



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:26 AM GMT

PDB ID : 2AGV
Title : Crystal structure of the SR CA₂⁺-ATPASE with BHQ and TG
Authors : Toyoshima, C.; Obara, K.; Norimatsu, Y.
Deposited on : 2005-07-27
Resolution : 2.40 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

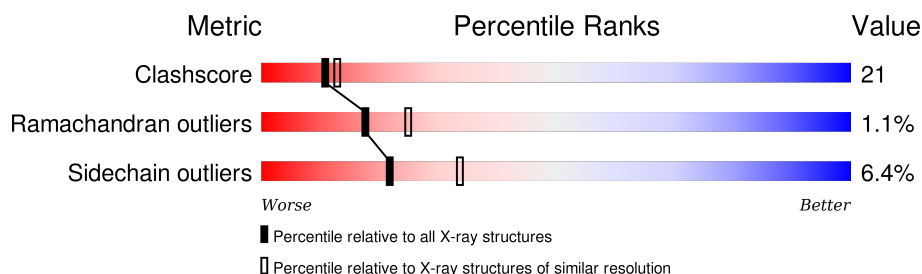
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	 60% 36% .
1	B	994	 61% 35% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15830 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

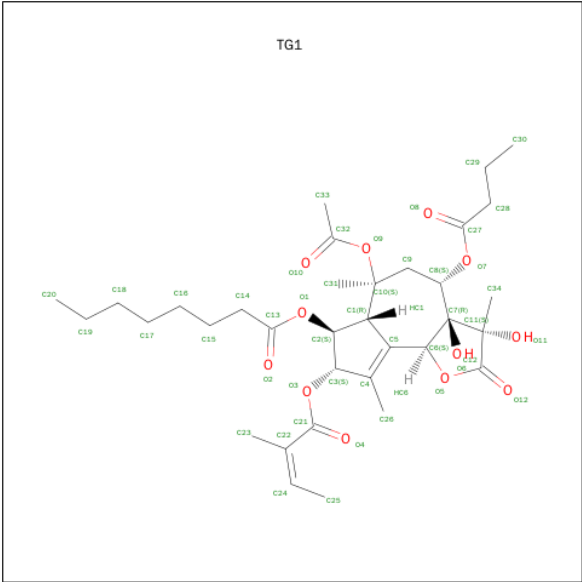
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191
B	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

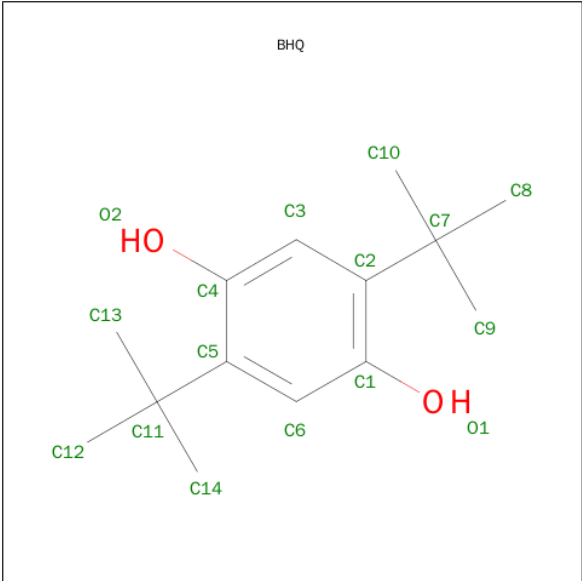
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BAPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C₃₄H₅₀O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			46	34	12		
3	B	1	Total	C	O	0	0
			46	34	12		

- Molecule 4 is 2,5-DITERT-BUTYLBENZENE-1,4-DIOL (three-letter code: BHQ) (formula: C₁₄H₂₂O₂).



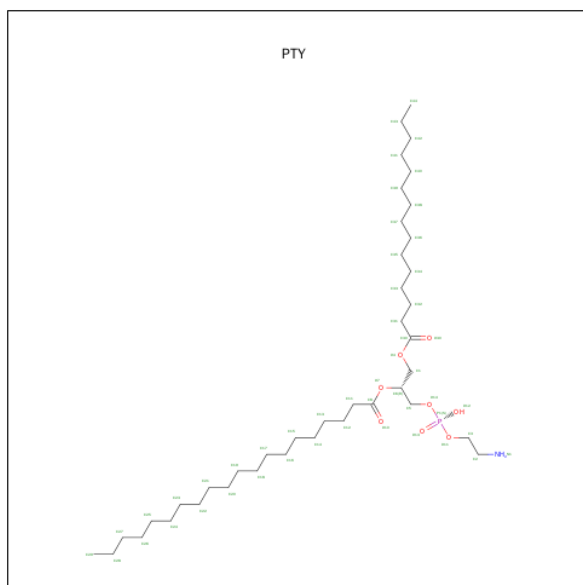
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	B	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	B	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	B	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 6 is water.

