



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N29  
Title : Crystal structure of carboxynorspermidine decarboxylase complexed with Norspermidine from Campylobacter jejuni  
Authors : Deng, X.; Lee, J.; Michael, A.J.; Tomchick, D.R.; Goldsmith, E.J.; Phillips, M.A.  
Deposited on : 2010-05-17  
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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

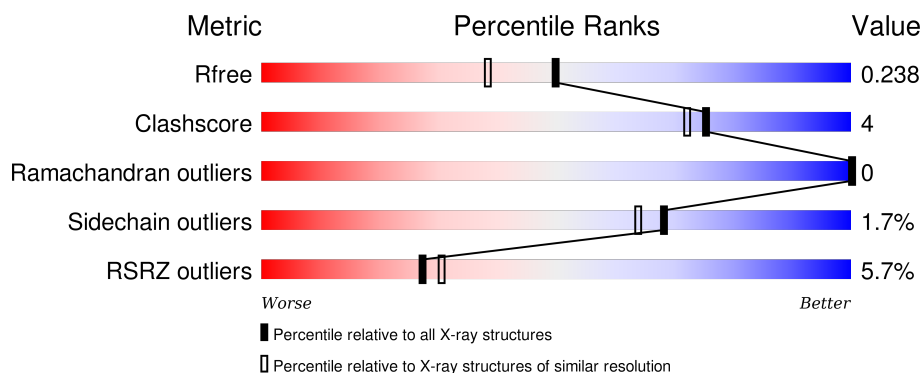
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	418	
1	B	418	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1003	-	-	-	X
4	GOL	B	1003	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6325 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 Carboxynorspermidine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	2	0
			2969	1904	494	555	16			
1	B	367	Total	C	N	O	S	0	1	0
			2921	1871	486	548	16			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP A3ZCM2
A	-34	ARG	-	EXPRESSION TAG	UNP A3ZCM2
A	-33	GLY	-	EXPRESSION TAG	UNP A3ZCM2
A	-32	SER	-	EXPRESSION TAG	UNP A3ZCM2
A	-31	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-30	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-29	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-28	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-27	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-26	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-25	GLY	-	EXPRESSION TAG	UNP A3ZCM2
A	-24	MET	-	EXPRESSION TAG	UNP A3ZCM2
A	-23	ALA	-	EXPRESSION TAG	UNP A3ZCM2
A	-22	SER	-	EXPRESSION TAG	UNP A3ZCM2
A	-21	MET	-	EXPRESSION TAG	UNP A3ZCM2
A	-20	THR	-	EXPRESSION TAG	UNP A3ZCM2
A	-19	GLY	-	EXPRESSION TAG	UNP A3ZCM2
A	-18	GLY	-	EXPRESSION TAG	UNP A3ZCM2
A	-17	GLN	-	EXPRESSION TAG	UNP A3ZCM2
A	-16	GLN	-	EXPRESSION TAG	UNP A3ZCM2
A	-15	MET	-	EXPRESSION TAG	UNP A3ZCM2
A	-14	GLY	-	EXPRESSION TAG	UNP A3ZCM2
A	-13	ARG	-	EXPRESSION TAG	UNP A3ZCM2
A	-12	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-11	LEU	-	EXPRESSION TAG	UNP A3ZCM2

