



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NOJ  
Title : COMPLEX OF GLYCOGEN PHOSPHORYLASE WITH A TRANSITION  
STATE ANALOGUE NOJIRIMYCIN TETRAZOLE AND PHOSPHATE IN  
THE T STATE  
Authors : Johnson, L.N.; Mitchell, E.P.  
Deposited on : 1996-03-12  
Resolution : 2.40 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) : **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

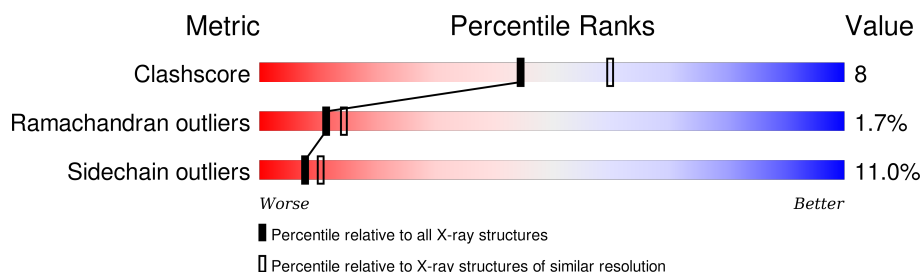
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	 68% 24% 5% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7187 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.

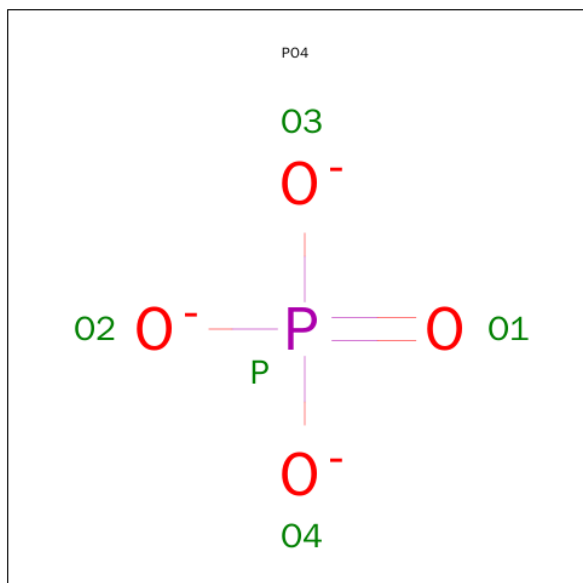
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	831	6759	4308	1191	1230	30	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

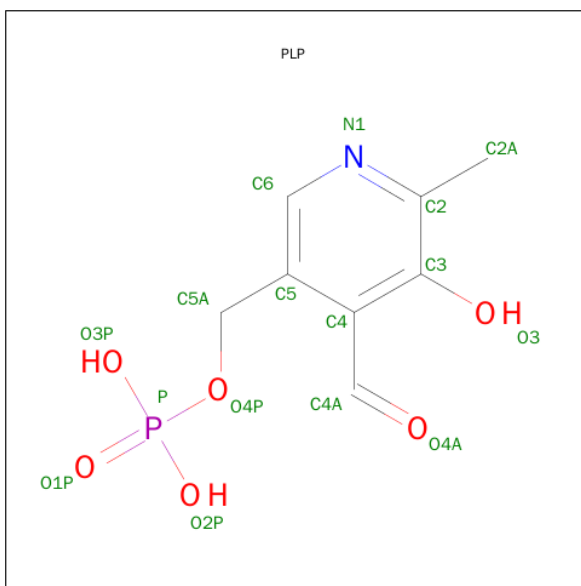
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
A	609	PRO	ALA	CONFLICT	UNP P00489

