



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:12 AM UTC

PDB ID : 4RLQ / pdb_00004rlq
Title : Crystal structure of a benzoate coenzyme A ligase with o-Toluic acid
Authors : Strom, S.; Nosrati, M.; Thornburg, C.; Walker, K.D.; Geiger, J.H.
Deposited on : 2014-10-17
Resolution : 1.63 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

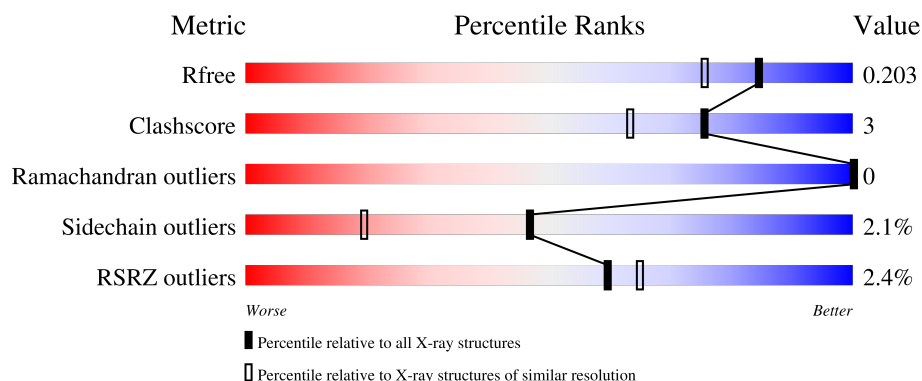
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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 $\leq 5\%$. 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	519	2% 94% 6%
1	B	519	3% 90% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8591 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.

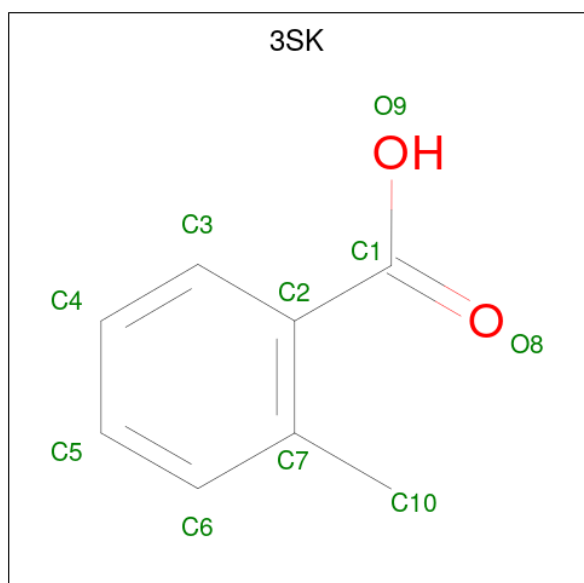
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	4	0
			3960	2534	685	731	10			
1	B	519	Total	C	N	O	S	0	4	0
			3981	2547	685	739	10			

There are 6 discrepancies between the modelled and reference sequences:

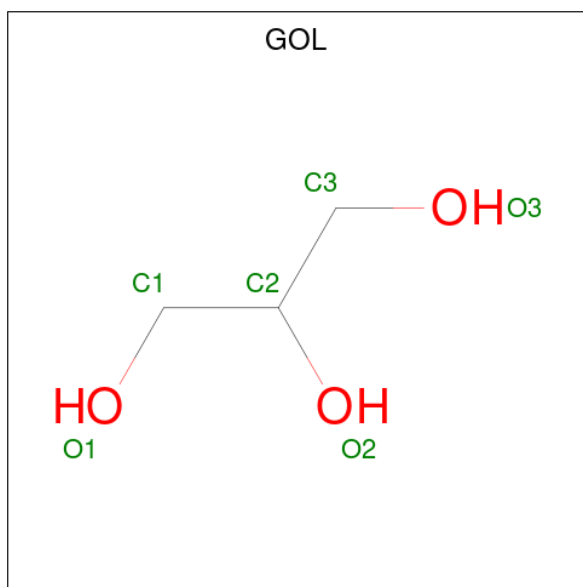
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0
B	524	GLY	-	expression tag	UNP Q93TK0

- Molecule 2 is 2-methylbenzoic acid (CCD ID: 3SK) (formula: C₈H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	8	2		
2	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