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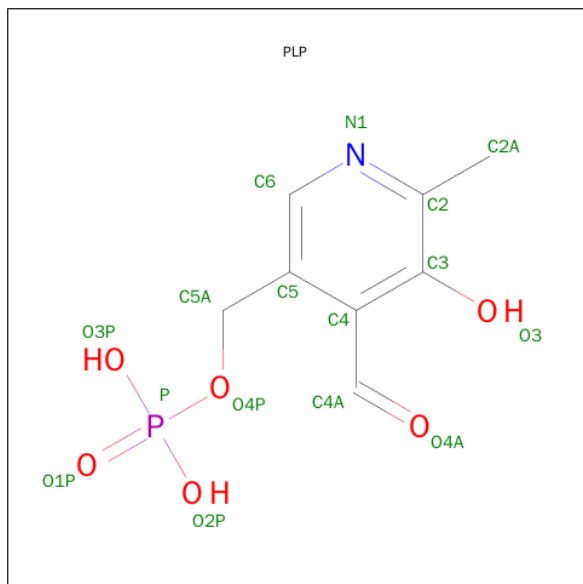
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	EXPRESSION TAG	UNP A3ZCM2
A	-9	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-8	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-7	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-6	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-5	LYS	-	EXPRESSION TAG	UNP A3ZCM2
A	-4	ASP	-	EXPRESSION TAG	UNP A3ZCM2
A	-3	HIS	-	EXPRESSION TAG	UNP A3ZCM2
A	-2	PRO	-	EXPRESSION TAG	UNP A3ZCM2
A	-1	PHE	-	EXPRESSION TAG	UNP A3ZCM2
A	0	THR	-	EXPRESSION TAG	UNP A3ZCM2
B	-35	MET	-	EXPRESSION TAG	UNP A3ZCM2
B	-34	ARG	-	EXPRESSION TAG	UNP A3ZCM2
B	-33	GLY	-	EXPRESSION TAG	UNP A3ZCM2
B	-32	SER	-	EXPRESSION TAG	UNP A3ZCM2
B	-31	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-30	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-29	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-28	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-27	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-26	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-25	GLY	-	EXPRESSION TAG	UNP A3ZCM2
B	-24	MET	-	EXPRESSION TAG	UNP A3ZCM2
B	-23	ALA	-	EXPRESSION TAG	UNP A3ZCM2
B	-22	SER	-	EXPRESSION TAG	UNP A3ZCM2
B	-21	MET	-	EXPRESSION TAG	UNP A3ZCM2
B	-20	THR	-	EXPRESSION TAG	UNP A3ZCM2
B	-19	GLY	-	EXPRESSION TAG	UNP A3ZCM2
B	-18	GLY	-	EXPRESSION TAG	UNP A3ZCM2
B	-17	GLN	-	EXPRESSION TAG	UNP A3ZCM2
B	-16	GLN	-	EXPRESSION TAG	UNP A3ZCM2
B	-15	MET	-	EXPRESSION TAG	UNP A3ZCM2
B	-14	GLY	-	EXPRESSION TAG	UNP A3ZCM2
B	-13	ARG	-	EXPRESSION TAG	UNP A3ZCM2
B	-12	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-11	LEU	-	EXPRESSION TAG	UNP A3ZCM2
B	-10	TYR	-	EXPRESSION TAG	UNP A3ZCM2
B	-9	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-8	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-7	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-6	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-5	LYS	-	EXPRESSION TAG	UNP A3ZCM2

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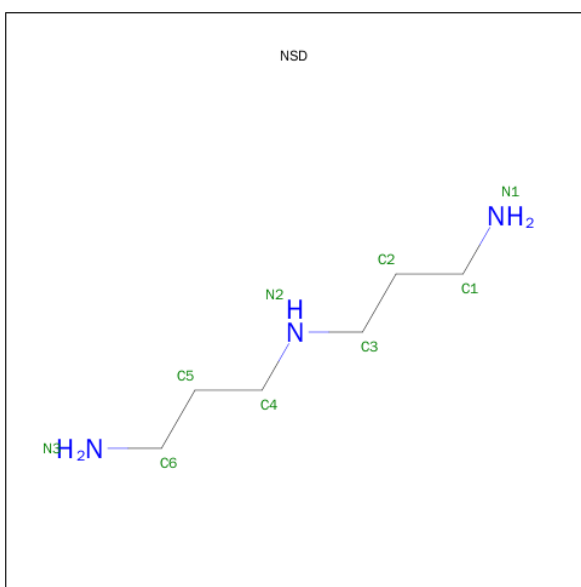
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	EXPRESSION TAG	UNP A3ZCM2
B	-3	HIS	-	EXPRESSION TAG	UNP A3ZCM2
B	-2	PRO	-	EXPRESSION TAG	UNP A3ZCM2
B	-1	PHE	-	EXPRESSION TAG	UNP A3ZCM2
B	0	THR	-	EXPRESSION TAG	UNP A3ZCM2

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



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 N-(3-AMINOPROPYL)PROPANE-1,3-DIAMINE (three-letter code: NSD) (formula:  $C_6H_{17}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	6	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	196	Total 196	O 196	0	0
5	B	188	Total 188	O 188	0	0



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 ( $RSRZ > 2$ ). 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.

