



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 06:34 PM EST

PDB ID : 3WQD
Title : D-threo-3-hydroxyaspartate dehydratase from *Delftia* sp. HT23 complexed with D-erythro-3-hydroxyaspartate
Authors : Yasutake, Y.; Matsumoto, Y.; Wada, M.
Deposited on : 2014-01-25
Resolution : 1.50 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

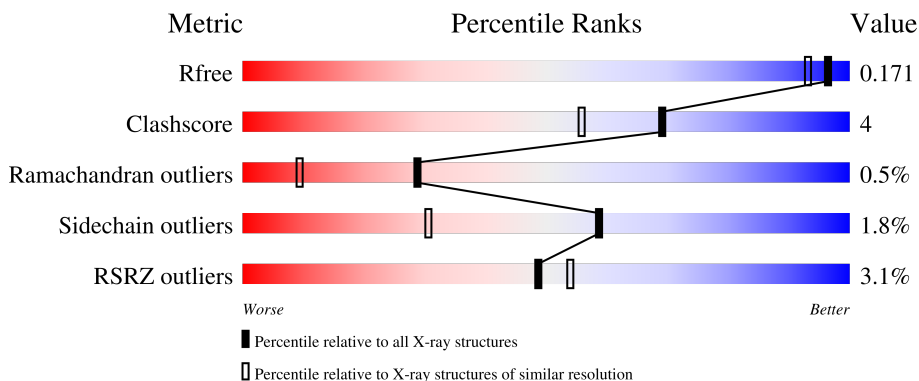
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	390	
1	B	390	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6559 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 D-threo-3-hydroxyaspartate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	379	2882	1789	541	537	15	0	8	0
1	B	389	2950	1832	555	545	18	0	7	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP B2DFG5
A	-8	HIS	-	expression tag	UNP B2DFG5
A	-7	HIS	-	expression tag	UNP B2DFG5
A	-6	HIS	-	expression tag	UNP B2DFG5
A	-5	HIS	-	expression tag	UNP B2DFG5
A	-4	HIS	-	expression tag	UNP B2DFG5
A	-3	HIS	-	expression tag	UNP B2DFG5
A	-2	ALA	-	expression tag	UNP B2DFG5
A	-1	MET	-	expression tag	UNP B2DFG5
A	0	SER	-	expression tag	UNP B2DFG5
B	-9	GLY	-	expression tag	UNP B2DFG5
B	-8	HIS	-	expression tag	UNP B2DFG5
B	-7	HIS	-	expression tag	UNP B2DFG5
B	-6	HIS	-	expression tag	UNP B2DFG5
B	-5	HIS	-	expression tag	UNP B2DFG5
B	-4	HIS	-	expression tag	UNP B2DFG5
B	-3	HIS	-	expression tag	UNP B2DFG5
B	-2	ALA	-	expression tag	UNP B2DFG5
B	-1	MET	-	expression tag	UNP B2DFG5
B	0	SER	-	expression tag	UNP B2DFG5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).

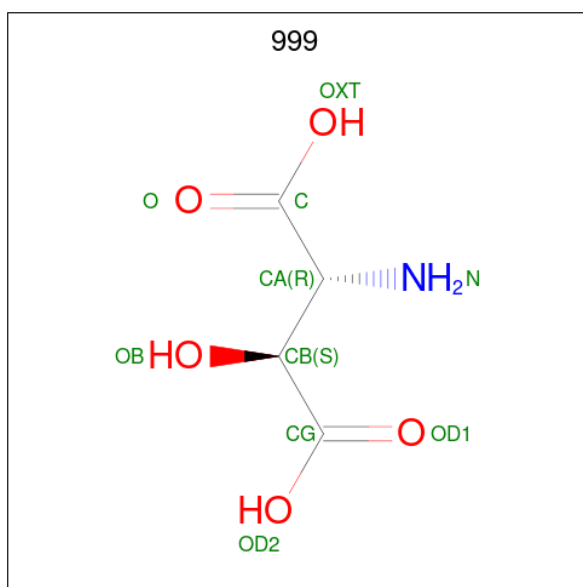


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	4	Total	Mg	0	0
			4	4		

- Molecule 4 is (3S)-3-hydroxy-D-aspartic acid (three-letter code: 999) (formula: C₄H₇NO₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	10	4	1	5	0	0
4	B	1	10	4	1	5	0	0