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



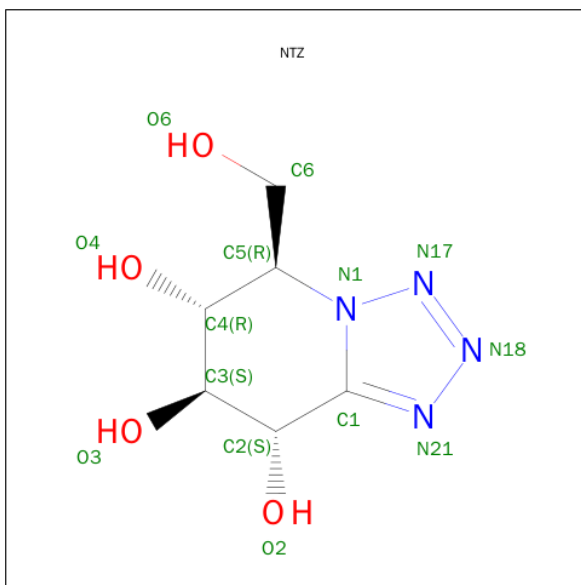
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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		

- Molecule 5 is water.

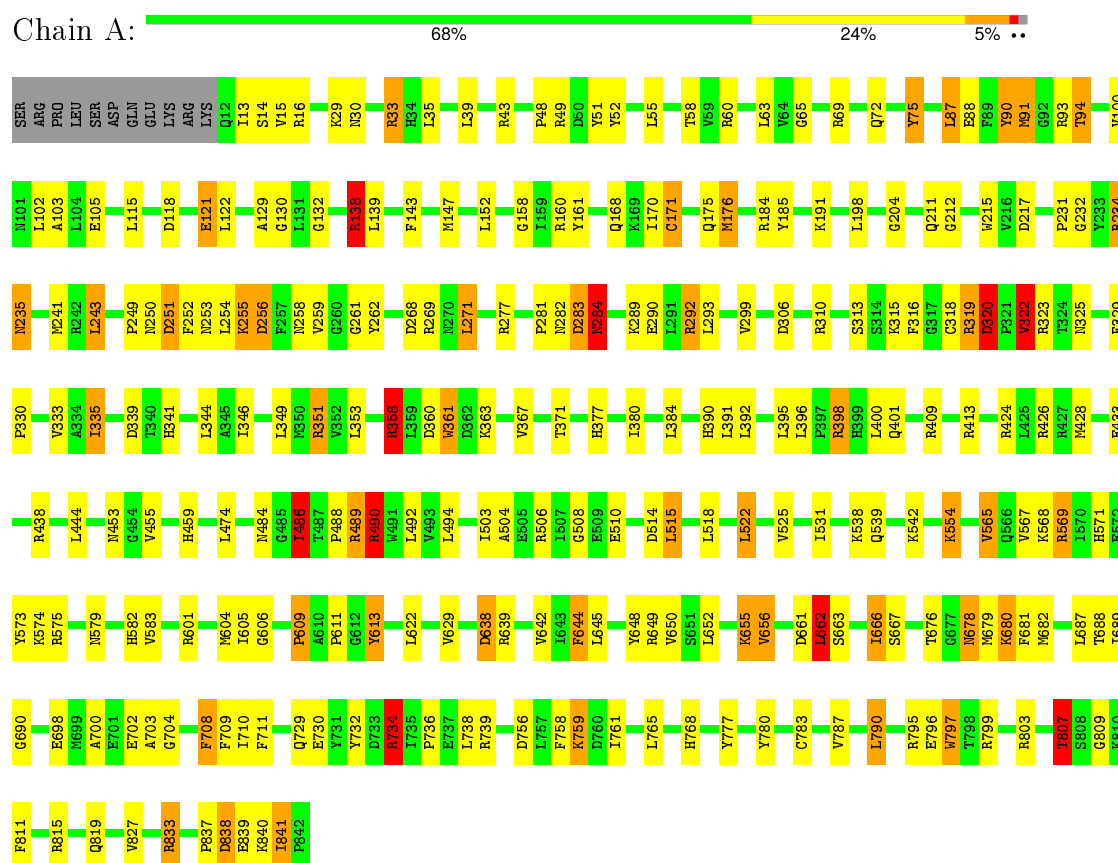
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	389	Total 389	O 389	0	0

### 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 ( $RSRZ > 2$ ). 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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.50 Å   128.50 Å   116.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.40)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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	0.79	1/6913 (0.0%)	1.58	86/9356 (0.9%)

