



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:17 AM UTC

PDB ID : 2ORD / pdb_00002ord
Title : Crystal structure of Acetylornithine aminotransferase (EC 2.6.1.11) (ACOAT) (TM1785) from *Thermotoga maritima* at 1.40 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-02-02
Resolution : 1.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

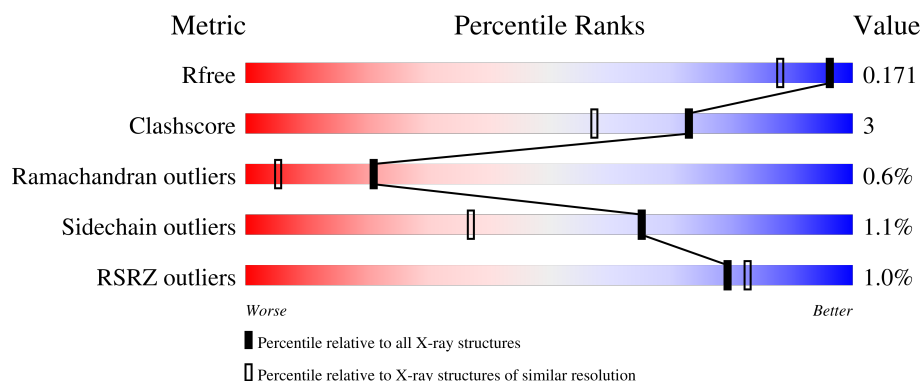
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
R_{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 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	397	% 90% 9% ..
1	B	397	% 92% 7% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7112 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 Acetylornithine aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	Se	0	19	0
			3176	2045	526	589	6	10			
1	B	393	Total	C	N	O	S	Se	0	10	0
			3129	2012	525	577	6	9			

There are 42 discrepancies between the modelled and reference sequences:

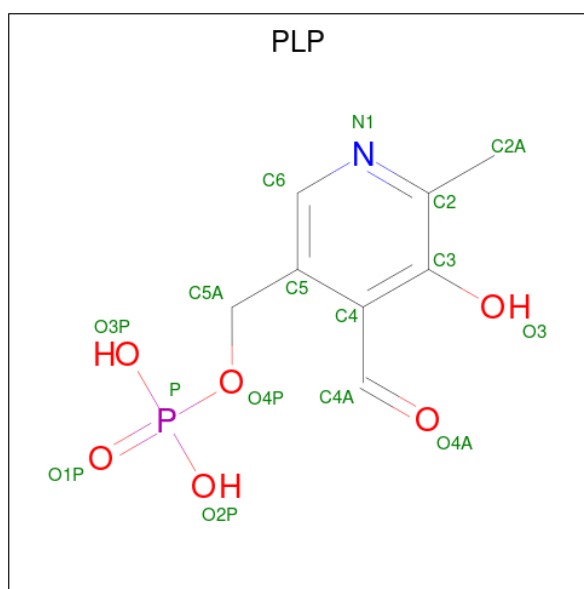
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q9X2A5
A	-10	GLY	-	expression tag	UNP Q9X2A5
A	-9	SER	-	expression tag	UNP Q9X2A5
A	-8	ASP	-	expression tag	UNP Q9X2A5
A	-7	LYS	-	expression tag	UNP Q9X2A5
A	-6	ILE	-	expression tag	UNP Q9X2A5
A	-5	HIS	-	expression tag	UNP Q9X2A5
A	-4	HIS	-	expression tag	UNP Q9X2A5
A	-3	HIS	-	expression tag	UNP Q9X2A5
A	-2	HIS	-	expression tag	UNP Q9X2A5
A	-1	HIS	-	expression tag	UNP Q9X2A5
A	0	HIS	-	expression tag	UNP Q9X2A5
A	1	MSE	MET	modified residue	UNP Q9X2A5
A	4	MSE	MET	modified residue	UNP Q9X2A5
A	73	MSE	MET	modified residue	UNP Q9X2A5
A	168	MSE	MET	modified residue	UNP Q9X2A5
A	217	MSE	MET	modified residue	UNP Q9X2A5
A	303	MSE	MET	modified residue	UNP Q9X2A5
A	309	MSE	MET	modified residue	UNP Q9X2A5
A	322	MSE	MET	modified residue	UNP Q9X2A5
A	325	MSE	MET	modified residue	UNP Q9X2A5
B	-11	MSE	-	expression tag	UNP Q9X2A5
B	-10	GLY	-	expression tag	UNP Q9X2A5
B	-9	SER	-	expression tag	UNP Q9X2A5
B	-8	ASP	-	expression tag	UNP Q9X2A5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	LYS	-	expression tag	UNP Q9X2A5
B	-6	ILE	-	expression tag	UNP Q9X2A5
B	-5	HIS	-	expression tag	UNP Q9X2A5
B	-4	HIS	-	expression tag	UNP Q9X2A5
B	-3	HIS	-	expression tag	UNP Q9X2A5
B	-2	HIS	-	expression tag	UNP Q9X2A5
B	-1	HIS	-	expression tag	UNP Q9X2A5
B	0	HIS	-	expression tag	UNP Q9X2A5
B	1	MSE	MET	modified residue	UNP Q9X2A5
B	4	MSE	MET	modified residue	UNP Q9X2A5
B	73	MSE	MET	modified residue	UNP Q9X2A5
B	168	MSE	MET	modified residue	UNP Q9X2A5
B	217	MSE	MET	modified residue	UNP Q9X2A5
B	303	MSE	MET	modified residue	UNP Q9X2A5
B	309	MSE	MET	modified residue	UNP Q9X2A5
B	322	MSE	MET	modified residue	UNP Q9X2A5
B	325	MSE	MET	modified residue	UNP Q9X2A5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- 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
			5	3	2		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			5	3	2		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
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		

