



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:07 PM GMT

PDB ID : 2O2Y
Title : The crystal structure of P. falciparum enoyl acyl carrier protein reductase
Authors : Muench, S.P.; Prigge, S.T.; McLeod, R.; Rafferty, J.B.; Kirisits, M.J.; Roberts, C.W.; Mui, E.J.; Rice, D.W.
Deposited on : 2006-11-30
Resolution : 2.20 Å(reported)

This is a wwPDB validation summary 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>

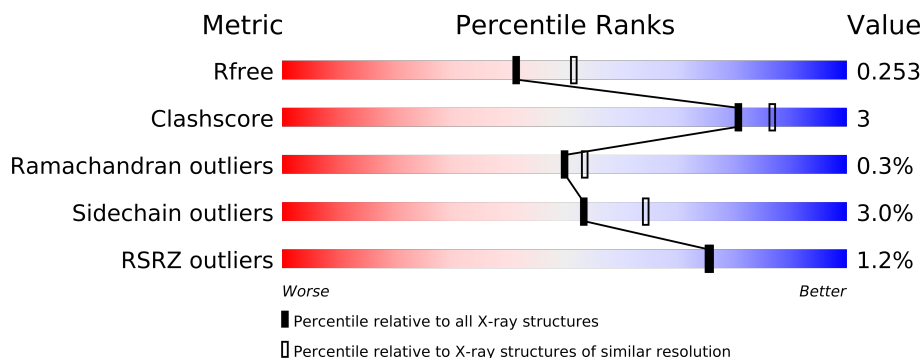
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
1	C	349	
1	D	349	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	D	713	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9909 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 Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2288	1460	385	432	11			
1	B	290	Total	C	N	O	S	13	0	0
			2293	1463	385	434	11			
1	C	293	Total	C	N	O	S	18	0	0
			2310	1474	386	440	10			
1	D	288	Total	C	N	O	S	4	0	0
			2270	1451	378	430	11			

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

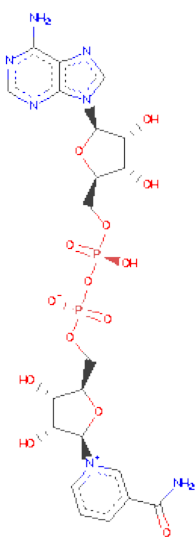
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



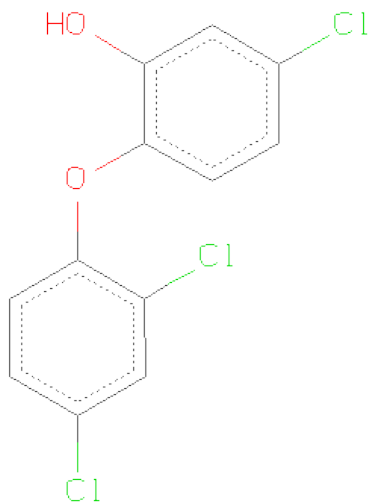
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 5 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
5	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
5	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
5	C	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 6 is water.

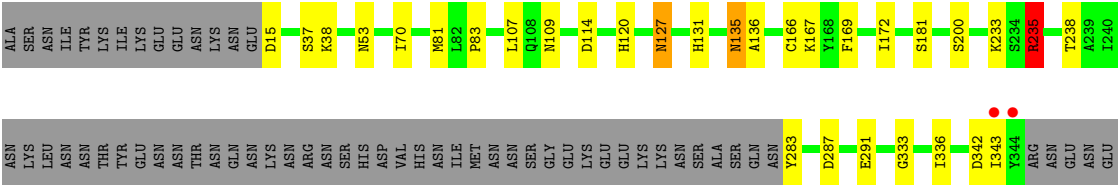
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	130	Total	O	0	0
			130	130		
6	C	109	Total	O	0	0
			109	109		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	150	Total 150	O 150	0	0