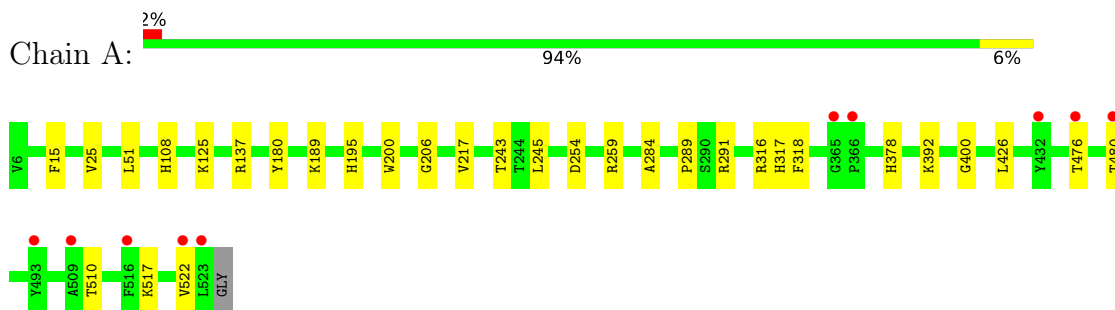
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	301	Total 301	O 301	0	0
4	B	275	Total 275	O 275	0	0

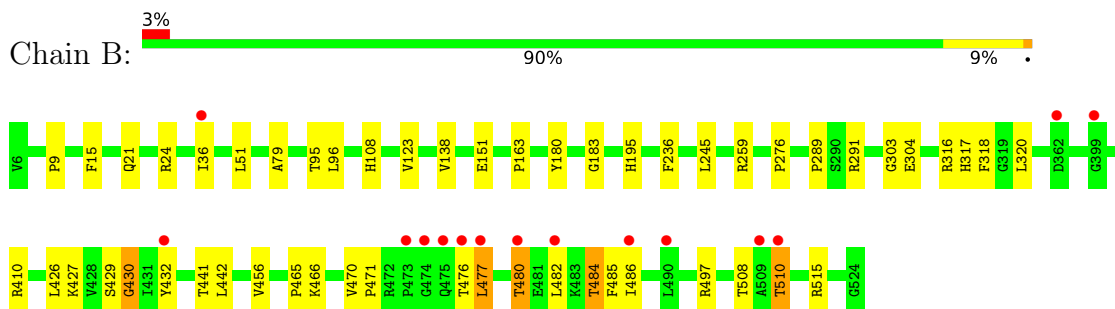
3 Residue-property plots

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: Benzoate-coenzyme A ligase



- Molecule 1: Benzoate-coenzyme A ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.66Å 94.81Å 95.35Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	33.04 – 1.63 33.04 – 1.63	Depositor EDS
% Data completeness (in resolution range)	96.9 (33.04-1.63) 96.9 (33.04-1.63)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.158 , 0.193 0.170 , 0.203	Depositor DCC
R_{free} test set	6135 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8591	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 4.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3SK, 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	1.24	4/4071 (0.1%)	1.11	1/5552 (0.0%)
1	B	1.27	6/4086 (0.1%)	1.12	3/5575 (0.1%)
All	All	1.26	10/8157 (0.1%)	1.11	4/11127 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	PRO	CA-C	-6.33	1.44	1.52
1	A	316	ARG	N-CA	6.16	1.53	1.46
1	B	183	GLY	N-CA	5.77	1.50	1.44
1	A	284	ALA	N-CA	5.76	1.53	1.46
1	B	470	VAL	N-CA	5.65	1.50	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	THR	N-CA-C	5.83	117.44	111.14
1	B	9	PRO	O-C-N	5.20	123.70	121.31
1	A	254	ASP	N-CA-C	5.04	116.78	111.28
1	B	485	PHE	N-CA-C	-5.04	105.79	111.28

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	3960	0	3901	13	1
1	B	3981	0	3912	34	1
2	A	10	0	7	0	0
2	B	10	0	7	0	0
3	A	12	0	16	0	0
3	B	42	0	56	3	0
4	A	301	0	0	2	0
4	B	275	0	0	4	0
All	All	8591	0	7899	47	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 3.