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	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ASN	CA-CB	6.40	1.69	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	A	490	ARG	NE-CZ-NH2	-15.31	112.64	120.30
1	A	575	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	A	490	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	A	428	MET	CA-CB-CG	10.40	130.98	113.30
1	A	75	TYR	CB-CG-CD2	-9.95	115.03	121.00
1	A	413	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	90	TYR	CB-CG-CD2	-8.98	115.61	121.00
1	A	807	THR	N-CA-CB	-8.82	93.55	110.30
1	A	283	ASP	N-CA-C	-8.38	88.37	111.00
1	A	90	TYR	CB-CG-CD1	8.08	125.85	121.00
1	A	413	ARG	NE-CZ-NH1	8.07	124.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	TYR	CB-CG-CD1	7.82	125.69	121.00
1	A	666	ILE	N-CA-CB	-7.79	92.88	110.80
1	A	569	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	A	650	VAL	CG1-CB-CG2	-7.61	98.72	110.90
1	A	486	ILE	CA-CB-CG1	-7.46	96.82	111.00
1	A	93	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	438	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	138	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	682	MET	CG-SD-CE	7.17	111.68	100.20
1	A	184	ARG	CA-CB-CG	7.16	129.15	113.40
1	A	424	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	575	ARG	CB-CG-CD	-6.90	93.66	111.60
1	A	333	VAL	CG1-CB-CG2	-6.74	100.11	110.90
1	A	51	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	A	121	GLU	CA-CB-CG	6.55	127.80	113.40
1	A	734	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	184	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	601	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	253	ASN	N-CA-C	-6.38	93.77	111.00
1	A	656	VAL	CB-CA-C	-6.35	99.34	111.40
1	A	413	ARG	CB-CG-CD	-6.32	95.16	111.60
1	A	841	ILE	N-CA-C	-6.30	94.00	111.00
1	A	777	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	251	ASP	CA-C-N	6.27	130.99	117.20
1	A	234	ARG	CG-CD-NE	6.26	124.94	111.80
1	A	351	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	486	ILE	CA-CB-CG2	6.17	123.23	110.90
1	A	249	PRO	N-CD-CG	-6.12	94.02	103.20
1	A	171	CYS	CA-CB-SG	6.09	124.96	114.00
1	A	358	ARG	CA-CB-CG	6.09	126.79	113.40
1	A	234	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	284	ASN	CA-C-N	-5.99	104.02	117.20
1	A	185	TYR	CB-CG-CD2	5.99	124.59	121.00
1	A	663	SER	CA-C-N	5.95	130.28	117.20
1	A	569	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
1	A	322	VAL	N-CA-C	5.93	127.00	111.00
1	A	506	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	33	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	170	ILE	N-CA-C	-5.89	95.11	111.00
1	A	613	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	565	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	A	310	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	91	MET	CG-SD-CE	5.68	109.30	100.20
1	A	215	TRP	N-CA-C	-5.60	95.88	111.00
1	A	663	SER	O-C-N	-5.57	113.79	122.70
1	A	255	LYS	CA-CB-CG	5.57	125.64	113.40
1	A	256	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	283	ASP	CA-CB-CG	5.51	125.52	113.40
1	A	398	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	662	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	A	277	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	649	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	14	SER	N-CA-C	-5.39	96.44	111.00
1	A	63	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	489	ARG	NE-CZ-NH2	5.37	122.99	120.30
1	A	490	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	401	GLN	N-CA-CB	-5.35	100.97	110.60
1	A	15	VAL	N-CA-C	-5.34	96.58	111.00
1	A	506	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	361	TRP	CG-CD2-CE3	-5.31	129.12	133.90
1	A	284	ASN	C-N-CA	5.29	134.92	121.70
1	A	609	PRO	N-CA-CB	5.28	109.63	103.30
1	A	367	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	A	680	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	613	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	87	LEU	CA-CB-CG	-5.15	103.46	115.30
1	A	573	TYR	CB-CG-CD2	5.15	124.09	121.00
1	A	629	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	A	161	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	292	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	655	LYS	CA-CB-CG	-5.10	102.18	113.40
1	A	90	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	346	ILE	CA-C-O	-5.02	109.56	120.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ASN	Mainchain
1	A	262	TYR	Sidechain
1	A	320	ASP	Peptide
1	A	341	HIS	Sidechain
1	A	52	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	644	PHE	Sidechain
1	A	681	PHE	Sidechain
1	A	711	PHE	Sidechain
1	A	75	TYR	Sidechain
1	A	811	PHE	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	6759	0	6699	107	0
2	A	10	0	0	0	0
3	A	15	0	7	0	0
4	A	14	0	10	0	0
5	A	389	0	0	9	0
All	All	7187	0	6716	107	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 8.

