



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:33 PM GMT

PDB ID : 1CDH
Title : STRUCTURES OF AN HIV AND MHC BINDING FRAGMENT FROM HUMAN CD4 AS REFINED IN TWO CRYSTAL LATTICES
Authors : Ryu, S.E.; Truneh, A.; Sweet, R.W.; Hendrickson, W.A.
Deposited on : 1994-01-26
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

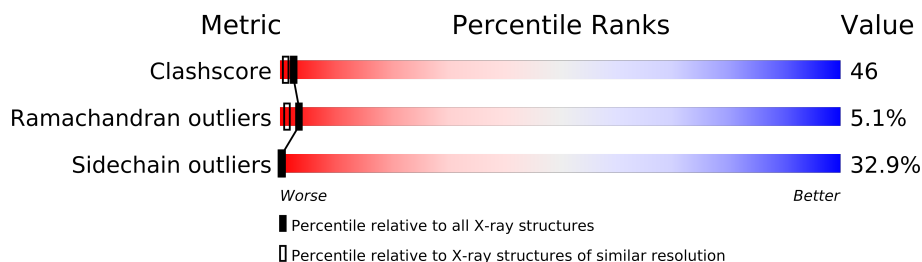
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	178	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1469 atoms, of which 0 are hydrogen and 0 are deuterium.

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 T CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total 1383	C 865	N 242	O 272	S 4	0	0	0

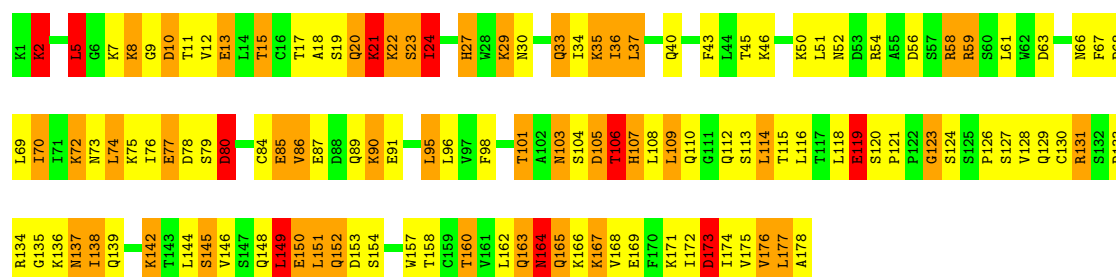
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total 86	O 86	0	0

i

Note EDS was not executed.

- Chain A:



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.71Å 30.01Å 87.54Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1469	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	0.99	0/1402	2.01	38/1891 (2.0%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ARG	CD-NE-CZ	16.09	146.13	123.60
1	A	54	ARG	NE-CZ-NH1	-13.85	113.37	120.30
1	A	43	PHE	CA-CB-CG	10.05	138.01	113.90
1	A	54	ARG	NE-CZ-NH2	9.97	125.28	120.30
1	A	58	ARG	CD-NE-CZ	8.86	136.00	123.60
1	A	59	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	A	87	GLU	OE1-CD-OE2	8.66	133.69	123.30
1	A	131	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	A	78	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	13	GLU	OE1-CD-OE2	7.34	132.11	123.30
1	A	2	LYS	CA-CB-CG	7.12	129.06	113.40
1	A	173	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	8	LYS	C-N-CA	6.99	136.97	122.30
1	A	37	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	5	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	58	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	A	106	THR	CB-CA-C	6.48	129.09	111.60
1	A	29	LYS	CA-CB-CG	6.47	127.64	113.40
1	A	56	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	74	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	173	ASP	O-C-N	5.89	132.13	122.70
1	A	56	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	77	GLU	CG-CD-OE1	-5.68	106.93	118.30
1	A	105	ASP	N-CA-C	-5.62	95.82	111.00
1	A	37	LEU	CB-CA-C	5.62	120.88	110.20
1	A	80	ASP	N-CA-CB	-5.62	100.49	110.60
1	A	105	ASP	N-CA-CB	5.47	120.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	CA-CB-CG2	5.45	119.07	110.90
1	A	17	THR	CA-CB-CG2	5.42	119.98	112.40
1	A	105	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	21	LYS	N-CA-CB	5.38	120.28	110.60
1	A	59	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	87	GLU	CG-CD-OE2	-5.18	107.94	118.30
1	A	36	ILE	O-C-N	5.10	130.85	122.70
1	A	128	VAL	CB-CA-C	5.08	121.05	111.40
1	A	149	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	119	GLU	CG-CD-OE2	-5.03	108.25	118.30
1	A	24	ILE	CA-C-N	5.01	128.23	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1383	0	1414	128	0
2	A	86	0	0	8	0
All	All	1469	0	1414	128	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

