



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 01:21 PM EDT

PDB ID : 2Z9V
Title : Crystal structure of pyridoxamine-pyruvate aminotransferase complexed with pyridoxamine
Authors : Yoshikane, Y.; Yokochi, N.; Yamasaki, M.; Mizutani, K.; Ohnishi, K.; Mikami, B.; Hayashi, H.; Yagi, T.
Deposited on : 2007-09-26
Resolution : 1.70 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

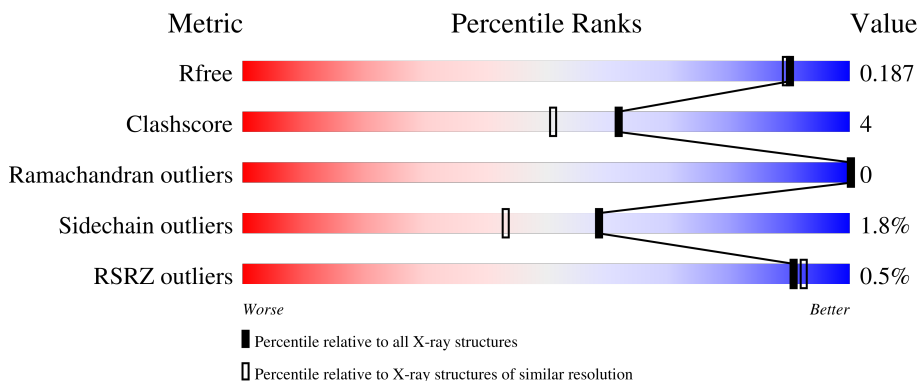
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

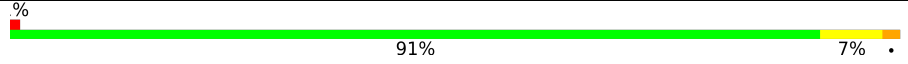
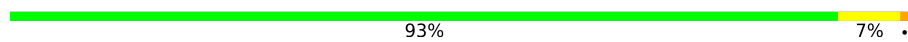
The reported resolution of this entry is 1.70 Å.

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	392	 91% 7% .
1	B	392	 93% 7% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6803 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 Aspartate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	2991	1904	515	557	15	0	12	0
1	B	392	2986	1904	511	556	15	0	10	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



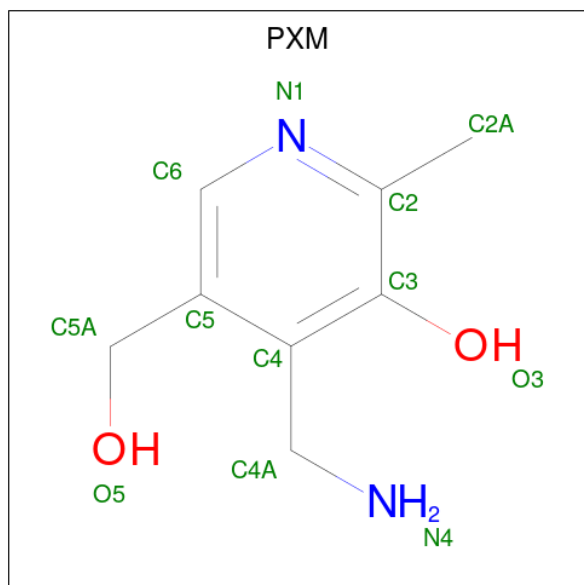
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 4-(AMINOMETHYL)-5-(HYDROXYMETHYL)-2-METHYLPYRIDIN-3-OL (three-letter code: PXM) (formula: C₈H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	8	2	2	0	0
3	B	1	12	8	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

