



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 AM UTC

PDB ID : 1NOJ / pdb_00001noj
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.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

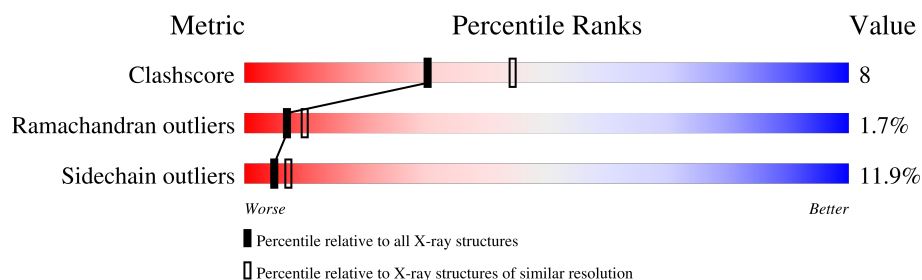
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	60%31%6% ..

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
2	PO4	A	996	-	X	-	-
2	PO4	A	997	-	X	-	-

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:

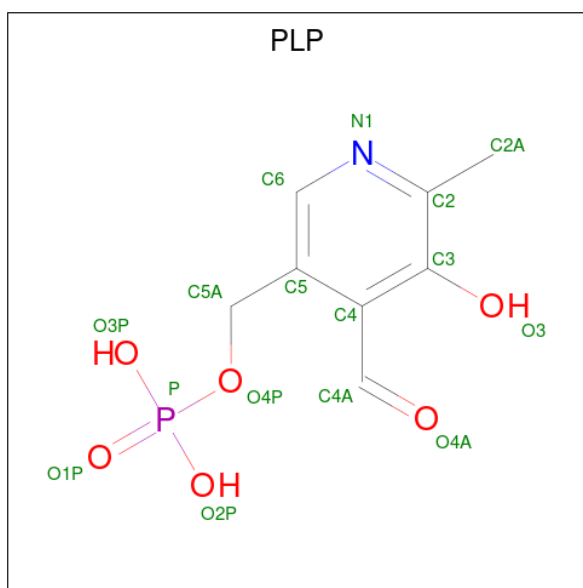
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
A	609	PRO	ALA	conflict	UNP P00489

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



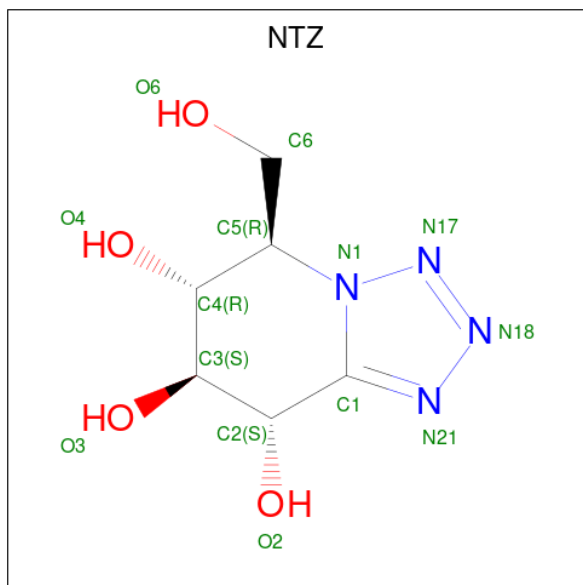
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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 (CCD ID: 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.