- Chain A:
- 
- 6% 78% 10% 11%
- Sequence: MET ARG GLY SER HIS HIS HIS HIS HIS MET GLY MET ALA SER MET THR THR GLY GLN GLN MET MET GLY ARG ASP LEU THR ASP ASP ASP LYS ASP HIS PRO PHE THR MET F2 Y3 E4 K5 I6 A10 Y11 S27 K31 K41 M49 Y73 Y81 S82 P83 A84 F85 E89 M103 Q107 F128 I129 LEU ALA PRO LYS SER MET THR THR ASN PRO CYS R141 R144 L145 G146 M154 V155 D156 C169 E170 E171 E204 K207 K208 G209 E213 E233 E236 K257 S265 A268 P271 Y278 R291 E292 S302 T312 T325 Q339 I340 R341 Y342 T343 I344 V345 K346 N347 T348 T349 F350 N351 G352 I353 R354 L355 P356 L367 N382

- Chain B:
- 
- | Position | Amino Acid | Frequency (bits) |
|----------|------------|------------------|
| 1        | MET        | 0.58             |
| 2        | ARG        | 0.58             |
| 3        | GLY        | 0.58             |
| 4        | SER        | 0.58             |
| 5        | HIS        | 0.58             |
| 6        | MET        | 0.58             |
| 7        | MET        | 0.58             |
| 8        | THR        | 0.58             |
| 9        | GLY        | 0.58             |
| 10       | GLY        | 0.58             |
| 11       | GLN        | 0.58             |
| 12       | GLN        | 0.58             |
| 13       | MET        | 0.58             |
| 14       | GLY        | 0.58             |
| 15       | ARG        | 0.58             |
| 16       | ASP        | 0.58             |
| 17       | LEU        | 0.58             |
| 18       | THR        | 0.58             |
| 19       | ASP        | 0.58             |
| 20       | ASP        | 0.58             |
| 21       | LYS        | 0.58             |
| 22       | HIS        | 0.58             |
| 23       | PRO        | 0.58             |
| 24       | PHE        | 0.58             |
| 25       | THR        | 0.58             |
| 26       | MET        | 0.58             |
| 27       | PHE        | 0.58             |
| 28       | THR        | 0.58             |
| 29       | GLU        | 0.58             |
| 30       | LYS        | 0.58             |
| 31       | LEU        | 0.58             |
| 32       | K17        | 0.58             |
| 33       | L18        | 0.58             |
| 34       | A39        | 0.58             |
| 35       | L40        | 0.58             |
| 36       | K41        | 0.58             |
| 37       | A48        | 0.58             |
| 38       | S62        | 0.58             |
| 39       | E72        | 0.58             |
| 40       | Y73        | 0.58             |
| 41       | Y81        | 0.58             |
| 42       | F96        | 0.58             |

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.50 Å   144.50 Å   79.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	102.06 – 1.90 37.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (102.06-1.90) 99.7 (37.21-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.179   ,   0.219 0.202   ,   0.238	Depositor DCC
$R_{free}$ test set	3376 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66670 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: GOL, NSD, 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	1.17	8/3034 (0.3%)	0.90	3/4080 (0.1%)
1	B	1.14	5/2980 (0.2%)	0.91	5/4009 (0.1%)
All	All	1.16	13/6014 (0.2%)	0.90	8/8089 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLU	CB-CG	7.37	1.66	1.52
1	B	346	LYS	CB-CG	-7.22	1.33	1.52
1	B	292	GLU	CB-CG	7.03	1.65	1.52
1	A	301	GLU	CG-CD	6.88	1.62	1.51
1	B	220	LYS	CE-NZ	6.36	1.65	1.49
1	A	292	GLU	CG-CD	6.21	1.61	1.51
1	A	4	GLU	CB-CG	5.99	1.63	1.52
1	A	292	GLU	CB-CG	5.90	1.63	1.52
1	B	72	GLU	CD-OE1	-5.80	1.19	1.25
1	A	10	ALA	CA-CB	5.57	1.64	1.52
1	A	41	LYS	CE-NZ	5.31	1.62	1.49
1	B	72	GLU	CD-OE2	-5.24	1.19	1.25
1	A	171	GLU	CG-CD	5.23	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	148	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	220	LYS	CD-CE-NZ	6.95	127.69	111.70
1	B	73	TYR	N-CA-C	6.47	128.48	111.00
1	A	73	TYR	N-CA-C	6.21	127.75	111.00
1	A	89	GLU	OE1-CD-OE2	5.66	130.09	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	LYS	CB-CA-C	-5.25	99.90	110.40
1	A	49	MET	CG-SD-CE	-5.17	91.92	100.20

