W O R L D W I D E

wwPDB

P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2022 – 04:07 PM EDT

PDB ID	:	6EFF
Title	:	NCTC10712
Authors	:	Iverson, T.M.
Deposited on	:	2018-08-16
Resolution	:	1.60 Å(reported)

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	Percentile Ranks	Value
Rfree		0.208
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		1.0%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
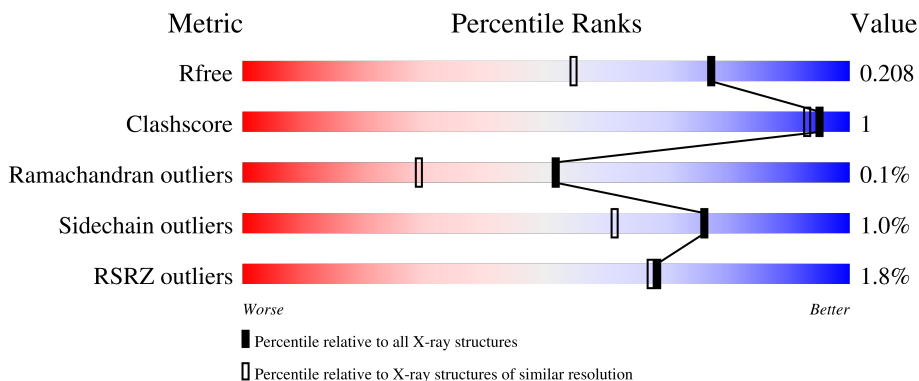
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	210	% 94%
1	B	210	3% 92% 6% ·
1	C	210	2% 94%
1	D	210	% 95%

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
3	GOL	D	509	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13908 atoms, of which 6382 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 NCTC10712 Siglec.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total 3118	C 981	H 1535	N 273	O 327	S 2	2	4	0
1	B	206	Total 3218	C 1009	H 1592	N 280	O 335	S 2	2	9	0
1	C	205	Total 3133	C 985	H 1540	N 275	O 330	S 3	3	3	0
1	D	205	Total 3184	C 1001	H 1568	N 279	O 334	S 2	0	6	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
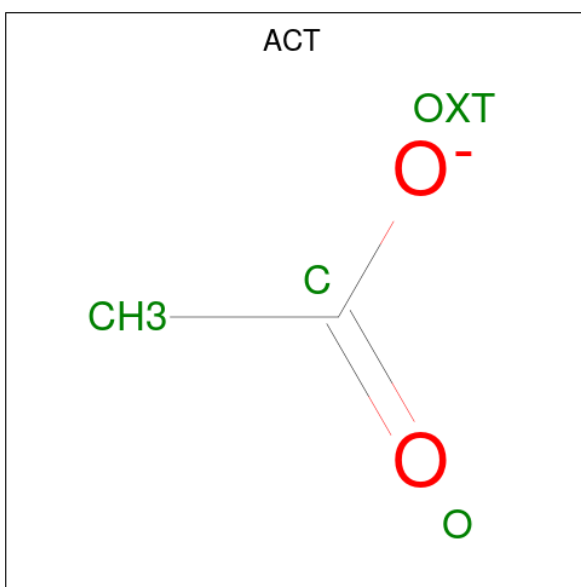
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 7	C 2	H 3	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	248	Total 248	O 248	0	0
5	B	234	Total 234	O 234	0	0
5	C	254	Total 254	O 254	0	0
5	D	252	Total 252	O 252	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
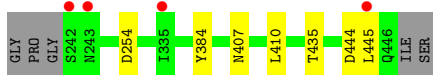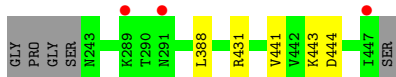
- Molecule 1: NCTC10712 Siglec

Chain A:

- Molecule 1: NCTC10712 Siglec

Chain B:
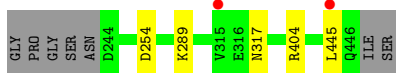
- Molecule 1: NCTC10712 Siglec

Chain C:

- Molecule 1: NCTC10712 Siglec

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.79Å 48.27Å 99.82Å 101.84° 91.39° 89.90°	Depositor
Resolution (Å)	47.24 – 1.60 47.24 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.4 (47.24-1.60) 87.7 (47.24-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.180 , 0.208 0.180 , 0.208	Depositor DCC
R_{free} test set	4402 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-l 0.076 for -h,k,-k-l 0.063 for -h,-k,k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13908	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 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, ACT, GOL

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	0.32	0/1622	0.55	0/2226
1	B	0.35	0/1685	0.57	0/2310
1	C	0.31	0/1629	0.53	0/2235
1	D	0.30	0/1652	0.55	0/2267
All	All	0.32	0/6588	0.55	0/9038

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	1583	1535	1524	1	0
1	B	1626	1592	1562	8	0
1	C	1593	1540	1530	3	0
1	D	1616	1568	1554	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	24	32	32	0	0

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	40	40	0	0
3	C	12	16	16	0	0
3	D	42	56	56	0	0
4	B	4	3	3	0	0
5	A	248	0	0	0	0
5	B	234	0	0	0	1
5	C	254	0	0	1	0
5	D	252	0	0	0	1
All	All	7526	6382	6317	16	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 1.

