



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:42 pm GMT

PDB ID : 1OC4
Title : LACTATE DEHYDROGENASE FROM PLASMODIUM BERGHEI
Authors : Winter, V.J.; Brady, R.L.
Deposited on : 2003-02-05
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

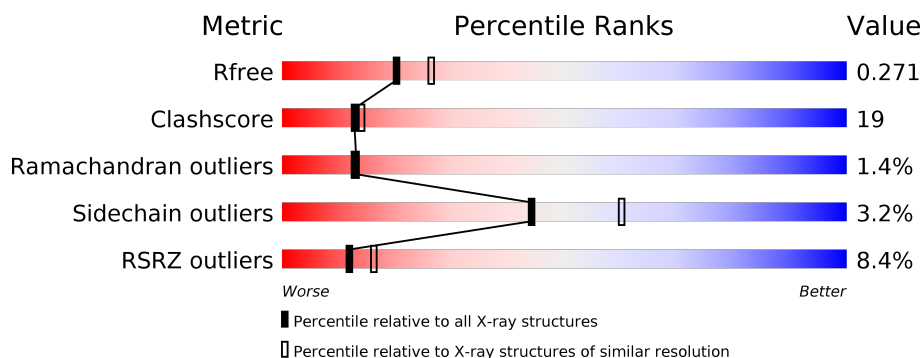
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	322	<div> <div>8%</div> <div>65%</div> <div>29%</div> <div>...</div> </div>
1	B	322	<div> <div>8%</div> <div>77%</div> <div>16%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1332	-	-	X	-

2 Entry composition [i](#)

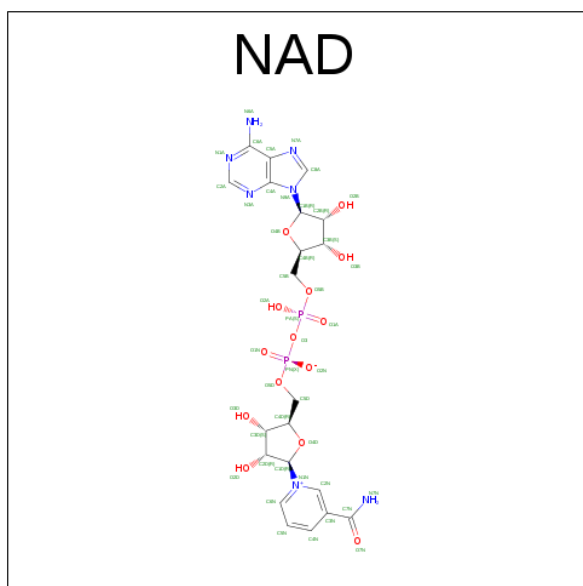
There are 5 unique types of molecules in this entry. The entry contains 5115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE.

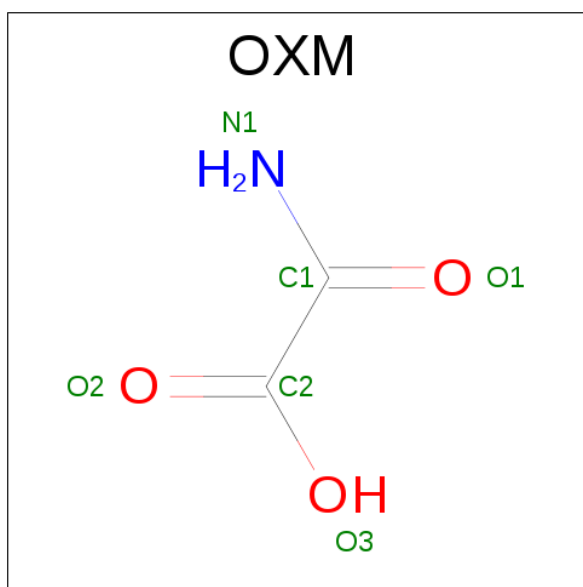
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	57	0	0
			2404	1527	415	448	14			
1	B	315	Total	C	N	O	S	38	0	0
			2404	1527	415	448	14			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