All (107) 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:252:PHE:HA	1:A:255:LYS:HB3	1.53	0.90
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.64	0.77
1:A:118:ASP:HB3	1:A:121:GLU:HG3	1.75	0.69
1:A:504:ALA:HA	1:A:508:GLY:O	1.94	0.68
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.77	0.65
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.79	0.65
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.79	0.63
1:A:662:LEU:HD22	1:A:689:ILE:HG22	1.80	0.62
1:A:486:ILE:HG12	1:A:680:LYS:HG2	1.83	0.60
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.66	0.60
1:A:569:ARG:HG3	1:A:571:HIS:CD2	2.36	0.59
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.85	0.58
1:A:758:PHE:HD1	1:A:761:ILE:HD12	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:O	1:A:138:ARG:HD3	2.04	0.56
1:A:283:ASP:HB3	1:A:569:ARG:HD2	1.87	0.56
1:A:455:VAL:H	1:A:459:HIS:HD2	1.53	0.56
1:A:678:ASN:HD22	1:A:679:MET:H	1.52	0.56
1:A:94:THR:HG21	5:A:1280:HOH:O	2.03	0.56
1:A:390:HIS:HD2	5:A:1181:HOH:O	1.88	0.56
1:A:488:PRO:O	1:A:492:LEU:HB3	2.05	0.56
1:A:690:GLY:O	1:A:710:ILE:HA	2.05	0.56
1:A:730:GLU:O	1:A:734:ARG:HG2	2.06	0.55
1:A:171:CYS:HB3	1:A:176:MET:HE2	1.88	0.55
1:A:799:ARG:O	1:A:803:ARG:HG3	2.06	0.54
1:A:293:LEU:HD21	1:A:392:LEU:HD23	1.90	0.54
1:A:13:ILE:H	1:A:13:ILE:HD12	1.73	0.54
1:A:129:ALA:HB2	5:A:1011:HOH:O	2.07	0.54
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.43	0.54
1:A:503:ILE:HD13	1:A:518:LEU:HD11	1.89	0.53
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.49	0.53
1:A:583:VAL:HG11	1:A:642:VAL:HG21	1.91	0.53
1:A:315:LYS:HB3	1:A:319:ARG:NH1	2.24	0.52
1:A:252:PHE:CE1	1:A:256:ASP:HB2	2.45	0.52
1:A:69:ARG:CZ	1:A:837:PRO:HA	2.41	0.51
1:A:708:PHE:CD2	1:A:710:ILE:HD13	2.45	0.51
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.93	0.51
1:A:833:ARG:N	1:A:833:ARG:HE	2.08	0.51
1:A:815:ARG:HH11	1:A:819:GLN:NE2	2.09	0.50
1:A:729:GLN:O	1:A:732:TYR:HB3	2.12	0.50
1:A:708:PHE:HD2	1:A:710:ILE:HD13	1.77	0.50
1:A:69:ARG:HA	1:A:72:GLN:HE21	1.76	0.50
1:A:490:ARG:HD2	5:A:1259:HOH:O	2.11	0.50
1:A:732:TYR:O	1:A:739:ARG:HG3	2.13	0.49
1:A:736:PRO:HG3	1:A:739:ARG:NH2	2.27	0.49
1:A:35:LEU:O	1:A:39:LEU:HB2	2.12	0.49
1:A:320:ASP:O	1:A:322:VAL:N	2.47	0.48
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.96	0.47
1:A:212:GLY:HA3	1:A:358:ARG:NH2	2.28	0.47
1:A:252:PHE:HA	1:A:255:LYS:CB	2.37	0.47
1:A:703:ALA:HB2	1:A:807:THR:CG2	2.44	0.47
1:A:525:VAL:O	1:A:531:ILE:HD11	2.15	0.46
1:A:152:LEU:HD22	1:A:827:VAL:HG11	1.98	0.46
1:A:698:GLU:O	1:A:702:GLU:HB2	2.16	0.45
1:A:569:ARG:HG2	1:A:574:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:O	1:A:103:ALA:HB3	2.17	0.45
