



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:46 am BST

PDB ID : 4PB5  
Title : D-threo-3-hydroxyaspartate dehydratase H351A mutant complexed with L-erythro-3-hydroxyaspartate  
Authors : Yasutake, Y.; Matsumoto, Y.; Wada, M.  
Deposited on : 2014-04-11  
Resolution : 1.90 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](mailto: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.

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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 : 2.11  
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) : 2.11

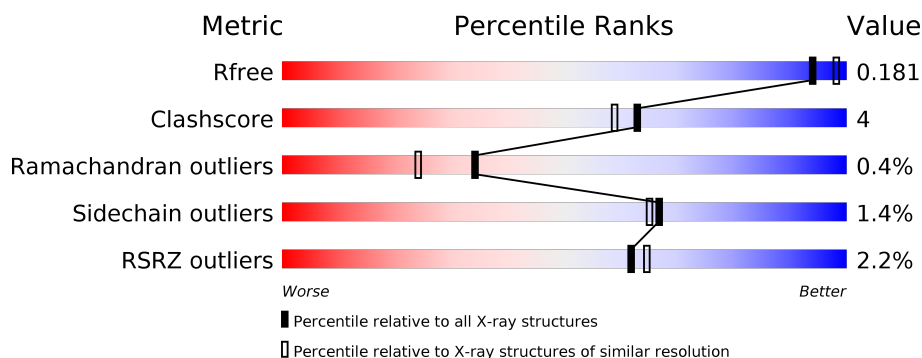
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 87%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>87%</span> <span>9%</span> </div> </div>
1	B	390	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 87%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>87%</span> <span>11%</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6314 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.

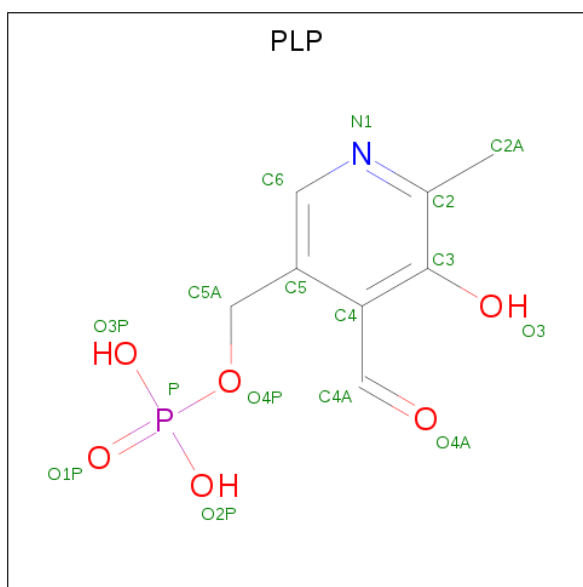
- Molecule 1 is a protein called D-threo-3-hydroxyaspartate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	6	0
			2857	1775	533	534	15			
1	B	388	Total	C	N	O	S	0	6	0
			2930	1820	549	543	18			

There are 22 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
A	351	ALA	HIS	engineered mutation	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
B	351	ALA	HIS	engineered mutation	UNP B2DFG5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).