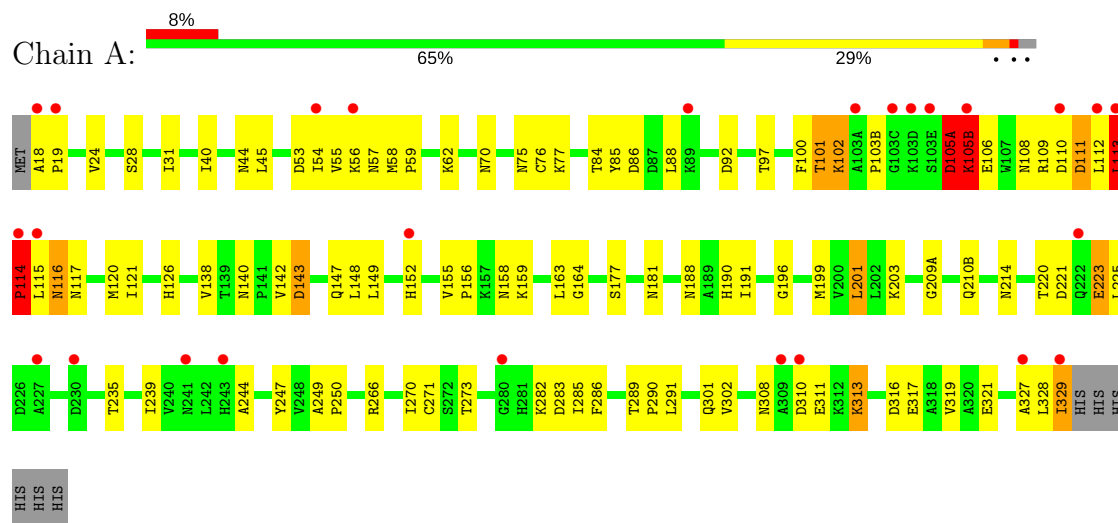
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total 64	O 64	0	0
5	B	131	Total 131	O 131	0	0

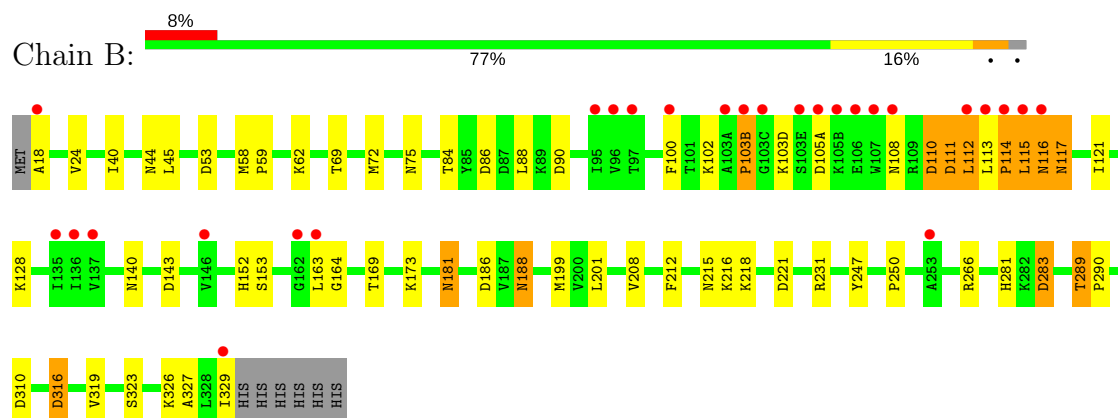
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.59Å 71.53Å 94.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.30 28.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.49-2.30) 94.7 (28.84-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.219 , 0.268 0.218 , 0.271	Depositor DCC
R_{free} test set	1536 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAD, OXM

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	1.41	13/2441 (0.5%)	1.18	24/3305 (0.7%)
1	B	0.77	9/2441 (0.4%)	0.95	17/3305 (0.5%)
All	All	1.13	22/4882 (0.5%)	1.07	41/6610 (0.6%)

