WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 02:32 am BST

PDB ID	:	6U3W
Title	:	Crystal structure of yeast alpha/epsilon-COP of the COPI vesicular coat
Authors	:	Travis, S.M.; Hughson, F.M.
Deposited on	:	2019-08-22
Resolution	:	2.39 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.39 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		0.238
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.7%
RSRZ outliers		8.1%

Worse   Better

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
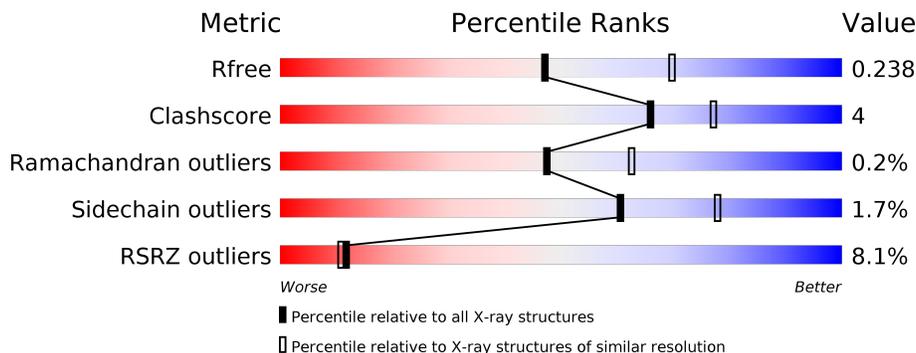
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	303	7% / 89% / 11%
2	B	310	9% / 82% / 11% / 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4915 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total 2384	C 1528	N 398	O 447	S 11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	899	MET	-	initiating methionine	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total 2343	C 1497	N 368	O 473	S 5	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P40509
B	2	GLY	-	expression tag	UNP P40509
B	3	SER	-	expression tag	UNP P40509
B	4	SER	-	expression tag	UNP P40509
B	5	HIS	-	expression tag	UNP P40509
B	6	HIS	-	expression tag	UNP P40509
B	7	HIS	-	expression tag	UNP P40509
B	8	HIS	-	expression tag	UNP P40509
B	9	HIS	-	expression tag	UNP P40509
B	10	HIS	-	expression tag	UNP P40509
B	11	SER	-	expression tag	UNP P40509
B	12	GLN	-	expression tag	UNP P40509
B	13	ASP	-	expression tag	UNP P40509
B	14	PRO	-	expression tag	UNP P40509

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
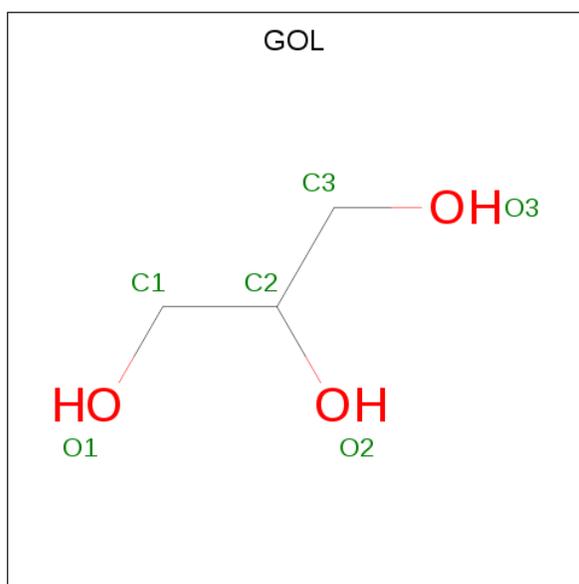
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total 118	O 118	0	0
4	B	64	Total 64	O 64	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: Coatomer subunit alpha

Chain A:
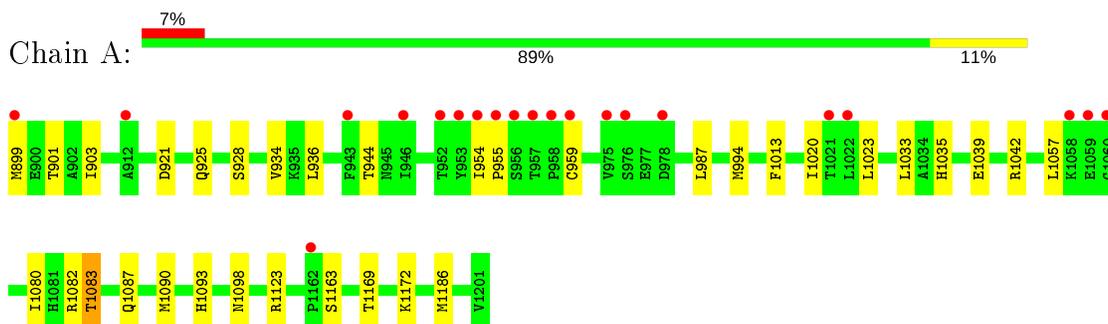
• Molecule 2: Coatomer subunit epsilon