The worst 5 of 16 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:D:388:LEU:HG	1:D:444:ASP:HB2	1.75	0.67
1:B:444:ASP:OD2	1:B:447:ILE:N	2.29	0.66
1:B:388:LEU:HG	1:B:444:ASP:HB2	1.77	0.65
1:C:384:TYR:HB3	1:C:445:LEU:HG	1.94	0.50
1:C:435:THR:HG22	5:C:605:HOH:O	2.11	0.49

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)
5:B:786:HOH:O	5:D:741:HOH:O[1_454]	2.11	0.09

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	205/210 (98%)	194 (95%)	10 (5%)	1 (0%)	29	11
1	B	211/210 (100%)	205 (97%)	6 (3%)	0	100	100
1	C	206/210 (98%)	200 (97%)	6 (3%)	0	100	100
1	D	209/210 (100%)	201 (96%)	8 (4%)	0	100	100
All	All	831/840 (99%)	800 (96%)	30 (4%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	LYS

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	180/184 (98%)	177 (98%)	3 (2%)	60	38
1	B	188/184 (102%)	187 (100%)	1 (0%)	88	80
1	C	181/184 (98%)	179 (99%)	2 (1%)	73	57
1	D	184/184 (100%)	183 (100%)	1 (0%)	88	80
All	All	733/736 (100%)	726 (99%)	7 (1%)	76	61

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	440	ARG
1	C	254	ASP
1	D	431	ARG
1	C	444	ASP
1	A	445	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 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	ACT	B	501	-	1,3,3	1.00	0	0,3,3	-	-
3	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.24	0
3	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.22	0
3	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.18	0
3	GOL	B	505	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	D	509	-	5,5,5	0.33	0	5,5,5	0.29	0
3	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	B	508	-	5,5,5	0.37	0	5,5,5	0.23	0
3	GOL	D	503	-	5,5,5	0.41	0	5,5,5	0.24	0
3	GOL	B	504	-	5,5,5	0.34	0	5,5,5	0.44	0
3	GOL	B	507	-	5,5,5	0.11	0	5,5,5	0.54	0
3	GOL	D	507	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	D	504	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	C	503	-	5,5,5	0.41	0	5,5,5	0.31	0
3	GOL	C	504	-	5,5,5	0.41	0	5,5,5	0.09	0
3	GOL	D	505	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
3	GOL	D	508	-	5,5,5	0.39	0	5,5,5	0.19	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
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	A	506	-	-	0/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	B	507	-	-	4/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	D	506	-	-	2/4/4/4	-
3	GOL	A	505	-	-	0/4/4/4	-
3	GOL	D	509	-	-	4/4/4/4	-
3	GOL	D	504	-	-	2/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	B	508	-	-	1/4/4/4	-
3	GOL	D	508	-	-	2/4/4/4	-
3	GOL	D	507	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	GOL	O1-C1-C2-C3
3	B	507	GOL	O1-C1-C2-O2
3	B	507	GOL	O1-C1-C2-C3
3	B	507	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	203/210 (96%)	-0.09	2 (0%)	82	82	10, 16, 33, 55	2 (0%)
1	B	206/210 (98%)	0.00	6 (2%)	51	49	10, 16, 31, 64	1 (0%)
1	C	205/210 (97%)	-0.07	4 (1%)	65	64	11, 15, 32, 46	1 (0%)
1	D	205/210 (97%)	-0.00	3 (1%)	73	73	10, 16, 33, 62	0
All	All	819/840 (97%)	-0.04	15 (1%)	68	67	10, 16, 33, 64	4 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	447	ILE	7.3
1	D	289	LYS	5.3
1	B	447	ILE	5.0
1	B	292	MET	3.6
1	B	291	ASN	3.3

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	GOL	D	509	6/6	0.39	0.42	33,41,49,50	0
3	GOL	D	506	6/6	0.52	0.32	31,40,44,48	0
4	ACT	B	501	4/4	0.65	0.29	30,36,38,38	0
3	GOL	D	503	6/6	0.73	0.19	31,41,46,50	0
3	GOL	C	504	6/6	0.80	0.21	18,41,51,55	0
3	GOL	D	504	6/6	0.81	0.19	28,37,47,52	0
3	GOL	B	506	6/6	0.82	0.20	32,38,42,45	0
3	GOL	A	506	6/6	0.83	0.18	21,37,44,49	0
3	GOL	D	508	6/6	0.83	0.26	23,32,42,46	0
3	GOL	D	507	6/6	0.85	0.16	27,40,48,53	0
3	GOL	C	503	6/6	0.85	0.20	17,32,43,51	0
3	GOL	B	504	6/6	0.86	0.18	17,28,33,39	0
3	GOL	B	507	6/6	0.87	0.14	26,33,44,53	0
3	GOL	B	508	6/6	0.88	0.23	22,37,45,51	0
3	GOL	A	505	6/6	0.88	0.23	20,31,39,39	0
3	GOL	D	505	6/6	0.89	0.17	18,32,39,39	0
3	GOL	A	504	6/6	0.89	0.12	16,22,26,31	0
3	GOL	B	505	6/6	0.94	0.13	17,23,28,34	0
3	GOL	A	503	6/6	0.94	0.10	15,20,28,29	0
2	CA	B	503	1/1	0.97	0.16	31,31,31,31	0
2	CA	D	502	1/1	0.98	0.18	33,33,33,33	0
2	CA	A	502	1/1	0.98	0.17	29,29,29,29	0
2	CA	B	502	1/1	0.99	0.07	13,13,13,13	0
2	CA	A	501	1/1	0.99	0.09	18,18,18,18	0
2	CA	C	501	1/1	0.99	0.07	15,15,15,15	0
2	CA	C	502	1/1	0.99	0.23	33,33,33,33	0
2	CA	D	501	1/1	0.99	0.07	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.