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	1	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105(B)	LYS	CA-CB	-39.23	0.67	1.53
1	A	113	LEU	C-N	31.01	1.93	1.34
1	A	105(B)	LYS	N-CA	21.00	1.88	1.46
1	A	282	LYS	CB-CG	16.66	1.97	1.52
1	A	105(B)	LYS	CA-C	15.09	1.92	1.52
1	A	102	LYS	N-CA	13.50	1.73	1.46
1	B	102	LYS	C-N	-11.22	1.08	1.34
1	A	101	THR	C-N	10.92	1.59	1.34
1	B	103(B)	PRO	C-N	10.43	1.51	1.33
1	A	113	LEU	CA-C	10.21	1.79	1.52
1	B	102	LYS	CA-CB	9.93	1.75	1.53
1	A	103(B)	PRO	N-CD	-9.31	1.34	1.47
1	B	108	ASN	CB-CG	9.16	1.72	1.51
1	A	102	LYS	CA-CB	-8.70	1.34	1.53
1	B	18	ALA	C-N	8.41	1.50	1.34
1	A	77	LYS	CG-CD	-8.00	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	LEU	CB-CG	7.87	1.75	1.52
1	A	105(A)	ASP	C-N	-7.12	1.17	1.34
1	B	103(D)	LYS	CA-CB	-6.92	1.38	1.53
1	B	18	ALA	N-CA	-6.87	1.32	1.46
1	B	18	ALA	CA-C	6.39	1.69	1.52
1	A	109	ARG	N-CA	-5.39	1.35	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105(A)	ASP	O-C-N	-17.60	94.53	122.70
1	B	102	LYS	N-CA-CB	-17.48	79.14	110.60
1	A	105(B)	LYS	N-CA-CB	17.32	141.79	110.60
1	A	105(B)	LYS	CB-CA-C	17.02	144.45	110.40
1	A	113	LEU	CB-CG-CD2	15.30	137.01	111.00
1	A	105(B)	LYS	N-CA-C	-13.79	73.76	111.00
1	A	102	LYS	CB-CA-C	13.49	137.38	110.40
1	B	110	ASP	CB-CG-OD1	11.59	128.73	118.30
1	A	113	LEU	C-N-CD	-11.48	95.34	120.60
1	B	112	LEU	CB-CA-C	8.82	126.97	110.20
1	A	103(B)	PRO	N-CA-CB	8.25	113.20	103.30
1	A	113	LEU	O-C-N	-7.80	106.27	121.10
1	A	113	LEU	CA-C-N	-7.60	95.83	117.10
1	B	18	ALA	N-CA-CB	7.56	120.69	110.10
1	B	102	LYS	CA-CB-CG	-7.08	97.83	113.40
1	A	105(A)	ASP	CA-C-N	7.08	132.77	117.20
1	A	101	THR	CA-C-N	-7.00	101.79	117.20
1	A	283	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	110	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	B	186	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	310	ASP	CB-CG-OD2	6.48	124.14	118.30
1	B	283	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	106	GLU	C-N-CA	-6.38	105.76	121.70
1	B	53	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	329	ILE	CB-CA-C	-6.22	99.17	111.60
1	A	103(B)	PRO	CA-N-CD	-6.17	102.87	111.50
1	B	316	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	92	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	106	GLU	O-C-N	5.91	132.16	122.70
1	A	316	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	221	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	143	ASP	CB-CG-OD2	5.53	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	105(A)	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	111	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	111	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	221	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	310	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	116	ASN	N-CA-C	5.29	125.28	111.00
1	B	90	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	106	GLU	CA-C-N	-5.22	105.72	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	105(B)	LYS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	THR	Mainchain
1	A	102	LYS	Mainchain
1	A	105(A)	ASP	Mainchain,Peptide
1	A	105(B)	LYS	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	2404	0	2485	133	0
1	B	2404	0	2484	50	0
2	A	44	0	26	7	0
2	B	44	0	26	3	0
3	A	6	0	2	1	0
3	B	6	0	2	0	0
4	A	6	0	8	0	0
4	B	6	0	8	4	0
5	A	64	0	0	5	0
5	B	131	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5115	0	5041	180	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 19.

