



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:58 PM GMT

PDB ID : 1I49
Title : CRYSTAL STRUCTURE ANALYSIS OF ARFAPTIN
Authors : Tarricone, C.; Xiao, B.; Justin, N.; Gamblin, S.J.; Smerdon, S.J.
Deposited on : 2001-02-20
Resolution : 2.80 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

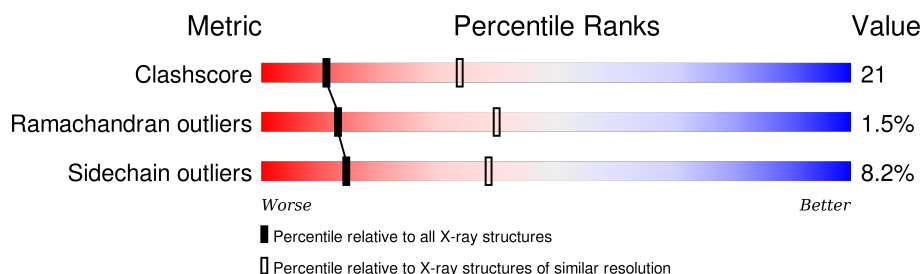
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	224	
1	B	224	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3442 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 ARFAPTIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1607	1012	280	311	4			
1	B	201	Total	C	N	O	S	0	0	0
			1610	1015	280	311	4			

- Molecule 2 is water.

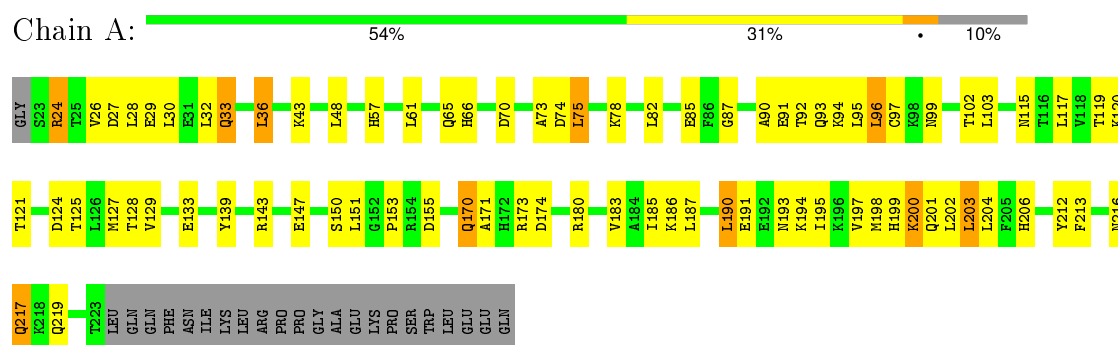
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	128	Total	O	0	0
			128	128		

3 Residue-property plots

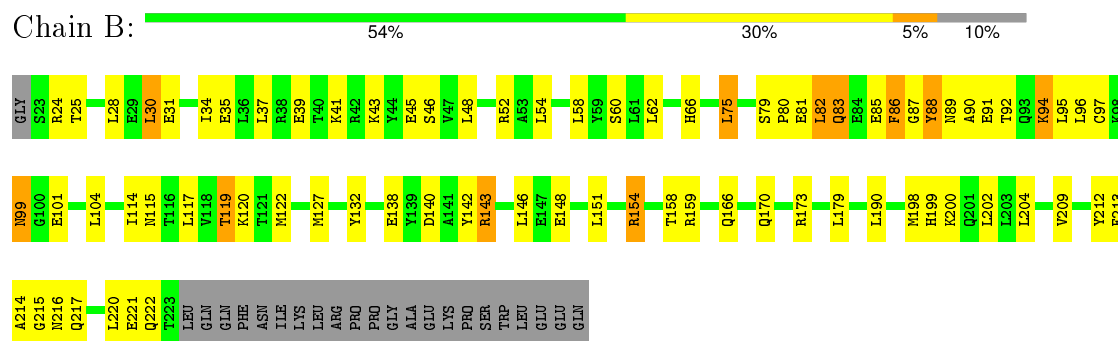
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ARFAPTIN 2



• Molecule 1: ARFAPTIN 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.33Å 146.33Å 82.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3442	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	0.41	0/1629	0.58	0/2192
1	B	0.42	0/1632	0.60	0/2196
All	All	0.41	0/3261	0.59	0/4388

There are no bond length outliers.

There are no bond angle outliers.