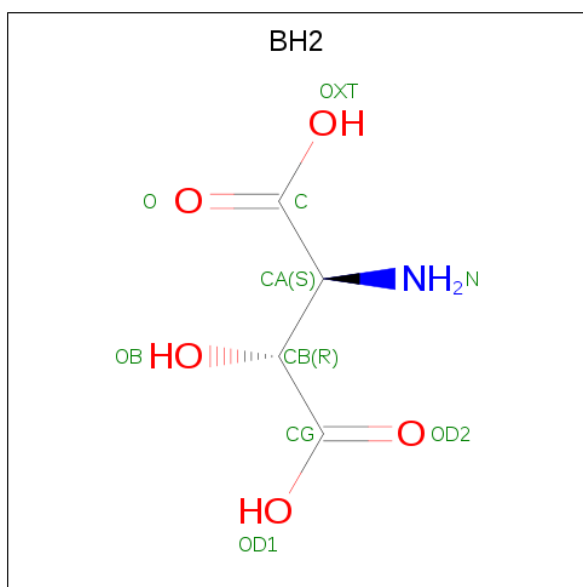


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

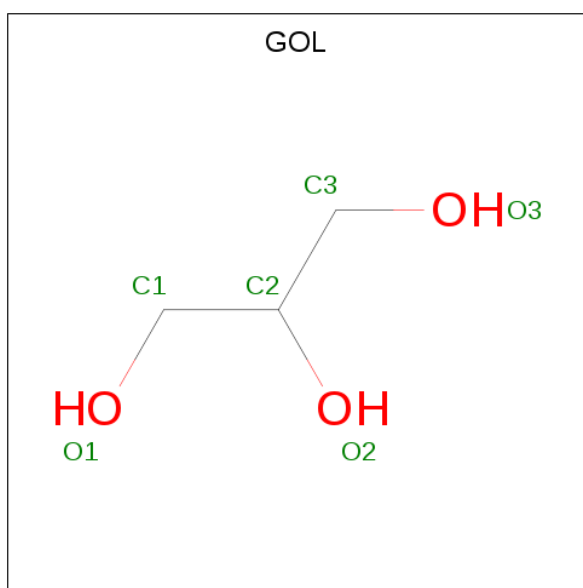
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (3R)-3-hydroxy-L-aspartic acid (three-letter code: BH2) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>5</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

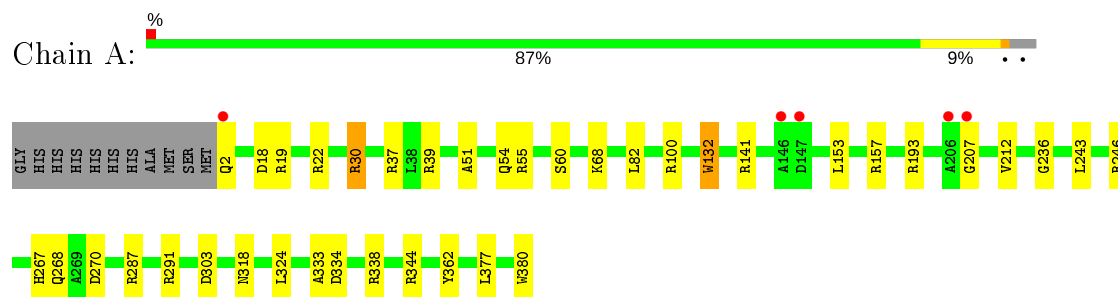
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	240	Total 240	O 240	0	0
6	B	229	Total 229	O 229	0	0

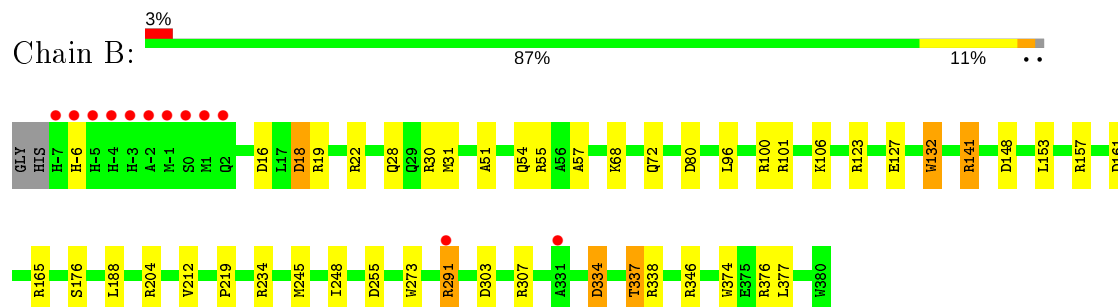
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.63Å 157.63Å 157.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.46 – 1.90 39.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.46-1.90) 99.8 (39.41-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.157 , 0.183 0.155 , 0.181	Depositor DCC
$R_{free}$ test set	3835 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h 0.004 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: GOL, MG, BH2, PLP