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	2969	0	2961	26	0
1	B	2921	0	2914	24	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
3	A	9	0	16	4	0
4	A	6	0	8	2	0
4	B	6	0	8	1	0
5	A	196	0	0	1	0
5	B	188	0	0	1	0
All	All	6325	0	5921	46	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 (46) 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:291[B]:ARG:HD2	1:A:292:GLU:OE2	1.80	0.82
1:B:85:PHE:H	1:B:107:GLN:HE22	1.36	0.74
1:A:103:ASN:HD21	1:A:146:GLY:H	1.39	0.70
1:B:278:TYR:OH	4:B:1003:GOL:H32	1.93	0.69
1:A:103:ASN:ND2	1:A:146:GLY:H	1.94	0.65
1:B:314:LEU:HD11	1:B:350:PHE:HE2	1.61	0.64
1:A:348:THR:HG22	1:B:348:THR:HG22	1.82	0.61
1:A:169:CYS:SG	3:A:1002:NSD:H2A	2.41	0.61
1:A:85:PHE:H	1:A:107:GLN:HE22	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:ND2	1:B:146:GLY:H	2.01	0.58
1:A:3:TYR:O	1:A:6:ILE:HG12	2.04	0.57
1:A:144:ARG:HA	1:B:253:ILE:HD11	1.88	0.55
1:A:350:PHE:CD1	1:B:346:LYS:HG3	2.44	0.53
1:A:89:GLU:OE1	1:B:354:ARG:NH2	2.41	0.52
1:A:204:HIS:CD2	1:A:207:LYS:HD3	2.45	0.52
5:A:437:HOH:O	1:B:148:ARG:HD2	2.11	0.50
1:B:103:ASN:HD21	1:B:146:GLY:H	1.58	0.50
1:A:268:ALA:O	1:A:347:ASN:HB2	2.12	0.49
1:B:153:GLU:O	1:B:154:ASN:HB2	2.12	0.49
1:B:41:LYS:NZ	2:B:1001:PLP:O3	2.47	0.48
1:B:85:PHE:N	1:B:107:GLN:HE22	2.08	0.47
1:B:197:VAL:HG21	1:B:222:PHE:CE2	2.49	0.47
1:A:278:TYR:OH	4:A:1003:GOL:H31	2.15	0.46
1:A:103:ASN:HD21	1:A:145:LEU:HA	1.81	0.46
1:B:153:GLU:O	1:B:154:ASN:CB	2.64	0.46
1:B:268:ALA:O	1:B:347:ASN:HB2	2.16	0.46
1:A:265:SER:HB2	1:A:312:THR:HG23	1.98	0.45
1:A:339:GLN:HE21	1:A:343:THR:HG21	1.82	0.45
1:A:27:SER:OG	1:A:31:LYS:HE3	2.17	0.45
1:A:312:THR:HG22	1:A:353:ILE:HG13	2.00	0.44
1:B:225:LYS:HD2	1:B:226:TYR:CE2	2.54	0.43
1:B:354:ARG:HD3	5:B:485:HOH:O	2.18	0.43
1:A:342:TYR:HD1	3:A:1002:NSD:HN3	1.66	0.43
1:A:6:ILE:HG21	1:A:367:LEU:HD21	2.01	0.42
1:A:169:CYS:SG	3:A:1002:NSD:C2	3.07	0.42
1:B:370:ILE:HD13	1:B:370:ILE:HA	1.91	0.42
1:B:18:LEU:CD2	1:B:48:ALA:HB1	2.50	0.42
1:A:11:TYR:CD2	1:A:356:PRO:HB2	2.55	0.42
1:A:236:GLU:OE1	3:A:1002:NSD:N1	2.54	0.41
1:B:62:SER:HA	1:B:81:TYR:O	2.20	0.41
1:A:271:PRO:HG2	1:A:346:LYS:HG3	2.02	0.41
1:B:85:PHE:H	1:B:107:GLN:NE2	2.09	0.41
1:B:89:GLU:HG3	1:B:93:ILE:HD12	2.01	0.41
1:B:103:ASN:HD21	1:B:145:LEU:HA	1.85	0.41
1:A:341:HIS:O	4:A:1003:GOL:H2	2.22	0.40
1:A:233:GLU:O	2:A:1001:PLP:H6	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	369/418 (88%)	358 (97%)	11 (3%)	0	100	100
1	B	364/418 (87%)	356 (98%)	8 (2%)	0	100	100
All	All	733/836 (88%)	714 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	319/357 (89%)	313 (98%)	6 (2%)	65	59
1	B	314/357 (88%)	309 (98%)	5 (2%)	70	66
All	All	633/714 (89%)	622 (98%)	11 (2%)	68	64

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

Mol	Chain	Res	Type
1	A	5	LYS
1	A	107	GLN
1	A	204	HIS
1	A	257	LYS
1	A	351	ASN
1	A	354	ARG
1	B	17	LYS
1	B	107	GLN

