



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:09 PM GMT

PDB ID : 1NOI
Title : COMPLEX OF GLYCOGEN PHOSPHORYLASE WITH A TRANSITION
STATE ANALOGUE NOJIRIMYCIN TETRAZOLE AND PHOSPHATE IN
THE T AND R STATES
Authors : Johnson, L.N.; Mitchell, E.P.
Deposited on : 1996-03-12
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

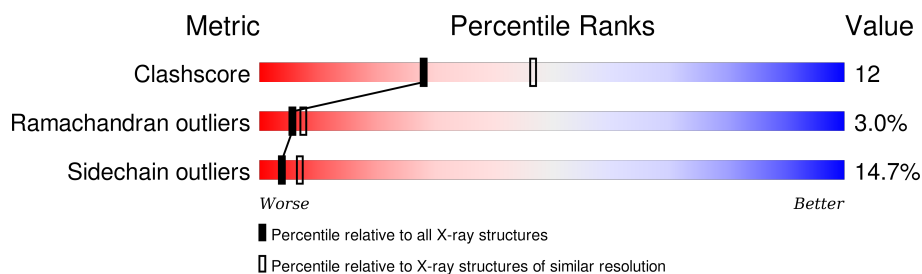
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27788 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 GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	B	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	C	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	D	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			

There are 8 discrepancies between the modelled and reference sequences:

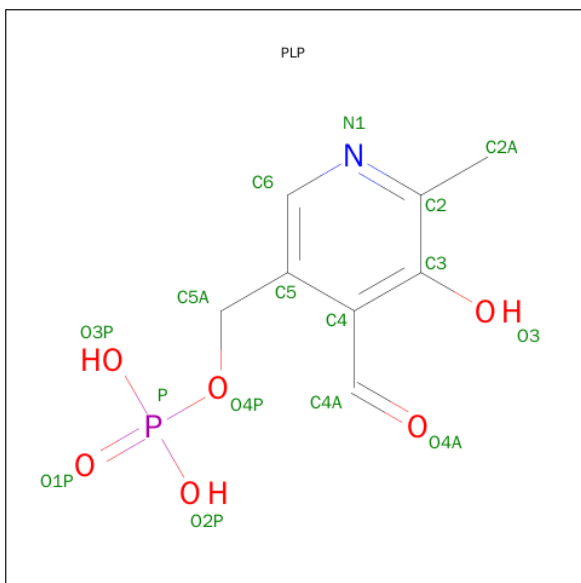
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
A	609	PRO	ALA	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
B	609	PRO	ALA	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
C	609	PRO	ALA	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489
D	609	PRO	ALA	CONFLICT	UNP P00489

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



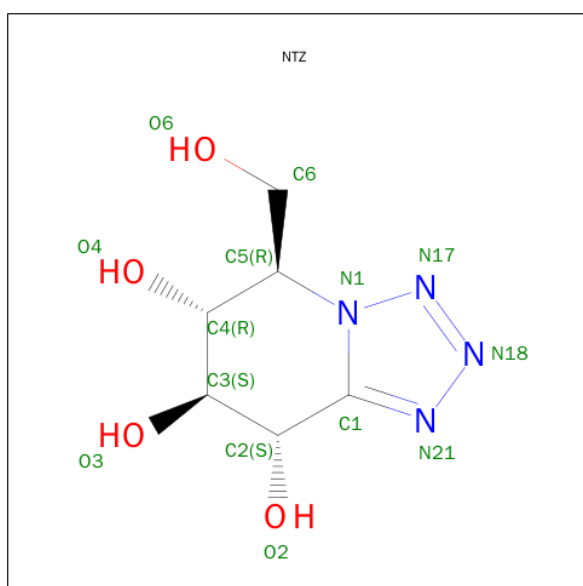
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is NOJIRIMYCINE TETRAZOLE (three-letter code: NTZ) (formula: $C_6H_{10}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	6	4	4		
4	B	1	Total	C	N	O	0	0
			14	6	4	4		
4	C	1	Total	C	N	O	0	0
			14	6	4	4		
4	D	1	Total	C	N	O	0	0
			14	6	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	222	Total	O	0	0
			222	222		

