



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:31 PM UTC

PDB ID : 1NOK / pdb_00001nok
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

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

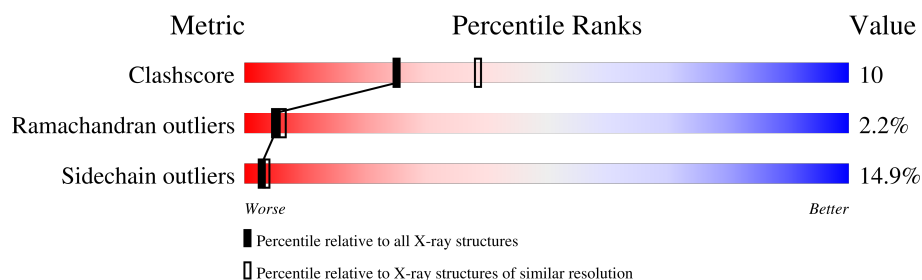
1 Overall quality at a glance

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	59% 29% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7230 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.

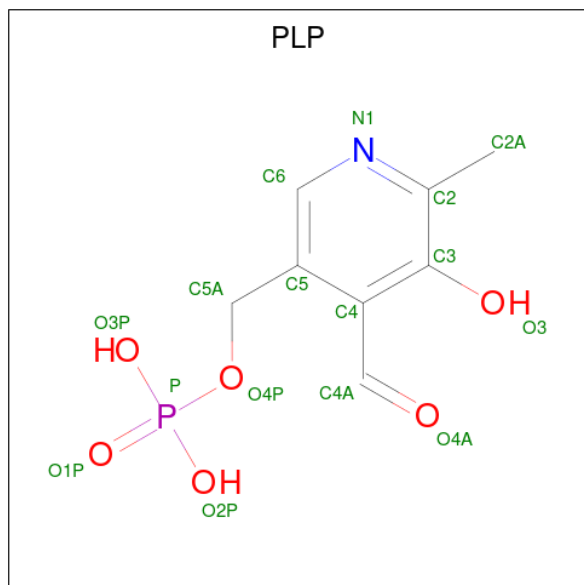
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

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:

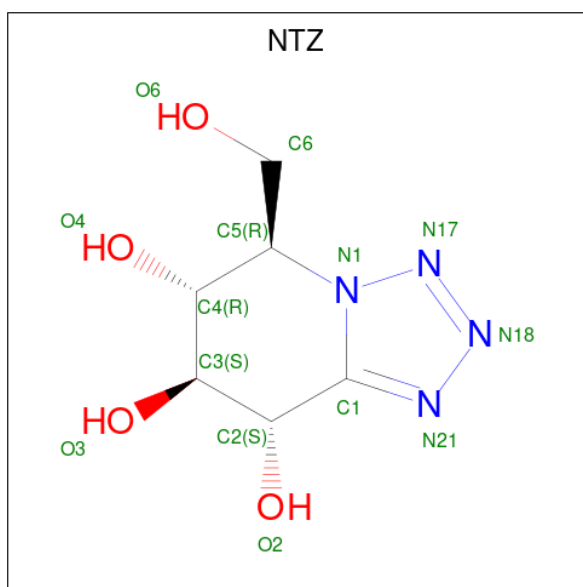
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
A	609	PRO	ALA	conflict	UNP P00489

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



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

- Molecule 3 is NOJIRIMYCINE TETRAZOLE (CCD ID: NTZ) (formula: $C_6H_{10}N_4O_4$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	442	Total	O	0	0
			442	442		

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}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7230	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 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	1.08	17/6913 (0.2%)	1.96	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	6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	CA-CB	11.71	1.68	1.54
1	A	787	VAL	CA-CB	7.79	1.65	1.54
1	A	371	THR	CA-CB	7.58	1.66	1.53
1	A	165	ILE	CA-CB	6.86	1.62	1.54
1	A	94	THR	CA-CB	6.74	1.64	1.53
1	A	379	VAL	CA-CB	6.59	1.62	1.54
1	A	629	VAL	CA-CB	6.50	1.61	1.54
1	A	369	VAL	CA-CB	6.03	1.62	1.54
1	A	322	VAL	CA-CB	5.86	1.62	1.54
1	A	319	ARG	NE-CZ	5.80	1.39	1.33
1	A	59	VAL	CA-CB	5.46	1.61	1.54
1	A	320	ASP	CA-CB	5.40	1.61	1.53
1	A	40	VAL	CA-CB	5.29	1.61	1.54
1	A	802	ILE	CA-CB	5.24	1.61	1.54
1	A	603	VAL	CA-CB	5.23	1.60	1.54
1	A	333	VAL	CA-CB	5.19	1.61	1.54
1	A	368	THR	CA-CB	5.00	1.61	1.53