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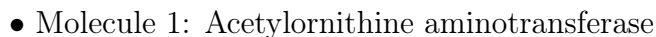
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	353	Total	O	0	2
			355	355		
4	B	317	Total	O	0	2
			320	320		

- Molecule 1: Acetylornithine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.95Å 95.63Å 96.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.80 – 1.40 42.80 – 1.40	Depositor EDS
% Data completeness (in resolution range)	84.2 (42.80-1.40) 84.1 (42.80-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.148 , 0.170 0.149 , 0.171	Depositor DCC
R_{free} test set	6909 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7112	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: PLP, 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	0.79	5/3294 (0.2%)	0.76	0/4429
1	B	0.76	3/3217 (0.1%)	0.77	0/4322
All	All	0.78	8/6511 (0.1%)	0.77	0/8751

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	MSE	SE-CE	-10.61	1.63	1.95
1	A	73	MSE	SE-CE	-8.15	1.71	1.95
1	B	4	MSE	SE-CE	-7.83	1.72	1.95
1	B	303	MSE	SE-CE	-5.75	1.78	1.95
1	A	322	MSE	SE-CE	-5.61	1.78	1.95
1	A	217	MSE	CG-SE	-5.29	1.79	1.95
1	A	303	MSE	SE-CE	-5.29	1.79	1.95
1	B	217	MSE	SE-CE	-5.08	1.80	1.95

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	3176	0	3177	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3129	0	3124	18	2
2	A	16	0	8	0	0
2	B	16	0	8	0	0
3	A	64	0	82	2	0
3	B	36	0	48	0	0
4	A	355	0	0	9	2
4	B	320	0	0	1	0
All	All	7112	0	6447	41	2

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.