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	1607	0	1611	77	0
1	B	1610	0	1620	83	1
2	A	97	0	0	0	0
2	B	128	0	0	2	0
All	All	3442	0	3231	135	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 21.

All (135) 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:A:33:GLN:HG2	1:A:187:LEU:HD13	1.43	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HE21	1:A:173:ARG:NH2	1.62	0.98
1:B:80:PRO:HA	1:B:83:GLN:HG3	1.47	0.93
1:A:170:GLN:HE21	1:A:173:ARG:HH22	0.95	0.91
1:A:170:GLN:NE2	1:A:173:ARG:HH22	1.76	0.79
1:B:115:ASN:O	1:B:119:THR:HB	1.82	0.79
1:B:212:TYR:O	1:B:216:ASN:HB2	1.83	0.78
1:B:90:ALA:O	1:B:94:LYS:HD2	1.87	0.74
1:A:191:GLU:OE1	1:A:194:LYS:HD3	1.86	0.74
1:A:48:LEU:HD21	1:A:115:ASN:HD22	1.54	0.72
1:B:75:LEU:O	1:B:79:SER:HB3	1.90	0.72
1:A:85:GLU:OE1	1:B:199:HIS:HD2	1.73	0.72
1:B:214:ALA:C	1:B:216:ASN:H	1.91	0.71
1:A:195:ILE:HD11	1:B:81:GLU:HB3	1.71	0.71
1:A:33:GLN:CG	1:A:187:LEU:HD13	2.20	0.70
1:B:146:LEU:HD21	1:B:166:GLN:NE2	2.05	0.70
1:B:198:MET:O	1:B:202:LEU:HB2	1.92	0.69
1:A:153:PRO:HG2	1:A:155:ASP:OD1	1.92	0.69
1:A:48:LEU:HD21	1:A:115:ASN:HA	1.75	0.68
1:A:119:THR:HG22	1:A:120:LYS:HG3	1.74	0.68
1:B:217:GLN:O	1:B:221:GLU:HB3	1.93	0.68
1:A:27:ASP:OD2	1:A:180:ARG:HD3	1.93	0.68
1:A:33:GLN:HG2	1:A:187:LEU:CD1	2.21	0.67
1:B:158:THR:O	1:B:158:THR:HG22	1.95	0.66
1:A:91:GLU:HA	1:A:91:GLU:OE1	1.95	0.66
1:B:66:HIS:CE1	1:B:97:CYS:HB3	2.31	0.66
1:A:185:ILE:HG22	1:A:186:LYS:N	2.11	0.66
1:B:75:LEU:HB3	1:B:86:PHE:CE1	2.32	0.65
1:B:213:PHE:O	1:B:216:ASN:HB3	1.96	0.65
1:A:124:ASP:O	1:A:127:MET:HB3	1.97	0.65
1:A:43:LYS:HB3	1:B:75:LEU:HD11	1.81	0.63
1:B:119:THR:HG22	1:B:120:LYS:HG3	1.81	0.62
1:A:61:LEU:O	1:A:65:GLN:HG3	1.99	0.62
1:A:95:LEU:HD13	1:A:219:GLN:HG2	1.82	0.61
1:A:202:LEU:HD13	1:B:85:GLU:O	2.02	0.60
1:B:214:ALA:C	1:B:216:ASN:N	2.55	0.59
1:A:24:ARG:O	1:A:26:VAL:HG23	2.03	0.59
1:B:62:LEU:HD21	1:B:101:GLU:HA	1.87	0.57
1:B:143:ARG:HB3	1:B:143:ARG:HH11	1.69	0.57
1:B:91:GLU:OE1	1:B:94:LYS:HD3	2.05	0.57
1:B:41:LYS:O	1:B:45:GLU:HG3	2.04	0.57
1:A:199:HIS:CD2	1:B:85:GLU:OE1	2.57	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:HB3	1:A:216:ASN:HD21	1.70	0.55
1:B:154:ARG:HD2	1:B:154:ARG:H	1.71	0.55
1:B:114:ILE:HD12	1:B:198:MET:SD	2.46	0.55
1:A:213:PHE:HB3	1:B:217:GLN:NE2	2.22	0.54
1:A:129:VAL:O	1:A:133:GLU:HG3	2.08	0.54
1:A:217:GLN:NE2	1:B:214:ALA:HA	2.23	0.54
1:A:125:THR:CB	1:A:190:LEU:HD12	2.38	0.54
1:A:195:ILE:HG23	1:B:82:LEU:HD11	1.90	0.54
1:B:148:GLU:O	1:B:151:LEU:HB3	2.08	0.54
1:B:95:LEU:C	1:B:97:CYS:H	2.11	0.53
1:A:202:LEU:HD11	1:B:86:PHE:CD2	2.43	0.53
1:B:39:GLU:O	1:B:43:LYS:HG2	2.08	0.53
1:A:92:THR:O	1:A:95:LEU:HB3	2.08	0.52
1:A:195:ILE:CD1	1:B:81:GLU:HB3	2.39	0.52
1:B:82:LEU:HG	1:B:85:GLU:HG3	1.92	0.52
1:A:115:ASN:O	1:A:119:THR:HB	2.10	0.52
1:A:70:ASP:O	1:A:73:ALA:HB3	2.10	0.52
1:B:48:LEU:HD21	1:B:115:ASN:HA	1.91	0.51
1:A:99:ASN:HD22	1:A:216:ASN:ND2	2.09	0.51
1:A:128:THR:HG22	1:A:183:VAL:HG22	1.92	0.51
1:A:30:LEU:HD12	1:A:180:ARG:HG3	1.93	0.51
1:A:139:TYR:CE1	1:A:173:ARG:HG3	2.46	0.51