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	291	ARG
1	B	351	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	107	GLN
1	A	229	GLN
1	A	339	GLN
1	A	341	HIS
1	B	103	ASN
1	B	107	GLN
1	B	118	ASN
1	B	158	ASN
1	B	203	HIS
1	B	241	GLN
1	B	382	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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
2	PLP	A	1001	1	15,15,16	1.42	2 (13%)	21,22,23	0.84	0
3	NSD	A	1002	-	8,8,8	3.08	2 (25%)	7,7,7	1.97	2 (28%)
4	GOL	A	1003	-	5,5,5	1.07	0	5,5,5	1.64	2 (40%)
2	PLP	B	1001	1	15,15,16	1.62	5 (33%)	21,22,23	1.40	4 (19%)
4	GOL	B	1003	-	5,5,5	0.59	0	5,5,5	0.39	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	A	1001	1	-	0/6/6/8	0/1/1/1
3	NSD	A	1002	-	-	0/6/6/6	0/0/0/0
4	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
2	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
4	GOL	B	1003	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NSD	C4-N2	-6.16	1.27	1.46
3	A	1002	NSD	C3-N2	-6.12	1.27	1.46
2	A	1001	PLP	P-O3P	-2.27	1.46	1.54
2	B	1001	PLP	P-O2P	-2.10	1.47	1.54
2	B	1001	PLP	O3-C3	2.20	1.42	1.37
2	B	1001	PLP	C2-N1	2.22	1.38	1.34
2	B	1001	PLP	C5-C4	2.93	1.43	1.40
2	B	1001	PLP	C3-C2	3.45	1.43	1.40
2	A	1001	PLP	C3-C2	3.79	1.43	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	GOL	O2-C2-C1	-2.56	96.92	108.65
4	A	1003	GOL	O2-C2-C3	-2.05	99.23	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PLP	C4-C3-C2	-2.01	116.62	120.05
2	B	1001	PLP	O3-C3-C2	2.39	121.81	117.66
2	B	1001	PLP	O3P-P-O4P	2.56	113.92	106.56
2	B	1001	PLP	C3-C4-C5	2.77	121.80	118.78
3	A	1002	NSD	C2-C3-N2	3.24	120.06	111.96
3	A	1002	NSD	C4-N2-C3	3.73	126.57	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PLP	1	0
3	A	1002	NSD	4	0
4	A	1003	GOL	2	0
2	B	1001	PLP	1	0
4	B	1003	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 ⓘ

### 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	371/418 (88%)	0.41	24 (6%) 22 25	2, 16, 30, 66	0
1	B	367/418 (87%)	0.37	18 (4%) 33 36	3, 17, 31, 47	0
All	All	738/836 (88%)	0.39	42 (5%) 27 30	2, 16, 31, 66	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	SER	8.3
1	A	129	SER	7.9
1	A	128	PHE	5.4
1	B	6	ILE	4.2
1	A	4	GLU	4.1
1	B	128	PHE	4.1
1	B	268	ALA	3.7
1	A	302	ASN	3.4
1	A	5	LYS	3.3
1	A	345	VAL	3.1
1	B	345	VAL	2.9
1	A	208	LYS	2.8
1	A	154	ASN	2.7
1	B	208	LYS	2.7
1	A	349	THR	2.7
1	A	141	ARG	2.7
1	B	313	CYS	2.6
1	A	301	GLU	2.6
1	A	348	THR	2.6
1	A	81	TYR	2.5
1	B	344	ILE	2.4
1	B	350	PHE	2.4
1	A	268	ALA	2.4
1	A	3	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	349	THR	2.3
1	B	353	ILE	2.3
1	B	348	THR	2.3
1	A	2	PHE	2.3
1	A	355	LEU	2.3
1	B	363	HIS	2.3
1	B	39	ALA	2.2
1	A	156	ASP	2.2
1	A	41	LYS	2.2
1	A	83	PRO	2.2
1	A	213	GLU	2.1
1	A	209	GLY	2.1
1	B	312	THR	2.1
1	A	350	PHE	2.1
1	A	325	ASP	2.1
1	B	355	LEU	2.1
1	B	261	ILE	2.0
1	B	142	TYR	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(Å <sup>2</sup> )	Q<0.9
4	GOL	B	1003	6/6	0.62	0.50	10.40	45,55,57,58	0
4	GOL	A	1003	6/6	0.84	0.29	4.08	38,44,46,50	0
3	NSD	A	1002	9/9	0.79	0.28	1.97	52,56,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	A	1001	15/16	0.97	0.14	-0.06	19,25,32,32	0
2	PLP	B	1001	15/16	0.97	0.12	-0.40	22,25,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.