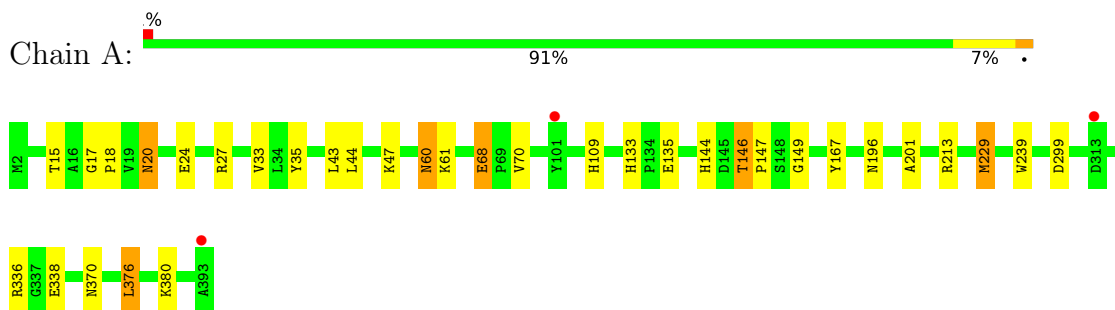
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	377	Total O 377 377	0	0
5	B	376	Total O 376 376	0	0

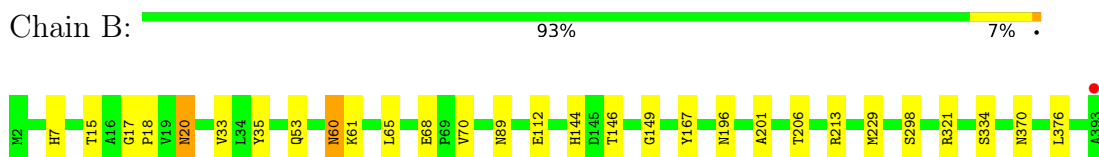
3 Residue-property plots [i](#)

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: Aspartate aminotransferase



- Molecule 1: Aspartate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.63Å 68.63Å 312.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 1.70 48.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (14.94-1.70) 98.4 (48.53-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.03 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.156 , 0.186 0.156 , 0.187	Depositor DCC
R_{free} test set	4106 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtrriage
Anisotropy	0.568	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PXM, 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	0.48	0/3094	0.59	0/4215
1	B	0.49	0/3080	0.61	0/4198
All	All	0.48	0/6174	0.60	0/8413