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	N-CA-C	12.00	127.03	109.14
1	A	413	ARG	CB-CG-CD	-11.26	85.39	111.30
1	A	838	ASP	CA-CB-CG	-11.04	101.56	112.60
1	A	666	ILE	N-CA-CB	-10.51	93.89	111.23
1	A	656	VAL	CB-CA-C	-9.80	96.38	112.26
1	A	724	ARG	CA-CB-CG	9.35	132.81	114.10
1	A	807	THR	N-CA-CB	-9.33	96.27	110.73
1	A	259	VAL	O-C-N	9.32	134.22	122.57
1	A	717	ASP	CA-CB-CG	9.25	121.85	112.60
1	A	734	ARG	CA-CB-CG	9.01	132.13	114.10
1	A	499	LEU	N-CA-C	-8.79	100.68	111.40
1	A	490	ARG	CB-CA-C	-8.63	96.17	110.85
1	A	556	HIS	N-CA-C	8.50	128.91	110.80
1	A	486	ILE	CA-CB-CG2	8.42	124.81	110.50
1	A	486	ILE	CA-CB-CG1	-8.31	96.27	110.40
1	A	320	ASP	CA-CB-CG	-8.30	104.30	112.60
1	A	128	ASP	CA-CB-CG	8.22	120.83	112.60
1	A	575	ARG	CB-CG-CD	-7.97	92.96	111.30
1	A	484	ASN	OD1-CG-ND2	-7.95	114.66	122.60
1	A	507	ILE	N-CA-C	7.94	120.52	112.90
1	A	189	TRP	CA-C-O	-7.94	110.41	119.14
1	A	23	ASN	CA-CB-CG	-7.85	104.75	112.60
1	A	256	ASP	N-CA-C	-7.84	91.57	107.41
1	A	319	ARG	CA-CB-CG	7.70	129.50	114.10
1	A	763	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	A	469	LYS	CA-CB-CG	7.59	129.29	114.10
1	A	713	MET	CG-SD-CE	-7.55	84.29	100.90
1	A	105	GLU	N-CA-C	7.55	119.50	111.28
1	A	15	VAL	CA-C-O	7.43	130.07	120.78
1	A	490	ARG	N-CA-CB	7.39	121.10	110.16
1	A	763	ASN	CB-CG-ND2	7.38	127.46	116.40
1	A	101	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	119	MET	CB-CA-C	-7.30	98.67	110.79
1	A	666	ILE	CA-CB-CG2	7.17	122.68	110.50
1	A	575	ARG	N-CA-C	7.14	121.09	111.24
1	A	553	TYR	CA-CB-CG	7.12	126.71	113.90
1	A	838	ASP	O-C-N	7.12	132.06	122.59
1	A	16	ARG	CB-CG-CD	7.03	127.48	111.30
1	A	549	LEU	CA-C-O	-7.02	113.63	121.00
1	A	253	ASN	O-C-N	6.99	131.44	122.71
1	A	712	GLY	O-C-N	6.94	131.22	122.68
1	A	264	GLN	CA-C-O	-6.91	113.50	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	VAL	N-CA-CB	-6.91	100.84	112.44
1	A	768	HIS	CA-CB-CG	6.88	120.67	113.80
1	A	405	GLU	CB-CG-CD	6.87	124.28	112.60
1	A	529	ALA	N-CA-C	-6.82	103.77	111.14
1	A	501	GLU	CB-CA-C	-6.80	100.41	110.95
1	A	78	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	840	LYS	O-C-N	6.75	131.57	122.59
1	A	458	ILE	CB-CG1-CD1	-6.71	99.70	113.80
1	A	661	ASP	N-CA-C	-6.69	104.76	113.12
1	A	666	ILE	CB-CA-C	6.68	122.25	111.29
1	A	554	LYS	O-C-N	6.68	131.37	122.96
1	A	458	ILE	CB-CA-C	-6.63	103.07	112.22
1	A	253	ASN	CA-C-N	6.62	134.19	121.54
1	A	253	ASN	C-N-CA	6.62	134.19	121.54
1	A	734	ARG	CB-CG-CD	6.62	126.53	111.30
1	A	97	ASN	CA-CB-CG	-6.61	105.99	112.60
1	A	609	PRO	N-CA-CB	6.60	110.18	103.25
1	A	184	ARG	CA-CB-CG	6.59	127.28	114.10
1	A	455	VAL	N-CA-C	6.59	119.22	112.90
1	A	271	LEU	N-CA-C	-6.57	96.80	110.80
1	A	13	ILE	N-CA-C	-6.57	105.34	111.45
1	A	320	ASP	CA-C-O	-6.55	111.18	120.16