Chain B:
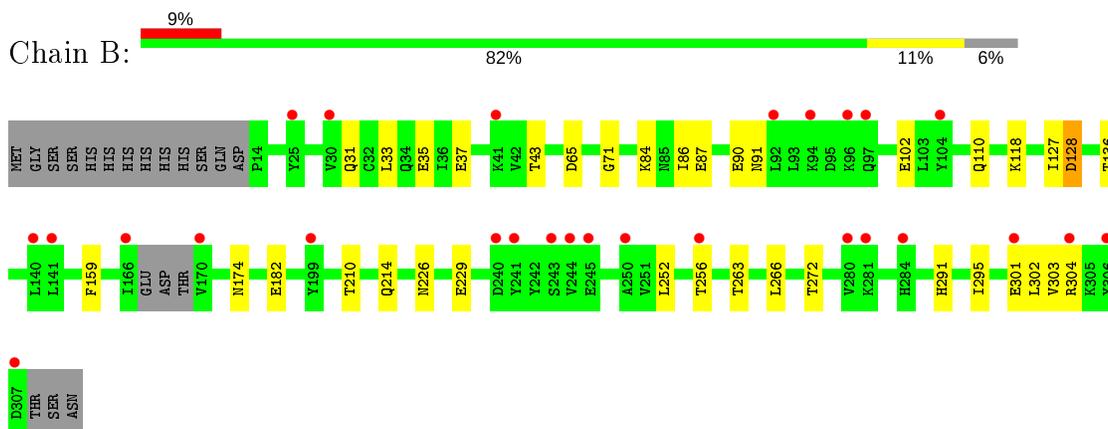
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.26Å　　84.59Å　　117.84Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	29.46　–　2.39 29.46　–　2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.46-2.39) 93.9 (29.46-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.178　,　0.238 0.178　,　0.238	Depositor DCC
R_{free} test set	1997 reflections (6.90%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.8	EDS
L-test for twinning[1]	$<|L|>$ = (Not available), $<L^2>$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4915	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

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[1]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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/2431	0.57	0/3287
2	B	0.37	0/2382	0.52	0/3232
All	All	0.40	0/4813	0.55	0/6519

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 (i)

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	2384	0	2427	20	0
2	B	2343	0	2295	20	0
3	A	6	0	8	0	0
4	A	118	0	0	4	0
4	B	64	0	0	1	0
All	All	4915	0	4730	38	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 4.

All (38) 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:994:MET:HE1	1:A:1013:PHE:HD1	1.22	1.01
1:A:994:MET:HE1	1:A:1013:PHE:CD1	2.15	0.75
2:B:33:LEU:O	2:B:37:GLU:HG2	1.91	0.70
2:B:86:ILE:HG23	2:B:90:GLU:HG3	1.75	0.69
1:A:1163:SER:OG	1:A:1172:LYS:NZ	2.38	0.57
2:B:301:GLU:OE1	2:B:304:ARG:NH2	2.39	0.56
1:A:987:LEU:HD13	1:A:1033:LEU:HD23	1.86	0.56
1:A:1082:ARG:HD3	4:A:1409:HOH:O	2.05	0.55
1:A:921:ASP:OD1	1:A:925:GLN:NE2	2.38	0.55
1:A:1123:ARG:NH1	4:A:1404:HOH:O	2.42	0.53
2:B:136:THR:HG21	2:B:174:ASN:HB3	1.91	0.53
1:A:1042:ARG:HD3	1:A:1169:THR:O	2.08	0.52
1:A:954:ILE:HG13	1:A:955:PRO:HD2	1.93	0.50
1:A:1082:ARG:HG2	4:A:1426:HOH:O	2.11	0.49
2:B:210:THR:O	2:B:214:GLN:HB2	2.13	0.49
2:B:266:LEU:HG	2:B:272:THR:HG21	1.95	0.48
2:B:87:GLU:O	2:B:91:ASN:ND2	2.42	0.48
2:B:31:GLN:O	2:B:35:GLU:HG2	2.14	0.47
2:B:102:GLU:OE2	4:B:401:HOH:O	2.20	0.47
2:B:127:ILE:HG22	2:B:127:ILE:O	2.14	0.47
1:A:1080:ILE:O	1:A:1083:THR:HB	2.15	0.46
1:A:1035:HIS:O	1:A:1039:GLU:HG3	2.16	0.46
1:A:1093:HIS:HD2	1:A:1098:ASN:HD22	1.64	0.45
1:A:899:MET:O	1:A:903:ILE:HG13	2.15	0.45
2:B:252:LEU:HA	2:B:252:LEU:HD12	1.80	0.44
1:A:1087:GLN:HA	1:A:1090:MET:HE3	1.98	0.44
1:A:955:PRO:HD3	2:B:256:THR:HG21	2.00	0.44
2:B:110:GLN:NE2	2:B:118:LYS:HE3	2.33	0.44
1:A:1186:MET:HE3	4:A:1518:HOH:O	2.17	0.43
2:B:291:HIS:O	2:B:295:ILE:HG12	2.19	0.43
2:B:226:ASN:HB3	2:B:229:GLU:OE2	2.19	0.43
1:A:936:LEU:HB2	2:B:303:VAL:HG22	2.00	0.42
1:A:1020:ILE:HA	1:A:1023:LEU:HG	2.00	0.42
2:B:302:LEU:HA	2:B:302:LEU:HD23	1.91	0.42
2:B:84:LYS:HA	2:B:84:LYS:HD3	1.90	0.41
1:A:1057:LEU:HD23	1:A:1057:LEU:HA	1.92	0.41
2:B:65:ASP:O	2:B:71:GLY:HA3	2.20	0.41
2:B:159:PHE:CZ	2:B:182:GLU:HB2	2.56	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	301/303 (99%)	291 (97%)	10 (3%)	0	100	100
2	B	287/310 (93%)	276 (96%)	10 (4%)	1 (0%)	41	55
All	All	588/613 (96%)	567 (96%)	20 (3%)	1 (0%)	47	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	128	ASP

