



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 07:34 PM EDT

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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

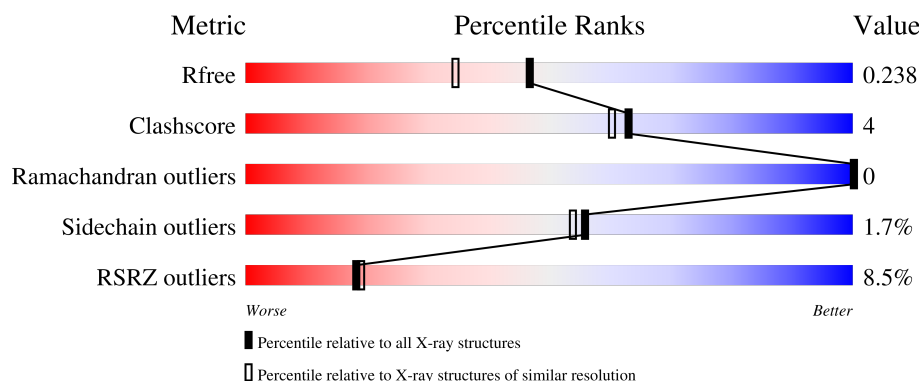
1 Overall quality at a glance

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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 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	418	<div> <div>7%</div> <div>78%</div> <div>10%</div> <div>11%</div> </div>
1	B	418	<div> <div>8%</div> <div>79%</div> <div>8%</div> <div>12%</div> </div>

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	-	-

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

Continued on next page...

Continued from previous page...

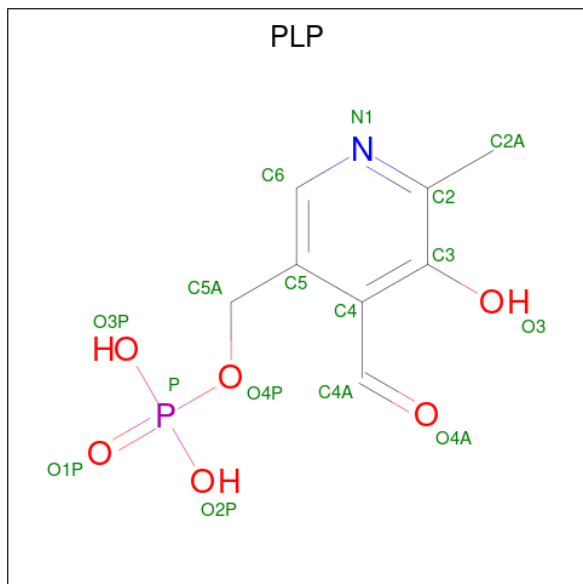
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	expression tag	UNP A3ZCM2
A	-9	ASP	-	expression tag	UNP A3ZCM2
A	-8	ASP	-	expression tag	UNP A3ZCM2
A	-7	ASP	-	expression tag	UNP A3ZCM2
A	-6	ASP	-	expression tag	UNP A3ZCM2
A	-5	LYS	-	expression tag	UNP A3ZCM2
A	-4	ASP	-	expression tag	UNP 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

Continued on next page...

Continued from previous page...

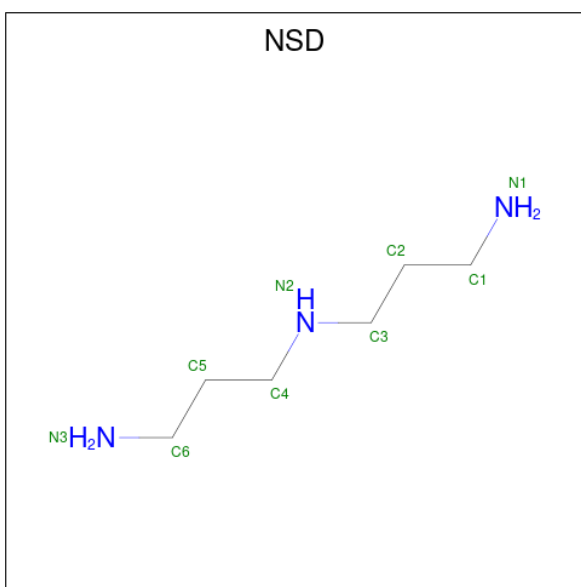
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	expression tag	UNP A3ZCM2
B	-3	HIS	-	expression tag	UNP A3ZCM2
B	-2	PRO	-	expression tag	UNP A3ZCM2
B	-1	PHE	-	expression tag	UNP A3ZCM2
B	0	THR	-	expression tag	UNP A3ZCM2

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



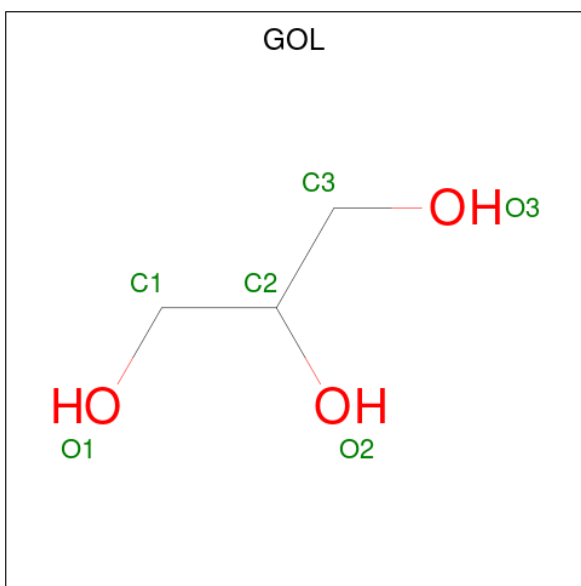
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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: C₃H₈O₃).