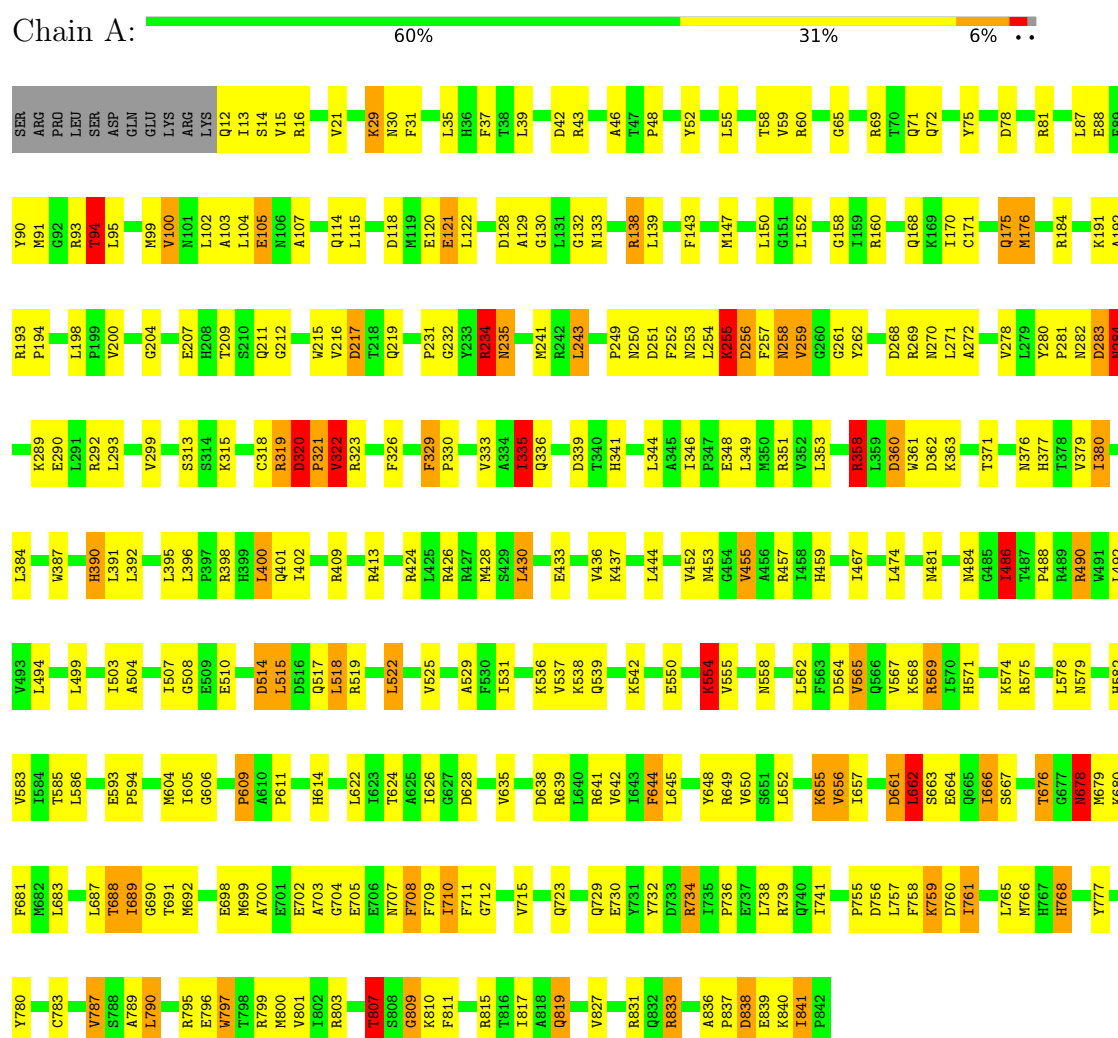
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	389	Total 389	O 389	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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 is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 128.50Å 116.30Å 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 ²)	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: PLP, PO4, NTZ

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	1.03	14/6913 (0.2%)	1.92	186/9356 (2.0%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ASN	CA-CB	9.66	1.69	1.53
1	A	335	ILE	CA-CB	8.31	1.64	1.54
1	A	841	ILE	CA-CB	7.93	1.64	1.54
1	A	379	VAL	CA-CB	6.76	1.62	1.54
1	A	689	ILE	CA-CB	6.48	1.61	1.54
1	A	94	THR	CA-CB	6.42	1.63	1.53
1	A	787	VAL	CA-CB	6.26	1.62	1.54
1	A	21	VAL	CA-CB	5.40	1.60	1.54
1	A	380	ILE	CA-CB	5.30	1.61	1.53
1	A	284	ASN	N-CA	5.28	1.53	1.46
1	A	283	ASP	CA-CB	5.27	1.62	1.53
1	A	657	ILE	CA-CB	5.12	1.57	1.53
1	A	320	ASP	CA-CB	5.05	1.61	1.53
1	A	258	ASN	N-CA	5.05	1.53	1.46

