



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:33 PM UTC

PDB ID : 9GPB / pdb_00009gpb
Title : THE ALLOSTERIC TRANSITION OF GLYCOGEN PHOSPHORYLASE
Authors : Barford, D.; Johnson, L.N.
Deposited on : 1990-12-17
Resolution : 2.90 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

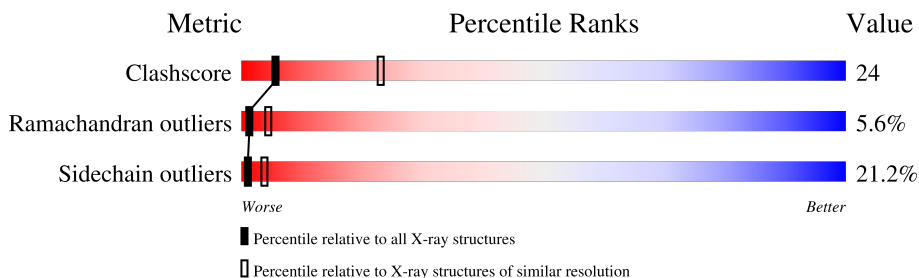
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	30% 39% 22% 7% .
1	B	842	32% 41% 19% 6% .
1	C	842	32% 39% 22% 5% .
1	D	842	24% 41% 26% 8% .

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
2	SO4	C	900	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26873 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	823	6703	4272	1185	1215	1	30	0	0	0
1	B	823	6703	4272	1185	1215	1	30	0	0	0
1	C	823	6703	4271	1185	1216	1	30	0	0	0
1	D	823	6704	4272	1185	1216	1	30	0	0	0

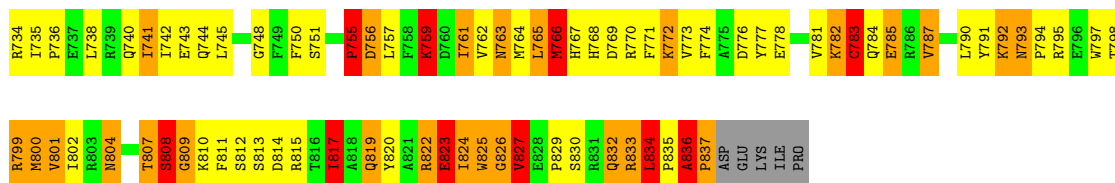
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