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	1.21	6/2921 (0.2%)	1.13	15/3962 (0.4%)
1	B	1.24	5/2999 (0.2%)	1.12	17/4065 (0.4%)
All	All	1.23	11/5920 (0.2%)	1.12	32/8027 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-6	HIS	CE1-NE2	9.37	1.54	1.32
1	B	132	TRP	CD2-CE2	7.23	1.50	1.41
1	A	19	ARG	CZ-NH1	6.28	1.41	1.33
1	B	374	TRP	CD2-CE2	5.74	1.48	1.41
1	A	132	TRP	CD2-CE2	5.63	1.48	1.41
1	B	273	TRP	CD2-CE2	5.39	1.47	1.41
1	A	267	HIS	CG-CD2	5.34	1.44	1.35
1	A	362	TYR	CG-CD2	5.34	1.46	1.39
1	B	-6	HIS	CG-ND1	5.29	1.50	1.38
1	A	380	TRP	CD2-CE2	5.28	1.47	1.41
1	A	207	GLY	N-CA	5.22	1.53	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	A	19	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	55	ARG	NE-CZ-NH2	9.65	125.13	120.30
1	B	30	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	100	ARG	NE-CZ-NH1	-7.63	116.48	120.30
1	A	303	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	19	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	18	ASP	CB-CG-OD1	7.28	124.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	B	376	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	B	234	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	16	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	82	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	B	55	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	55	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	193	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	106	LYS	CD-CE-NZ	-5.93	98.06	111.70
1	A	193	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	123	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	B	346	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	246	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	344	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	80	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	287	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	31	MET	CG-SD-CE	5.34	108.75	100.20
1	B	19	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	55	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	101	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	39	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	243	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	B	148	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	255	ASP	CB-CG-OD2	5.06	122.85	118.30

