



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DJ0
Title : THE CRYSTAL STRUCTURE OF E. COLI PSEUDOURIDINE SYNTHASE
I AT 1.5 ANGSTROM RESOLUTION
Authors : Foster, P.G.; Huang, L.; Santi, D.V.; Stroud, R.M.
Deposited on : 1999-11-30
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

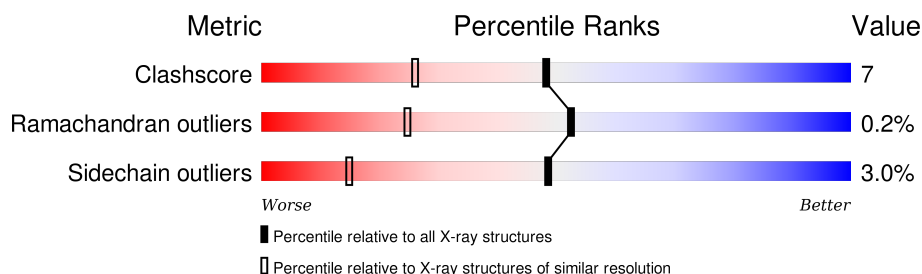
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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	264	 79% 16% • •
1	B	264	 81% 15% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4663 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 PSEUDOURIDINE SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2097	1333	382	374	8			
1	B	264	Total	C	N	O	S	0	0	0
			2097	1333	382	374	8			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

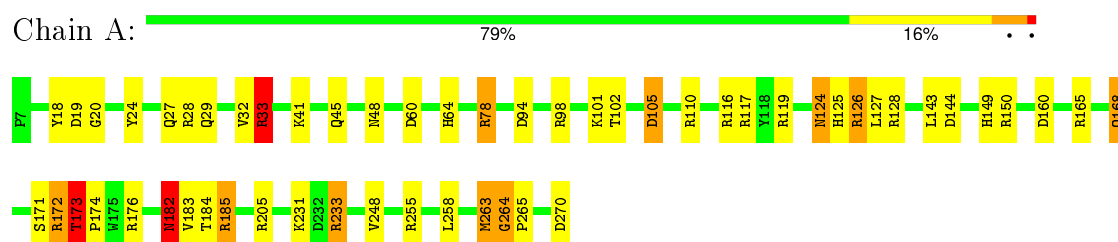
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	255	Total	O	0	0
			255	255		
3	B	212	Total	O	0	0
			212	212		

3 Residue-property plots [i](#)

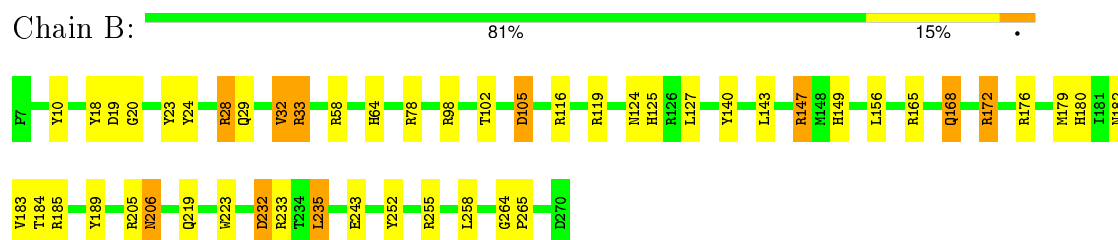
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PSEUDOURIDINE SYNTHASE I



• Molecule 1: PSEUDOURIDINE SYNTHASE I



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.08 Å 37.40 Å 103.48 Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	38.00 – 1.50	Depositor
% Data completeness (in resolution range)	95.2 (38.00-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4663	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.63	0/2153	1.50	40/2929 (1.4%)
1	B	0.57	0/2153	1.47	33/2929 (1.1%)
All	All	0.60	0/4306	1.49	73/5858 (1.2%)