All (128) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:ARG:HH11	1:A:137:ASN:HB3	1.07	1.11
1:A:20:GLN:HE22	1:A:86:VAL:HG12	0.93	1.08
1:A:20:GLN:NE2	1:A:86:VAL:HG12	1.69	1.06
1:A:103:ASN:HD21	1:A:115:THR:HB	1.17	1.05
1:A:136:LYS:HD2	1:A:137:ASN:H	1.26	0.99
1:A:30:ASN:HD21	1:A:34:ILE:HD12	1.29	0.95
1:A:20:GLN:HE22	1:A:86:VAL:CG1	1.79	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:GLN:HE21	1:A:45:THR:HG21	1.33	0.92
1:A:106:THR:HG22	1:A:174:ILE:HD13	1.50	0.91
1:A:131:ARG:NH1	1:A:137:ASN:HB3	1.87	0.89
1:A:79:SER:O	1:A:80:ASP:HB2	1.73	0.88
1:A:10:ASP:O	1:A:74:LEU:HB2	1.76	0.84
1:A:104:SER:HB2	1:A:108:LEU:HD21	1.60	0.83
1:A:22:LYS:HB3	1:A:63:ASP:O	1.80	0.82
1:A:114:LEU:HD12	1:A:149:LEU:HD21	1.59	0.82
1:A:106:THR:O	1:A:175:VAL:N	2.13	0.82
1:A:106:THR:HG22	1:A:174:ILE:CD1	2.11	0.80
1:A:30:ASN:HD21	1:A:34:ILE:CD1	1.94	0.80
1:A:133:PRO:HG2	1:A:154:SER:O	1.81	0.80
1:A:114:LEU:HD23	1:A:116:LEU:HD21	1.64	0.79
1:A:20:GLN:HG2	2:A:183:HOH:O	1.83	0.79
1:A:136:LYS:HD2	1:A:137:ASN:N	1.97	0.78
1:A:101:THR:O	1:A:116:LEU:HA	1.82	0.78
1:A:5:LEU:HD22	1:A:166:LYS:HB3	1.66	0.77
1:A:20:GLN:NE2	1:A:86:VAL:CG1	2.43	0.77
1:A:131:ARG:HH11	1:A:137:ASN:CB	1.94	0.77
1:A:118:LEU:HD21	1:A:126:PRO:HG2	1.65	0.77
1:A:23:SER:OG	1:A:23:SER:O	1.97	0.76
1:A:114:LEU:CD2	1:A:116:LEU:HD21	2.14	0.76
1:A:30:ASN:ND2	1:A:34:ILE:HD12	1.99	0.76
1:A:103:ASN:ND2	1:A:115:THR:HB	1.98	0.75
1:A:138:ILE:HD13	1:A:146:VAL:HG22	1.69	0.73
1:A:40:GLN:NE2	1:A:45:THR:HG21	2.04	0.71
1:A:114:LEU:O	1:A:145:SER:HA	1.91	0.71
1:A:163:GLN:O	1:A:165:GLN:N	2.24	0.71
1:A:109:LEU:HD12	1:A:177:LEU:HB3	1.72	0.70
1:A:104:SER:CB	1:A:108:LEU:HD21	2.21	0.69
1:A:67:PHE:CE1	1:A:86:VAL:HG11	2.30	0.67
1:A:163:GLN:O	1:A:164:ASN:C	2.32	0.66
1:A:20:GLN:OE1	1:A:24:ILE:HG13	1.96	0.66
1:A:160:THR:HG23	1:A:169:GLU:HG3	1.78	0.65
1:A:106:THR:HB	1:A:173:ASP:O	1.98	0.64
1:A:134:ARG:HG3	1:A:152:GLN:HB3	1.78	0.63
1:A:107:HIS:HA	1:A:175:VAL:O	1.99	0.62
1:A:84:CYS:O	1:A:90:LYS:HA	2.01	0.61
1:A:119:GLU:HG2	2:A:197:HOH:O	2.00	0.60
1:A:79:SER:HA	1:A:95:LEU:O	2.01	0.60
1:A:152:GLN:O	1:A:153:ASP:OD1	2.20	0.59
1:A:176:VAL:HG12	1:A:176:VAL:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:SER:HB2	1:A:121:PRO:HD2	1.85	0.58
1:A:58:ARG:HD2	1:A:61:LEU:HD12	1.85	0.57
1:A:33:GLN:N	1:A:33:GLN:HE21	2.00	0.57
1:A:114:LEU:HD23	1:A:116:LEU:CD2	2.33	0.57
1:A:8:LYS:HD3	1:A:9:GLY:N	2.20	0.57
1:A:167:LYS:O	1:A:167:LYS:HG3	2.03	0.56
1:A:40:GLN:NE2	1:A:45:THR:CG2	2.70	0.55
1:A:108:LEU:HD13	1:A:114:LEU:HD12	1.89	0.55
1:A:20:GLN:HB3	2:A:247:HOH:O	2.07	0.54
1:A:107:HIS:HA	1:A:175:VAL:HB	1.89	0.54
1:A:27:HIS:CE1	1:A:85:GLU:HB2	2.43	0.54
1:A:116:LEU:N	1:A:116:LEU:HD23	2.22	0.54
1:A:107:HIS:ND1	1:A:107:HIS:N	2.56	0.54
1:A:164:ASN:O	1:A:166:LYS:N	2.31	0.53
1:A:115:THR:C	1:A:116:LEU:HD23	2.30	0.52
1:A:59:ARG:HB2	1:A:59:ARG:HH11	1.75	0.51
1:A:163:GLN:CG	1:A:164:ASN:H	2.24	0.51