1:A:252:PHE:CZ	1:A:256:ASP:HB2	2.52	0.45
1:A:538:LYS:O	1:A:542:LYS:HG3	2.16	0.45
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.98	0.45
1:A:490:ARG:HA	1:A:494:LEU:CB	2.47	0.45
1:A:703:ALA:CB	1:A:807:THR:HG21	2.47	0.44
1:A:283:ASP:HB3	1:A:569:ARG:CD	2.46	0.44
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.52	0.44
1:A:250:ASN:CA	1:A:269:ARG:HH12	2.30	0.44
1:A:567:VAL:HA	1:A:606:GLY:O	2.18	0.44
1:A:486:ILE:CD1	1:A:676:THR:HB	2.47	0.44
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.82	0.44
1:A:105:GLU:HG2	5:A:1142:HOH:O	2.17	0.44
1:A:395:LEU:HG	1:A:396:LEU:HG	2.00	0.44
1:A:351:ARG:HG2	1:A:351:ARG:HH11	1.83	0.44
1:A:661:ASP:HB3	1:A:797:TRP:CZ3	2.53	0.44
1:A:100:VAL:O	1:A:234:ARG:NH1	2.51	0.44
1:A:289:LYS:HD3	1:A:289:LYS:HA	1.90	0.43
1:A:211:GLN:NE2	1:A:211:GLN:HA	2.33	0.43
1:A:158:GLY:O	1:A:243:LEU:HA	2.18	0.43
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.54	0.43
1:A:283:ASP:CB	1:A:569:ARG:HD2	2.48	0.43
1:A:700:ALA:O	1:A:704:GLY:N	2.52	0.43
1:A:795:ARG:O	1:A:799:ARG:HG3	2.19	0.43
1:A:319:ARG:HD3	1:A:320:ASP:OD1	2.19	0.43
1:A:143:PHE:O	1:A:147:MET:HG3	2.19	0.43
1:A:290:GLU:HG3	1:A:391:LEU:HD11	2.00	0.43
1:A:709:PHE:HZ	1:A:790:LEU:HD12	1.84	0.43
1:A:565:VAL:HA	1:A:604:MET:O	2.19	0.43
1:A:91:MET:HE3	1:A:241:MET:SD	2.59	0.42
1:A:282:ASN:O	1:A:284:ASN:N	2.51	0.42
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.99	0.42
1:A:329:PHE:HB3	1:A:330:PRO:HD3	2.01	0.42
1:A:35:LEU:CD2	1:A:43:ARG:HG2	2.50	0.42
1:A:261:GLY:HA3	5:A:1173:HOH:O	2.18	0.42
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.84	0.42
1:A:335:ILE:HG23	1:A:371:THR:HG22	2.01	0.42
1:A:16:ARG:HA	5:A:1070:HOH:O	2.18	0.42
1:A:538:LYS:HE2	1:A:538:LYS:HB2	1.96	0.42
1:A:756:ASP:O	1:A:759:LYS:HB2	2.20	0.42
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:C	1:A:837:PRO:HG2	2.40	0.41
1:A:204:GLY:HA2	1:A:217:ASP:O	2.21	0.41
1:A:130:GLY:N	5:A:1160:HOH:O	2.52	0.41
1:A:234:ARG:CG	1:A:234:ARG:HH11	2.33	0.41
1:A:87:LEU:HD11	1:A:299:VAL:HG11	2.02	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.16	0.41
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	0.41
1:A:349:LEU:O	1:A:353:LEU:HG	2.22	0.41
1:A:139:LEU:CD2	1:A:377:HIS:HE1	2.34	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.95	0.41
1:A:484:ASN:ND2	5:A:1036:HOH:O	2.55	0.40
1:A:688:THR:HB	1:A:708:PHE:CE2	2.57	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	829/842 (98%)	749 (90%)	66 (8%)	14 (2%)	11	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	LEU
1	A	313	SER
1	A	318	CYS
1	A	320	ASP
1	A	322	VAL
1	A	838	ASP
1	A	259	VAL
1	A	254	LEU
1	A	339	ASP