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ASP	CA-CB-CG	12.92	125.52	112.60
1	A	841	ILE	N-CA-C	-12.74	94.00	107.89
1	A	666	ILE	N-CA-CB	-11.12	92.88	111.23
1	A	807	THR	N-CA-CB	-10.70	93.55	111.20
1	A	283	ASP	N-CA-C	-10.53	88.37	110.80
1	A	360	ASP	CA-CB-CG	10.07	122.67	112.60
1	A	656	VAL	CB-CA-C	-9.87	99.34	111.97
1	A	676	THR	N-CA-C	-9.61	103.67	114.62
1	A	253	ASN	N-CA-C	-9.29	93.77	108.63
1	A	170	ILE	N-CA-C	-8.75	95.11	107.80
1	A	14	SER	N-CA-C	-8.54	96.44	108.23
1	A	322	VAL	N-CA-C	8.49	127.00	109.34
1	A	657	ILE	O-C-N	-8.45	114.07	120.07
1	A	428	MET	CA-CB-CG	8.44	130.98	114.10
1	A	575	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	430	LEU	N-CA-C	-8.05	102.91	112.89
1	A	251	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	486	ILE	CA-CB-CG1	-7.99	96.82	110.40
1	A	575	ARG	N-CA-C	7.95	122.36	111.39
1	A	656	VAL	N-CA-CB	7.84	119.73	110.55
1	A	663	SER	O-C-N	-7.79	113.79	123.05
1	A	284	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	A	346	ILE	CA-C-O	-7.75	109.56	119.95
1	A	215	TRP	N-CA-C	-7.75	95.88	108.52
1	A	575	ARG	CB-CG-CD	-7.67	93.66	111.30
1	A	184	ARG	CA-CB-CG	7.52	129.15	114.10
1	A	486	ILE	CA-CB-CG2	7.49	123.23	110.50
1	A	562	LEU	N-CA-C	-7.43	97.89	109.25
1	A	402	ILE	N-CA-C	-7.36	103.61	110.53
1	A	270	ASN	CA-CB-CG	-7.34	105.25	112.60
1	A	216	VAL	N-CA-CB	-7.34	102.25	112.52
1	A	284	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	507	ILE	N-CA-C	7.29	120.04	112.83
1	A	490	ARG	NE-CZ-NH2	-7.28	112.64	119.20
1	A	272	ALA	N-CA-C	-7.22	104.27	113.23
1	A	761	ILE	N-CA-C	-7.20	103.83	110.82
1	A	579	ASN	CB-CG-ND2	7.13	127.09	116.40
1	A	807	THR	CB-CA-C	7.09	122.51	111.02
1	A	114	GLN	OE1-CD-NE2	-7.05	115.55	122.60
1	A	413	ARG	CB-CG-CD	-7.02	95.16	111.30
1	A	46	ALA	N-CA-C	6.98	120.06	108.96
1	A	424	ARG	O-C-N	6.93	129.57	122.09
1	A	579	ASN	OD1-CG-ND2	-6.88	115.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	CA-CB-CG	6.85	127.80	114.10
1	A	209	THR	N-CA-C	-6.82	101.34	110.55
1	A	348	GLU	CA-C-O	-6.78	113.72	120.70
1	A	31	PHE	N-CA-C	-6.70	103.91	111.14
1	A	564	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	529	ALA	N-CA-C	-6.62	103.99	111.14
1	A	193	ARG	CA-C-N	6.61	127.14	119.47
1	A	193	ARG	C-N-CA	6.61	127.14	119.47
1	A	757	LEU	N-CA-C	6.58	119.29	111.33
1	A	656	VAL	CA-C-N	6.57	124.38	120.24
1	A	656	VAL	C-N-CA	6.57	124.38	120.24
1	A	278	VAL	N-CA-C	6.56	118.16	108.45
1	A	683	LEU	N-CA-C	6.53	120.34	112.38
1	A	789	ALA	N-CA-C	-6.45	103.94	110.97
1	A	21	VAL	N-CA-CB	-6.45	103.59	110.62
1	A	284	ASN	CA-C-N	6.41	134.92	121.91
1	A	284	ASN	C-N-CA	6.41	134.92	121.91
1	A	257	PHE	CA-CB-CG	6.41	120.20	113.80
1	A	284	ASN	CB-CG-ND2	6.35	125.92	116.40