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		

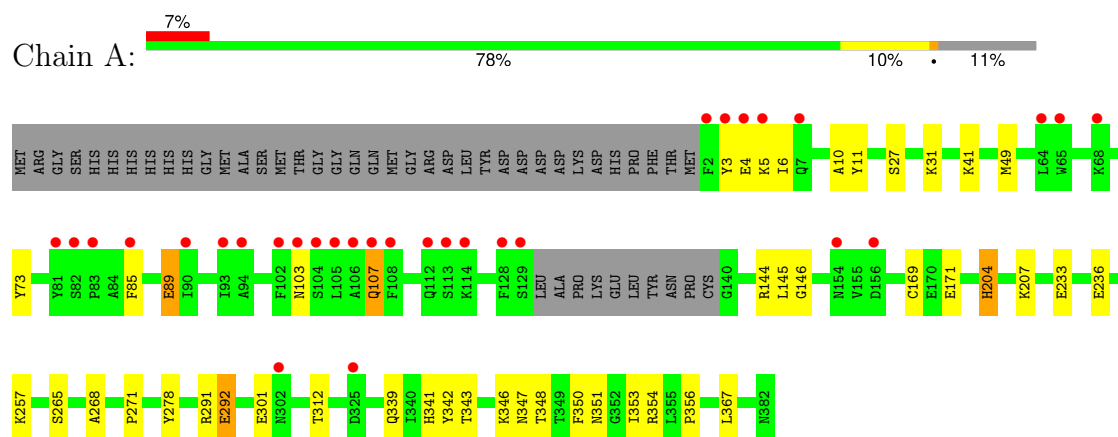
- Molecule 5 is water.

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

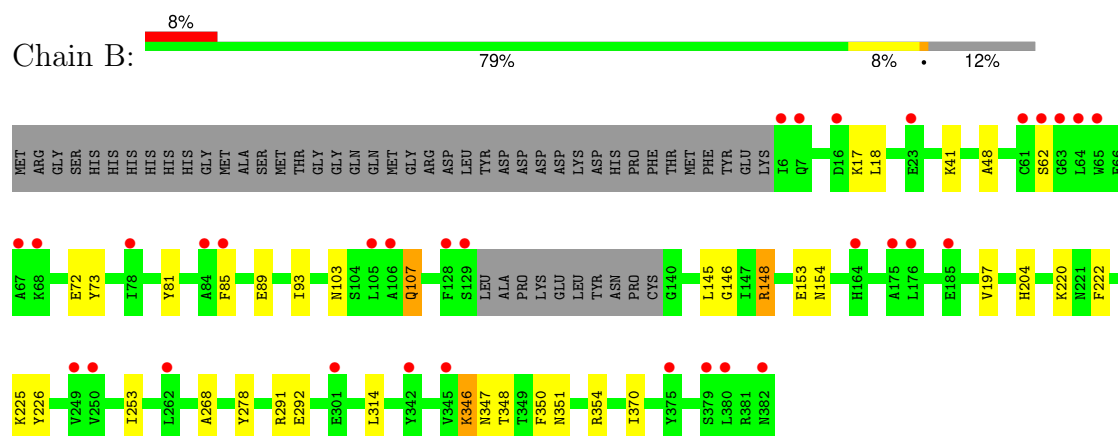
3 Residue-property plots [i](#)

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: Carboxynorspermidine decarboxylase



• Molecule 1: Carboxynorspermidine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.50Å 144.50Å 79.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.06 – 1.90 102.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (102.06-1.90) 99.7 (102.06-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.89Å)	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 (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, GOL, NSD

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	52	49
1	B	314/357 (88%)	309 (98%)	5 (2%)	58	56
All	All	633/714 (89%)	622 (98%)	11 (2%)	56	54