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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	A	263	MET	CA-CB-CG	12.24	134.11	113.30
1	A	128	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	B	58	ARG	CD-NE-CZ	10.07	137.69	123.60
1	B	176	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	150	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	28	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	33	ARG	CD-NE-CZ	9.07	136.30	123.60
1	A	110	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	150	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	185	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	128	ARG	NE-CZ-NH2	-8.44	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	116	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	98	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	78	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	A	255	ARG	CD-NE-CZ	7.49	134.08	123.60
1	A	270	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	173	THR	CA-C-O	7.26	135.34	120.10
1	B	32	VAL	CA-CB-CG2	7.07	121.50	110.90
1	B	165	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	185	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	165	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	116	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	105	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	28	ARG	CD-NE-CZ	6.63	132.88	123.60
1	B	19	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	105	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	116	ARG	NH1-CZ-NH2	6.54	126.60	119.40
1	B	19	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	182	ASN	CA-CB-CG	6.43	127.56	113.40
1	A	233	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	264	GLY	CA-C-O	-6.43	109.03	120.60
1	B	32	VAL	CA-CB-CG1	-6.42	101.26	110.90
1	A	165	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	176	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	255	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	116	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	172	ARG	N-CA-CB	6.08	121.54	110.60
1	B	140	TYR	CA-CB-CG	6.06	124.92	113.40
1	A	94	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	263	MET	CG-SD-CE	-5.92	90.73	100.20
1	B	98	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	105	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	18	TYR	CB-CG-CD2	5.90	124.54	121.00
1	A	33	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	94	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	B	265	PRO	CA-N-CD	-5.71	103.51	111.50
1	A	265	PRO	N-CA-CB	5.68	110.11	103.30
1	B	189	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	117	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	119	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	205	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	78	ARG	NE-CZ-NH2	-5.55	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	B	255	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	205	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	18	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	172	ARG	N-CA-C	-5.46	96.27	111.00
1	B	78	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	144	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	232	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	206	ASN	O-C-N	-5.40	114.05	122.70
1	B	23	TYR	CB-CG-CD1	5.38	124.23	121.00
1	B	10	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	B	165	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	144	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	60	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	147	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	33	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	105	ASP	CA-CB-CG	-5.12	102.13	113.40
1	A	28	ARG	NH1-CZ-NH2	-5.06	113.84	119.40
1	A	19	ASP	CB-CG-OD2	-5.02	113.79	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASN	Mainchain
1	A	264	GLY	Mainchain,Peptide
1	B	264	GLY	Mainchain,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	2097	0	2066	33	0
1	B	2097	0	2066	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	255	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	212	0	0	3	0
All	All	4663	0	4132	61	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 7.

