



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:34 PM GMT

PDB ID : 4PB4  
Title : D-threo-3-hydroxyaspartate dehydratase H351A mutant complexed with  
2-amino maleic acid  
Authors : Yasutake, Y.; Matsumoto, Y.; Wada, M.  
Deposited on : 2014-04-11  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

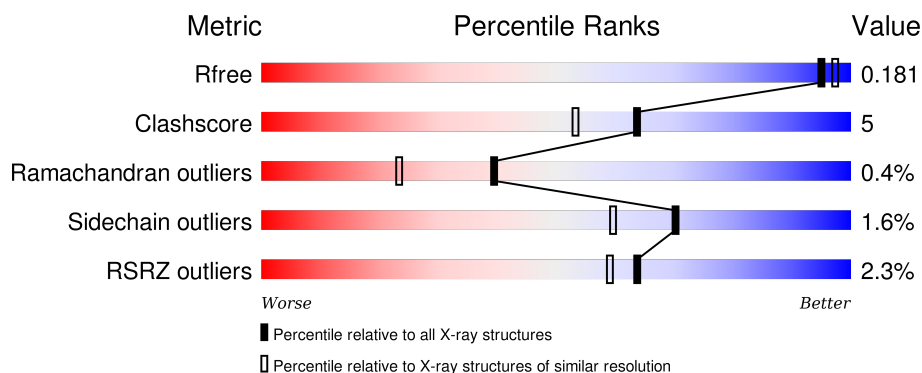
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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 0%, red 4%, orange 4%, yellow 11%, green 87%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>87%</span> <span>9%</span> <span>••</span> </div> </div>
1	B	390	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, yellow 11%, green 87%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>87%</span> <span>11%</span> <span>•</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6277 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	389	Total	C	N	O	S	0	6	0
			2940	1826	552	544	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).

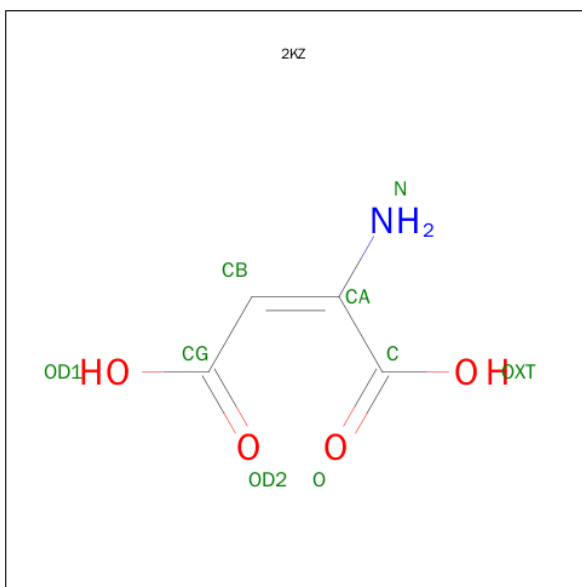


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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 2-amino maleic acid (three-letter code: 2KZ) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	1	4		
4	B	1	Total	C	N	O	0	0
			9	4	1	4		

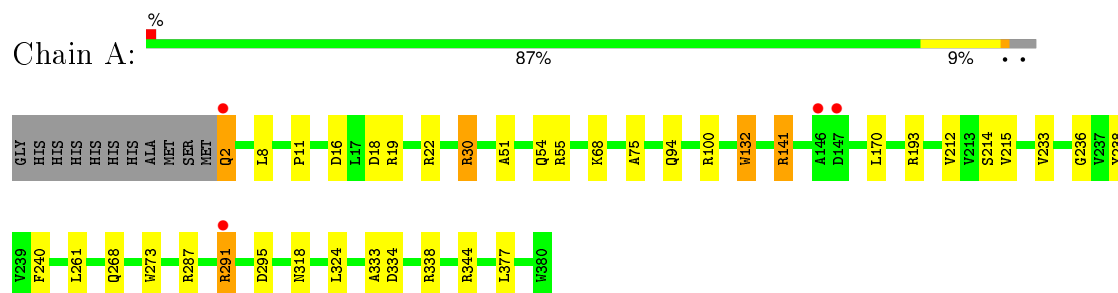
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	215	Total	O	0	0
			215	215		