1:A:170:GLN:NE2	1:A:173:ARG:NH2	2.45	0.51
1:B:35:GLU:HG2	2:B:248:HOH:O	2.11	0.51
1:B:214:ALA:O	1:B:216:ASN:N	2.44	0.50
1:A:74:ASP:OD1	1:A:78:LYS:NZ	2.44	0.50
1:B:24:ARG:NH2	1:B:31:GLU:OE2	2.44	0.50
1:A:195:ILE:HG23	1:B:82:LEU:CD1	2.42	0.50
1:A:61:LEU:CD1	1:B:54:LEU:HD12	2.42	0.50
1:B:87:GLY:C	1:B:89:ASN:H	2.16	0.49
1:A:99:ASN:O	1:A:212:TYR:HD1	1.95	0.49
1:A:206:HIS:HE1	1:B:92:THR:OG1	1.94	0.49
1:B:48:LEU:HD21	1:B:115:ASN:HD22	1.78	0.49
1:B:25:THR:OG1	1:B:140:ASP:OD1	2.24	0.49
1:A:202:LEU:HD11	1:B:86:PHE:CE2	2.47	0.49
1:B:97:CYS:O	1:B:101:GLU:HB2	2.11	0.49
1:B:138:GLU:O	1:B:142:TYR:HD1	1.95	0.49
1:B:30:LEU:O	1:B:34:ILE:HG13	2.12	0.49
1:A:199:HIS:HD2	1:B:85:GLU:OE1	1.95	0.49
1:A:200:LYS:O	1:A:204:LEU:HG	2.13	0.49
1:B:95:LEU:O	1:B:97:CYS:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HD23	1:B:220:LEU:HD13	1.95	0.48
1:B:170:GLN:HG2	1:B:173:ARG:NH1	2.27	0.48
1:A:87:GLY:O	1:A:91:GLU:HG2	2.14	0.48
1:A:27:ASP:OD2	1:A:180:ARG:CD	2.59	0.47
1:A:128:THR:HG22	1:A:183:VAL:CG2	2.43	0.47
1:A:57:HIS:CE1	1:B:60:SER:HB3	2.49	0.47
1:B:200:LYS:O	1:B:204:LEU:HG	2.15	0.47
1:B:170:GLN:HG2	1:B:173:ARG:HH12	1.78	0.47
1:A:206:HIS:CE1	1:B:92:THR:OG1	2.67	0.47
1:B:127:MET:HE2	2:B:325:HOH:O	2.14	0.47
1:B:99:ASN:O	1:B:99:ASN:ND2	2.48	0.47
1:A:43:LYS:CB	1:B:75:LEU:HD11	2.44	0.47
1:B:90:ALA:C	1:B:94:LYS:HD2	2.35	0.47
1:A:32:LEU:O	1:A:36:LEU:HD23	2.14	0.47
1:B:117:LEU:O	1:B:122:MET:HG3	2.15	0.47
1:A:213:PHE:CB	1:B:217:GLN:HE22	2.27	0.46
1:A:203:LEU:HD23	1:B:88:TYR:OH	2.15	0.46
1:A:92:THR:HG21	1:B:209:VAL:HG11	1.97	0.46
1:B:95:LEU:C	1:B:97:CYS:N	2.70	0.44
1:A:117:LEU:O	1:A:121:THR:HB	2.17	0.44
1:A:194:LYS:O	1:A:198:MET:HB2	2.17	0.44
1:B:58:LEU:HB3	1:B:104:LEU:HD13	2.00	0.44
1:A:99:ASN:HD22	1:A:216:ASN:CG	2.22	0.44
1:A:185:ILE:CG2	1:A:186:LYS:N	2.81	0.43
1:A:99:ASN:O	1:A:212:TYR:CD1	2.71	0.43
1:A:212:TYR:HD2	1:A:213:PHE:CD1	2.36	0.43
1:A:66:HIS:CE1	1:A:97:CYS:HB3	2.54	0.43
1:A:197:VAL:O	1:A:201:GLN:HG2	2.19	0.43
1:A:202:LEU:HD13	1:B:85:GLU:C	2.39	0.43
1:B:82:LEU:O	1:B:83:GLN:C	2.57	0.43
1:B:81:GLU:H	1:B:81:GLU:CD	2.23	0.42
1:B:82:LEU:O	1:B:85:GLU:HG2	2.19	0.42
1:B:24:ARG:HH22	1:B:31:GLU:CD	2.23	0.42
1:A:61:LEU:HD11	1:B:54:LEU:CD1	2.49	0.42
1:A:143:ARG:O	1:A:147:GLU:HG3	2.20	0.42
1:B:75:LEU:O	1:B:86:PHE:CD1	2.73	0.42
1:A:61:LEU:HD11	1:B:54:LEU:HD12	2.02	0.42
1:A:102:THR:HG22	1:A:103:LEU:N	2.34	0.42
1:A:202:LEU:HD22	1:B:85:GLU:O	2.19	0.42
1:A:171:ALA:O	1:A:174:ASP:HB2	2.20	0.41
1:B:37:LEU:HD13	1:B:190:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD12	1:A:216:ASN:OD1	2.20	0.41
1:A:48:LEU:CD2	1:A:115:ASN:HD22	2.27	0.41
1:B:75:LEU:HB3	1:B:86:PHE:CD1	2.55	0.41
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.85	0.41
1:B:166:GLN:OE1	1:B:170:GLN:NE2	2.53	0.40
1:A:147:GLU:O	1:A:150:SER:HB2	2.21	0.40
1:B:52:ARG:HH22	1:B:115:ASN:ND2	2.19	0.40
1:A:90:ALA:O	1:A:94:LYS:HG3	2.22	0.40
1:B:179:LEU:HA	1:B:179:LEU:HD23	1.96	0.40
1:B:217:GLN:O	1:B:221:GLU:CB	2.67	0.40
1:A:75:LEU:HD13	1:A:75:LEU:HA	1.88	0.40