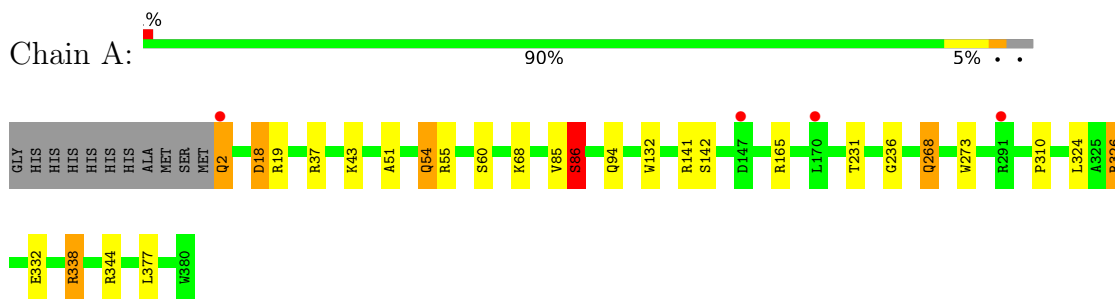
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	348	348	348	0	0
5	B	324	324	324	0	0

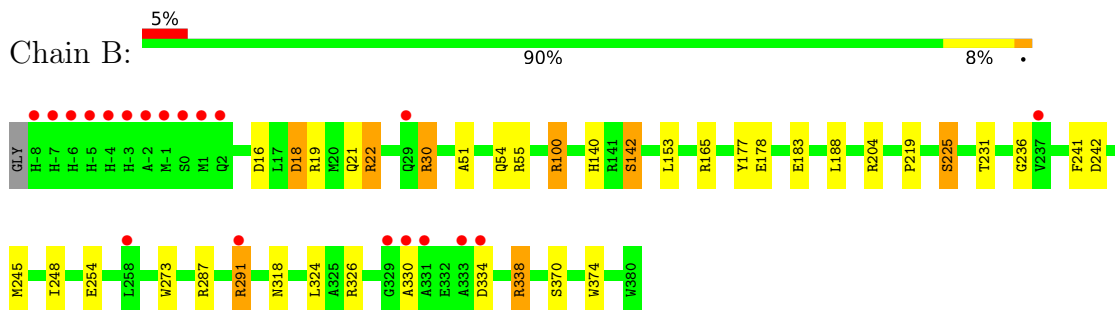
3 Residue-property plots [i](#)

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: D-threo-3-hydroxyaspartate dehydratase



- Molecule 1: D-threo-3-hydroxyaspartate dehydratase



4 Data and refinement statistics i

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.83Å 157.83Å 158.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.88 – 1.50 28.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (28.88-1.50) 98.7 (28.87-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.87 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.144 , 0.176 0.137 , 0.171	Depositor DCC
R_{free} test set	7785 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -l,-k,-h 0.004 for -h,l,k	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6559	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, MG, 999