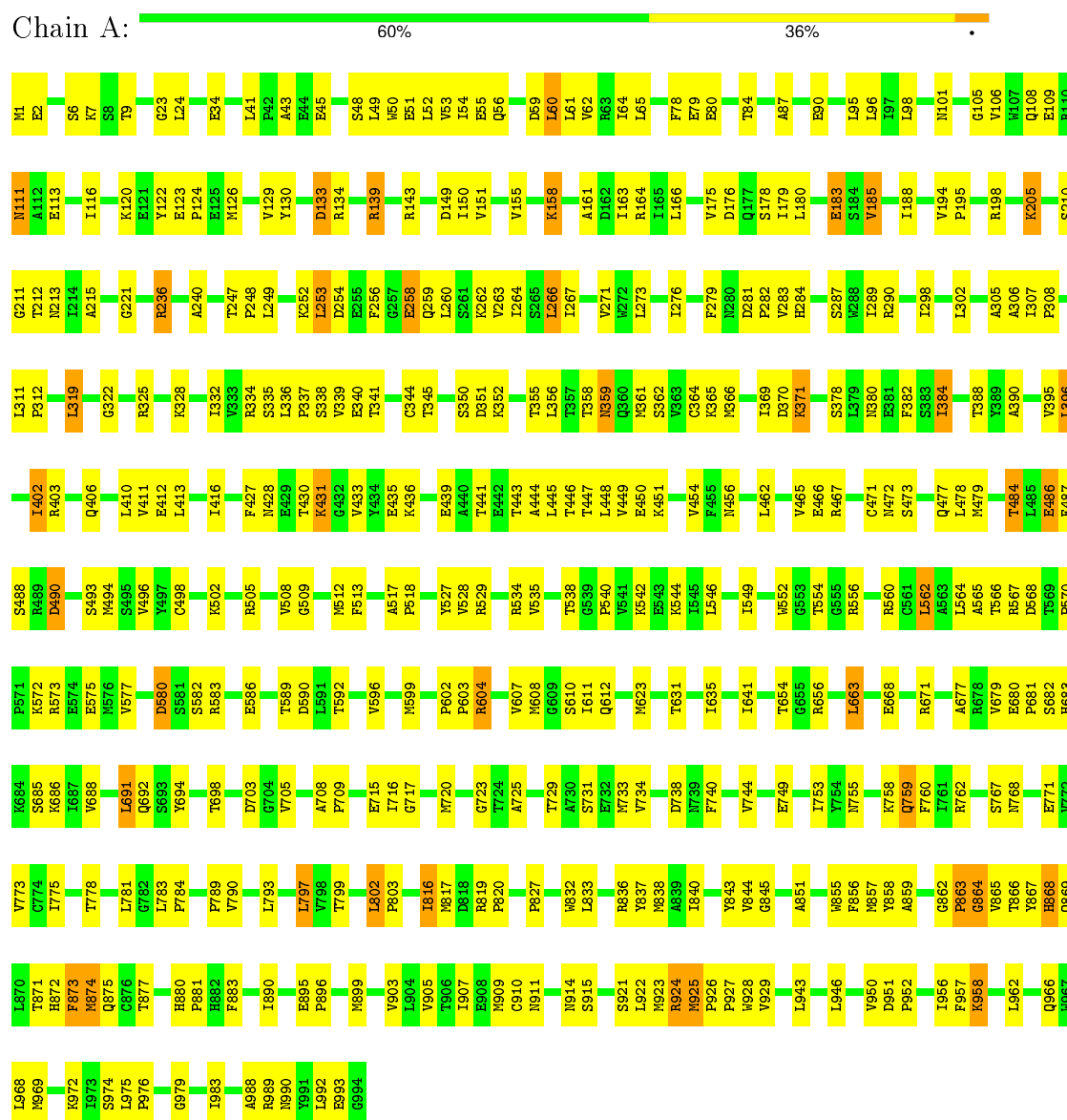
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	124	Total	O	0	0
			124	124		
6	B	124	Total	O	0	0
			124	124		

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 errors 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.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Response	Percentage
Yes	61%
No	35%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	71.39 Å 71.39 Å 591.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (14.98-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15830	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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: BHQ, NA, TG1, PTY

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	0.42	0/7812	0.64	1/10592 (0.0%)
1	B	0.41	0/7812	0.64	2/10592 (0.0%)
All	All	0.42	0/15624	0.64	3/21184 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	505	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	512	MET	CG-SD-CE	5.91	109.65	100.20

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	7671	0	7764	331	0
1	B	7671	0	7764	330	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	46	0	50	3	0
3	B	46	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	0	22	1	0
4	B	16	0	22	1	0
5	A	57	0	33	2	0
5	B	57	0	33	2	0
6	A	124	0	0	7	0
6	B	124	0	0	7	0
All	All	15830	0	15738	660	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 21.