All (180) 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:100:PHE:CD1	1:A:115:LEU:HG	1.35	1.54
1:A:112:LEU:C	1:A:114:PRO:HD2	1.33	1.43
1:A:100:PHE:CD1	1:A:115:LEU:CG	2.14	1.21
1:A:113:LEU:N	1:A:114:PRO:CD	2.08	1.17
1:A:113:LEU:N	1:A:114:PRO:HD2	1.58	1.16
1:A:121:ILE:HD13	1:A:152:HIS:CE1	1.82	1.14
1:A:112:LEU:C	1:A:114:PRO:CD	2.16	1.12
1:A:117:ASN:HD21	1:A:329:ILE:CD1	1.68	1.06
1:A:329:ILE:O	1:A:329:ILE:HG23	1.32	1.05
1:A:18:ALA:HB3	1:A:19:PRO:HD3	1.36	1.05
1:A:114:PRO:HG2	1:A:115:LEU:H	1.25	1.02
1:A:117:ASN:HD21	1:A:329:ILE:HD12	1.24	1.00
1:A:191:ILE:HG12	1:A:201:LEU:HD22	1.45	0.98
1:A:329:ILE:CG2	1:A:329:ILE:O	2.08	0.98
1:B:100:PHE:HD1	1:B:116:ASN:HD21	1.06	0.93
1:A:313:LYS:HE2	1:A:317:GLU:OE2	1.69	0.92
1:A:121:ILE:CD1	1:A:152:HIS:CE1	2.51	0.92
1:B:121:ILE:HD12	1:B:152:HIS:NE2	1.87	0.89
1:B:121:ILE:HD12	1:B:152:HIS:CD2	2.09	0.87
1:A:220:THR:OG1	1:A:223:GLU:HG2	1.74	0.86
1:A:18:ALA:HB3	1:A:19:PRO:CD	2.05	0.86
1:A:114:PRO:HG2	1:A:115:LEU:N	1.91	0.83
1:A:121:ILE:HD13	1:A:152:HIS:NE2	1.94	0.82
1:A:84:THR:HG22	1:A:86:ASP:H	1.45	0.82
1:A:112:LEU:O	1:A:114:PRO:HD2	1.80	0.81
1:B:69:THR:HA	1:B:72:MET:HE2	1.63	0.81
1:A:113:LEU:N	1:A:114:PRO:HD3	1.93	0.80
1:A:100:PHE:CG	1:A:115:LEU:HD23	2.17	0.80
1:A:100:PHE:CD1	1:A:115:LEU:CD2	2.65	0.80
1:A:120:MET:CE	1:A:149:LEU:HD12	2.12	0.80
1:B:100:PHE:HD1	1:B:116:ASN:ND2	1.79	0.79
1:A:18:ALA:CB	1:A:19:PRO:HD3	2.14	0.78
1:A:117:ASN:ND2	1:A:329:ILE:CD1	2.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:HD1	1:A:115:LEU:O	1.66	0.78
1:B:121:ILE:CD1	1:B:152:HIS:CD2	2.67	0.77
1:A:155:VAL:CG2	5:A:2022:HOH:O	2.33	0.77
1:A:100:PHE:CG	1:A:115:LEU:CD2	2.66	0.77
1:A:285:ILE:HD13	1:A:319:VAL:HG13	1.65	0.77
1:A:117:ASN:HD21	1:A:329:ILE:HD13	1.50	0.75
1:B:100:PHE:CG	1:B:115:LEU:HD12	2.20	0.75
1:B:69:THR:HA	1:B:72:MET:CE	2.17	0.74
1:B:121:ILE:CD1	1:B:152:HIS:NE2	2.52	0.73
1:A:273:THR:HG21	1:A:291:LEU:HD21	1.72	0.72
1:A:120:MET:HE1	1:A:149:LEU:HD12	1.72	0.70
1:A:117:ASN:ND2	1:A:329:ILE:HD13	2.05	0.70
1:A:155:VAL:HG22	1:A:156:PRO:HD2	1.74	0.70
1:B:103(B):PRO:HD2	1:B:115:LEU:HD21	1.73	0.69
1:B:327:ALA:C	1:B:329:ILE:H	1.96	0.68
1:A:56:LYS:O	1:A:57:ASN:HB2	1.92	0.68
1:A:70:ASN:HD21	1:A:76:CYS:H	1.41	0.68
1:A:105(A):ASP:C	1:A:105(B):LYS:CA	2.61	0.68
1:B:121:ILE:HD12	1:B:152:HIS:CE1	2.30	0.67
1:A:266:ARG:HH11	1:B:181:ASN:HD21	1.42	0.67
1:A:327:ALA:C	1:A:329:ILE:H	1.98	0.67
1:A:112:LEU:CA	1:A:114:PRO:CD	2.73	0.66
1:A:121:ILE:CD1	1:A:152:HIS:NE2	2.57	0.66
1:A:291:LEU:CD2	1:A:302:VAL:HG22	2.26	0.66
1:A:53:ASP:OD1	1:A:54:ILE:N	2.29	0.66
1:A:271:CYS:HB2	1:A:291:LEU:HD12	1.78	0.65