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	2991	0	3027	37	0
1	B	2986	0	3019	25	0
2	A	10	0	0	1	0
2	B	15	0	0	1	0
3	A	12	0	11	1	0
3	B	12	0	12	0	0
4	A	12	0	16	3	0
4	B	12	0	16	1	0
5	A	377	0	0	6	0
5	B	376	0	0	1	0
All	All	6803	0	6101	53	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 (53) 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:299:ASP:H	4:A:953:GOL:H32	1.11	1.08
1:A:299:ASP:N	4:A:953:GOL:H32	1.94	0.81
1:B:370:ASN:HD21	1:B:376:LEU:H	1.25	0.81
1:A:338[A]:GLU:HG2	5:A:1766:HOH:O	1.80	0.81
1:A:370:ASN:HD21	1:A:376:LEU:H	1.30	0.78
1:A:43:LEU:HG	1:A:47[A]:LYS:HE2	1.66	0.78
1:A:44:LEU:HA	1:A:47[A]:LYS:HE3	1.69	0.74
1:A:144:HIS:HE1	1:A:149:GLY:HA2	1.56	0.69
1:B:144:HIS:HE1	1:B:149:GLY:HA2	1.57	0.68
1:A:70:VAL:HG23	1:B:229:MET:CE	2.26	0.64
1:A:33:VAL:H	1:B:20:ASN:ND2	1.98	0.61
1:A:70:VAL:HG23	1:B:229:MET:HE3	1.81	0.61
1:A:299:ASP:H	4:A:953:GOL:C3	2.02	0.60
1:A:20:ASN:ND2	1:B:33:VAL:H	2.00	0.60
1:A:229:MET:HA	1:A:229:MET:HE2	1.82	0.60
1:B:167:TYR:CE2	1:B:213:ARG:HG2	2.38	0.59
1:B:370:ASN:ND2	1:B:376:LEU:H	2.00	0.57
1:A:336[B]:ARG:HD2	2:A:1601:SO4:O3	2.07	0.55
1:B:298:SER:HB2	4:B:954:GOL:H2	1.88	0.54
1:A:147:PRO:HG3	1:A:336[B]:ARG:HD3	1.89	0.54
1:A:213[B]:ARG:HD3	5:A:1882:HOH:O	2.07	0.54
1:A:370:ASN:ND2	1:A:376:LEU:H	2.03	0.50
1:A:133:HIS:HD2	1:A:135:GLU:OE1	1.95	0.49
1:A:370:ASN:HD21	1:A:376:LEU:HB2	1.78	0.49
1:A:68[B]:GLU:CD	1:A:70:VAL:HG22	2.33	0.49
1:A:196:ASN:HA	1:A:201:ALA:O	2.14	0.48
1:A:229:MET:HE1	1:B:70:VAL:HG23	1.96	0.48
1:B:7:HIS:ND1	2:B:2602:SO4:O1	2.47	0.47
1:B:17:GLY:HA2	1:B:18:PRO:C	2.35	0.47
1:A:229:MET:HE3	5:B:2656:HOH:O	2.16	0.46
1:A:43:LEU:HD11	1:A:47[B]:LYS:HE2	1.98	0.46
1:A:15:THR:HG21	1:B:35:TYR:CG	2.51	0.45
1:B:321:ARG:CZ	1:B:334:SER:HB3	2.47	0.45
1:B:60:ASN:H	1:B:60:ASN:HD22	1.65	0.44
1:A:167:TYR:CE2	1:A:213[B]:ARG:HG2	2.52	0.44
1:A:229:MET:HE2	1:A:229:MET:CA	2.46	0.44
5:A:1688:HOH:O	1:B:229:MET:HE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:HE1	5:A:1842:HOH:O	2.01	0.44
5:A:1688:HOH:O	1:B:229:MET:CE	2.65	0.44
1:A:70:VAL:HG23	1:B:229:MET:HE1	1.96	0.44
1:A:35:TYR:CG	1:B:15:THR:HG21	2.53	0.43
1:A:47[B]:LYS:HD2	5:A:1867:HOH:O	2.18	0.43
1:B:89:ASN:O	1:B:112[B]:GLU:HG3	2.19	0.43
1:A:146:THR:OG1	3:A:1501:PXM:H2A1	2.18	0.42
1:A:229:MET:CE	1:B:70:VAL:HG23	2.49	0.42
1:B:196:ASN:HA	1:B:201:ALA:O	2.20	0.42
1:B:196:ASN:H	1:B:196:ASN:ND2	2.17	0.42
1:A:60:ASN:H	1:A:60:ASN:HD22	1.68	0.41
1:B:53:GLN:HE22	1:B:61:LYS:HE2	1.85	0.41
1:A:24:GLU:HG3	1:A:27:ARG:HH22	1.85	0.41
1:A:17:GLY:HA2	1:A:18:PRO:C	2.41	0.41
1:A:61:LYS:HD3	1:A:239:TRP:CD2	2.56	0.40
1:B:65:LEU:HB2	1:B:206:THR:HB	2.03	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	402/392 (103%)	395 (98%)	7 (2%)	0	100	100
1	B	400/392 (102%)	394 (98%)	6 (2%)	0	100	100
All	All	802/784 (102%)	789 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/299 (104%)	303 (97%)	8 (3%)	46	28
1	B	309/299 (103%)	304 (98%)	5 (2%)	62	48
All	All	620/598 (104%)	607 (98%)	13 (2%)	59	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	60	ASN
1	A	68[A]	GLU
1	A	68[B]	GLU
1	A	146	THR
1	A	229	MET
1	A	376	LEU
1	A	380	LYS
1	B	20	ASN
1	B	60	ASN
1	B	68[A]	GLU
1	B	68[B]	GLU
1	B	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	53	GLN
1	A	60	ASN
1	A	89	ASN
1	A	109	HIS
1	A	124	GLN
1	A	133	HIS
1	A	144	HIS
1	A	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	ASN
1	A	322	GLN
1	A	354	GLN
1	A	370	ASN
1	B	20	ASN
1	B	53	GLN
1	B	60	ASN
1	B	89	ASN
1	B	124	GLN
1	B	144	HIS
1	B	196	ASN
1	B	237	ASN
1	B	255	ASN
1	B	322	GLN
1	B	370	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	GOL	A	953	-	5,5,5	0.40	0	5,5,5	0.40	0
4	GOL	A	955	-	5,5,5	0.38	0	5,5,5	0.22	0
2	SO4	A	1603	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	B	2602	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	B	2604	-	4,4,4	0.11	0	6,6,6	0.20	0
4	GOL	B	954	-	5,5,5	0.38	0	5,5,5	0.57	0
2	SO4	B	2601	-	4,4,4	0.29	0	6,6,6	0.56	0
3	PXM	B	2501	-	12,12,12	0.79	0	16,16,16	1.69	3 (18%)
4	GOL	B	956	-	5,5,5	0.36	0	5,5,5	0.23	0
2	SO4	A	1601	-	4,4,4	0.34	0	6,6,6	0.35	0
3	PXM	A	1501	-	12,12,12	0.88	1 (8%)	16,16,16	1.60	4 (25%)