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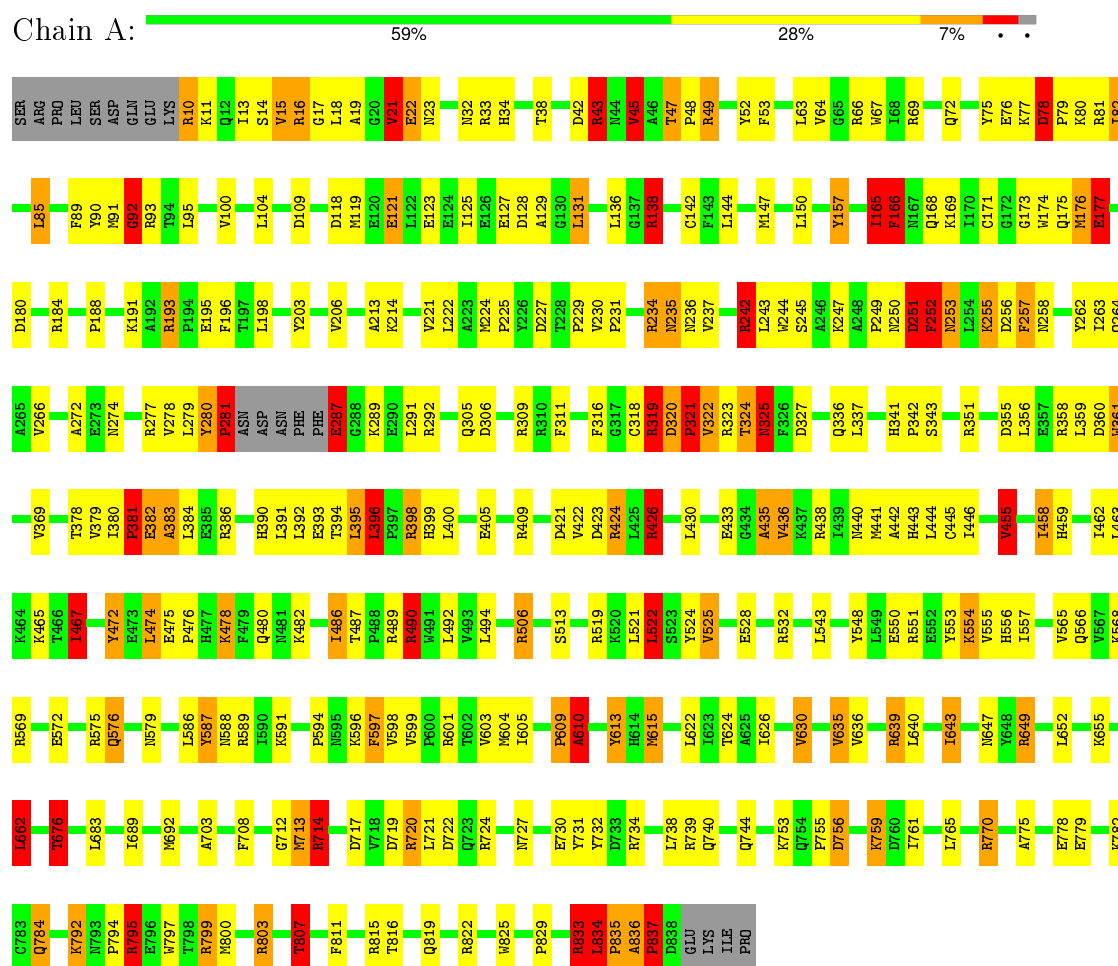
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	218	Total 218	O 218	0	0
5	D	221	Total 221	O 221	0	0

3 Residue-property plots

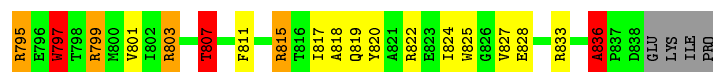
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE