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.18Å 82.37Å 94.82Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.20) 97.7 (29.89-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.246 0.209 , 0.253	Depositor DCC
R_{free} test set	3374 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.2	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 67485 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9909	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TCL, SO4, NAD, 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	0.48	0/2331	0.61	0/3147
1	B	0.61	3/2336 (0.1%)	0.77	6/3154 (0.2%)
1	C	0.61	5/2353 (0.2%)	0.79	8/3178 (0.3%)
1	D	0.58	1/2313 (0.0%)	0.70	3/3124 (0.1%)
All	All	0.57	9/9333 (0.1%)	0.72	17/12603 (0.1%)

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
1	C	0	2
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	LYS	CA-CB	-14.15	1.22	1.53
1	C	117	ASN	CG-OD1	-11.33	0.99	1.24
1	D	166	CYS	CB-SG	-10.70	1.64	1.82
1	C	42	LYS	CG-CD	-8.06	1.25	1.52
1	C	86	ALA	CA-CB	6.71	1.66	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	MET	CG-SD-CE	20.00	132.19	100.20
1	D	81	MET	CG-SD-CE	15.30	124.68	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	MET	CG-SD-CE	13.58	121.92	100.20
1	B	198	MET	CG-SD-CE	12.95	120.92	100.20
1	C	53	ASN	OD1-CG-ND2	-10.96	96.68	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	LEU	Mainchain
1	C	117	ASN	Sidechain
1	C	53	ASN	Sidechain

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	2288	0	2286	20	0
1	B	2293	0	2291	17	0
1	C	2310	0	2295	15	0
1	D	2270	0	2263	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	5	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	1	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
5	A	17	0	6	0	0
5	B	17	0	6	0	0
5	C	17	0	6	0	0
5	D	17	0	6	0	0
6	A	106	0	0	2	0
6	B	130	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	109	0	0	3	0
6	D	150	0	0	1	0
All	All	9909	0	9263	60	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 3.

The worst 5 of 60 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:339:LEU:HD22	1:C:292:TYR:CE1	2.23	0.73
1:B:292:TYR:CD1	1:C:339:LEU:HD22	2.31	0.65
1:A:319:GLU:OE1	1:C:39:ARG:NH2	2.30	0.65
1:D:283:TYR:CE2	1:D:291:GLU:OE1	2.51	0.64
1:B:292:TYR:CE1	1:C:339:LEU:HD22	2.34	0.62

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	286/349 (82%)	272 (95%)	13 (4%)	1 (0%)	50	53
1	B	286/349 (82%)	276 (96%)	9 (3%)	1 (0%)	50	53
1	C	289/349 (83%)	277 (96%)	10 (4%)	2 (1%)	30	28
1	D	284/349 (81%)	274 (96%)	10 (4%)	0	100	100
All	All	1145/1396 (82%)	1099 (96%)	42 (4%)	4 (0%)	50	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	LYS
1	C	14	GLU
1	B	72	LYS

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Mol	Chain	Res	Type
1	A	240	ILE

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	248/307 (81%)	240 (97%)	8 (3%)	51	62
1	B	249/307 (81%)	243 (98%)	6 (2%)	61	73
1	C	249/307 (81%)	240 (96%)	9 (4%)	47	56
1	D	246/307 (80%)	239 (97%)	7 (3%)	56	67
All	All	992/1228 (81%)	962 (97%)	30 (3%)	53	64

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	334	LEU
1	C	102	LYS
1	D	200	SER
1	C	77	ASN
1	C	135	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	301	GLN
1	C	135	ASN
1	D	135	ASN
1	C	66	ASN
1	C	101	ASN