1:A:24:VAL:HG11	1:A:88:LEU:HD23	1.79	0.65
1:A:120:MET:HB2	1:A:148:LEU:HD23	1.78	0.64
1:A:58:MET:HB3	1:A:59:PRO:HD3	1.78	0.64
1:A:313:LYS:CE	1:A:317:GLU:OE2	2.46	0.63
1:A:113:LEU:CA	1:A:114:PRO:CD	2.76	0.63
1:A:120:MET:HA	1:A:120:MET:HE3	1.80	0.63
1:A:28:SER:O	1:A:62:LYS:NZ	2.25	0.63
1:A:44:ASN:ND2	1:A:75:ASN:H	1.97	0.62
1:B:169:THR:HB	1:B:173:LYS:HE3	1.80	0.62
1:A:100:PHE:CD1	1:A:115:LEU:CB	2.82	0.62
1:A:114:PRO:CG	1:A:115:LEU:H	1.90	0.61
1:B:215:ASN:O	1:B:216:LYS:HB2	1.99	0.61
1:A:142:VAL:HG13	1:A:143:ASP:N	2.16	0.60
1:A:181:ASN:HD21	1:B:266:ARG:NH1	2.00	0.60
1:A:321:GLU:HA	1:A:321:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASN:OD1	1:A:308:ASN:C	2.40	0.59
1:B:84:THR:HG22	1:B:86:ASP:H	1.67	0.59
1:A:115:LEU:O	1:A:116:ASN:CG	2.42	0.58
1:A:140:ASN:ND2	2:A:1330:NAD:O2D	2.37	0.58
1:B:113:LEU:HB2	1:B:114:PRO:HD3	1.84	0.57
1:A:113:LEU:CA	1:A:114:PRO:HD2	2.31	0.57
1:A:100:PHE:CD1	1:A:115:LEU:O	2.53	0.57
1:A:112:LEU:CA	1:A:114:PRO:HD2	2.29	0.56
1:A:58:MET:N	1:A:59:PRO:HD2	2.20	0.56
1:A:155:VAL:HG23	5:A:2022:HOH:O	1.99	0.56
1:A:220:THR:H	1:A:223:GLU:HG3	1.70	0.56
1:A:110:ASP:C	1:A:112:LEU:H	2.07	0.56
1:A:210(B):GLN:HE21	1:A:214:ASN:HD21	1.54	0.55
1:A:147:GLN:HB2	1:A:286:PHE:CD1	2.42	0.55
1:B:188:ASN:HD21	4:B:1332:GOL:H2	1.71	0.55
1:A:85:TYR:CG	1:A:126:HIS:ND1	2.76	0.54
1:A:273:THR:HB	1:A:291:LEU:HD11	1.89	0.54
1:B:113:LEU:O	1:B:117:ASN:ND2	2.41	0.54
1:A:114:PRO:CG	1:A:115:LEU:N	2.52	0.53
1:B:44:ASN:ND2	1:B:75:ASN:H	2.06	0.53
1:A:54:ILE:HG13	1:A:55:VAL:N	2.23	0.52
1:A:201:LEU:HD23	1:A:201:LEU:N	2.24	0.52
1:A:100:PHE:CD2	1:A:115:LEU:HD21	2.44	0.52
1:A:110:ASP:O	1:A:112:LEU:N	2.43	0.52
1:A:70:ASN:ND2	1:A:76:CYS:H	2.04	0.52
1:A:108:ASN:OD1	1:A:110:ASP:N	2.33	0.51
1:A:108:ASN:OD1	1:A:110:ASP:HB2	2.11	0.51
1:A:190:HIS:CD2	1:A:270:ILE:HD11	2.46	0.51
1:A:100:PHE:CD2	1:A:115:LEU:CD2	2.93	0.51
1:A:158:ASN:OD1	1:A:159:LYS:HG2	2.10	0.51
1:A:285:ILE:HD13	1:A:319:VAL:CG1	2.40	0.50
1:B:110:ASP:C	1:B:112:LEU:H	2.14	0.50
1:A:220:THR:OG1	1:A:223:GLU:CG	2.56	0.50
1:A:239:ILE:HG22	1:A:244:ALA:O	2.11	0.50
1:B:327:ALA:C	1:B:329:ILE:N	2.63	0.50
1:A:289:THR:OG1	1:A:290:PRO:HD2	2.12	0.49
1:A:138:VAL:O	2:A:1330:NAD:H2N	2.13	0.49
1:A:155:VAL:CG2	1:A:156:PRO:HD2	2.42	0.49
1:A:291:LEU:HD23	1:A:302:VAL:HA	1.95	0.49
1:A:329:ILE:O	1:A:329:ILE:HG12	2.09	0.49
1:A:117:ASN:ND2	1:A:329:ILE:HG21	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:CE	1:A:120:MET:HA	2.43	0.49
1:A:113:LEU:CA	1:A:114:PRO:N	2.76	0.49
1:A:112:LEU:HA	1:A:114:PRO:CG	2.43	0.49
1:B:140:ASN:OD1	2:B:1330:NAD:C2N	2.61	0.49