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Mol	Chain	Res	Type
1	A	554	LYS
1	A	268	ASP
1	A	638	ASP
1	A	284	ASN
1	A	609	PRO

### 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	720/732 (98%)	641 (89%)	79 (11%)	8 10

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	33	ARG
1	A	48	PRO
1	A	49	ARG
1	A	55	LEU
1	A	60	ARG
1	A	90	TYR
1	A	94	THR
1	A	115	LEU
1	A	122	LEU
1	A	138	ARG
1	A	176	MET
1	A	191	LYS
1	A	198	LEU
1	A	231	PRO
1	A	235	ASN
1	A	243	LEU
1	A	251	ASP
1	A	281	PRO
1	A	292	ARG
1	A	306	ASP

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Mol	Chain	Res	Type
1	A	316	PHE
1	A	319	ARG
1	A	323	ARG
1	A	325	ASN
1	A	335	ILE
1	A	344	LEU
1	A	358	ARG
1	A	360	ASP
1	A	363	LYS
1	A	380	ILE
1	A	384	LEU
1	A	398	ARG
1	A	400	LEU
1	A	426	ARG
1	A	433	GLU
1	A	444	LEU
1	A	453	ASN
1	A	474	LEU
1	A	486	ILE
1	A	489	ARG
1	A	490	ARG
1	A	510	GLU
1	A	514	ASP
1	A	515	LEU
1	A	522	LEU
1	A	539	GLN
1	A	554	LYS
1	A	568	LYS
1	A	579	ASN
1	A	611	PRO
1	A	613	TYR
1	A	622	LEU
1	A	638	ASP
1	A	639	ARG
1	A	645	LEU
1	A	655	LYS
1	A	656	VAL
1	A	662	LEU
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	687	LEU

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Mol	Chain	Res	Type
1	A	708	PHE
1	A	734	ARG
1	A	738	LEU
1	A	759	LYS
1	A	765	LEU
1	A	768	HIS
1	A	787	VAL
1	A	790	LEU
1	A	796	GLU
1	A	797	TRP
1	A	807	THR
1	A	833	ARG
1	A	838	ASP
1	A	839	GLU
1	A	840	LYS
1	A	841	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	72	GLN
1	A	114	GLN
1	A	211	GLN
1	A	235	ASN
1	A	390	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	819	GLN

### 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 ⓘ

4 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	996	-	4,4,4	2.92	3 (75%)	6,6,6	0.42	0
2	PO4	A	997	-	4,4,4	2.50	3 (75%)	6,6,6	0.59	0
4	NTZ	A	998	-	12,15,15	1.82	3 (25%)	12,22,22	2.49	1 (8%)
3	PLP	A	999	1	15,15,16	1.97	3 (20%)	21,22,23	1.39	4 (19%)

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	996	-	-	0/0/0/0	0/0/0/0
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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-5.65	1.36	1.40
2	A	996	PO4	P-O4	-3.95	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	PO4	P-O2	-3.31	1.41	1.53
2	A	996	PO4	P-O3	-2.79	1.43	1.53
2	A	996	PO4	P-O1	-2.75	1.40	1.52
2	A	997	PO4	P-O3	-2.63	1.43	1.53
3	A	999	PLP	P-O3P	-2.62	1.45	1.54
2	A	997	PO4	P-O4	-2.44	1.44	1.53
3	A	999	PLP	C5-C4	-2.39	1.37	1.40
4	A	998	NTZ	N17-N1	2.46	1.39	1.34
4	A	998	NTZ	N21-N18	2.50	1.38	1.34
4	A	998	NTZ	N17-N18	4.12	1.40	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	C4A-C4-C5	-2.79	117.98	120.88
3	A	999	PLP	C5-C6-N1	-2.47	119.57	123.86
3	A	999	PLP	C6-C5-C4	2.39	120.18	118.15
3	A	999	PLP	O3P-P-O1P	2.40	118.32	110.58
4	A	998	NTZ	N18-N17-N1	7.90	110.26	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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