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	2857	0	2868	14	0
1	B	2930	0	2933	35	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	10	0	3	1	0
4	B	10	0	2	1	0
5	B	6	0	8	2	0
6	A	240	0	0	1	0
6	B	229	0	0	2	0
All	All	6314	0	5826	50	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 (50) 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:245[B]:MET:HA	1:B:245[B]:MET:CE	1.62	1.30
1:B:100[B]:ARG:CG	1:B:100[B]:ARG:HH11	1.55	1.16
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:HG2	1.03	1.14
1:B:245[B]:MET:HA	1:B:245[B]:MET:HE3	1.11	1.10
1:A:30:ARG:HH11	1:A:30:ARG:HG3	0.90	1.04
1:A:30:ARG:CG	1:A:30:ARG:HH11	1.73	0.99
1:A:30:ARG:NH1	1:A:30:ARG:HG3	1.56	0.96
1:B:245[B]:MET:HE3	1:B:245[B]:MET:CA	1.96	0.95
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG2	1.81	0.91
1:B:245[B]:MET:HA	1:B:245[B]:MET:HE2	1.54	0.89
1:B:245[B]:MET:CA	1:B:245[B]:MET:CE	2.43	0.75
1:B:68[A]:LYS:HG2	1:B:377:LEU:HD21	1.74	0.70
1:B:100[B]:ARG:CG	1:B:100[B]:ARG:NH1	2.32	0.69
1:B:303:ASP:OD2	1:B:307:ARG:NH1	2.24	0.69
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.59	0.68
1:B:245[B]:MET:HE3	1:B:248:ILE:HD12	1.75	0.68
1:B:334:ASP:OD2	1:B:337:THR:HG23	1.94	0.68
4:A:403:BH2:HA	6:A:739:HOH:O	1.95	0.66
1:B:100[B]:ARG:NH1	1:B:127:GLU:OE2	2.29	0.66
1:B:291:ARG:HD2	1:B:291:ARG:H	1.63	0.64
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:HG3	1.59	0.63
1:B:307:ARG:HH11	1:B:307:ARG:HB2	1.63	0.63
1:B:245[B]:MET:CE	1:B:248:ILE:HD12	2.31	0.61
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.66	0.60
1:B:245[B]:MET:HE2	1:B:245[B]:MET:CA	2.20	0.57
4:B:403:BH2:HA	6:B:662:HOH:O	2.05	0.56
1:B:18:ASP:HB3	1:B:22:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:N	1:B:291:ARG:HD2	2.23	0.53
1:A:153:LEU:O	1:A:157[B]:ARG:HG3	2.09	0.53
1:B:157:ARG:HB3	5:B:404:GOL:H32	1.92	0.52
1:B:219:PRO:HG3	1:B:245[B]:MET:HE1	1.95	0.49
1:A:132:TRP:CH2	1:A:212:VAL:HG11	2.50	0.46
1:B:132:TRP:CH2	1:B:212:VAL:HG11	2.51	0.46
1:A:338:ARG:HG3	1:A:338:ARG:O	2.15	0.46
1:A:18:ASP:HB3	1:A:22:ARG:NH2	2.32	0.44
1:A:37[B]:ARG:HD3	1:A:60:SER:OG	2.17	0.44
1:A:318:ASN:OD1	1:B:141:ARG:HD3	2.17	0.43
1:B:307:ARG:HH11	1:B:307:ARG:CB	2.30	0.43
1:A:333:ALA:O	1:A:334:ASP:C	2.56	0.42
1:B:28:GLN:HG2	1:B:57:ALA:O	2.18	0.42
1:B:176:SER:HB3	1:B:188:LEU:HD23	2.01	0.42
1:B:161:ASP:HB2	5:B:404:GOL:H12	2.01	0.42
1:B:96:LEU:O	1:B:100[A]:ARG:HG3	2.19	0.41
1:B:165:ARG:HD3	6:B:542:HOH:O	2.20	0.41
1:A:68:LYS:HG2	1:A:377:LEU:HD21	2.01	0.41
1:B:96:LEU:HD21	1:B:100[A]:ARG:CZ	2.51	0.41
1:B:72:GLN:OE1	1:B:377:LEU:HD13	2.20	0.41
1:A:324:LEU:C	1:A:324:LEU:HD23	2.41	0.40
1:A:30:ARG:CG	1:A:30:ARG:NH1	2.40	0.40
1:B:338:ARG:HD2	1:B:338:ARG:HH11	1.74	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	383/390 (98%)	375 (98%)	6 (2%)	2 (0%)	29	18
1	B	392/390 (100%)	382 (97%)	9 (2%)	1 (0%)	41	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	775/780 (99%)	757 (98%)	15 (2%)	3 (0%)	34 24

All (3) Ramachandran outliers are listed below:

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

### 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	285/288 (99%)	281 (99%)	4 (1%)	67 65
1	B	293/288 (102%)	289 (99%)	4 (1%)	67 65
All	All	578/576 (100%)	570 (99%)	8 (1%)	67 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	30	ARG
1	A	268	GLN
1	A	291	ARG
1	B	153	LEU
1	B	291	ARG
1	B	334	ASP
1	B	337	THR