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 oligosaccharides 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	B	1001	1	15,15,16	1.57	5 (33%)	21,22,23	1.40	4 (19%)
4	GOL	A	1003	-	5,5,5	1.10	1 (20%)	5,5,5	1.85	2 (40%)
2	PLP	A	1001	1	15,15,16	1.27	2 (13%)	21,22,23	0.88	1 (4%)
3	NSD	A	1002	-	8,8,8	2.99	2 (25%)	7,7,7	1.65	2 (28%)
4	GOL	B	1003	-	5,5,5	0.64	0	5,5,5	0.35	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	1001	1	-	0/6/6/8	0/1/1/1
4	GOL	A	1003	-	-	3/4/4/4	-
2	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
3	NSD	A	1002	-	-	2/6/6/6	-
4	GOL	B	1003	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NSD	C4-N2	-5.97	1.27	1.47
3	A	1002	NSD	C3-N2	-5.93	1.27	1.47
2	B	1001	PLP	C5-C4	3.00	1.43	1.40
2	B	1001	PLP	C2-N1	2.77	1.38	1.33
2	A	1001	PLP	C3-C2	2.33	1.43	1.41
2	B	1001	PLP	O3-C3	2.33	1.42	1.36
2	A	1001	PLP	P-O3P	-2.22	1.46	1.54
2	B	1001	PLP	C3-C2	2.11	1.43	1.41
2	B	1001	PLP	P-O2P	-2.05	1.47	1.54
4	A	1003	GOL	O2-C2	2.05	1.49	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NSD	C2-C3-N2	2.98	120.06	112.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	GOL	O2-C2-C1	-2.96	96.92	109.18
3	A	1002	NSD	C4-N2-C3	2.78	126.57	113.40
2	B	1001	PLP	O3P-P-O4P	2.78	113.92	106.67
2	B	1001	PLP	C3-C4-C5	2.68	121.80	118.59
4	A	1003	GOL	O2-C2-C3	-2.40	99.23	109.18
2	B	1001	PLP	C4-C3-C2	-2.18	116.62	119.89
2	A	1001	PLP	C3-C2-N1	-2.17	118.23	120.96
2	B	1001	PLP	O3-C3-C2	2.04	121.81	117.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NSD	C2-C3-N2-C4
4	A	1003	GOL	O1-C1-C2-C3
4	A	1003	GOL	C1-C2-C3-O3
4	A	1003	GOL	O2-C2-C3-O3
3	A	1002	NSD	C4-C5-C6-N3
4	B	1003	GOL	C1-C2-C3-O3
4	B	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PLP	1	0
4	A	1003	GOL	2	0
2	A	1001	PLP	1	0
3	A	1002	NSD	4	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, 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	371/418 (88%)	0.44	31 (8%) 18 19	2, 16, 30, 66	2 (0%)
1	B	367/418 (87%)	0.68	32 (8%) 17 18	3, 16, 31, 47	1 (0%)
All	All	738/836 (88%)	0.56	63 (8%) 18 19	2, 16, 31, 66	3 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	ASN	7.3
1	B	6	ILE	4.8
1	A	2	PHE	4.4
1	B	65	TRP	4.4
1	B	64	LEU	4.2
1	A	3	TYR	4.0
1	A	128	PHE	4.0
1	B	129	SER	3.8
1	A	85	PHE	3.6
1	A	105	LEU	3.5
1	A	90	ILE	3.4
1	A	106	ALA	3.4
1	A	129	SER	3.4
1	A	83	PRO	3.3
1	B	128	PHE	3.2
1	A	104	SER	3.2
1	A	5	LYS	3.2
1	B	78	ILE	3.2
1	B	61	CYS	3.1
1	B	85	PHE	3.0
1	A	94	ALA	3.0
1	A	64	LEU	3.0
1	A	154	ASN	2.9
1	A	4	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	250	VAL	2.9
1	B	68	LYS	2.9
1	B	67	ALA	2.7
1	B	62	SER	2.7
1	B	105	LEU	2.7
1	B	7	GLN	2.6
1	A	103	ASN	2.6
1	B	379	SER	2.6
1	B	106	ALA	2.6
1	B	342	TYR	2.6
1	B	175	ALA	2.6
1	A	114	LYS	2.5
1	B	345	VAL	2.5
1	B	301	GLU	2.5
1	A	81	TYR	2.4
1	A	108	PHE	2.4
1	A	302	ASN	2.4
1	A	82	SER	2.4
1	B	63	GLY	2.4
1	A	65	TRP	2.4
1	B	164	HIS	2.3
1	A	7	GLN	2.3
1	B	176	LEU	2.3
1	A	113	SER	2.3
1	A	156	ASP	2.3
1	B	375	TYR	2.3
1	A	102	PHE	2.2
1	A	93	ILE	2.2
1	B	249	VAL	2.2
1	B	262	LEU	2.1
1	A	68	LYS	2.1
1	B	16	ASP	2.1
1	B	84	ALA	2.1
1	A	112	GLN	2.0
1	B	23	GLU	2.0
1	A	325	ASP	2.0
1	A	107	GLN	2.0
1	B	185	GLU	2.0
1	B	380	LEU	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(\AA^2)	Q<0.9
4	GOL	B	1003	6/6	0.57	0.24	45,55,57,58	0
3	NSD	A	1002	9/9	0.73	0.23	52,56,61,62	0
4	GOL	A	1003	6/6	0.75	0.17	38,44,46,50	0
2	PLP	B	1001	15/16	0.96	0.07	22,25,31,31	0
2	PLP	A	1001	15/16	0.96	0.08	19,25,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.