1	A	167	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	386	ARG	CB-CG-CD	-6.47	96.42	111.30
1	A	831	ARG	N-CA-C	-6.45	102.69	110.44
1	A	170	ILE	CA-C-O	-6.44	113.27	120.74
1	A	574	LYS	CA-CB-CG	6.43	126.96	114.10
1	A	576	GLN	N-CA-C	-6.42	104.71	112.54
1	A	436	VAL	N-CA-C	-6.41	99.26	108.48
1	A	638	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	838	ASP	N-CA-C	6.37	124.37	110.80
1	A	389	VAL	CA-C-O	-6.35	114.66	121.27
1	A	807	THR	CB-CA-C	6.35	121.46	110.72
1	A	251	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	735	ILE	CA-C-N	6.32	125.81	119.24
1	A	735	ILE	C-N-CA	6.32	125.81	119.24
1	A	467	ILE	N-CA-CB	-6.30	101.97	110.54
1	A	666	ILE	CA-CB-CG1	-6.29	99.71	110.40
1	A	469	LYS	CB-CG-CD	6.19	125.53	111.30
1	A	61	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	107	ALA	CA-C-O	-6.17	114.34	120.82
1	A	554	LYS	CA-C-N	6.14	133.02	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	C-N-CA	6.14	133.02	121.97
1	A	318	CYS	N-CA-C	-6.12	97.75	110.80
1	A	253	ASN	N-CA-C	-6.07	100.52	109.62
1	A	338	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	758	PHE	N-CA-C	6.04	120.27	113.02
1	A	718	VAL	N-CA-C	-6.02	104.87	110.53
1	A	392	LEU	CA-C-N	5.99	128.23	120.44
1	A	392	LEU	C-N-CA	5.99	128.23	120.44
1	A	156	GLY	CA-C-O	-5.99	115.91	121.18
1	A	510	GLU	CA-CB-CG	5.99	126.07	114.10
1	A	16	ARG	N-CA-C	-5.98	102.60	111.81
1	A	501	GLU	CA-CB-CG	5.96	126.02	114.10
1	A	833	ARG	CA-CB-CG	5.94	125.98	114.10
1	A	727	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	656	VAL	N-CA-CB	5.89	121.43	110.77
1	A	692	MET	N-CA-CB	-5.87	102.64	110.57
1	A	743	GLU	CB-CG-CD	5.86	122.57	112.60
1	A	564	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	644	PHE	CA-C-O	5.82	126.95	120.43
1	A	796	GLU	N-CA-CB	-5.79	101.38	110.30
1	A	678	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	772	LYS	CA-CB-CG	5.77	125.64	114.10
1	A	119	MET	N-CA-CB	5.76	118.58	110.12
1	A	352	VAL	N-CA-CB	-5.73	103.85	110.55
1	A	171	CYS	N-CA-CB	5.71	119.51	110.55
1	A	431	VAL	CA-C-O	-5.69	114.38	120.59
1	A	457	ARG	CA-C-O	-5.69	114.52	120.55
1	A	599	VAL	CA-C-N	5.68	125.44	119.76
1	A	599	VAL	C-N-CA	5.68	125.44	119.76
1	A	255	LYS	N-CA-C	5.68	122.89	110.80
1	A	729	GLN	CA-C-O	-5.67	114.41	120.42
1	A	393	GLU	CA-CB-CG	5.65	125.41	114.10
1	A	575	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	93	ARG	CG-CD-NE	5.60	124.33	112.00
1	A	402	ILE	CA-C-O	-5.59	114.84	121.05
1	A	338	ASN	CB-CG-ND2	5.58	124.78	116.40
1	A	360	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	413	ARG	N-CA-C	-5.55	104.86	111.69
1	A	633	ASP	CA-C-N	5.55	125.08	119.19
1	A	633	ASP	C-N-CA	5.55	125.08	119.19
1	A	323	ARG	N-CA-C	-5.55	98.98	110.80
1	A	510	GLU	CB-CG-CD	5.54	122.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	ARG	CG-CD-NE	-5.54	99.82	112.00