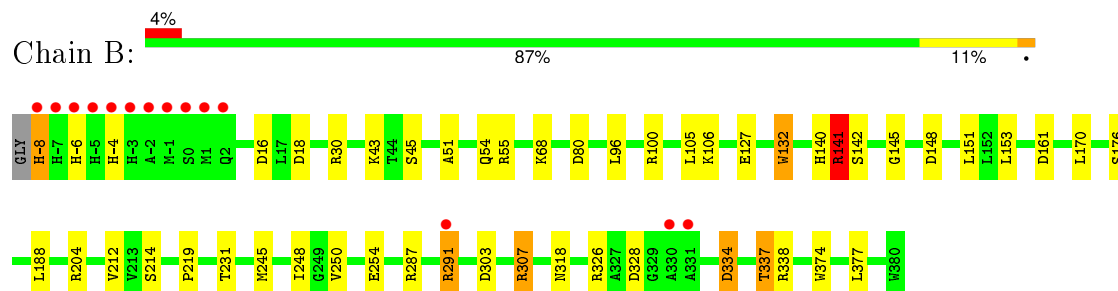
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	157.75Å 157.75Å 158.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.21 – 1.80 37.21 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.21-1.80) 99.6 (37.21-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.06 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.164 , 0.183 0.163 , 0.181	Depositor DCC
$R_{free}$ test set	4544 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.4	EDS
Estimated twinning fraction	0.002 for -l,-k,-h 0.004 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 91217 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6277	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 2KZ, 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	1.25	5/2921 (0.2%)	1.15	12/3962 (0.3%)
1	B	1.28	9/3010 (0.3%)	1.21	18/4080 (0.4%)
All	All	1.27	14/5931 (0.2%)	1.18	30/8042 (0.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-6	HIS	CG-CD2	7.88	1.49	1.35
1	A	132	TRP	CD2-CE2	6.48	1.49	1.41
1	B	204	ARG	CD-NE	-6.40	1.35	1.46
1	A	273	TRP	CD2-CE2	5.91	1.48	1.41
1	B	145	GLY	N-CA	5.86	1.54	1.46
1	B	374	TRP	CD2-CE2	5.76	1.48	1.41
1	B	132	TRP	CD2-CE2	5.76	1.48	1.41
1	A	240	PHE	CE1-CZ	5.38	1.47	1.37
1	B	141	ARG	CZ-NH2	5.38	1.40	1.33
1	B	45	SER	CA-CB	5.26	1.60	1.52
1	B	142	SER	CB-OG	5.21	1.49	1.42
1	A	238	TYR	CG-CD2	5.12	1.45	1.39
1	B	254	GLU	CD-OE1	5.10	1.31	1.25
1	A	287	ARG	CZ-NH2	5.05	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	-16.81	111.89	120.30
1	B	18	ASP	CB-CG-OD1	11.34	128.51	118.30
1	B	204	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	55	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	A	19	ARG	NE-CZ-NH2	-8.18	116.21	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	287	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	B	106	LYS	CD-CE-NZ	-7.17	95.20	111.70
1	B	30	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	A	344	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	55	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	A	100	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	231	THR	OG1-CB-CG2	-6.17	95.82	110.00
1	A	324	LEU	CB-CG-CD1	-6.11	100.62	111.00
1	B	328	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	287	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	8	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	B	55	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	A	295	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	148	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	193	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	307	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	B	105	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	B	80	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	338	ARG	CG-CD-NE	-5.36	100.55	111.80
1	B	151	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	161	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	80	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	16	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	326	ARG	NE-CZ-NH1	-5.10	117.75	120.30

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	21	0
1	B	2940	0	2940	38	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	1	2	0
4	B	9	0	1	2	0
5	A	215	0	0	5	0
5	B	215	0	0	4	0
All	All	6277	0	5822	61	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 5.