1	A	100	VAL	CA-C-O	-6.34	114.50	121.29
1	A	358	ARG	CA-CB-CG	6.34	126.79	114.10
1	A	712	GLY	O-C-N	6.28	128.88	122.91
1	A	424	ARG	N-CA-C	-6.26	104.38	111.14
1	A	251	ASP	CA-C-O	-6.26	111.56	120.51
1	A	707	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	579	ASN	CA-CB-CG	6.25	118.85	112.60
1	A	578	LEU	N-CA-C	-6.24	104.56	111.36
1	A	499	LEU	N-CA-C	-6.22	104.42	111.07
1	A	666	ILE	CB-CA-C	6.22	121.49	111.29
1	A	128	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	401	GLN	N-CA-CB	-6.20	100.97	110.20
1	A	326	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	481	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	15	VAL	N-CA-C	-6.13	96.58	109.34
1	A	249	PRO	N-CD-CG	-6.12	94.02	103.20
1	A	217	ASP	N-CA-C	6.10	120.04	112.24
1	A	626	ILE	N-CA-C	-6.08	104.81	110.53
1	A	650	VAL	CA-C-O	-6.08	114.95	121.27
1	A	609	PRO	N-CA-CB	6.08	109.63	103.25
1	A	336	GLN	CA-C-O	-6.05	113.88	120.36
1	A	678	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	255	LYS	N-CA-C	-6.03	106.56	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	ILE	N-CA-CB	-5.98	100.86	111.93
1	A	800	MET	N-CA-C	-5.97	104.68	111.07
1	A	436	VAL	N-CA-C	-5.97	99.04	107.75
1	A	655	LYS	CA-CB-CG	-5.96	102.18	114.10
1	A	234	ARG	CG-CD-NE	5.88	124.94	112.00
1	A	518	LEU	N-CA-C	-5.87	105.38	112.54
1	A	817	ILE	CA-C-O	-5.86	114.64	120.85
1	A	329	PHE	CA-C-N	5.80	125.42	119.56
1	A	329	PHE	C-N-CA	5.80	125.42	119.56
1	A	777	TYR	CA-C-O	-5.78	114.93	121.00
1	A	514	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	255	LYS	CA-CB-CG	5.77	125.64	114.10
1	A	59	VAL	N-CA-C	-5.73	105.26	110.82
1	A	741	ILE	CB-CA-C	-5.73	104.64	111.97
1	A	320	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	624	THR	N-CA-C	-5.67	105.18	111.36
1	A	175	GLN	O-C-N	5.67	129.80	122.89
1	A	517	GLN	CA-CB-CG	-5.65	102.81	114.10
1	A	42	ASP	CA-CB-CG	5.64	118.25	112.60
1	A	575	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	A	121	GLU	CB-CA-C	-5.62	102.06	110.88
1	A	94	THR	O-C-N	-5.60	115.41	122.19
1	A	554	LYS	N-CA-C	5.59	122.70	110.80
1	A	249	PRO	N-CA-C	-5.57	102.38	110.80
1	A	121	GLU	CA-C-N	5.57	127.74	120.28
1	A	121	GLU	C-N-CA	5.57	127.74	120.28
1	A	691	THR	O-C-N	-5.56	115.81	122.65
1	A	376	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	387	TRP	N-CA-C	5.52	119.44	109.44
1	A	284	ASN	N-CA-C	5.52	122.56	110.80
1	A	455	VAL	N-CA-C	5.52	117.51	111.77
1	A	71	GLN	N-CA-C	5.51	117.29	111.28
1	A	452	VAL	N-CA-C	-5.51	100.24	108.46
1	A	107	ALA	N-CA-C	-5.51	105.19	111.14
1	A	120	GLU	CA-C-O	-5.50	113.88	120.10
1	A	801	VAL	CA-C-O	-5.50	115.56	121.27
1	A	650	VAL	CG1-CB-CG2	-5.49	98.72	110.80
1	A	569	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	A	258	ASN	N-CA-C	-5.46	103.91	111.28