1:A:7:LYS:HG2	1:A:168:VAL:HG11	1.93	0.50
1:A:59:ARG:O	1:A:59:ARG:CG	2.60	0.50
1:A:151:LEU:HD21	1:A:178:ALA:HB2	1.92	0.50
1:A:8:LYS:C	1:A:8:LYS:CD	2.80	0.50
1:A:58:ARG:HG3	2:A:185:HOH:O	2.11	0.50
1:A:130:CYS:HA	1:A:158:THR:O	2.12	0.49
1:A:144:LEU:O	1:A:145:SER:HB2	2.12	0.49
1:A:157:TRP:CD1	1:A:174:ILE:HG12	2.48	0.48
1:A:164:ASN:C	1:A:166:LYS:H	2.12	0.48
1:A:109:LEU:CD1	1:A:177:LEU:HB3	2.42	0.48
1:A:85:GLU:HG3	1:A:90:LYS:HB2	1.96	0.48
1:A:124:SER:HB2	1:A:163:GLN:HE22	1.79	0.48
1:A:70:ILE:HG21	1:A:72:LYS:HZ3	1.78	0.48
1:A:112:GLN:O	1:A:149:LEU:HD22	2.14	0.47
1:A:5:LEU:HB3	1:A:168:VAL:HG22	1.96	0.47
1:A:133:PRO:CG	1:A:154:SER:O	2.56	0.47
1:A:15:THR:CG2	2:A:258:HOH:O	2.61	0.47
1:A:23:SER:C	1:A:24:ILE:HG12	2.34	0.47
1:A:130:CYS:SG	1:A:144:LEU:CD2	3.03	0.47
1:A:121:PRO:O	1:A:123:GLY:N	2.48	0.47
1:A:127:SER:O	1:A:162:LEU:HD12	2.15	0.47
1:A:103:ASN:HD21	1:A:115:THR:CB	2.07	0.46
1:A:108:LEU:C	1:A:109:LEU:HD13	2.36	0.46
1:A:124:SER:CB	1:A:163:GLN:HE22	2.28	0.46
1:A:36:ILE:HD13	1:A:51:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:LEU:HB3	1:A:176:VAL:HG21	1.98	0.45
1:A:22:LYS:O	1:A:23:SER:HB3	2.16	0.45
1:A:151:LEU:HA	1:A:176:VAL:CG1	2.45	0.45
1:A:12:VAL:HG23	2:A:245:HOH:O	2.17	0.45
1:A:8:LYS:C	1:A:8:LYS:HD2	2.37	0.45
1:A:150:GLU:O	1:A:176:VAL:HG11	2.18	0.44
1:A:30:ASN:C	1:A:30:ASN:OD1	2.55	0.44
1:A:70:ILE:CG2	1:A:72:LYS:HZ3	2.31	0.44
1:A:11:THR:HG23	1:A:72:LYS:HA	1.99	0.44
1:A:157:TRP:O	1:A:171:LYS:HA	2.17	0.44
1:A:59:ARG:HH11	1:A:59:ARG:CB	2.30	0.44
1:A:101:THR:O	1:A:116:LEU:CA	2.60	0.43
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.77	0.43
1:A:104:SER:HA	2:A:262:HOH:O	2.18	0.43
1:A:98:PHE:HZ	1:A:163:GLN:OE1	2.01	0.43
1:A:22:LYS:HE3	1:A:63:ASP:O	2.19	0.43
1:A:2:LYS:HZ1	1:A:15:THR:HB	1.83	0.42
1:A:108:LEU:HD23	1:A:112:GLN:OE1	2.19	0.42
1:A:2:LYS:NZ	1:A:15:THR:HG22	2.34	0.42
1:A:18:ALA:HB2	1:A:86:VAL:HG21	2.02	0.42
1:A:104:SER:C	1:A:105:ASP:O	2.57	0.42
1:A:7:LYS:O	1:A:8:LYS:C	2.58	0.42
1:A:163:GLN:HG2	1:A:164:ASN:OD1	2.20	0.42
1:A:35:LYS:HB2	2:A:182:HOH:O	2.20	0.42
1:A:134:ARG:CG	1:A:152:GLN:HB3	2.49	0.42
1:A:138:ILE:CD1	1:A:146:VAL:HG22	2.43	0.41
1:A:59:ARG:NH1	1:A:59:ARG:CB	2.84	0.41
1:A:68:PRO:HB2	1:A:70:ILE:CD1	2.50	0.41
1:A:75:LYS:HB3	1:A:77:GLU:OE2	2.21	0.41
1:A:164:ASN:C	1:A:166:LYS:N	2.73	0.41
1:A:13:GLU:HG3	1:A:70:ILE:HD12	2.03	0.41
1:A:46:LYS:HE3	1:A:52:ASN:O	2.20	0.41
1:A:27:HIS:HD1	1:A:27:HIS:C	2.22	0.41
1:A:85:GLU:HG3	1:A:90:LYS:CB	2.51	0.41
1:A:21:LYS:O	1:A:22:LYS:C	2.60	0.40
1:A:29:LYS:HA	1:A:34:ILE:O	2.22	0.40
1:A:7:LYS:O	1:A:10:ASP:HB2	2.21	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	176/178 (99%)	149 (85%)	18 (10%)	9 (5%)	3 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	22	LYS
1	A	80	ASP
1	A	142	LYS
1	A	164	ASN
1	A	21	LYS
1	A	145	SER
1	A	135	GLY
1	A	123	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	161/161 (100%)	108 (67%)	53 (33%)	0 0