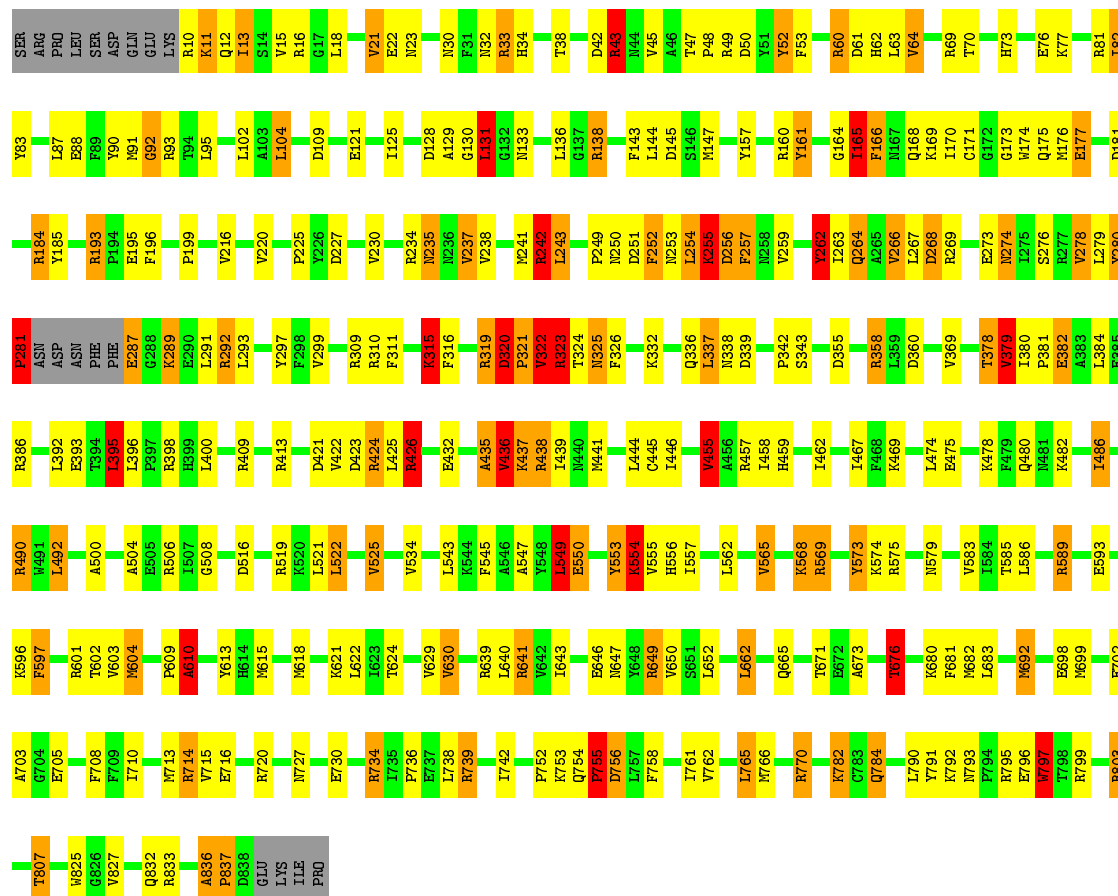






• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain D: 61% 26% 9% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00 Å 190.00 Å 88.20 Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27788	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NTZ, 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	0.91	4/6843 (0.1%)	1.80	148/9261 (1.6%)
1	B	0.89	2/6843 (0.0%)	1.77	154/9261 (1.7%)
1	C	0.88	2/6843 (0.0%)	1.71	120/9261 (1.3%)
1	D	0.91	6/6843 (0.1%)	1.83	151/9261 (1.6%)
All	All	0.90	14/27372 (0.1%)	1.78	573/37044 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	4
1	C	0	7
1	D	0	6
All	All	0	26

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	322	VAL	CA-CB	7.96	1.71	1.54
1	A	78	ASP	CA-CB	6.40	1.68	1.53
1	B	100	VAL	CA-CB	6.23	1.67	1.54
1	D	237	VAL	CA-CB	5.88	1.67	1.54
1	C	82	ILE	CA-CB	5.81	1.68	1.54

The worst 5 of 573 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	A	490	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	D	490	ARG	NE-CZ-NH2	-17.23	111.69	120.30
1	D	575	ARG	NE-CZ-NH1	15.58	128.09	120.30
1	D	575	ARG	NE-CZ-NH2	-14.13	113.23	120.30

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain
1	A	252	PHE	Sidechain
1	A	262	TYR	Sidechain
1	A	472	TYR	Sidechain
1	A	52	TYR	Sidechain

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	6692	0	6650	150	0
1	B	6692	0	6650	162	1
1	C	6692	0	6650	181	0
1	D	6692	0	6650	158	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	6	1	0
3	C	15	0	7	1	0
3	D	15	0	6	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	223	0	0	14	1
5	B	222	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	218	0	0	16	1
5	D	221	0	0	16	1
All	All	27788	0	26666	625	2

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 12.