1:B:58:MET:SD	1:B:62:LYS:HE3	2.53	0.49
1:A:191:ILE:CG1	1:A:201:LEU:HD22	2.32	0.49
2:A:1330:NAD:C4N	3:A:1331:OXM:C1	2.91	0.48
1:B:84:THR:HG23	5:B:2013:HOH:O	2.12	0.48
1:B:247:TYR:HA	1:B:250:PRO:HG2	1.96	0.48
1:A:18:ALA:CB	1:A:19:PRO:CD	2.74	0.48
1:B:112:LEU:CG	1:B:112:LEU:CA	2.92	0.48
1:B:281:HIS:CD2	1:B:319:VAL:HG11	2.48	0.48
1:A:196:GLY:O	1:A:199:MET:HG3	2.13	0.48
1:A:85:TYR:CD2	1:A:126:HIS:ND1	2.81	0.48
1:B:327:ALA:O	1:B:329:ILE:HG23	2.14	0.47
1:A:142:VAL:CG1	1:A:143:ASP:N	2.77	0.47
1:A:181:ASN:HD21	1:B:266:ARG:HH11	1.61	0.47
1:A:117:ASN:C	1:A:117:ASN:OD1	2.53	0.47
1:A:85:TYR:CD1	1:A:126:HIS:CE1	3.03	0.46
1:A:210(B):GLN:HE21	1:A:214:ASN:ND2	2.13	0.46
1:B:113:LEU:HB2	1:B:114:PRO:CD	2.46	0.46
1:A:311:GLU:OE2	5:A:2061:HOH:O	2.21	0.46
1:A:327:ALA:C	1:A:329:ILE:N	2.67	0.46
1:B:283:ASP:O	1:B:326:LYS:NZ	2.48	0.46
1:A:249:ALA:N	1:A:250:PRO:CD	2.78	0.46
1:B:163:LEU:HD23	2:B:1330:NAD:C7N	2.46	0.46
1:B:100:PHE:CD1	1:B:116:ASN:ND2	2.70	0.45
1:A:203:LYS:NZ	5:A:2036:HOH:O	2.47	0.45
1:B:208:VAL:HB	1:B:212:PHE:CE1	2.52	0.45
1:B:215:ASN:O	1:B:216:LYS:CB	2.62	0.45
1:A:285:ILE:HG12	1:A:286:PHE:N	2.32	0.44
1:A:58:MET:N	1:A:59:PRO:CD	2.79	0.44
1:A:44:ASN:HD21	1:A:75:ASN:H	1.65	0.44
1:A:266:ARG:NH1	1:B:181:ASN:HD21	2.11	0.44
1:B:128:LYS:HE3	1:B:128:LYS:HB2	1.85	0.44
1:A:301:GLN:NE2	1:B:218:LYS:HE2	2.33	0.44
1:A:113:LEU:H	1:A:114:PRO:HD3	1.80	0.44
1:A:54:ILE:HG23	2:A:1330:NAD:C5A	2.48	0.43
1:B:188:ASN:HD21	4:B:1332:GOL:C2	2.29	0.43
1:B:289:THR:OG1	1:B:290:PRO:HD2	2.17	0.43
1:A:163:LEU:HD23	2:A:1330:NAD:C7N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209(A):GLY:O	4:B:1332:GOL:H32	2.19	0.43
1:A:100:PHE:CD1	1:A:115:LEU:HD23	2.45	0.42
1:A:97:THR:HB	2:A:1330:NAD:H51N	2.00	0.42
1:A:58:MET:HB3	1:A:59:PRO:CD	2.46	0.42
1:A:40:ILE:HG23	1:A:45:LEU:HB3	2.00	0.42
1:B:24:VAL:HG11	1:B:88:LEU:HD23	2.01	0.42
1:A:53:ASP:HB3	1:A:59:PRO:HG3	2.00	0.42
1:B:188:ASN:ND2	4:B:1332:GOL:H2	2.34	0.42
1:B:40:ILE:HG23	1:B:45:LEU:HB3	2.01	0.42
1:A:120:MET:HB3	1:A:120:MET:HE2	1.77	0.42
1:A:112:LEU:HA	1:A:114:PRO:CD	2.46	0.41
1:A:220:THR:H	1:A:223:GLU:CG	2.31	0.41
1:A:203:LYS:HE3	1:A:225:LEU:HD23	2.01	0.41
1:A:247:TYR:C	1:A:250:PRO:HD2	2.40	0.41
1:B:212:PHE:HD2	1:B:218:LYS:HD3	1.85	0.41
1:A:58:MET:SD	1:A:62:LYS:HD2	2.60	0.41
2:B:1330:NAD:H6N	5:B:2097:HOH:O	2.20	0.41
1:A:329:ILE:HD12	5:A:2021:HOH:O	2.20	0.41
1:A:110:ASP:C	1:A:112:LEU:N	2.73	0.41
1:B:58:MET:N	1:B:59:PRO:HD2	2.36	0.41
1:B:199:MET:HG3	1:B:201:LEU:CD1	2.50	0.41
1:A:31:ILE:HG13	2:A:1330:NAD:PN	2.61	0.41
1:B:281:HIS:CE1	1:B:316:ASP:OD1	2.74	0.40
1:B:181:ASN:HD22	1:B:181:ASN:HA	1.71	0.40