1	A	519	ARG	CA-CB-CG	-5.45	103.20	114.10
1	A	550	GLU	CA-C-N	5.44	127.89	120.54
1	A	550	GLU	C-N-CA	5.44	127.89	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	760	ASP	N-CA-C	5.43	118.11	111.82
1	A	133	ASN	N-CA-C	-5.39	106.76	113.55
1	A	558	ASN	O-C-N	-5.38	116.36	121.20
1	A	400	LEU	N-CA-C	-5.38	106.22	112.89
1	A	768	HIS	CA-CB-CG	5.37	119.17	113.80
1	A	467	ILE	N-CA-CB	-5.37	104.27	110.55
1	A	284	ASN	O-C-N	5.36	129.72	122.59
1	A	499	LEU	CA-C-O	-5.36	115.20	120.82
1	A	585	THR	N-CA-C	-5.34	105.36	111.07
1	A	333	VAL	N-CA-C	5.33	115.80	108.12
1	A	253	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	105	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	558	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	662	LEU	CA-C-O	-5.30	114.64	120.36
1	A	688	THR	N-CA-C	5.29	117.85	109.24
1	A	321	PRO	O-C-N	5.27	129.76	122.64
1	A	219	GLN	N-CA-C	-5.26	101.88	110.20
1	A	555	VAL	N-CA-C	5.25	117.42	109.12
1	A	402	ILE	CA-C-O	-5.23	115.25	121.05
1	A	280	TYR	CA-C-N	5.22	126.37	119.84
1	A	280	TYR	C-N-CA	5.22	126.37	119.84
1	A	362	ASP	N-CA-C	5.22	118.43	111.75
1	A	390	HIS	CA-CB-CG	5.21	119.01	113.80
1	A	614	HIS	CA-C-O	-5.21	115.33	120.90
1	A	467	ILE	CA-C-O	-5.20	115.66	121.17
1	A	437	LYS	N-CA-C	-5.20	102.59	110.28
1	A	594	PRO	N-CA-C	5.19	120.59	113.84
1	A	819	GLN	CA-CB-CG	-5.19	103.72	114.10
1	A	661	ASP	N-CA-C	-5.17	106.66	113.12
1	A	270	ASN	N-CA-C	-5.17	98.27	107.98
1	A	635	VAL	CA-C-O	-5.16	115.71	121.17
1	A	649	ARG	CA-C-O	-5.16	115.89	121.36
1	A	628	ASP	O-C-N	5.14	127.37	122.07
1	A	256	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	628	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	194	PRO	CA-N-CD	-5.13	104.82	112.00
1	A	78	ASP	N-CA-C	5.12	121.13	109.81
1	A	664	GLU	N-CA-C	5.12	116.61	108.67
1	A	666	ILE	CA-CB-CG2	5.11	119.19	110.50
1	A	809	GLY	N-CA-C	5.11	119.06	112.83
1	A	192	ALA	CA-C-N	-5.10	116.76	123.34
1	A	192	ALA	C-N-CA	-5.10	116.76	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	ALA	CA-C-N	5.09	124.70	119.05
1	A	836	ALA	C-N-CA	5.09	124.70	119.05
1	A	635	VAL	N-CA-C	-5.08	105.54	110.42
1	A	593	GLU	CA-C-N	5.08	124.75	119.56
1	A	593	GLU	C-N-CA	5.08	124.75	119.56
1	A	90	TYR	CA-CB-CG	5.08	123.04	113.90
1	A	200	VAL	N-CA-C	-5.07	101.01	108.11
1	A	715	VAL	CA-C-O	-5.07	115.48	120.85
1	A	467	ILE	N-CA-C	5.06	115.28	110.42
1	A	207	GLU	N-CA-C	-5.05	101.17	109.40
1	A	37	PHE	N-CA-C	5.04	116.77	111.28
1	A	93	ARG	CB-CG-CD	-5.04	99.71	111.30
1	A	413	ARG	CA-CB-CG	5.04	124.17	114.10
1	A	387	TRP	CA-C-N	5.03	126.13	119.84
1	A	387	TRP	C-N-CA	5.03	126.13	119.84
1	A	29	LYS	N-CA-C	-5.02	105.70	111.07
1	A	831	ARG	CA-CB-CG	5.01	124.12	114.10