All (41) 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:305[B]:LYS:HE3	1:A:372[B]:ASP:OD1	1.19	1.24
1:B:305[B]:LYS:HE3	1:B:372[B]:ASP:OD1	1.35	1.22
1:A:305[B]:LYS:CE	1:A:372[B]:ASP:OD1	1.96	1.14
1:B:305[B]:LYS:CE	1:B:372[B]:ASP:OD1	2.06	1.03
1:A:333[B]:GLU:OE1	4:A:618:HOH:O	2.08	0.67
1:B:305[B]:LYS:NZ	1:B:372[B]:ASP:OD1	2.31	0.63
1:B:305[B]:LYS:NZ	1:B:372[B]:ASP:CG	2.56	0.63
1:B:305[B]:LYS:NZ	1:B:372[B]:ASP:OD2	2.32	0.62
1:A:305[B]:LYS:NZ	1:A:372[B]:ASP:OD1	2.33	0.62
1:B:305[B]:LYS:HZ1	1:B:372[B]:ASP:CG	2.09	0.60
1:A:111:LYS:HG3	4:A:668:HOH:O	2.01	0.59
3:A:402:GOL:C1	3:A:410:GOL:O2	2.51	0.58
1:B:35:SER:HA	4:B:585[C]:HOH:O	2.02	0.57
1:B:161:VAL:HG13	1:B:196:GLU:HG2	1.88	0.56
1:A:161:VAL:HG13	1:A:196:GLU:HG2	1.88	0.56
3:A:405:GOL:C1	4:A:493:HOH:O	2.54	0.56
1:A:-2:HIS:O	1:A:1[A]:MSE:SE	2.74	0.56
1:A:305[B]:LYS:HZ1	1:A:372[B]:ASP:CG	2.15	0.55
1:A:255:GLU:HG2	4:A:762[B]:HOH:O	2.11	0.51
1:A:51[A]:GLU:HG2	4:A:534:HOH:O	2.11	0.51
1:B:86:GLY:HA3	1:B:253:VAL:O	2.11	0.50
1:A:72[B]:GLN:HE22	1:B:9:ARG:HH12	1.59	0.50
1:A:167:LYS:NZ	4:A:552:HOH:O	2.44	0.50
1:B:302:LEU:HD13	1:B:371:ILE:HG23	1.95	0.49
1:A:72[B]:GLN:NE2	4:A:604:HOH:O	2.45	0.49
1:A:-4:HIS:HB3	1:B:68:TRP:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72[B]:GLN:CD	4:A:604:HOH:O	2.57	0.48
1:B:111:LYS:HE3	1:B:112[B]:LYS:NZ	2.30	0.46
1:A:58:GLU:HG2	4:A:705:HOH:O	2.14	0.46
1:A:4:MSE:HE2	1:B:253:VAL:HG22	1.97	0.46
1:A:305[B]:LYS:NZ	1:A:372[B]:ASP:CG	2.74	0.44
1:A:165:ARG:HG3	1:A:200:LEU:HD21	2.01	0.43
1:A:333[B]:GLU:H	1:A:333[B]:GLU:HG3	1.47	0.43
1:A:302:LEU:HD13	1:A:371:ILE:HG23	2.00	0.42
1:B:111:LYS:HE3	1:B:112[B]:LYS:HZ2	1.83	0.42
1:B:121:SER:O	1:B:155:TYR:HA	2.20	0.41
1:B:333:GLU:CD	1:B:333:GLU:H	2.27	0.41
1:A:74:GLU:HB2	1:B:-6:ILE:HD13	2.02	0.41
1:A:307:GLN:NE2	1:A:319[B]:VAL:HG23	2.34	0.41
1:A:121:SER:O	1:A:155:TYR:HA	2.21	0.41
1:A:86:GLY:HA3	1:A:253:VAL:O	2.20	0.40

All (2) 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:B:18[B]:LYS:NZ	4:A:443:HOH:O[3_655]	1.62	0.58
1:B:162[B]:GLU:OE1	4:A:629:HOH:O[3_555]	1.91	0.29

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	411/397 (104%)	398 (97%)	10 (2%)	3 (1%)	18	4
1	B	401/397 (101%)	387 (96%)	12 (3%)	2 (0%)	24	7
All	All	812/794 (102%)	785 (97%)	22 (3%)	5 (1%)	21	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	ALA
1	B	239	ALA
1	A	186	ILE
1	B	186	ILE
1	A	37	ILE

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	338/322 (105%)	333 (98%)	5 (2%)	57	26
1	B	329/322 (102%)	325 (99%)	4 (1%)	63	34
All	All	667/644 (104%)	658 (99%)	9 (1%)	65	30

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

Mol	Chain	Res	Type
1	A	72[A]	GLN
1	A	72[B]	GLN
1	A	110	LYS
1	A	166	ARG
1	A	367	GLU
1	B	72[A]	GLN
1	B	72[B]	GLN
1	B	267	THR
1	B	367	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	383	GLN
1	B	-3	HIS