1	A	772	LYS	N-CA-CB	-5.54	101.13	110.49
1	A	710	ILE	CB-CG1-CD1	-5.54	102.17	113.80
1	A	235	ASN	CA-CB-CG	5.50	118.11	112.60
1	A	213	ALA	N-CA-C	-5.50	101.31	110.17
1	A	724	ARG	CB-CA-C	-5.47	102.28	110.88
1	A	643	ILE	N-CA-CB	-5.42	103.61	111.52
1	A	31	PHE	N-CA-C	-5.41	104.80	111.40
1	A	251	ASP	CA-C-O	-5.39	112.81	120.51
1	A	467	ILE	CA-C-O	-5.38	115.36	120.95
1	A	322	VAL	CA-CB-CG2	-5.37	101.27	110.40
1	A	453	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	614	HIS	CA-C-O	-5.37	115.16	120.90
1	A	501	GLU	N-CA-CB	5.36	117.76	109.98
1	A	455	VAL	N-CA-CB	-5.35	105.36	112.26
1	A	317	GLY	CA-C-N	5.33	131.73	121.54
1	A	317	GLY	C-N-CA	5.33	131.73	121.54
1	A	407	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	322	VAL	CA-CB-CG1	5.32	119.45	110.40
1	A	595	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	553	TYR	O-C-N	-5.32	115.56	121.84
1	A	162	GLU	CA-CB-CG	5.30	124.70	114.10
1	A	91	MET	N-CA-C	5.24	117.90	111.82
1	A	610	ALA	CA-C-N	5.24	125.29	119.32
1	A	610	ALA	C-N-CA	5.24	125.29	119.32
1	A	590	ILE	CA-CB-CG2	-5.24	101.60	110.50
1	A	367	VAL	CA-C-O	-5.21	115.64	121.17
1	A	29	LYS	CB-CA-C	-5.21	102.70	110.88
1	A	579	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	366	GLU	CA-CB-CG	5.20	124.50	114.10
1	A	764	MET	CG-SD-CE	-5.20	89.47	100.90
1	A	170	ILE	O-C-N	-5.19	115.13	122.76
1	A	643	ILE	CA-CB-CG1	-5.18	101.60	110.40
1	A	697	VAL	CA-C-O	-5.18	115.68	121.17
1	A	360	ASP	N-CA-C	-5.16	103.72	110.53
1	A	171	CYS	CB-CA-C	-5.16	101.73	110.19
1	A	408	GLN	CB-CG-CD	-5.16	103.83	112.60
1	A	645	LEU	N-CA-CB	-5.16	102.67	110.35
1	A	370	LYS	CG-CD-CE	5.15	123.15	111.30
1	A	93	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	317	GLY	O-C-N	5.15	129.39	122.70
1	A	796	GLU	CB-CG-CD	5.14	121.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	LEU	CA-CB-CG	5.14	134.29	116.30
1	A	176	MET	N-CA-C	-5.11	100.13	108.76
1	A	576	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	268	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	675	GLY	O-C-N	-5.08	116.09	122.70
1	A	772	LYS	CA-C-N	5.08	127.42	120.46
1	A	772	LYS	C-N-CA	5.08	127.42	120.46
1	A	573	TYR	CA-CB-CG	5.08	123.04	113.90
1	A	840	LYS	CA-CB-CG	5.06	124.21	114.10
1	A	797	TRP	CD2-CE2-CZ2	5.05	127.45	122.40
1	A	135	GLY	N-CA-C	5.05	118.75	112.64
1	A	430	LEU	N-CA-C	-5.04	106.39	112.54
1	A	412	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	412	ASN	CB-CG-ND2	5.03	123.94	116.40
1	A	71	GLN	CA-C-O	-5.02	115.55	120.82
1	A	684	ASN	OD1-CG-ND2	-5.01	117.58	122.60
1	A	555	VAL	CA-C-N	5.01	131.12	121.54
1	A	555	VAL	C-N-CA	5.01	131.12	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain
1	A	404	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	524	TYR	Sidechain
1	A	573	TYR	Sidechain
1	A	841	ILE	Peptide