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	5	LEU
1	A	10	ASP
1	A	15	THR
1	A	19	SER

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Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	LYS
1	A	23	SER
1	A	24	ILE
1	A	27	HIS
1	A	33	GLN
1	A	35	LYS
1	A	37	LEU
1	A	50	LYS
1	A	66	ASN
1	A	69	LEU
1	A	70	ILE
1	A	72	LYS
1	A	73	ASN
1	A	76	ILE
1	A	85	GLU
1	A	89	GLN
1	A	90	LYS
1	A	91	GLU
1	A	95	LEU
1	A	96	LEU
1	A	101	THR
1	A	103	ASN
1	A	106	THR
1	A	107	HIS
1	A	109	LEU
1	A	110	GLN
1	A	113	SER
1	A	114	LEU
1	A	119	GLU
1	A	129	GLN
1	A	137	ASN
1	A	138	ILE
1	A	139	GLN
1	A	142	LYS
1	A	148	GLN
1	A	149	LEU
1	A	150	GLU
1	A	151	LEU
1	A	152	GLN
1	A	160	THR
1	A	163	GLN

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	167	LYS
1	A	172	ILE
1	A	173	ASP
1	A	176	VAL
1	A	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	GLN
1	A	40	GLN
1	A	73	ASN
1	A	103	ASN
1	A	129	GLN
1	A	152	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.