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:B:151:LEU:O	1:B:151:LEU:O[6_554]	1.74	0.46

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	199/224 (89%)	174 (87%)	23 (12%)	2 (1%)	19	52
1	B	199/224 (89%)	179 (90%)	16 (8%)	4 (2%)	9	30
All	All	398/448 (89%)	353 (89%)	39 (10%)	6 (2%)	13	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	GLN
1	B	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	28	LEU
1	A	96	LEU
1	B	159	ARG
1	B	215	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	171/193 (89%)	157 (92%)	14 (8%)	14	38
1	B	172/193 (89%)	158 (92%)	14 (8%)	15	39
All	All	343/386 (89%)	315 (92%)	28 (8%)	14	38

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	29	GLU
1	A	33	GLN
1	A	36	LEU
1	A	75	LEU
1	A	82	LEU
1	A	93	GLN
1	A	151	LEU
1	A	170	GLN
1	A	190	LEU
1	A	193	ASN
1	A	200	LYS
1	A	203	LEU
1	A	217	GLN
1	B	28	LEU
1	B	30	LEU
1	B	46	SER
1	B	75	LEU
1	B	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	86	PHE
1	B	88	TYR
1	B	94	LYS
1	B	99	ASN
1	B	119	THR
1	B	132	TYR
1	B	143	ARG
1	B	154	ARG
1	B	222	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	108	ASN
1	A	115	ASN
1	A	170	GLN
1	A	193	ASN
1	A	199	HIS
1	A	206	HIS
1	A	219	GLN
1	B	66	HIS
1	B	93	GLN
1	B	115	ASN
1	B	199	HIS
1	B	206	HIS
1	B	217	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

There are no ligands in this entry.

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.