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	131	0
2	A	15	0	7	0	0
3	A	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	442	0	0	12	0
All	All	7230	0	6716	131	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 10.

All (131) 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:713:MET:HE1	1:A:775:ALA:HB1	1.61	0.83
1:A:764:MET:HE2	1:A:769:ASP:HA	1.62	0.81
1:A:571:HIS:HB2	1:A:574:LYS:HG2	1.63	0.80
1:A:319:ARG:NE	1:A:320:ASP:H	1.87	0.72
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.73	0.70
1:A:764:MET:CE	1:A:769:ASP:HA	2.20	0.70
1:A:365:TRP:O	1:A:369:VAL:HG12	1.93	0.68
1:A:703:ALA:HA	1:A:807:THR:HG21	1.79	0.65
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.79	0.65
1:A:320:ASP:HB3	1:A:321:PRO:HD3	1.78	0.65
1:A:803:ARG:O	1:A:807:THR:HB	2.00	0.61
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.65	0.60
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.83	0.60
1:A:169:LYS:HB2	1:A:176:MET:HB2	1.84	0.60
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.68	0.58
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.37	0.58
1:A:550:GLU:HA	1:A:554:LYS:HB2	1.85	0.58
1:A:95:LEU:HG	1:A:99:MET:HE2	1.86	0.57
1:A:592:LYS:HG3	1:A:593:GLU:HG2	1.86	0.57
1:A:703:ALA:CA	1:A:807:THR:HG21	2.35	0.55
1:A:678:ASN:HD22	1:A:679:MET:H	1.54	0.55
1:A:519:ARG:O	1:A:522:LEU:HB2	2.06	0.55
1:A:314:SER:HB3	1:A:316:PHE:HD1	1.71	0.54
1:A:320:ASP:HB3	1:A:321:PRO:CD	2.37	0.54
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.48	0.53
1:A:795:ARG:O	1:A:799:ARG:HG3	2.09	0.53
1:A:144:LEU:HA	1:A:147:MET:HE3	1.90	0.53
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.89	0.53
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.73	0.53
1:A:568:LYS:HG3	1:A:574:LYS:HE3	1.89	0.53
1:A:94:THR:HG22	4:A:1424:HOH:O	2.10	0.52
1:A:181:ASP:HB3	1:A:184:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:TYR:HA	1:A:551:ARG:HD3	1.91	0.52
1:A:251:ASP:CG	1:A:252:PHE:H	2.17	0.52
1:A:690:GLY:O	1:A:710:ILE:HA	2.09	0.52
1:A:312:LYS:HE2	1:A:324:THR:HG21	1.92	0.52
1:A:778:GLU:O	1:A:782:LYS:HD3	2.10	0.51
1:A:144:LEU:HD12	1:A:147:MET:CE	2.41	0.51
1:A:730:GLU:O	1:A:734:ARG:HG2	2.10	0.51
1:A:521:LEU:HD22	1:A:530:PHE:CZ	2.46	0.51
1:A:469:LYS:HE3	1:A:470:ASP:H	1.76	0.51
1:A:351:ARG:O	1:A:355:ASP:HB2	2.10	0.50
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.93	0.50
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.12	0.49
1:A:349:LEU:O	1:A:353:LEU:HG	2.11	0.49
1:A:525:VAL:O	1:A:531:ILE:HD11	2.13	0.49
1:A:172:GLY:O	1:A:621:LYS:NZ	2.45	0.49
1:A:257:PHE:O	1:A:258:ASN:HB2	2.13	0.48
1:A:839:GLU:O	1:A:840:LYS:NZ	2.45	0.48
1:A:519:ARG:NH1	4:A:1060:HOH:O	2.45	0.48
1:A:66:ARG:HG3	1:A:837:PRO:HB3	1.96	0.47
1:A:601:ARG:HD2	4:A:1137:HOH:O	2.14	0.47
1:A:181:ASP:O	1:A:184:ARG:NH1	2.48	0.47
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.95	0.47
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.23	0.47
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.14	0.47
1:A:329:PHE:HD2	1:A:371:THR:HG21	1.79	0.47
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.50	0.47
1:A:515:LEU:HD13	1:A:809:GLY:HA2	1.97	0.47
1:A:193:ARG:HB3	1:A:196:PHE:CD2	2.50	0.47
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.97	0.46
1:A:15:VAL:HG13	1:A:15:VAL:O	2.16	0.46
1:A:749:PHE:HB2	4:A:1538:HOH:O	2.16	0.46
1:A:390:HIS:HD2	4:A:1265:HOH:O	1.98	0.46
1:A:58:THR:O	1:A:62:HIS:HD2	1.99	0.46
1:A:81:ARG:HG3	1:A:155:TYR:HE1	1.81	0.46