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
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	114	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	114	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 (114) 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:171:CYS:HB3	1:A:176:MET:HE2	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:699:MET:HE2	1:A:708:PHE:HZ	1.67	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
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:95:LEU:HG	1:A:99:MET:HE2	1.87	0.55
1:A:799:ARG:O	1:A:803:ARG:HG3	2.06	0.54
1:A:171:CYS:SG	1:A:176:MET:HE2	2.48	0.54
1:A:293:LEU:HD21	1:A:392:LEU:HD23	1.90	0.54
1:A:13:ILE:HD12	1:A:13:ILE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:LEU:O	1:A:39:LEU:HB2	2.12	0.49
1:A:736:PRO:HG3	1:A:739:ARG:NH2	2.27	0.49
1:A:320:ASP:O	1:A:322:VAL:N	2.47	0.48
1:A:212:GLY:HA3	1:A:358:ARG:NH2	2.28	0.47
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.96	0.47
1:A:252:PHE:HA	1:A:255:LYS:CB	2.37	0.47
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.96	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:65:GLY:C	1:A:837:PRO:HG2	2.40	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
1:A:102:LEU:O	1:A:103:ALA:HB3	2.17	0.45
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.98	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:171:CYS:CB	1:A:176:MET:HE2	2.45	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:91:MET:HE3	1:A:241:MET:SD	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:105:GLU:HG2	5:A:1142:HOH:O	2.17	0.44
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.82	0.44
1:A:351:ARG:HH11	1:A:351:ARG:HG2	1.83	0.44
1:A:395:LEU:HG	1:A:396:LEU:HG	2.00	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:HA	1:A:289:LYS:HD3	1.90	0.43
1:A:320:ASP:CG	1:A:321:PRO:HD3	2.42	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:211:GLN:HA	1:A:211:GLN:NE2	2.33	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:319:ARG:HD3	1:A:320:ASP:OD1	2.19	0.43
1:A:795:ARG:O	1:A:799:ARG:HG3	2.19	0.43
1:A:565:VAL:HA	1:A:604:MET:O	2.19	0.43
1:A:709:PHE:HZ	1:A:790:LEU:HD12	1.84	0.43
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:12:GLN:CD	1:A:12:GLN:N	2.78	0.42
1:A:16:ARG:HA	5:A:1070:HOH:O	2.18	0.42
1:A:335:ILE:HG23	1:A:371:THR:HG22	2.01	0.42
1:A:538:LYS:HB2	1:A:538:LYS:HE2	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
1:A:130:GLY:N	5:A:1160:HOH:O	2.52	0.41
1:A:204:GLY:HA2	1:A:217:ASP:O	2.21	0.41
1:A:87:LEU:HD11	1:A:299:VAL:HG11	2.02	0.41
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.33	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.16	0.41
1:A:139:LEU:CD2	1:A:377:HIS:HE1	2.34	0.41
1:A:349:LEU:O	1:A:353:LEU:HG	2.22	0.41
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	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 [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	829/842 (98%)	749 (90%)	66 (8%)	14 (2%)	7	10