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	1.27	8/2947 (0.3%)	1.16	13/3996 (0.3%)
1	B	1.33	15/3024 (0.5%)	1.21	17/4099 (0.4%)
All	All	1.30	23/5971 (0.4%)	1.18	30/8095 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	GLU	CD-OE2	16.13	1.43	1.25
1	B	183	GLU	CD-OE1	12.08	1.39	1.25
1	A	86	SER	CB-OG	-9.08	1.30	1.42
1	B	204	ARG	CD-NE	-7.20	1.34	1.46
1	A	132	TRP	CG-CD1	7.18	1.46	1.36
1	B	178	GLU	CD-OE2	-6.94	1.18	1.25
1	A	19	ARG	CZ-NH1	6.77	1.41	1.33
1	A	132	TRP	CD2-CE2	6.64	1.49	1.41
1	A	273	TRP	CD2-CE2	6.24	1.48	1.41
1	A	142	SER	CB-OG	6.20	1.50	1.42
1	B	30	ARG	CZ-NH2	6.12	1.41	1.33
1	B	370	SER	CB-OG	-6.09	1.34	1.42
1	B	142	SER	CB-OG	5.67	1.49	1.42
1	B	273	TRP	CD2-CE2	5.66	1.48	1.41
1	B	55	ARG	CZ-NH2	5.63	1.40	1.33
1	B	374	TRP	CD2-CE2	5.58	1.48	1.41
1	B	204	ARG	CG-CD	5.38	1.65	1.51
1	A	60	SER	CB-OG	-5.37	1.35	1.42
1	B	254	GLU	CD-OE2	5.30	1.31	1.25
1	B	21	GLN	CD-OE1	-5.16	1.12	1.24
1	A	54	GLN	CD-OE1	5.01	1.34	1.24
1	B	100[A]	ARG	CZ-NH2	5.00	1.39	1.33
1	B	100[B]	ARG	CZ-NH2	5.00	1.39	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	A	19	ARG	NE-CZ-NH1	17.43	129.02	120.30
1	A	326	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	B	204	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	B	30	ARG	NE-CZ-NH1	-12.00	114.30	120.30
1	B	55	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	A	19	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	B	55	ARG	NE-CZ-NH2	9.17	124.89	120.30
1	B	165	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	55	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	A	338[A]	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	338[B]	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	287	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	18	ASP	CB-CG-OD2	7.75	125.28	118.30
1	A	338[A]	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	338[B]	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	30	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	A	344	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	18	ASP	CB-CG-OD1	6.72	124.34	118.30
1	B	16	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	19	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	231	THR	OG1-CB-CG2	-5.75	96.77	110.00
1	A	310	PRO	C-N-CA	-5.69	110.34	122.30
1	B	177	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	188	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	B	183	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	37[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	37[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	225	SER	N-CA-CB	5.04	118.06	110.50
1	B	22	ARG	CG-CD-NE	-5.01	101.27	111.80

