



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G8Q
Title : CRYSTAL STRUCTURE OF HUMAN CD81 EXTRACELLULAR DOMAIN, A RECEPTOR FOR HEPATITIS C VIRUS
Authors : Kitadokoro, K.; Bolognesi, M.; Bordo, D.; Grandi, G.; Galli, G.; Petracca, R.; Falugi, F.
Deposited on : 2000-11-20
Resolution : 1.60 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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

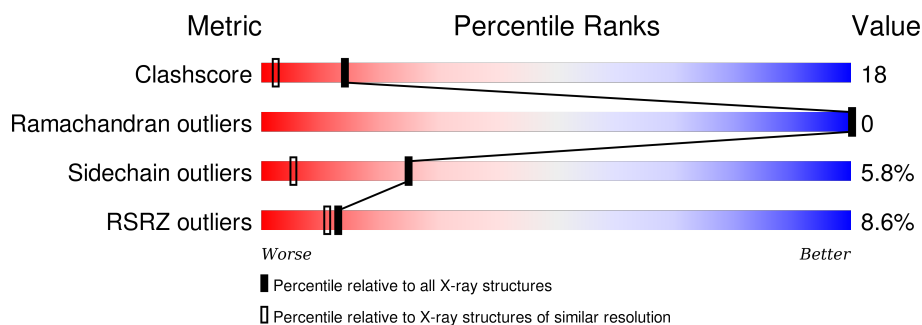
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	90	<div> <div>3%</div> <div>63%</div> <div>26%</div> <div>9%</div> <div>.</div> </div>
1	B	90	<div> <div>13%</div> <div>58%</div> <div>31%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1550 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 CD81 ANTIGEN, EXTRACELLULAR DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	3	0	0
			693	430	118	141	4			
1	B	86	Total	C	N	O	S	17	0	0
			663	414	113	132	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	LEU	CONFLICT	UNP P60033
B	302	HIS	LEU	CONFLICT	UNP P60033

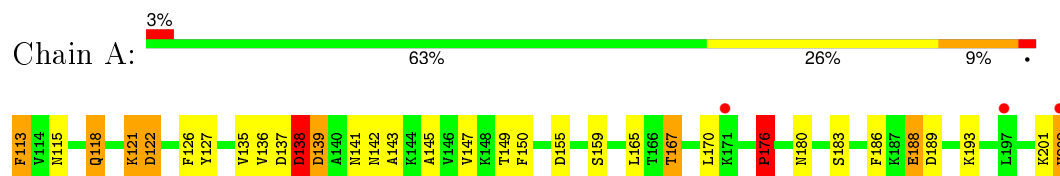
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total	O	0	0
			104	104		
2	B	90	Total	O	0	0
			90	90		

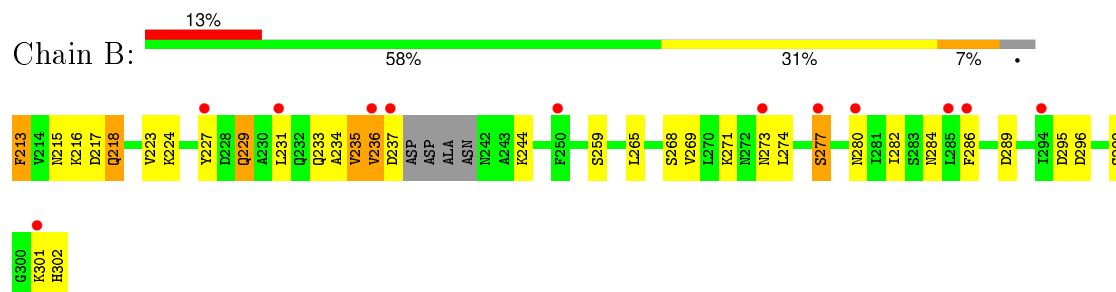
3 Residue-property plots [i](#)

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.