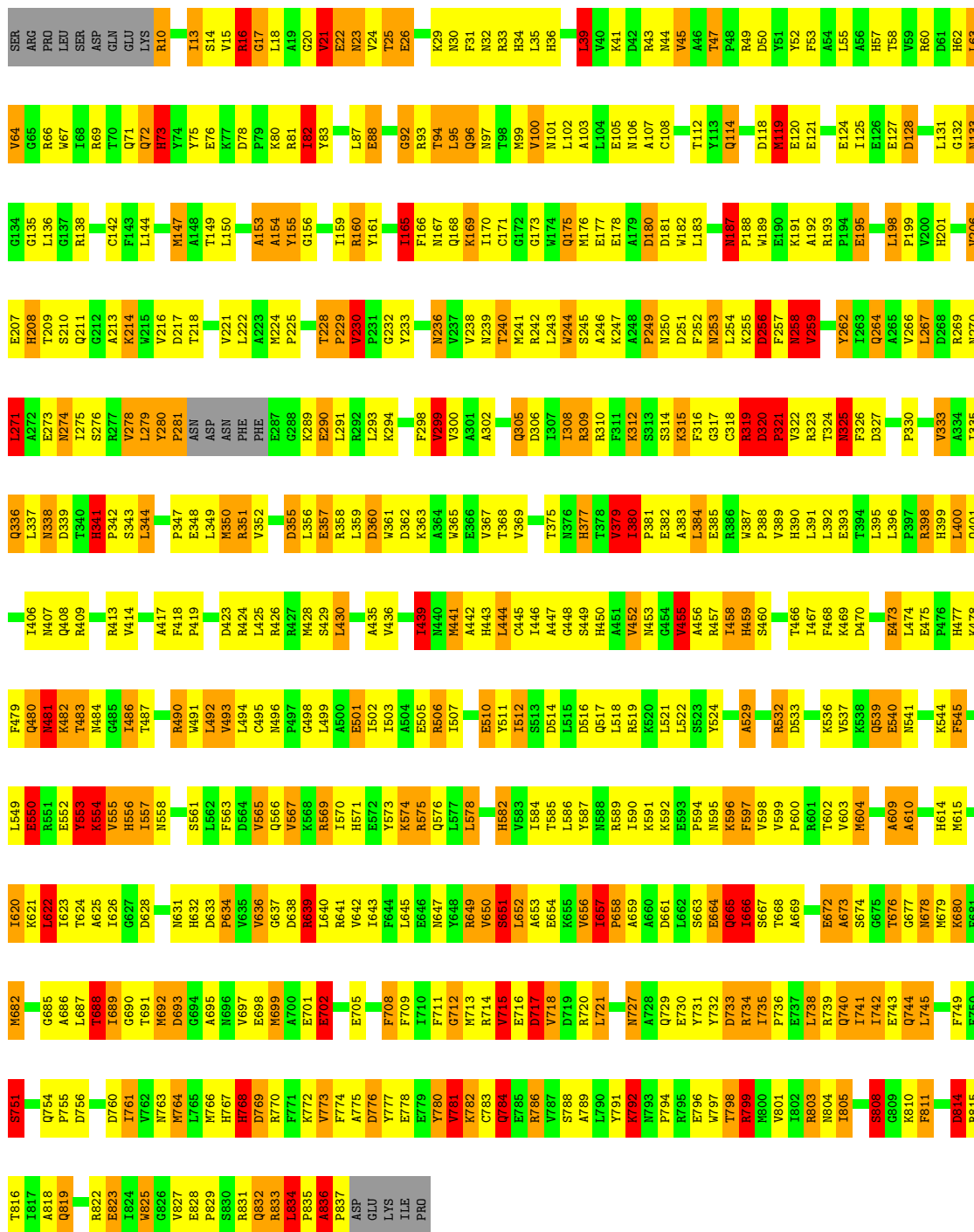
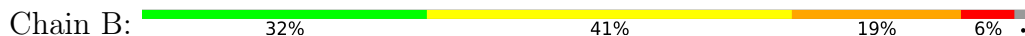
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		



● Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26873	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: SO4, LLP

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	1.26	36/6827 (0.5%)	2.34	427/9236 (4.6%)
1	B	1.27	41/6827 (0.6%)	2.33	384/9236 (4.2%)
1	C	1.28	48/6827 (0.7%)	2.34	396/9237 (4.3%)
1	D	1.26	41/6829 (0.6%)	2.34	426/9240 (4.6%)
All	All	1.27	166/27310 (0.6%)	2.34	1633/36949 (4.4%)

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	A	0	9
1	B	0	8
1	C	0	10
1	D	0	6
All	All	0	33

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	VAL	CA-CB	15.48	1.67	1.54
1	C	18	LEU	N-CA	-11.57	1.32	1.46
1	C	565	VAL	CA-CB	9.31	1.66	1.54
1	C	17	GLY	C-N	-8.88	1.21	1.33
1	C	406	ILE	CA-CB	8.77	1.64	1.54

The worst 5 of 1633 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	GLY	O-C-N	26.32	153.18	122.64
1	B	266	VAL	N-CA-C	-15.28	96.17	110.53
1	A	575	ARG	N-CA-C	15.16	132.75	111.52
1	A	128	ASP	CA-CB-CG	14.59	127.19	112.60
1	D	533	ASP	CA-CB-CG	13.61	126.21	112.60

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	256	ASP	Mainchain
1	A	51	TYR	Sidechain

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	6703	0	6658	316	0
1	B	6703	0	6659	296	0
1	C	6703	0	6653	297	0
1	D	6704	0	6659	397	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	4	0
2	D	15	0	0	2	0
All	All	26873	0	26629	1259	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 24.