All (61) 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:B:182:ASN:HD21	1:B:184:THR:HG23	1.11	1.06
1:B:125:HIS:HD2	1:B:127:LEU:H	1.21	0.88
1:B:182:ASN:ND2	1:B:184:THR:HG23	1.90	0.87
1:A:124:ASN:HD21	1:A:143:LEU:H	1.27	0.82
1:A:125:HIS:HD2	1:A:127:LEU:H	1.27	0.82
1:B:20:GLY:H	1:B:64:HIS:HD2	1.28	0.79
1:A:182:ASN:HD21	1:A:184:THR:HG23	1.47	0.78
1:A:20:GLY:H	1:A:64:HIS:HD2	1.31	0.78
1:B:124:ASN:HD22	1:B:185:ARG:HH22	1.30	0.78
1:A:124:ASN:HD22	1:A:185:ARG:HH22	1.31	0.77
1:B:149:HIS:HD2	1:B:183:VAL:H	1.32	0.75
1:B:182:ASN:HD21	1:B:184:THR:CG2	1.96	0.75
1:B:20:GLY:H	1:B:64:HIS:CD2	2.04	0.74
1:A:20:GLY:H	1:A:64:HIS:CD2	2.05	0.73
1:B:125:HIS:CD2	1:B:127:LEU:H	2.09	0.69
1:A:182:ASN:ND2	1:A:184:THR:HG23	2.09	0.67
1:B:124:ASN:HD21	1:B:143:LEU:H	1.43	0.66
1:A:41:LYS:O	1:A:45:GLN:HG3	1.98	0.64
1:A:149:HIS:HD2	1:A:183:VAL:H	1.45	0.63
1:B:24:TYR:CD1	1:B:32:VAL:HG11	2.34	0.63
1:A:125:HIS:CD2	1:A:127:LEU:H	2.13	0.60
1:A:182:ASN:HD21	1:A:184:THR:CG2	2.17	0.57
1:B:32:VAL:HG12	1:B:33:ARG:N	2.22	0.54
1:A:126:ARG:HG3	3:A:761:HOH:O	2.06	0.54
1:B:149:HIS:CD2	1:B:183:VAL:H	2.19	0.53
1:B:232:ASP:HB3	1:B:235:LEU:CD2	2.39	0.53
1:B:32:VAL:HG12	1:B:33:ARG:H	1.74	0.52
1:A:168:GLN:HB2	3:A:780:HOH:O	2.09	0.51
1:A:182:ASN:ND2	3:A:616:HOH:O	2.44	0.50
1:B:102:THR:HG23	3:B:791:HOH:O	2.12	0.49
1:B:156:LEU:HD21	1:B:180:HIS:HA	1.94	0.49
1:B:168:GLN:HB2	3:B:792:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:C	1:A:172:ARG:O	2.45	0.48
1:B:179:MET:O	1:B:180:HIS:HB3	2.14	0.48
1:A:172:ARG:O	1:A:173:THR:O	2.31	0.48
1:A:126:ARG:HD2	3:A:623:HOH:O	2.13	0.48
1:A:172:ARG:O	1:A:173:THR:C	2.53	0.48
1:B:20:GLY:N	1:B:64:HIS:HD2	2.05	0.47
1:B:147:ARG:HD2	1:B:147:ARG:HH11	1.55	0.47
1:A:48:ASN:HD22	1:A:78:ARG:HH21	1.63	0.46
1:B:219:GLN:HG3	1:B:223:TRP:CE3	2.51	0.46
1:A:24:TYR:HE1	1:A:33:ARG:HH11	1.64	0.46
1:B:64:HIS:HE1	1:B:243:GLU:O	1.99	0.46
1:A:173:THR:HA	1:A:174:PRO:HD3	1.80	0.45
1:B:232:ASP:HB3	1:B:235:LEU:HD23	1.98	0.45
1:A:149:HIS:CD2	1:A:183:VAL:H	2.31	0.45
1:A:124:ASN:ND2	1:A:143:LEU:H	2.06	0.45
1:A:248:VAL:HB	1:A:263:MET:HB2	1.99	0.45
1:B:206:ASN:HB3	3:B:703:HOH:O	2.17	0.44
1:A:101:LYS:HD3	1:A:258:LEU:HD23	2.00	0.43
1:A:27:GLN:HE21	1:A:29:GLN:HB2	1.82	0.43
1:A:160:ASP:OD2	1:A:231:LYS:HE3	2.18	0.42
1:A:102:THR:HB	3:A:807:HOH:O	2.20	0.42
1:A:149:HIS:HE1	3:A:746:HOH:O	2.01	0.42
1:A:149:HIS:CD2	1:A:182:ASN:HA	2.55	0.42
1:B:252:TYR:CD2	1:B:258:LEU:HD12	2.55	0.41
1:B:64:HIS:CE1	1:B:243:GLU:O	2.73	0.41
1:A:32:VAL:HG23	3:A:676:HOH:O	2.21	0.41
1:B:24:TYR:CD1	1:B:32:VAL:CG1	3.03	0.41
1:A:124:ASN:ND2	1:A:185:ARG:HH22	2.10	0.40
1:A:126:ARG:NE	3:A:735:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	262/264 (99%)	252 (96%)	9 (3%)	1 (0%)	39	14
1	B	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
All	All	524/528 (99%)	509 (97%)	14 (3%)	1 (0%)	52	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR

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	217/217 (100%)	211 (97%)	6 (3%)	51	17
1	B	217/217 (100%)	210 (97%)	7 (3%)	46	13
All	All	434/434 (100%)	421 (97%)	13 (3%)	48	15

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	105	ASP
1	A	126	ARG
1	A	168	GLN
1	A	182	ASN
1	A	233	ARG
1	B	28	ARG
1	B	29	GLN
1	B	105	ASP
1	B	168	GLN
1	B	172	ARG
1	B	233	ARG
1	B	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	48	ASN
1	A	64	HIS
1	A	124	ASN
1	A	125	HIS
1	A	149	HIS
1	A	182	ASN
1	A	186	HIS
1	A	218	ASN
1	B	64	HIS
1	B	124	ASN
1	B	125	HIS
1	B	149	HIS
1	B	182	ASN
1	B	186	HIS
1	B	218	ASN

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 ⓘ

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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