- Molecule 1: CD81 ANTIGEN, EXTRACELLULAR DOMAIN



- Molecule 1: CD81 ANTIGEN, EXTRACELLULAR DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	31.48Å 77.17Å 38.46Å 90.00° 107.39° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 21.07 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-1.60) 88.0 (21.07-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.238 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 95.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21557 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1550	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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	1.31	1/702 (0.1%)	2.16	26/948 (2.7%)
1	B	1.33	3/671 (0.4%)	2.61	16/902 (1.8%)
All	All	1.32	4/1373 (0.3%)	2.39	42/1850 (2.3%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	SER	C-N	19.72	1.68	1.33
1	A	138	ASP	CB-CG	14.00	1.81	1.51
1	B	280	ASN	N-CA	5.34	1.57	1.46
1	B	299	SER	CA-CB	5.02	1.60	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	SER	O-C-N	-54.77	30.09	123.20
1	A	189	ASP	CB-CG-OD2	16.58	133.22	118.30
1	A	127	TYR	CB-CG-CD2	-11.23	114.26	121.00
1	A	127	TYR	CB-CG-CD1	9.47	126.68	121.00
1	A	147	VAL	CA-CB-CG2	-9.47	96.70	110.90
1	A	189	ASP	OD1-CG-OD2	-8.39	107.35	123.30
1	A	165	LEU	CB-CG-CD2	8.25	125.02	111.00
1	B	296	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	B	213	PHE	CA-CB-CG	7.58	132.09	113.90
1	B	268	SER	CB-CA-C	7.45	124.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASN	O-C-N	7.36	134.47	122.70
1	A	138	ASP	CA-CB-CG	-7.18	97.61	113.40
1	A	186	PHE	CB-CG-CD2	-6.86	116.00	120.80
1	A	167	THR	CA-C-O	6.46	133.67	120.10
1	A	126	PHE	CB-CG-CD1	-6.42	116.30	120.80
1	A	159	SER	N-CA-CB	6.40	120.11	110.50
1	B	286	PHE	CG-CD1-CE1	6.03	127.43	120.80
1	B	223	VAL	CA-CB-CG2	-5.96	101.95	110.90
1	A	150	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	B	227	TYR	CB-CG-CD2	5.83	124.50	121.00
1	A	137	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	301	LYS	CB-CA-C	-5.57	99.27	110.40
1	A	135	VAL	CA-CB-CG2	5.56	119.24	110.90
1	A	147	VAL	CA-CB-CG1	5.53	119.19	110.90
1	B	284	ASN	CA-CB-CG	-5.47	101.38	113.40
1	A	143	ALA	O-C-N	-5.46	113.96	122.70
1	A	113	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	B	235	VAL	CG1-CB-CG2	5.39	119.53	110.90
1	A	136	VAL	O-C-N	-5.36	114.13	122.70
1	A	122	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	229	GLN	O-C-N	-5.27	114.27	122.70
1	B	231	LEU	O-C-N	5.27	131.13	122.70
1	A	145	ALA	O-C-N	5.26	131.11	122.70
1	A	115	ASN	O-C-N	5.25	131.10	122.70
1	A	176	PRO	O-C-N	5.25	131.09	122.70
1	B	231	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	218	GLN	N-CA-CB	5.20	119.96	110.60
1	A	139	ASP	N-CA-CB	5.13	119.83	110.60
1	A	188	GLU	O-C-N	5.10	130.85	122.70
1	A	170	LEU	CB-CG-CD1	-5.06	102.41	111.00
1	B	234	ALA	CB-CA-C	-5.03	102.56	110.10
1	B	289	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	259	SER	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	693	0	672	32	1
1	B	663	0	648	18	8
2	A	104	0	0	18	9
2	B	90	0	0	7	2
All	All	1550	0	1320	48	10

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 18.