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.98	0.45
1:A:69:ARG:HD3	1:A:837:PRO:HA	1.98	0.45
1:A:367:VAL:O	1:A:371:THR:HG23	2.17	0.45
1:A:487:THR:O	1:A:491:TRP:HB2	2.16	0.45
1:A:548:TYR:HA	1:A:551:ARG:HH11	1.81	0.45
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.51	0.45
1:A:388:PRO:HG2	1:A:391:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD11	1:A:303:THR:HG21	1.97	0.45
1:A:455:VAL:H	1:A:459:HIS:HD2	1.62	0.45
1:A:554:LYS:HD3	1:A:555:VAL:H	1.80	0.45
1:A:738:LEU:HD12	1:A:777:TYR:CD2	2.52	0.45
1:A:809:GLY:HA3	4:A:1060:HOH:O	2.17	0.45
1:A:335:ILE:HD11	1:A:337:LEU:HD11	1.98	0.45
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.50	0.45
1:A:798:THR:O	1:A:802:ILE:HG13	2.16	0.45
1:A:322:VAL:O	1:A:323:ARG:NH1	2.51	0.44
1:A:329:PHE:CD2	1:A:371:THR:HG21	2.51	0.44
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.52	0.44
1:A:177:GLU:HG2	1:A:611:PRO:HG3	1.99	0.44
1:A:66:ARG:HA	1:A:69:ARG:HG2	2.00	0.44
1:A:247:LYS:NZ	4:A:1395:HOH:O	2.50	0.44
1:A:423:ASP:O	1:A:426:ARG:HG3	2.18	0.44
1:A:469:LYS:HD3	4:A:1171:HOH:O	2.17	0.44
1:A:316:PHE:HA	1:A:320:ASP:HB2	2.00	0.44
1:A:16:ARG:HD2	4:A:1430:HOH:O	2.18	0.43
1:A:519:ARG:NH1	1:A:807:THR:HA	2.32	0.43
1:A:72:GLN:O	1:A:75:TYR:HB3	2.18	0.43
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.25	0.43
1:A:777:TYR:O	1:A:781:VAL:HG13	2.18	0.43
1:A:519:ARG:NH2	4:A:1061:HOH:O	2.44	0.43
1:A:411:LEU:HD22	1:A:425:LEU:HD12	1.99	0.43
1:A:549:LEU:C	1:A:554:LYS:HB2	2.44	0.43
1:A:764:MET:HE2	1:A:769:ASP:CA	2.41	0.43
1:A:486:ILE:CD1	1:A:676:THR:HB	2.49	0.42
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.55	0.42
1:A:16:ARG:HB3	1:A:105:GLU:HB3	2.02	0.42
1:A:303:THR:O	1:A:307:ILE:HG13	2.18	0.42
1:A:594:PRO:O	1:A:639:ARG:NH2	2.50	0.42
1:A:90:TYR:HE1	4:A:1212:HOH:O	2.02	0.42
1:A:251:ASP:CG	1:A:252:PHE:N	2.77	0.42
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.55	0.42
1:A:366:GLU:O	1:A:370:LYS:HB2	2.18	0.42
1:A:542:LYS:HE2	1:A:559:PRO:O	2.20	0.42
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.50	0.42
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.52	0.42
1:A:515:LEU:HB3	1:A:809:GLY:HA2	2.01	0.42
1:A:599:VAL:HA	1:A:600:PRO:HD3	1.92	0.42
1:A:803:ARG:HB2	1:A:803:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLY:HA2	1:A:217:ASP:O	2.20	0.42
1:A:423:ASP:O	1:A:427:ARG:HB2	2.19	0.42
1:A:335:ILE:O	1:A:335:ILE:HG13	2.16	0.41
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.02	0.41
1:A:403:ILE:HG21	1:A:403:ILE:HD13	1.87	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.18	0.41
1:A:23:ASN:O	1:A:27:LEU:HD22	2.20	0.41
1:A:466:THR:O	1:A:469:LYS:HE2	2.20	0.41
1:A:319:ARG:HE	1:A:320:ASP:H	1.68	0.41
1:A:764:MET:HE3	4:A:1278:HOH:O	2.20	0.41
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.86	0.41
1:A:680:LYS:O	1:A:683:LEU:HD12	2.19	0.41
1:A:144:LEU:HD12	1:A:147:MET:HE1	2.02	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.86	0.41
1:A:196:PHE:HB2	1:A:225:PRO:HG2	2.03	0.41
1:A:761:ILE:HG22	1:A:765:LEU:HD22	2.01	0.41
1:A:386:ARG:HA	1:A:439:ILE:O	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	829/842 (98%)	770 (93%)	41 (5%)	18 (2%)	5 6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	SER
1	A	252	PHE
1	A	254	LEU
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	320	ASP
1	A	551	ARG
1	A	556	HIS
1	A	839	GLU
1	A	840	LYS
1	A	259	VAL
1	A	318	CYS
1	A	323	ARG
1	A	836	ALA
1	A	251	ASP
1	A	322	VAL
1	A	835	PRO
1	A	838	ASP
1	A	14	SER