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 ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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$
4	NAD	A	650	-	48,48,48	1.37	4 (8%)	73,73,73	1.82	6 (8%)
5	TCL	A	705	-	18,18,18	1.73	2 (11%)	25,25,25	0.96	1 (4%)
4	NAD	B	1450	-	48,48,48	1.37	3 (6%)	73,73,73	1.67	6 (8%)
5	TCL	B	706	-	18,18,18	1.63	2 (11%)	25,25,25	1.12	2 (8%)
5	TCL	C	708	-	18,18,18	1.79	4 (22%)	25,25,25	1.12	1 (4%)
4	NAD	C	750	-	48,48,48	1.31	3 (6%)	73,73,73	1.81	8 (10%)
4	NAD	D	550	-	48,48,48	1.34	4 (8%)	73,73,73	1.98	13 (17%)
5	TCL	D	707	-	18,18,18	1.84	2 (11%)	25,25,25	0.96	1 (4%)
3	SO4	D	713	1	4,4,4	0.39	0	6,6,6	0.34	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
4	NAD	A	650	-	-	0/30/62/62	0/3/5/5
5	TCL	A	705	-	-	0/4/4/4	0/2/2/2
4	NAD	B	1450	-	-	0/30/62/62	0/3/5/5
5	TCL	B	706	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TCL	C	708	-	-	0/4/4/4	0/2/2/2
4	NAD	C	750	-	-	0/30/62/62	0/3/5/5
4	NAD	D	550	-	-	0/30/62/62	0/3/5/5
5	TCL	D	707	-	-	0/4/4/4	0/2/2/2
3	SO4	D	713	1	-	0/0/0/0	0/0/0/0

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	650	NAD	O7N-C7N	7.10	1.40	1.24
4	B	1450	NAD	O7N-C7N	6.80	1.40	1.24
4	C	750	NAD	O7N-C7N	6.46	1.39	1.24
4	D	550	NAD	O7N-C7N	6.40	1.39	1.24
5	D	707	TCL	C6-C5	5.17	1.48	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	750	NAD	N3A-C2A-N1A	-11.42	119.16	128.71
4	A	650	NAD	N3A-C2A-N1A	-11.27	119.29	128.71
4	D	550	NAD	N3A-C2A-N1A	-10.69	119.77	128.71
4	B	1450	NAD	N3A-C2A-N1A	-10.04	120.32	128.71
4	D	550	NAD	C3N-C7N-N7N	4.87	123.31	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	290/349 (83%)	-0.37	5 (1%) 67 68	17, 21, 25, 30	0
1	B	290/349 (83%)	-0.47	2 (0%) 84 86	17, 20, 25, 32	11 (3%)
1	C	293/349 (83%)	-0.31	5 (1%) 67 68	17, 21, 26, 33	15 (5%)
1	D	288/349 (82%)	-0.56	2 (0%) 84 86	17, 20, 25, 30	4 (1%)
All	All	1161/1396 (83%)	-0.43	14 (1%) 75 76	17, 20, 25, 33	30 (2%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	TYR	4.5
1	A	283	TYR	4.1
1	D	343	ILE	4.1
1	A	345	ARG	3.8
1	A	241	ASN	3.7

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 ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	D	713	5/5	0.24	6.97	46,47,48,49	0
4	NAD	D	550	44/44	0.13	1.51	20,22,25,28	0
5	TCL	D	707	17/17	0.11	0.95	21,23,26,27	0
2	CL	A	710	1/1	0.15	0.92	14,14,14,14	0
4	NAD	B	1450	44/44	0.12	0.88	18,22,25,26	0
4	NAD	A	650	44/44	0.11	0.76	20,21,24,24	0
5	TCL	A	705	17/17	0.10	0.15	21,22,22,24	0
5	TCL	B	706	17/17	0.10	-0.14	22,23,24,25	0
2	CL	C	712	1/1	0.10	-0.15	23,23,23,23	0
4	NAD	C	750	44/44	0.10	-0.20	17,21,24,26	0
2	CL	B	711	1/1	0.08	-0.55	22,22,22,22	0
2	CL	D	709	1/1	0.10	-0.71	16,16,16,16	0
5	TCL	C	708	17/17	0.09	-1.08	21,22,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.