All (48) 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:229:GLN:HG2	2:B:194:HOH:O	1.24	1.28
1:A:202:HIS:HA	2:A:306:HOH:O	1.71	0.89
1:B:216:LYS:HE3	2:B:138:HOH:O	1.76	0.84
1:A:118:GLN:HG3	1:A:121:LYS:NZ	1.93	0.83
1:A:155:ASP:OD2	2:A:292:HOH:O	2.03	0.75
1:B:269:VAL:HG12	1:B:274:LEU:HD12	1.71	0.72
1:A:202:HIS:O	2:A:216:HOH:O	2.08	0.71
1:A:149:THR:HA	2:A:279:HOH:O	1.91	0.70
1:B:236:VAL:HG23	1:B:237:ASP:N	2.05	0.69
1:A:113:PHE:CD1	2:A:250:HOH:O	2.45	0.68
1:A:118:GLN:NE2	2:A:205:HOH:O	2.27	0.68
1:A:113:PHE:N	2:A:276:HOH:O	2.28	0.67
1:A:118:GLN:HG3	1:A:121:LYS:HZ2	1.60	0.65
1:B:271:LYS:NZ	2:B:154:HOH:O	2.10	0.65
1:A:113:PHE:CD1	2:A:271:HOH:O	2.51	0.61
1:A:201:LYS:O	1:A:202:HIS:C	2.38	0.60
1:A:180:ASN:ND2	1:A:183:SER:H	2.00	0.58
1:B:273:ASN:HA	2:B:22:HOH:O	2.03	0.58
1:B:244:LYS:HG3	2:B:12:HOH:O	2.02	0.58
1:A:118:GLN:O	1:A:121:LYS:HD3	2.03	0.58
1:A:113:PHE:CG	2:A:271:HOH:O	2.57	0.57
1:A:188:GLU:HG3	2:A:245:HOH:O	2.05	0.56
1:A:149:THR:HG23	2:A:279:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HA	2:A:286:HOH:O	2.04	0.55
1:B:236:VAL:HG23	1:B:237:ASP:HB2	1.88	0.54
1:A:118:GLN:CG	1:A:121:LYS:NZ	2.70	0.53
1:B:215:ASN:HD22	1:B:218:GLN:H	1.55	0.52
1:A:149:THR:HG23	1:B:302:HIS:HB3	1.92	0.51
1:B:216:LYS:NZ	2:B:150:HOH:O	2.45	0.50
1:A:118:GLN:CG	1:A:121:LYS:HZ1	2.26	0.47
1:A:118:GLN:HG3	1:A:121:LYS:HZ1	1.72	0.47
1:A:121:LYS:HE2	2:A:247:HOH:O	2.14	0.47
1:A:121:LYS:CE	1:A:122:ASP:OD1	2.64	0.46
1:B:236:VAL:O	1:B:237:ASP:O	2.33	0.46
1:B:235:VAL:HG21	1:B:265:LEU:CD2	2.46	0.46
1:A:121:LYS:HG2	2:A:247:HOH:O	2.16	0.45
1:A:149:THR:CG2	1:B:302:HIS:HB3	2.46	0.45
1:A:149:THR:CA	2:A:279:HOH:O	2.59	0.44
1:B:233:GLN:CD	2:B:194:HOH:O	2.55	0.43
1:A:202:HIS:CE1	2:A:284:HOH:O	2.72	0.43
1:B:215:ASN:HD21	1:B:217:ASP:HB2	1.83	0.43
1:B:235:VAL:HG21	1:B:265:LEU:HD22	2.01	0.42
1:A:149:THR:CB	2:A:279:HOH:O	2.67	0.41
1:A:193:LYS:HB3	1:A:202:HIS:NE2	2.35	0.41
1:B:224:LYS:CE	1:B:295:ASP:OD1	2.68	0.41
1:A:176:PRO:HD2	2:A:252:HOH:O	2.21	0.41
1:A:180:ASN:HD21	1:A:183:SER:H	1.66	0.41
1:A:142:ASN:HD22	1:A:142:ASN:HA	1.79	0.40

All (10) 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:213:PHE:CZ	2:A:300:HOH:O[1_655]	0.78	1.42
1:A:138:ASP:OD1	2:B:180:HOH:O[2_646]	1.37	0.83
1:B:213:PHE:CE1	2:A:300:HOH:O[1_655]	1.43	0.77
1:B:213:PHE:CE2	2:A:300:HOH:O[1_655]	1.66	0.54
1:B:282:ILE:C	2:A:285:HOH:O[2_556]	1.83	0.37
1:B:282:ILE:CG2	2:A:285:HOH:O[2_556]	1.87	0.33
2:A:245:HOH:O	2:B:143:HOH:O[1_455]	2.15	0.05
1:B:213:PHE:CE2	2:A:223:HOH:O[1_655]	2.15	0.05
1:B:282:ILE:O	2:A:285:HOH:O[2_556]	2.17	0.03
1:B:282:ILE:CB	2:A:285:HOH:O[2_556]	2.17	0.03

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	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
1	B	82/90 (91%)	78 (95%)	4 (5%)	0	100	100
All	All	170/180 (94%)	163 (96%)	7 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	80/80 (100%)	73 (91%)	7 (9%)	12	1
1	B	76/80 (95%)	74 (97%)	2 (3%)	54	25
All	All	156/160 (98%)	147 (94%)	9 (6%)	25	5

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	121	LYS
1	A	138	ASP
1	A	139	ASP
1	A	167	THR
1	A	176	PRO
1	A	202	HIS
1	B	236	VAL

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Mol	Chain	Res	Type
1	B	277	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	180	ASN
1	B	215	ASN
1	B	272	ASN
1	B	302	HIS

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 [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	90/90 (100%)	0.26	3 (3%)	50	47	21, 31, 46, 68	1 (1%)
1	B	84/90 (93%)	0.58	12 (14%)	4	3	22, 30, 51, 73	2 (2%)
All	All	174/180 (96%)	0.41	15 (8%)	13	11	21, 31, 49, 73	3 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	ASP	5.1
1	B	236	VAL	5.0
1	B	277	SER	3.9
1	B	280	ASN	3.7
1	A	171	LYS	3.0
1	B	250	PHE	3.0
1	B	231	LEU	2.9
1	B	227	TYR	2.8
1	B	273	ASN	2.6
1	B	294	ILE	2.6
1	B	286	PHE	2.5
1	B	285	LEU	2.4
1	A	197	LEU	2.3
1	B	301	LYS	2.1
1	A	202	HIS	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.