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	313/322 (97%)	292 (93%)	15 (5%)	6 (2%)	9 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	313/322 (97%)	298 (95%)	12 (4%)	3 (1%)	18	20
All	All	626/644 (97%)	590 (94%)	27 (4%)	9 (1%)	13	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105(A)	ASP
1	A	114	PRO
1	A	116	ASN
1	A	111	ASP
1	A	328	LEU
1	B	111	ASP
1	A	164	GLY
1	B	164	GLY
1	B	114	PRO

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	266/273 (97%)	257 (97%)	9 (3%)	42	57
1	B	266/273 (97%)	258 (97%)	8 (3%)	46	63
All	All	532/546 (97%)	515 (97%)	17 (3%)	44	60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105(B)	LYS
1	A	113	LEU
1	A	114	PRO
1	A	177	SER
1	A	188	ASN
1	A	201	LEU
1	A	223	GLU

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Mol	Chain	Res	Type
1	A	235	THR
1	A	313	LYS
1	B	115	LEU
1	B	117	ASN
1	B	153	SER
1	B	181	ASN
1	B	188	ASN
1	B	231	ARG
1	B	289	THR
1	B	323	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	57	ASN
1	A	70	ASN
1	A	75	ASN
1	A	83	ASN
1	A	117	ASN
1	A	140	ASN
1	A	152	HIS
1	A	181	ASN
1	A	188	ASN
1	A	190	HIS
1	A	214	ASN
1	B	44	ASN
1	B	83	ASN
1	B	117	ASN
1	B	126	HIS
1	B	129	ASN
1	B	181	ASN
1	B	188	ASN
1	B	210(B)	GLN
1	B	241	ASN
1	B	281	HIS