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	305	GLN
1	B	-4	HIS
1	B	54	GLN
1	B	94	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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$
2	PLP	B	401	4	15,15,16	2.38	4 (26%)	20,22,23	1.94	8 (40%)
2	PLP	A	401	4	15,15,16	2.46	5 (33%)	20,22,23	2.32	11 (55%)
5	GOL	B	404	-	5,5,5	1.20	1 (20%)	5,5,5	0.98	0
4	BH2	A	403	3,2	3,9,9	1.52	1 (33%)	4,12,12	0.72	0
4	BH2	B	403	3,2	3,9,9	1.88	1 (33%)	4,12,12	0.64	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
2	PLP	B	401	4	-	0/6/6/8	0/1/1/1
2	PLP	A	401	4	-	0/6/6/8	0/1/1/1
5	GOL	B	404	-	-	2/4/4/4	-
4	BH2	A	403	3,2	-	0/4/12/12	-
4	BH2	B	403	3,2	-	0/4/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C3-C2	6.60	1.47	1.40
2	A	401	PLP	C3-C2	5.58	1.46	1.40
2	B	401	PLP	C3-C4	4.41	1.49	1.40
2	A	401	PLP	C5-C4	4.30	1.45	1.40
2	A	401	PLP	C3-C4	4.14	1.48	1.40
2	B	401	PLP	C5-C4	3.49	1.44	1.40
4	B	403	BH2	CA-CB	-3.20	1.51	1.54
2	A	401	PLP	C4A-C4	-2.96	1.45	1.51
5	B	404	GOL	O3-C3	2.41	1.52	1.42
4	A	403	BH2	CA-N	-2.41	1.43	1.47
2	B	401	PLP	C6-C5	2.06	1.42	1.37
2	A	401	PLP	C6-C5	2.05	1.42	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C4A-C4-C5	-4.41	116.39	120.94
2	A	401	PLP	C6-N1-C2	3.86	126.31	119.17
2	A	401	PLP	C2A-C2-N1	3.53	124.57	117.67
2	B	401	PLP	C2A-C2-N1	3.13	123.77	117.67
2	B	401	PLP	C6-N1-C2	3.10	124.91	119.17
2	A	401	PLP	O3-C3-C4	3.01	126.02	118.10
2	B	401	PLP	C4A-C4-C5	-2.89	117.96	120.94
2	A	401	PLP	C3-C4-C5	2.88	121.86	118.74
2	B	401	PLP	O2P-P-O4P	-2.78	99.34	106.73
2	A	401	PLP	C2A-C2-C3	-2.71	117.54	120.89
2	A	401	PLP	C4-C3-C2	-2.57	116.27	120.07
2	A	401	PLP	C6-C5-C4	-2.47	116.21	118.16
2	B	401	PLP	O2P-P-O1P	2.38	120.01	110.68
2	B	401	PLP	C3-C2-N1	-2.35	117.73	120.77
2	A	401	PLP	C3-C2-N1	-2.26	117.85	120.77
2	A	401	PLP	O3P-P-O2P	2.16	115.90	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	401	PLP	O2P-P-O1P	2.12	118.98	110.68
2	B	401	PLP	C5A-C5-C6	2.11	122.84	119.37
2	B	401	PLP	O3P-P-O2P	2.06	115.52	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	GOL	2	0
4	A	403	BH2	1	0
4	B	403	BH2	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	379/390 (97%)	-0.43	5 (1%) 77 79	9, 19, 36, 57	0
1	B	388/390 (99%)	-0.16	12 (3%) 49 51	10, 19, 42, 88	0
All	All	767/780 (98%)	-0.30	17 (2%) 62 64	9, 19, 39, 88	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	HIS	6.1
1	B	-1	MET	5.9
1	B	-4	HIS	5.7
1	B	1	MET	5.5
1	B	-2	ALA	4.3
1	B	0	SER	4.2
1	B	-6	HIS	4.0
1	B	2	GLN	3.8
1	A	2	GLN	3.8
1	B	291	ARG	3.6
1	B	-3	HIS	3.4
1	B	-7	HIS	3.1
1	A	147	ASP	2.8
1	B	331	ALA	2.4
1	A	146	ALA	2.4
1	A	206	ALA	2.2
1	A	207	GLY	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	404	6/6	0.84	0.17	29,32,34,40	0
3	MG	B	402	1/1	0.91	0.11	29,29,29,29	0
4	BH2	A	403	10/10	0.93	0.12	22,27,30,30	0
4	BH2	B	403	10/10	0.95	0.12	20,23,31,33	0
3	MG	A	402	1/1	0.98	0.06	31,31,31,31	0
2	PLP	A	401	15/16	0.98	0.09	15,16,18,21	0
2	PLP	B	401	15/16	0.99	0.09	13,15,17,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.