-N	15.12	1.68	1.34
1	C	242	LEU	C-O	15.06	1.51	1.23
1	C	241	PHE	C-N	-14.68	1.00	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GLN	O-C-N	-52.77	38.27	122.70
1	C	241	PHE	O-C-N	-22.84	86.16	122.70
1	D	237	ASN	O-C-N	-19.61	91.33	122.70
1	C	241	PHE	CA-C-N	19.11	159.24	117.20
1	C	242	LEU	CA-C-O	17.56	156.98	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	180	GLN	Mainchain
1	C	241	PHE	Mainchain,Peptide
1	D	237	ASN	Mainchain

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	1941	0	1950	87	0
1	B	1941	0	1950	94	0
1	C	1926	0	1920	112	0
1	D	1924	0	1916	98	0
1	E	1956	0	1959	70	0
1	F	1939	0	1943	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	11633	0	11638	508	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 22.

The worst 5 of 508 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:241:PHE:C	1:D:242:LEU:N	1.68	1.44
1:C:98:ARG:HH21	1:C:193:ARG:CZ	1.35	1.38
1:D:182:PRO:C	1:D:183:LEU:N	1.74	1.37
1:C:227:THR:CG2	1:C:229:ARG:HG3	1.62	1.29
1:C:98:ARG:NE	1:C:193:ARG:HD2	1.43	1.29

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	237/279 (85%)	214 (90%)	18 (8%)	5 (2%)	9	40
1	B	237/279 (85%)	208 (88%)	21 (9%)	8 (3%)	5	25
1	C	237/279 (85%)	209 (88%)	21 (9%)	7 (3%)	5	29
1	D	237/279 (85%)	199 (84%)	28 (12%)	10 (4%)	3	20
1	E	240/279 (86%)	213 (89%)	19 (8%)	8 (3%)	5	26
1	F	237/279 (85%)	207 (87%)	24 (10%)	6 (2%)	7	34
All	All	1425/1674 (85%)	1250 (88%)	131 (9%)	44 (3%)	5	28

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLY
1	B	228	LYS
1	C	188	GLY
1	D	92	SER
1	D	188	GLY

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	219/256 (86%)	205 (94%)	14 (6%)	22	59
1	B	219/256 (86%)	197 (90%)	22 (10%)	9	34
1	C	215/256 (84%)	196 (91%)	19 (9%)	12	42
1	D	213/256 (83%)	193 (91%)	20 (9%)	11	39
1	E	219/256 (86%)	208 (95%)	11 (5%)	30	70
1	F	218/256 (85%)	203 (93%)	15 (7%)	19	56
All	All	1303/1536 (85%)	1202 (92%)	101 (8%)	16	49

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	HIS
1	D	28	GLU
1	F	124	ARG
1	C	191	GLN
1	C	211	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	C	69	GLN
1	D	194	GLN
1	B	191	GLN
1	D	232	ASN

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.