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	1330	-	41,48,48	1.57	3 (7%)	43,73,73	1.98	5 (11%)
3	OXM	A	1331	-	2,5,5	0.58	0	2,6,6	0.91	0
4	GOL	A	1332	-	5,5,5	0.17	0	5,5,5	0.58	0
2	NAD	B	1330	-	41,48,48	1.62	3 (7%)	43,73,73	1.84	3 (6%)
3	OXM	B	1331	-	2,5,5	0.53	0	2,6,6	0.91	0
4	GOL	B	1332	-	5,5,5	0.41	0	5,5,5	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1330	-	-	0/22/62/62	0/5/5/5
3	OXM	A	1331	-	-	0/0/4/4	0/0/0/0
4	GOL	A	1332	-	-	0/4/4/4	0/0/0/0
2	NAD	B	1330	-	-	0/22/62/62	0/5/5/5
3	OXM	B	1331	-	-	0/0/4/4	0/0/0/0
4	GOL	B	1332	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1330	NAD	C2A-N1A	2.20	1.38	1.33
2	A	1330	NAD	C2A-N1A	2.43	1.38	1.33
2	A	1330	NAD	C2A-N3A	3.59	1.38	1.32
2	B	1330	NAD	C2A-N3A	3.70	1.38	1.32
2	B	1330	NAD	O7N-C7N	8.05	1.40	1.24
2	A	1330	NAD	O7N-C7N	8.07	1.40	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1330	NAD	N3A-C2A-N1A	-9.99	120.15	128.86
2	B	1330	NAD	N3A-C2A-N1A	-9.88	120.25	128.86
2	A	1330	NAD	C4B-O4B-C1B	-4.45	105.03	109.77
2	B	1330	NAD	C1B-N9A-C4A	-3.43	120.71	126.64
2	A	1330	NAD	C4A-C5A-N7A	-2.65	106.85	109.41
2	B	1330	NAD	C4A-C5A-N7A	-2.30	107.19	109.41
2	A	1330	NAD	C1B-N9A-C4A	-2.24	122.77	126.64
2	A	1330	NAD	C3N-C7N-N7N	2.57	120.71	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1330	NAD	7	0
3	A	1331	OXM	1	0
2	B	1330	NAD	3	0
4	B	1332	GOL	4	0

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

6.1 Protein, DNA and RNA chains

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	314/322 (97%)	0.33	26 (8%)	12 16	22, 32, 66, 94	13 (4%)
1	B	315/322 (97%)	0.29	27 (8%)	11 16	20, 30, 70, 94	12 (3%)
All	All	629/644 (97%)	0.31	53 (8%)	12 16	20, 31, 70, 94	25 (3%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	10.2
1	A	114	PRO	6.5
1	A	103(A)	ALA	6.3
1	B	115	LEU	6.2
1	B	112	LEU	5.2
1	B	137	VAL	4.5
1	A	327	ALA	4.4
1	A	103(C)	GLY	3.9
1	A	112	LEU	3.7
1	B	105(B)	LYS	3.7
1	B	136	ILE	3.6
1	B	103(E)	SER	3.5
1	A	310	ASP	3.4
1	B	107	TRP	3.4
1	B	106	GLU	3.3
1	A	329	ILE	3.3
1	B	105(A)	ASP	3.2
1	A	113	LEU	3.2
1	A	54	ILE	3.1
1	B	103(B)	PRO	3.1
1	B	114	PRO	3.1
1	A	18	ALA	3.1
1	B	95	ILE	2.8
1	A	103(D)	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	243	HIS	2.8
1	A	56	LYS	2.7
1	B	113	LEU	2.7
1	B	329	ILE	2.7
1	B	18	ALA	2.6
1	A	19	PRO	2.6
1	B	146	VAL	2.5
1	B	116	ASN	2.4
1	B	103(C)	GLY	2.4
1	A	230	ASP	2.3
1	A	309	ALA	2.3
1	A	103(E)	SER	2.3
1	B	96	VAL	2.3
1	A	89	LYS	2.3
1	A	222	GLN	2.3
1	B	108	ASN	2.3
1	A	280	GLY	2.2
1	B	135	ILE	2.2
1	B	162	GLY	2.2
1	A	241	ASN	2.2
1	B	103(A)	ALA	2.2
1	B	97	THR	2.2
1	A	105(B)	LYS	2.1
1	A	152	HIS	2.1
1	A	110	ASP	2.1
1	B	253	ALA	2.1
1	B	100	PHE	2.0
1	A	227	ALA	2.0
1	B	163	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	1332	6/6	0.92	0.17	1.54	24,24,26,28	0
3	OXM	A	1331	6/6	0.88	0.17	0.36	49,50,50,50	0
2	NAD	A	1330	44/44	0.90	0.17	0.17	34,42,50,52	0
4	GOL	B	1332	6/6	0.98	0.16	-0.26	25,26,27,27	0
3	OXM	B	1331	6/6	0.96	0.13	-1.05	43,43,43,43	0
2	NAD	B	1330	44/44	0.97	0.10	-1.24	18,33,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.