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Mol	Chain	Res	Type
1	B	5	ASN
1	B	65	ASN
1	B	383	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	405	-	5,5,5	0.41	0	5,5,5	0.28	0
3	GOL	B	406	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	A	409	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	A	406	-	5,5,5	0.42	0	5,5,5	0.45	0
3	GOL	A	407	-	5,5,5	0.44	0	5,5,5	0.31	0
3	GOL	B	404	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	A	402	-	4,4,5	0.69	0	4,4,5	0.83	0
3	GOL	A	403	-	5,5,5	0.29	0	5,5,5	0.33	0
3	GOL	A	405	-	4,4,5	0.69	0	4,4,5	0.51	0
3	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	408	-	5,5,5	0.38	0	5,5,5	0.46	0
3	GOL	A	410	-	5,5,5	0.52	0	5,5,5	0.43	0
3	GOL	A	404	-	5,5,5	0.47	0	5,5,5	0.27	0
2	PLP	B	401	-	16,16,16	1.25	1 (6%)	20,23,23	1.14	2 (10%)
3	GOL	B	407	-	5,5,5	0.42	0	5,5,5	0.24	0
2	PLP	A	401	-	16,16,16	1.17	1 (6%)	20,23,23	1.23	2 (10%)
3	GOL	A	411	-	5,5,5	0.36	0	5,5,5	0.23	0
3	GOL	B	402	-	5,5,5	0.46	0	5,5,5	0.43	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	B	405	-	-	2/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	A	412	-	-	2/4/4/4	-
3	GOL	A	409	-	-	1/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	B	404	-	-	3/4/4/4	-
3	GOL	A	402	-	-	0/2/2/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	0/2/2/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	A	408	-	-	4/4/4/4	-
3	GOL	A	410	-	-	2/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
2	PLP	B	401	-	-	2/8/8/8	0/1/1/1
3	GOL	B	407	-	-	4/4/4/4	-
2	PLP	A	401	-	-	2/8/8/8	0/1/1/1
3	GOL	A	411	-	-	2/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C6-N1	4.08	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C6-N1	2.80	1.40	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	O4A-C4A-C4	-2.62	118.58	124.80
2	B	401	PLP	C5-C6-N1	-2.48	119.79	123.83
2	B	401	PLP	O4A-C4A-C4	-2.21	119.56	124.80
2	A	401	PLP	O3P-P-O2P	2.19	116.02	107.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	407	GOL	C1-C2-C3-O3
3	A	408	GOL	O1-C1-C2-C3
3	A	408	GOL	C1-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
2	A	401	PLP	C3-C4-C4A-O4A
2	A	401	PLP	C5-C4-C4A-O4A
2	B	401	PLP	C5-C4-C4A-O4A
2	B	401	PLP	C3-C4-C4A-O4A
3	A	404	GOL	C1-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	A	410	GOL	O1-C1-C2-C3
3	A	411	GOL	O1-C1-C2-C3
3	A	412	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	B	405	GOL	O1-C1-C2-C3
3	B	407	GOL	C1-C2-C3-O3
3	A	407	GOL	O2-C2-C3-O3
3	A	408	GOL	O1-C1-C2-O2
3	A	410	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	A	408	GOL	O2-C2-C3-O3
3	B	407	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3
3	A	412	GOL	O2-C2-C3-O3
3	A	411	GOL	O1-C1-C2-O2
3	B	405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	407	GOL	O2-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
3	A	405	GOL	1	0
3	A	410	GOL	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	384/397 (96%)	-0.28	4 (1%) 79 83	7, 12, 22, 41	18 (4%)
1	B	384/397 (96%)	-0.32	4 (1%) 79 83	6, 13, 24, 43	11 (2%)
All	All	768/794 (96%)	-0.30	8 (1%) 79 83	6, 12, 23, 43	29 (3%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2	HIS	3.2
1	A	385	ILE	3.1
1	B	-7	LYS	2.9
1	A	-7	LYS	2.8
1	B	85	GLY	2.6
1	B	-2	HIS	2.5
1	B	385	ILE	2.2
1	A	166	ARG	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 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(Å ²)	Q<0.9
3	GOL	A	409	6/6	0.64	0.23	67,69,70,70	0
3	GOL	A	410	6/6	0.64	0.25	56,57,62,63	0
3	GOL	B	405	6/6	0.71	0.24	60,62,63,64	0
3	GOL	A	411	6/6	0.73	0.21	71,72,73,73	0
3	GOL	A	405	5/6	0.75	0.21	43,49,50,53	0
3	GOL	A	407	6/6	0.76	0.17	46,51,52,53	0
3	GOL	A	403	6/6	0.77	0.16	43,50,53,54	0
3	GOL	B	407	6/6	0.77	0.22	65,65,66,68	0
3	GOL	A	412	6/6	0.79	0.22	73,76,76,78	0
3	GOL	B	404	6/6	0.81	0.23	66,67,69,71	0
3	GOL	A	408	6/6	0.83	0.16	44,50,53,53	0
3	GOL	B	406	6/6	0.84	0.20	53,58,60,62	0
3	GOL	A	406	6/6	0.85	0.16	43,50,50,56	0
3	GOL	B	403	6/6	0.85	0.15	26,39,42,42	0
3	GOL	B	402	6/6	0.88	0.13	19,34,39,47	0
3	GOL	A	404	6/6	0.91	0.13	13,30,39,45	0
3	GOL	A	402	5/6	0.92	0.11	16,21,34,35	0
2	PLP	B	401	16/16	0.96	0.09	10,16,32,36	16
2	PLP	A	401	16/16	0.97	0.08	9,13,31,36	16

6.5 Other polymers [i](#)

There are no such residues in this entry.