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
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%)	634 (88%)	86 (12%)	5 7

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	48	PRO
1	A	55	LEU
1	A	60	ARG
1	A	81	ARG
1	A	94	THR
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	138	ARG
1	A	150	LEU
1	A	176	MET
1	A	191	LYS
1	A	198	LEU
1	A	231	PRO
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	255	LYS
1	A	259	VAL
1	A	281	PRO
1	A	292	ARG
1	A	319	ARG
1	A	323	ARG
1	A	335	ILE
1	A	344	LEU
1	A	358	ARG
1	A	360	ASP
1	A	363	LYS
1	A	380	ILE

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	398	ARG
1	A	400	LEU
1	A	426	ARG
1	A	430	LEU
1	A	433	GLU
1	A	444	LEU
1	A	453	ASN
1	A	457	ARG
1	A	474	LEU
1	A	486	ILE
1	A	510	GLU
1	A	514	ASP
1	A	515	LEU
1	A	522	LEU
1	A	536	LYS
1	A	537	VAL
1	A	539	GLN
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	586	LEU
1	A	611	PRO
1	A	622	LEU
1	A	639	ARG
1	A	641	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
1	A	705	GLU
1	A	708	PHE
1	A	710	ILE
1	A	723	GLN
1	A	734	ARG
1	A	738	LEU
1	A	755	PRO
1	A	759	LYS

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	766	MET
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	810	LYS
1	A	833	ARG
1	A	838	ASP
1	A	839	GLU
1	A	840	LYS
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	32	ASN
1	A	34	HIS
1	A	71	GLN
1	A	72	GLN
1	A	114	GLN
1	A	211	GLN
1	A	235	ASN
1	A	270	ASN
1	A	390	HIS
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	678	ASN
1	A	763	ASN
1	A	768	HIS
1	A	793	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 [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](#)

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	$\# Z > 2$
3	PLP	A	999	1	15,15,16	1.73	5 (33%)	21,22,23	1.36	3 (14%)
4	NTZ	A	998	-	13,15,15	2.90	5 (38%)	14,22,22	4.22	5 (35%)
2	PO4	A	997	-	4,4,4	3.67	4 (100%)	6,6,6	3.33	6 (100%)
2	PO4	A	996	-	4,4,4	4.18	4 (100%)	6,6,6	2.38	4 (66%)

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
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
4	NTZ	A	998	-	-	1/2/22/22	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	NTZ	C1-N21	6.51	1.38	1.32
2	A	996	PO4	P-O4	-5.29	1.39	1.54
4	A	998	NTZ	C1-N1	5.22	1.38	1.34
4	A	998	NTZ	N17-N18	4.66	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	PO4	P-O2	-4.51	1.41	1.54
2	A	996	PO4	P-O1	-4.48	1.40	1.50
3	A	999	PLP	C3-C2	-3.96	1.36	1.41
2	A	996	PO4	P-O3	-3.86	1.43	1.54
2	A	997	PO4	P-O3	-3.67	1.43	1.54
2	A	997	PO4	P-O4	-3.43	1.44	1.54
2	A	997	PO4	P-O1	2.87	1.57	1.50
4	A	998	NTZ	N1-N17	2.84	1.39	1.35
2	A	996	PO4	P-O2	-2.66	1.46	1.54
3	A	999	PLP	P-O3P	-2.56	1.45	1.54
3	A	999	PLP	C5-C4	-2.47	1.37	1.40
4	A	998	NTZ	C3-C2	2.18	1.56	1.53
3	A	999	PLP	C2-N1	2.04	1.37	1.33
3	A	999	PLP	C5A-C5	2.02	1.56	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	NTZ	N1-C1-N21	11.51	114.02	108.45
4	A	998	NTZ	C1-N1-N17	-8.34	102.93	108.47
4	A	998	NTZ	N1-N17-N18	5.57	110.26	106.00
2	A	997	PO4	O3-P-O1	-4.72	94.25	110.95
2	A	996	PO4	O2-P-O1	-3.77	97.63	110.95
2	A	997	PO4	O4-P-O2	3.39	118.47	107.91
2	A	997	PO4	O4-P-O3	3.14	117.69	107.91
2	A	997	PO4	O4-P-O1	-2.95	100.53	110.95
3	A	999	PLP	C4A-C4-C5	-2.87	117.98	120.94
2	A	996	PO4	O4-P-O3	2.80	116.62	107.91
2	A	997	PO4	O3-P-O2	2.80	116.62	107.91
3	A	999	PLP	C5-C6-N1	-2.62	119.57	123.83
3	A	999	PLP	C6-C5-C4	2.54	120.18	118.10
2	A	997	PO4	O2-P-O1	-2.49	102.13	110.95
4	A	998	NTZ	C1-N21-N18	-2.41	104.18	105.81
2	A	996	PO4	O3-P-O2	-2.33	100.66	107.91
2	A	996	PO4	O4-P-O1	2.30	119.07	110.95
4	A	998	NTZ	N21-N18-N17	-2.22	108.62	111.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	998	NTZ	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.