The worst 5 of 47 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:15:PHE:H	1:B:195:HIS:HD2	1.18	0.87
1:A:15:PHE:H	1:A:195:HIS:HD2	1.19	0.87
1:B:429:SER:OG	1:B:429:SER:O	1.97	0.78
1:A:245:LEU:HD21	1:A:259:ARG:HG2	1.66	0.76
1:A:25:VAL:HG13	4:A:1269:HOH:O	1.86	0.73

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)
1:A:291:ARG:NH2	1:B:316:ARG:O[1_554]	2.11	0.09

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	520/519 (100%)	505 (97%)	15 (3%)	0	100	100
1	B	521/519 (100%)	510 (98%)	11 (2%)	0	100	100
All	All	1041/1038 (100%)	1015 (98%)	26 (2%)	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	407/412 (99%)	400 (98%)	7 (2%)	53	27
1	B	409/412 (99%)	399 (98%)	10 (2%)	43	15
All	All	816/824 (99%)	799 (98%)	17 (2%)	47	19

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	482	LEU
1	B	510	THR
1	B	36	ILE
1	B	320	LEU
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	HIS
1	B	195	HIS
1	B	460	HIS
1	B	317	HIS
1	A	378	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
3	GOL	B	1006	-	5,5,5	0.34	0	5,5,5	0.67	0
3	GOL	B	1001	-	5,5,5	0.77	0	5,5,5	1.44	2 (40%)
3	GOL	B	1002	-	5,5,5	0.53	0	5,5,5	0.52	0
3	GOL	B	1004	-	5,5,5	0.69	0	5,5,5	1.69	1 (20%)
3	GOL	B	1007	-	5,5,5	0.57	0	5,5,5	1.01	0
3	GOL	A	1001	-	5,5,5	0.96	0	5,5,5	0.72	0
3	GOL	B	1005	-	5,5,5	0.80	0	5,5,5	2.31	2 (40%)
3	GOL	B	1003	-	5,5,5	0.45	0	5,5,5	0.86	0
3	GOL	A	1002	-	5,5,5	0.70	0	5,5,5	0.86	0
2	3SK	B	1000	-	10,10,10	1.00	1 (10%)	13,13,13	1.21	2 (15%)
2	3SK	A	1000	-	10,10,10	0.74	0	13,13,13	1.14	1 (7%)

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	B	1006	-	-	2/4/4/4	-
3	GOL	B	1001	-	-	0/4/4/4	-
3	GOL	B	1002	-	-	0/4/4/4	-
3	GOL	B	1004	-	-	4/4/4/4	-
3	GOL	B	1007	-	-	0/4/4/4	-
3	GOL	A	1001	-	-	0/4/4/4	-
3	GOL	B	1005	-	-	2/4/4/4	-
3	GOL	B	1003	-	-	1/4/4/4	-
3	GOL	A	1002	-	-	0/4/4/4	-
2	3SK	B	1000	-	-	2/4/4/4	0/1/1/1
2	3SK	A	1000	-	-	2/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	3SK	C4-C3	2.03	1.42	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1005	GOL	O1-C1-C2	3.64	126.78	110.38
2	B	1000	3SK	C5-C4-C3	-3.32	116.14	120.24
3	B	1004	GOL	O3-C3-C2	-2.71	98.18	110.38
3	B	1005	GOL	C3-C2-C1	-2.46	102.76	111.80
2	A	1000	3SK	C7-C2-C1	-2.46	119.38	122.47

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1004	GOL	C1-C2-C3-O3
3	B	1005	GOL	C1-C2-C3-O3
3	B	1006	GOL	C1-C2-C3-O3
3	B	1004	GOL	O2-C2-C3-O3
3	B	1005	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1005	GOL	3	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 [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	518/519 (99%)	-0.21	10 (1%) 66 72	6, 19, 37, 58	4 (0%)
1	B	519/519 (100%)	-0.09	15 (2%) 53 59	7, 20, 37, 52	6 (1%)
All	All	1037/1038 (99%)	-0.15	25 (2%) 59 65	6, 19, 37, 58	10 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	GLY	8.5
1	B	476	THR	4.3
1	A	476	THR	3.7
1	B	475	GLN	3.4
1	A	523	LEU	3.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	GOL	B	1007	6/6	0.82	0.13	33,35,37,38	0
3	GOL	B	1005	6/6	0.83	0.14	22,31,38,40	0
3	GOL	B	1003	6/6	0.91	0.12	26,39,46,53	0
3	GOL	A	1002	6/6	0.92	0.10	24,30,38,45	0
3	GOL	B	1004	6/6	0.92	0.11	18,34,39,42	0
3	GOL	B	1001	6/6	0.93	0.09	23,27,31,38	0
3	GOL	A	1001	6/6	0.94	0.09	17,24,25,32	0
3	GOL	B	1006	6/6	0.95	0.08	24,31,41,53	0
3	GOL	B	1002	6/6	0.95	0.09	17,19,20,23	0
2	3SK	A	1000	10/10	0.96	0.06	11,12,13,14	0
2	3SK	B	1000	10/10	0.97	0.05	10,11,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.