All (61) 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:30:ARG:HH11	1:A:30:ARG:CG	1.53	1.20
1:B:245[B]:MET:CE	1:B:245[B]:MET:HA	1.72	1.17
4:B:403:2KZ:CB	5:B:712:HOH:O	1.90	1.17
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:CG	1.61	1.11
1:B:245[B]:MET:HE3	1:B:245[B]:MET:HA	1.14	1.11
4:A:403:2KZ:CB	5:A:709:HOH:O	2.02	1.07
1:A:30:ARG:NH1	1:A:30:ARG:HG3	1.33	1.03
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:HG2	0.86	1.01
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG2	1.67	0.97
1:B:245[B]:MET:HE3	1:B:245[B]:MET:CA	2.07	0.79
1:A:2:GLN:CA	1:A:2:GLN:HE21	1.95	0.77
1:A:2:GLN:HA	1:A:2:GLN:HE21	1.50	0.76
1:B:303:ASP:OD2	1:B:307:ARG:NH1	2.17	0.76
1:B:245[B]:MET:HE3	1:B:248:ILE:HD12	1.68	0.75
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:CG	2.33	0.74
1:A:2:GLN:HA	1:A:2:GLN:NE2	2.04	0.72
1:B:68[A]:LYS:HG2	1:B:377:LEU:HD21	1.70	0.72
1:B:307:ARG:HH11	1:B:307:ARG:HB2	1.55	0.71
1:A:94[A]:GLN:HG3	5:A:648:HOH:O	1.94	0.67
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.59	0.67
1:B:245[B]:MET:CA	1:B:245[B]:MET:CE	2.55	0.66
1:B:245[B]:MET:HA	1:B:245[B]:MET:HE2	1.72	0.63
1:A:18:ASP:HB3	1:A:22:ARG:NH2	2.14	0.62
1:B:245[B]:MET:CE	1:B:248:ILE:HD12	2.30	0.61
1:B:291:ARG:HD2	1:B:291:ARG:H	1.66	0.60
1:B:219:PRO:HG3	1:B:245[B]:MET:HE1	1.83	0.60
1:B:334:ASP:OD2	1:B:337:THR:HG23	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.65	0.60
1:A:2:GLN:CA	1:A:2:GLN:NE2	2.63	0.60
1:B:291:ARG:HD2	1:B:291:ARG:N	2.16	0.60
4:B:403:2KZ:CA	5:B:712:HOH:O	2.34	0.59
1:A:18:ASP:OD1	5:A:659:HOH:O	2.17	0.59
1:B:140:HIS:HD2	5:B:614:HOH:O	1.85	0.59
1:B:307:ARG:NH1	1:B:307:ARG:HB2	2.22	0.55
4:A:403:2KZ:CA	5:A:709:HOH:O	2.40	0.53
1:B:307:ARG:CB	1:B:307:ARG:HH11	2.20	0.53
1:A:30:ARG:NH1	1:A:30:ARG:CG	2.23	0.52
1:B:337:THR:HG23	5:B:693:HOH:O	2.10	0.52
1:B:245[B]:MET:CA	1:B:245[B]:MET:HE2	2.36	0.52
1:B:245[B]:MET:HE2	1:B:250:VAL:HG22	1.92	0.50
1:B:132:TRP:CH2	1:B:212:VAL:HG11	2.46	0.49
1:A:318:ASN:OD1	1:B:141:ARG:HD3	2.11	0.49
1:B:43:LYS:HE3	2:B:401:PLP:C4A	2.44	0.48
1:A:68:LYS:HG2	1:A:377:LEU:HD21	1.97	0.47
1:A:132:TRP:CH2	1:A:212:VAL:HG11	2.52	0.45
1:B:68[A]:LYS:HD3	1:B:377:LEU:HG	2.00	0.44
1:B:176:SER:HB3	1:B:188:LEU:HD23	2.00	0.44
1:A:333:ALA:O	1:A:334:ASP:C	2.55	0.44
1:A:11:PRO:HA	1:A:261:LEU:O	2.18	0.44
1:B:96:LEU:HD21	1:B:100[A]:ARG:CZ	2.47	0.44
1:A:75:ALA:HB2	5:A:507:HOH:O	2.18	0.44
1:A:291:ARG:H	1:A:291:ARG:HG2	1.49	0.43
1:A:215:VAL:O	1:A:233:VAL:HA	2.18	0.43
1:A:170:LEU:HA	1:A:214:SER:O	2.19	0.42
1:B:-8:HIS:O	1:B:-4:HIS:CD2	2.73	0.42
1:A:141:ARG:HD3	1:B:318:ASN:OD1	2.20	0.42
1:B:100[B]:ARG:NH1	1:B:127:GLU:OE2	2.52	0.41
1:B:-8:HIS:HB3	1:B:-4:HIS:CD2	2.56	0.41
1:B:338:ARG:HD3	1:B:338:ARG:HA	1.86	0.41
1:B:68[A]:LYS:CG	1:B:377:LEU:HD21	2.45	0.40
1:B:170:LEU:HA	1:B:214:SER:O	2.22	0.40

There are no symmetry-related clashes.