The worst 5 of 1259 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:C:37:PHE:CE2	1:D:18:LEU:HB3	1.46	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PHE:HE2	1:D:18:LEU:CB	1.32	1.42
1:C:37:PHE:CE2	1:D:18:LEU:CB	2.06	1.32
1:C:15:VAL:O	1:C:17:GLY:N	1.79	1.14
2:C:900:SO4:O3	1:D:43:ARG:NH2	1.79	1.13

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	816/842 (97%)	651 (80%)	112 (14%)	53 (6%)	1	3
1	B	816/842 (97%)	669 (82%)	107 (13%)	40 (5%)	1	6
1	C	818/842 (97%)	678 (83%)	102 (12%)	38 (5%)	2	7
1	D	818/842 (97%)	643 (79%)	124 (15%)	51 (6%)	1	3
All	All	3268/3368 (97%)	2641 (81%)	445 (14%)	182 (6%)	1	4

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	21	VAL
1	A	152	LEU
1	A	166	PHE
1	A	236	ASN

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	711/730 (97%)	578 (81%)	133 (19%)	1	5
1	B	711/730 (97%)	565 (80%)	146 (20%)	1	4
1	C	710/730 (97%)	575 (81%)	135 (19%)	1	5
1	D	711/730 (97%)	522 (73%)	189 (27%)	0	1
All	All	2843/2920 (97%)	2240 (79%)	603 (21%)	1	4

5 of 603 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	257	PHE
1	D	709	PHE
1	D	305	GLN
1	D	255	LYS
1	D	526	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	459	HIS
1	D	167	ASN
1	C	566	GLN
1	C	784	GLN
1	D	264	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	LLP	B	680	1	23,24,25	1.49	5 (21%)	25,32,34	1.47	3 (12%)
1	LLP	D	680	1	23,24,25	1.84	5 (21%)	25,32,34	1.34	2 (8%)
1	LLP	C	680	1	23,24,25	1.50	3 (13%)	25,32,34	2.12	2 (8%)
1	LLP	A	680	1	23,24,25	1.61	4 (17%)	25,32,34	1.21	5 (20%)

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
1	LLP	B	680	1	-	2/16/17/19	0/1/1/1
1	LLP	D	680	1	-	8/16/17/19	0/1/1/1
1	LLP	C	680	1	-	0/16/17/19	0/1/1/1
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	LLP	C3-C2	-5.61	1.35	1.41
1	A	680	LLP	C3-C2	-4.68	1.36	1.41
1	D	680	LLP	C4-C4'	3.43	1.53	1.46
1	A	680	LLP	C4-C5	-3.42	1.37	1.42
1	C	680	LLP	C3-C2	-3.30	1.37	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	LLP	OP4-C5'-C5	8.90	126.03	109.36
1	B	680	LLP	OP4-C5'-C5	5.13	118.98	109.36
1	D	680	LLP	OP4-C5'-C5	4.68	118.14	109.36
1	C	680	LLP	CD-CE-NZ	-3.23	102.28	110.83
1	A	680	LLP	CG-CD-CE	-2.55	104.49	113.38

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C4-C5-C5'-OP4
1	D	680	LLP	C5'-OP4-P-OP1
1	D	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C5'-OP4-P-OP3

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	680	LLP	2	0
1	D	680	LLP	4	0
1	C	680	LLP	2	0
1	A	680	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
2	SO4	C	902	-	4,4,4	0.29	0	6,6,6	0.67	0
2	SO4	A	901	-	4,4,4	0.58	0	6,6,6	0.37	0
2	SO4	D	902	-	4,4,4	0.45	0	6,6,6	0.30	0
2	SO4	B	901	-	4,4,4	0.69	0	6,6,6	0.25	0
2	SO4	C	901	-	4,4,4	0.40	0	6,6,6	0.32	0
2	SO4	D	901	-	4,4,4	0.61	0	6,6,6	0.52	0
2	SO4	C	900	-	4,4,4	0.63	0	6,6,6	0.33	0
2	SO4	B	902	-	4,4,4	0.28	0	6,6,6	0.51	0
2	SO4	D	900	-	4,4,4	0.54	0	6,6,6	0.41	0
2	SO4	B	900	-	4,4,4	0.35	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	900	-	4,4,4	0.31	0	6,6,6	0.47	0
2	SO4	A	902	-	4,4,4	0.53	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	1	0
2	D	902	SO4	1	0
2	C	900	SO4	4	0
2	B	902	SO4	1	0
2	D	900	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	18:LEU	C	19:ALA	N	22.68
1	B	18:LEU	C	19:ALA	N	19.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.