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	2882	0	2889	19	0
1	B	2950	0	2947	27	0
2	A	15	0	6	3	0
2	B	15	0	6	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	0	0
5	A	348	0	0	6	0
5	B	324	0	0	8	0
All	All	6559	0	5852	43	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 (43) 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:100[B]:ARG:HH11	1:B:100[B]:ARG:CG	1.11	1.48
1:B:100[B]:ARG:CG	1:B:100[B]:ARG:NH1	1.90	1.08
1:A:268[A]:GLN:HE21	1:B:142:SER:HA	1.14	1.06
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG2	1.50	1.05
1:B:291:ARG:HD2	1:B:291:ARG:H	1.29	0.97
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG3	1.85	0.90
1:A:231[B]:THR:HG22	5:A:843:HOH:O	1.74	0.88
1:B:245[B]:MET:HE3	1:B:245[B]:MET:HA	1.57	0.87
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:HG2	0.70	0.85
1:B:142:SER:HB2	5:B:807:HOH:O	1.81	0.81
1:A:43:LYS:NZ	2:A:401:PLP:C4A	2.49	0.76
1:B:291:ARG:HD2	1:B:291:ARG:N	2.00	0.76
1:A:268[A]:GLN:NE2	1:B:142:SER:HA	1.97	0.73
1:A:43:LYS:HZ1	2:A:401:PLP:C4A	2.01	0.73
1:A:268[A]:GLN:HE21	1:B:142:SER:CA	2.00	0.72
1:A:231[B]:THR:CG2	5:A:843:HOH:O	2.32	0.70
1:A:68:LYS:HG2	1:A:377:LEU:HD21	1.75	0.67
1:B:100[A]:ARG:HD2	5:B:694:HOH:O	1.93	0.67
1:B:338:ARG:NH2	5:B:768:HOH:O	2.31	0.64
1:B:140:HIS:HE1	5:B:735:HOH:O	1.81	0.64
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.66	0.61
1:B:245[B]:MET:HA	1:B:245[B]:MET:CE	2.28	0.58
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.68	0.57
1:A:94[A]:GLN:HG3	5:A:671:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HD3	1:B:330:ALA:HB3	1.87	0.56
1:A:43:LYS:HZ2	2:A:401:PLP:C4A	2.20	0.55
1:B:245[B]:MET:HE3	1:B:248:ILE:HD12	1.88	0.54
1:B:18:ASP:HB3	1:B:22:ARG:NH2	2.23	0.54
1:B:100[A]:ARG:CD	5:B:694:HOH:O	2.53	0.53
1:A:326:ARG:HD2	1:A:332:GLU:OE1	2.10	0.52
1:B:338:ARG:HD2	5:B:770:HOH:O	2.10	0.51
1:B:324:LEU:C	1:B:324:LEU:HD23	2.32	0.50
1:B:242:ASP:OD1	1:B:245[B]:MET:HG2	2.12	0.49
1:A:165:ARG:HD3	5:A:779:HOH:O	2.15	0.47
1:B:318[B]:ASN:ND2	5:B:700:HOH:O	2.46	0.47
1:A:324:LEU:HD23	1:A:324:LEU:C	2.36	0.46
1:A:268[A]:GLN:CD	5:A:747:HOH:O	2.53	0.46
1:A:338[B]:ARG:HA	1:A:338[B]:ARG:HD2	1.83	0.44
1:A:268[A]:GLN:NE2	5:A:747:HOH:O	2.51	0.42
1:A:85:VAL:O	1:A:86:SER:C	2.57	0.42
1:A:2:GLN:NE2	1:A:2:GLN:HA	2.35	0.42
1:B:140:HIS:HD2	5:B:533:HOH:O	2.03	0.41
1:B:219:PRO:HG3	1:B:245[B]:MET:HE1	2.02	0.41

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	385/390 (99%)	375 (97%)	8 (2%)	2 (0%)	29 9
1	B	394/390 (101%)	385 (98%)	7 (2%)	2 (0%)	29 9
All	All	779/780 (100%)	760 (98%)	15 (2%)	4 (0%)	29 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	B	241	PHE
1	A	236	GLY
1	B	236	GLY

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	288/289 (100%)	283 (98%)	5 (2%)	60	33
1	B	296/289 (102%)	290 (98%)	6 (2%)	55	25
All	All	584/578 (101%)	573 (98%)	11 (2%)	59	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	18	ASP
1	A	86	SER
1	A	268[A]	GLN
1	A	268[B]	GLN
1	B	30	ARG
1	B	153	LEU
1	B	225	SER
1	B	291	ARG
1	B	334	ASP
1	B	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	B	54	GLN
1	B	94	GLN
1	B	140	HIS

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](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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
4	999	A	403	2,3	7,9,9	1.54	1 (14%)	10,12,12	1.04	0
2	PLP	B	402	4	15,15,16	2.21	5 (33%)	20,22,23	2.10	5 (25%)
4	999	B	405	2,3	7,9,9	2.00	2 (28%)	10,12,12	1.39	2 (20%)
2	PLP	A	401	4	15,15,16	2.72	7 (46%)	20,22,23	1.86	7 (35%)