The worst 5 of 660 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:567:ARG:HD3	1:B:570:PRO:HA	1.42	1.01
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.42	1.01
1:B:865:VAL:HB	1:B:868:HIS:HB2	1.41	0.99
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.42	0.98
1:B:126:MET:HE2	1:B:139:ARG:HD3	1.49	0.94

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	992/994 (100%)	920 (93%)	61 (6%)	11 (1%)	17	25
1	B	992/994 (100%)	921 (93%)	60 (6%)	11 (1%)	17	25
All	All	1984/1988 (100%)	1841 (93%)	121 (6%)	22 (1%)	17	25

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PHE
1	B	883	PHE
1	A	185	VAL
1	A	663	LEU
1	A	866	THR

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	840/840 (100%)	785 (94%)	55 (6%)	21	33
1	B	840/840 (100%)	788 (94%)	52 (6%)	23	35
All	All	1680/1680 (100%)	1573 (94%)	107 (6%)	22	34

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	816	ILE
1	B	96	LEU
1	B	760	PHE
1	A	838	MET
1	A	968	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	919	ASN
1	B	108	GLN
1	B	875	GLN
1	A	880	HIS
1	A	914	ASN

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](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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$
3	TG1	A	1003	-	43,48,48	1.41	8 (18%)	42,72,72	1.66	8 (19%)
4	BHQ	A	1004	-	16,16,16	1.91	5 (31%)	26,26,26	1.20	2 (7%)
5	PTY	A	1011	-	17,18,49	1.04	2 (11%)	18,23,54	1.55	3 (16%)
5	PTY	A	1012	-	17,18,49	1.49	3 (17%)	18,23,54	1.65	1 (5%)
5	PTY	A	1013	-	17,18,49	1.19	3 (17%)	18,23,54	1.31	2 (11%)
3	TG1	B	1103	-	43,48,48	1.44	8 (18%)	42,72,72	1.67	8 (19%)
4	BHQ	B	1104	-	16,16,16	1.93	6 (37%)	26,26,26	1.21	2 (7%)
5	PTY	B	1111	-	17,18,49	1.07	3 (17%)	18,23,54	1.53	3 (16%)
5	PTY	B	1112	-	17,18,49	1.49	3 (17%)	18,23,54	1.64	2 (11%)
5	PTY	B	1113	-	17,18,49	1.19	3 (17%)	18,23,54	1.31	2 (11%)

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	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
4	BHQ	A	1004	-	-	0/12/12/12	0/1/1/1
5	PTY	A	1011	-	-	0/20/20/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
5	PTY	A	1013	-	-	0/20/20/53	0/0/0/0
3	TG1	B	1103	-	-	0/33/99/99	0/3/3/3
4	BHQ	B	1104	-	-	0/12/12/12	0/1/1/1
5	PTY	B	1111	-	-	0/20/20/53	0/0/0/0
5	PTY	B	1112	-	-	0/20/20/53	0/0/0/0
5	PTY	B	1113	-	-	0/20/20/53	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1103	TG1	C33-C32	-2.08	1.42	1.49
5	B	1113	PTY	P1-O13	2.03	1.58	1.51
5	B	1111	PTY	C5-C6	2.04	1.56	1.50
5	A	1013	PTY	P1-O13	2.05	1.58	1.51
5	A	1011	PTY	C1-C6	2.07	1.56	1.50

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	TG1	O12-C12-C11	-3.37	125.16	128.26
3	B	1103	TG1	O5-C6-C7	-3.10	101.34	104.08
3	A	1003	TG1	O5-C6-C7	-3.02	101.41	104.08
3	B	1103	TG1	O12-C12-C11	-2.99	125.51	128.26
5	A	1011	PTY	C5-C6-C1	-2.50	106.23	112.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	TG1	3	0
4	A	1004	BHQ	1	0
5	A	1012	PTY	2	0
3	B	1103	TG1	3	0
4	B	1104	BHQ	1	0
5	B	1112	PTY	2	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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.