## 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	383/390 (98%)	373 (97%)	8 (2%)	2 (0%)	34	17
1	B	393/390 (101%)	383 (98%)	9 (2%)	1 (0%)	46	29
All	All	776/780 (100%)	756 (97%)	17 (2%)	3 (0%)	39	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ARG
1	A	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%)	74	65
1	B	294/288 (102%)	289 (98%)	5 (2%)	68	57
All	All	579/576 (100%)	570 (98%)	9 (2%)	70	59

All (9) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	291	ARG
1	B	-8	HIS
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	54	GLN
1	A	140	HIS
1	B	-4	HIS
1	B	54	GLN
1	B	94	GLN
1	B	140	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	$\# Z  > 2$
2	PLP	A	401	4	15,15,16	2.78	5 (33%)	21,22,23	1.57	6 (28%)
4	2KZ	A	403	3,2	3,8,8	1.17	0	0,10,10	0.00	-
2	PLP	B	401	4	15,15,16	2.10	4 (26%)	21,22,23	1.63	5 (23%)
4	2KZ	B	403	3,2	3,8,8	1.36	0	0,10,10	0.00	-

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	A	401	4	-	0/6/6/8	0/1/1/1
4	2KZ	A	403	3,2	-	0/1/8/8	0/0/0/0
2	PLP	B	401	4	-	0/6/6/8	0/1/1/1
4	2KZ	B	403	3,2	-	0/1/8/8	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	O3-C3	-2.04	1.32	1.37
2	A	401	PLP	P-O1P	-2.02	1.44	1.51
2	B	401	PLP	C6-C5	2.03	1.42	1.37
2	B	401	PLP	C5-C4	2.61	1.43	1.40
2	B	401	PLP	C3-C4	2.78	1.47	1.40
2	A	401	PLP	C3-C4	2.92	1.47	1.40
2	A	401	PLP	C5-C4	5.66	1.47	1.40
2	B	401	PLP	C3-C2	6.26	1.45	1.40
2	A	401	PLP	C3-C2	7.79	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	C2A-C2-C3	-3.74	116.53	121.04
2	A	401	PLP	C2A-C2-C3	-2.79	117.67	121.04
2	A	401	PLP	C6-C5-C4	-2.72	115.84	118.15
2	A	401	PLP	O3-C3-C4	2.05	123.90	118.12
2	B	401	PLP	O3P-P-O2P	2.12	115.44	107.38
2	A	401	PLP	O3P-P-O2P	2.12	115.47	107.38
2	B	401	PLP	O2P-P-O1P	2.23	117.77	110.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	C6-N1-C2	2.51	124.40	119.28
2	A	401	PLP	C2A-C2-N1	2.61	123.73	117.95
2	A	401	PLP	C6-N1-C2	2.75	124.89	119.28
2	B	401	PLP	C2A-C2-N1	2.81	124.17	117.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	2KZ	2	0
2	B	401	PLP	1	0
4	B	403	2KZ	2	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, 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%)	-0.46	4 (1%) 82 80	9, 19, 37, 62	0
1	B	389/390 (99%)	-0.13	14 (3%) 46 40	9, 19, 41, 99	0
All	All	768/780 (98%)	-0.29	18 (2%) 64 59	9, 19, 38, 99	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-8	HIS	6.9
1	B	-5	HIS	6.2
1	B	-1	MET	6.0
1	B	-4	HIS	5.0
1	A	2	GLN	4.9
1	B	1	MET	4.5
1	B	0	SER	4.4
1	B	-2	ALA	3.7
1	B	-6	HIS	3.7
1	B	291	ARG	3.3
1	B	2	GLN	3.2
1	B	-3	HIS	3.2
1	A	147	ASP	2.8
1	B	331	ALA	2.7
1	A	291	ARG	2.6
1	B	-7	HIS	2.3
1	B	330	ALA	2.1
1	A	146	ALA	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	2KZ	A	403	9/9	0.93	0.14	1.41	22,25,34,34	0
2	PLP	A	401	15/16	0.98	0.09	-0.05	15,16,18,21	0
4	2KZ	B	403	9/9	0.92	0.12	-0.08	20,24,30,35	0
2	PLP	B	401	15/16	0.99	0.10	-0.43	13,14,17,20	0
3	MG	B	402	1/1	0.97	0.06	-	25,25,25,25	0
3	MG	A	402	1/1	0.94	0.10	-	25,25,25,25	0

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

There are no such residues in this entry.