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	999	A	403	2,3	-	1/12/12/12	-
2	PLP	B	402	4	-	0/6/6/8	0/1/1/1
4	999	B	405	2,3	-	1/12/12/12	-
2	PLP	A	401	4	-	0/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C3-C2	6.40	1.47	1.40
2	B	402	PLP	C5-C4	4.78	1.45	1.40
2	A	401	PLP	C5-C4	4.69	1.45	1.40
2	A	401	PLP	C4A-C4	-3.98	1.43	1.51
2	B	402	PLP	C3-C2	3.93	1.44	1.40
4	B	405	999	OB-CB	3.64	1.49	1.42
2	B	402	PLP	C4A-C4	-3.60	1.44	1.51
2	A	401	PLP	C6-C5	3.34	1.44	1.37
2	B	402	PLP	C3-C4	2.84	1.46	1.40
4	A	403	999	OB-CB	2.74	1.47	1.42
4	B	405	999	OXT-C	-2.58	1.22	1.30
2	A	401	PLP	P-O3P	-2.56	1.45	1.54
2	A	401	PLP	C3-C4	2.43	1.45	1.40
2	B	402	PLP	P-O3P	-2.33	1.45	1.54
2	A	401	PLP	O3-C3	-2.06	1.32	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	PLP	C6-C5-C4	4.71	121.87	118.16
2	B	402	PLP	C6-N1-C2	4.06	126.68	119.17
2	B	402	PLP	C5-C6-N1	-3.85	117.40	123.82
2	A	401	PLP	C6-N1-C2	3.50	125.64	119.17
2	A	401	PLP	C6-C5-C4	3.48	120.89	118.16
2	A	401	PLP	C5-C6-N1	-3.34	118.26	123.82
2	A	401	PLP	C2A-C2-N1	2.76	123.05	117.67
4	B	405	999	OXT-C-CA	2.36	122.47	114.22
2	B	402	PLP	O2P-P-O4P	-2.35	100.49	106.73
2	A	401	PLP	O3P-P-O2P	2.33	116.52	107.64
2	A	401	PLP	C2A-C2-C3	-2.25	118.11	120.89
2	B	402	PLP	O3P-P-O2P	2.23	116.17	107.64
4	B	405	999	OD2-CG-CB	2.07	118.86	113.27
2	A	401	PLP	C5A-C5-C6	-2.03	116.04	119.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	405	999	C-CA-CB-CG
4	A	403	999	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	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

6.1 Protein, DNA and RNA chains

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	379/390 (97%)	-0.16	4 (1%) 80 84	12, 20, 39, 80	0
1	B	389/390 (99%)	0.01	20 (5%) 28 30	12, 20, 44, 69	0
All	All	768/780 (98%)	-0.08	24 (3%) 49 54	12, 20, 42, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-8	HIS	5.1
1	B	1	MET	5.0
1	B	-1	MET	5.0
1	A	2	GLN	4.7
1	B	-5	HIS	4.6
1	B	-2	ALA	4.0
1	B	330	ALA	4.0
1	B	0	SER	3.8
1	B	-4	HIS	3.7
1	A	147	ASP	3.6
1	B	-6	HIS	3.4
1	B	291	ARG	3.2
1	B	-7	HIS	2.9
1	B	2	GLN	2.9
1	A	291	ARG	2.9
1	B	334	ASP	2.7
1	B	-3	HIS	2.7
1	B	333	ALA	2.5
1	B	329	GLY	2.4
1	B	331	ALA	2.4
1	B	237	VAL	2.3
1	A	170	LEU	2.2
1	B	258	LEU	2.2
1	B	29	GLN	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 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
3	MG	B	406	1/1	0.93	0.17	23,23,23,23	1
3	MG	B	404	1/1	0.95	0.09	22,22,22,22	1
4	999	A	403	10/10	0.97	0.06	17,19,21,22	0
2	PLP	A	401	15/16	0.98	0.11	15,17,21,21	0
4	999	B	405	10/10	0.98	0.05	16,17,19,20	0
2	PLP	B	402	15/16	0.99	0.09	13,16,19,19	0
3	MG	B	401	1/1	0.99	0.03	23,23,23,23	1
3	MG	A	402	1/1	1.00	0.04	17,17,17,17	0
3	MG	B	403	1/1	1.00	0.07	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.