5.3.2 Protein sidechains (i)

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	256/257 (100%)	250 (98%)	6 (2%)	50	70
2	B	260/279 (93%)	257 (99%)	3 (1%)	71	85
All	All	516/536 (96%)	507 (98%)	9 (2%)	60	78

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

Mol	Chain	Res	Type
1	A	901	THR
1	A	928	SER
1	A	934	VAL
1	A	944	THR
1	A	959	CYS

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Mol	Chain	Res	Type
1	A	1083	THR
2	B	43	THR
2	B	128	ASP
2	B	263	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	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)

1 ligand is 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	$\#|Z| > 2$
3	GOL	A	1301	-	5,5,5	0.68	0	5,5,5	1.21	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	A	1301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	GOL	O1-C1-C2-C3
3	A	1301	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	303/303 (100%)	0.33	21 (6%)	16	15	29, 40, 56, 86	0
2	B	291/310 (93%)	0.43	27 (9%)	8	8	31, 48, 70, 84	0
All	All	594/613 (96%)	0.38	48 (8%)	12	11	29, 43, 66, 86	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	244	VAL	6.2
1	A	975	VAL	5.5
1	A	1060	GLY	4.8
2	B	241	TYR	4.6
1	A	957	THR	4.3
2	B	170	VAL	3.8
1	A	958	PRO	3.7
1	A	954	ILE	3.6
1	A	955	PRO	3.6
2	B	304	ARG	3.5
1	A	1022	LEU	3.5
1	A	946	ILE	3.5
1	A	956	SER	3.2
1	A	912	ALA	3.1
1	A	1059	GLU	3.1
1	A	952	THR	3.1
2	B	94	LYS	3.0
2	B	166	ILE	2.9
2	B	281	LYS	2.9
2	B	140	LEU	2.8
1	A	978	ASP	2.8
2	B	284	HIS	2.7
2	B	104	TYR	2.7
2	B	245	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	141	LEU	2.6
2	B	307	ASP	2.5
2	B	240	ASP	2.5
2	B	30	VAL	2.4
2	B	301	GLU	2.4
1	A	976	SER	2.4
1	A	953	TYR	2.3
1	A	1058	LYS	2.3
2	B	306	TYR	2.3
2	B	92	LEU	2.2
2	B	96	LYS	2.2
2	B	256	THR	2.2
2	B	280	VAL	2.2
2	B	250	ALA	2.2
1	A	943	PHE	2.1
1	A	1021	THR	2.1
2	B	243	SER	2.1
1	A	959	CYS	2.1
2	B	199	TYR	2.1
2	B	41	LYS	2.1
2	B	97	GLN	2.1
1	A	1162	PRO	2.0
2	B	25	TYR	2.0
1	A	899	MET	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)

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	A	1301	6/6	0.96	0.10	36,43,46,51	0

6.5 Other polymers (i)

There are no such residues in this entry.