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
4	GOL	A	953	-	-	2/4/4/4	-
4	GOL	A	955	-	-	4/4/4/4	-
4	GOL	B	954	-	-	3/4/4/4	-
4	GOL	B	956	-	-	4/4/4/4	-
3	PXM	B	2501	-	-	1/4/4/4	0/1/1/1
3	PXM	A	1501	-	-	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)
3	A	1501	PXM	C2A-C2	2.10	1.53	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2501	PXM	C6-C5-C4	4.44	121.26	118.12
3	A	1501	PXM	C6-C5-C4	3.29	120.45	118.12
3	A	1501	PXM	C5A-C5-C6	-2.78	114.85	119.37
3	B	2501	PXM	C5A-C5-C6	-2.26	115.69	119.37
3	B	2501	PXM	C5-C6-N1	-2.18	120.19	123.82
3	A	1501	PXM	C3-C4-C5	-2.11	116.69	118.72
3	A	1501	PXM	C5-C6-N1	-2.05	120.41	123.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	953	GOL	O1-C1-C2-C3
4	A	955	GOL	O1-C1-C2-C3
4	B	956	GOL	O1-C1-C2-O2
4	B	956	GOL	O1-C1-C2-C3
4	B	954	GOL	O1-C1-C2-O2
4	A	955	GOL	C1-C2-C3-O3
4	B	954	GOL	O1-C1-C2-C3
4	B	956	GOL	C1-C2-C3-O3
4	A	953	GOL	O1-C1-C2-O2
4	A	955	GOL	O1-C1-C2-O2
3	A	1501	PXM	C5-C4-C4A-N4
3	B	2501	PXM	C5-C4-C4A-N4
4	A	955	GOL	O2-C2-C3-O3
3	A	1501	PXM	C3-C4-C4A-N4
4	B	956	GOL	O2-C2-C3-O3
4	B	954	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	953	GOL	3	0
2	B	2602	SO4	1	0
4	B	954	GOL	1	0
2	A	1601	SO4	1	0
3	A	1501	PXM	1	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	392/392 (100%)	-0.42	3 (0%) 86 88	10, 13, 20, 29	0
1	B	392/392 (100%)	-0.55	1 (0%) 94 94	9, 12, 17, 28	0
All	All	784/784 (100%)	-0.48	4 (0%) 91 92	9, 12, 19, 29	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	ALA	5.7
1	B	393	ALA	4.8
1	A	101	TYR	2.5
1	A	313	ASP	2.4

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 monosaccharides 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
4	GOL	A	953	6/6	0.72	0.20	35,39,41,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	954	6/6	0.83	0.18	32,39,40,41	0
4	GOL	B	956	6/6	0.83	0.18	34,37,38,38	0
4	GOL	A	955	6/6	0.87	0.13	36,36,37,38	0
2	SO4	B	2602	5/5	0.88	0.19	46,46,48,48	0
3	PXM	A	1501	12/12	0.94	0.09	14,15,16,19	0
2	SO4	A	1601	5/5	0.96	0.11	22,24,26,27	0
2	SO4	A	1603	5/5	0.97	0.09	24,25,26,28	0
3	PXM	B	2501	12/12	0.97	0.07	10,13,15,16	0
2	SO4	B	2604	5/5	0.97	0.13	29,32,33,34	0
2	SO4	B	2601	5/5	0.98	0.09	18,20,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.