The worst 5 of 625 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:D:322:VAL:HG13	1:D:325:ASN:HB3	1.43	0.98
1:C:171:CYS:SG	1:C:176:MET:HG3	2.09	0.92
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.54	0.90
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.58	0.86
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.58	0.84

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1030:HOH:O	5:D:1049:HOH:O[2_646]	1.46	0.74
1:B:550:GLU:OE2	5:C:1030:HOH:O[2_746]	2.04	0.16

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	822/842 (98%)	741 (90%)	52 (6%)	29 (4%)	4	6
1	B	822/842 (98%)	743 (90%)	59 (7%)	20 (2%)	7	11
1	C	822/842 (98%)	751 (91%)	46 (6%)	25 (3%)	5	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	822/842 (98%)	746 (91%)	51 (6%)	25 (3%)	5 7
All	All	3288/3368 (98%)	2981 (91%)	208 (6%)	99 (3%)	5 7

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	ALA
1	A	22	GLU
1	A	166	PHE
1	A	253	ASN

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	712/732 (97%)	592 (83%)	120 (17%)	2 4
1	B	712/732 (97%)	615 (86%)	97 (14%)	5 8
1	C	712/732 (97%)	617 (87%)	95 (13%)	5 9
1	D	712/732 (97%)	605 (85%)	107 (15%)	3 6
All	All	2848/2928 (97%)	2429 (85%)	419 (15%)	4 7

5 of 419 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	596	LYS
1	C	214	LYS
1	D	568	LYS
1	B	652	LEU
1	B	803	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	784	GLN
1	C	412	ASN
1	D	576	GLN
1	C	34	HIS
1	C	235	ASN

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 ⓘ

12 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	PO4	A	997	-	4,4,4	2.46	3 (75%)	6,6,6	0.51	0
4	NTZ	A	998	-	12,15,15	1.21	2 (16%)	12,22,22	2.99	3 (25%)
3	PLP	A	999	1	15,15,16	1.18	1 (6%)	21,22,23	1.24	4 (19%)
2	PO4	B	997	-	4,4,4	2.68	3 (75%)	6,6,6	0.44	0
4	NTZ	B	998	-	12,15,15	1.90	6 (50%)	12,22,22	2.38	4 (33%)
3	PLP	B	999	1	15,15,16	1.54	2 (13%)	21,22,23	1.19	2 (9%)
2	PO4	C	997	-	4,4,4	2.75	3 (75%)	6,6,6	0.48	0
4	NTZ	C	998	-	12,15,15	2.21	5 (41%)	12,22,22	2.81	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	C	999	1	15,15,16	1.92	3 (20%)	21,22,23	1.21	2 (9%)
2	PO4	D	997	-	4,4,4	2.61	3 (75%)	6,6,6	0.46	0
4	NTZ	D	998	-	12,15,15	1.90	4 (33%)	12,22,22	4.53	4 (33%)
3	PLP	D	999	1	15,15,16	1.92	1 (6%)	21,22,23	1.15	2 (9%)

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	PO4	A	997	-	-	0/0/0/0	0/0/0/0
4	NTZ	A	998	-	-	0/2/22/22	0/1/2/2
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
2	PO4	B	997	-	-	0/0/0/0	0/0/0/0
4	NTZ	B	998	-	-	0/2/22/22	0/1/2/2
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1
2	PO4	C	997	-	-	0/0/0/0	0/0/0/0
4	NTZ	C	998	-	-	0/2/22/22	0/1/2/2
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1
2	PO4	D	997	-	-	0/0/0/0	0/0/0/0
4	NTZ	D	998	-	-	0/2/22/22	0/1/2/2
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	PLP	C3-C2	-6.37	1.36	1.40
3	C	999	PLP	C3-C2	-5.25	1.37	1.40
3	B	999	PLP	C3-C2	-3.70	1.38	1.40
2	C	997	PO4	P-O2	-3.66	1.40	1.53
2	D	997	PO4	P-O2	-3.38	1.41	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	998	NTZ	N21-N18-N17	-5.02	104.04	110.09
4	B	998	NTZ	C1-C2-C3	-3.68	105.86	113.17
3	C	999	PLP	O4P-C5A-C5	-2.95	104.11	108.99
3	A	999	PLP	O2P-P-O4P	-2.91	98.19	106.56
4	A	998	NTZ	C1-C2-C3	-2.63	107.96	113.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	PLP	1	0
2	C	997	PO4	1	0
3	C	999	PLP	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.