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%)	613 (85%)	107 (15%)	3 3

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	33	ARG
1	A	48	PRO
1	A	55	LEU
1	A	93	ARG
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU

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Mol	Chain	Res	Type
1	A	138	ARG
1	A	144	LEU
1	A	195	GLU
1	A	198	LEU
1	A	211	GLN
1	A	231	PRO
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	251	ASP
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	258	ASN
1	A	264	GLN
1	A	271	LEU
1	A	287	GLU
1	A	292	ARG
1	A	314	SER
1	A	319	ARG
1	A	322	VAL
1	A	323	ARG
1	A	335	ILE
1	A	337	LEU
1	A	344	LEU
1	A	358	ARG
1	A	361	TRP
1	A	363	LYS
1	A	369	VAL
1	A	371	THR
1	A	382	GLU
1	A	384	LEU
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	413	ARG
1	A	422	VAL
1	A	425	LEU
1	A	430	LEU
1	A	433	GLU
1	A	437	LYS
1	A	444	LEU

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Mol	Chain	Res	Type
1	A	467	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	523	SER
1	A	528	GLU
1	A	536	LYS
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	565	VAL
1	A	568	LYS
1	A	569	ARG
1	A	574	LYS
1	A	586	LEU
1	A	590	ILE
1	A	593	GLU
1	A	596	LYS
1	A	603	VAL
1	A	611	PRO
1	A	622	LEU
1	A	639	ARG
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	658	PRO
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU
1	A	716	GLU
1	A	730	GLU
1	A	742	ILE
1	A	743	GLU
1	A	765	LEU
1	A	768	HIS

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Mol	Chain	Res	Type
1	A	770	ARG
1	A	787	VAL
1	A	790	LEU
1	A	796	GLU
1	A	797	TRP
1	A	803	ARG
1	A	807	THR
1	A	833	ARG
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	71	GLN
1	A	208	HIS
1	A	235	ASN
1	A	270	ASN
1	A	325	ASN
1	A	390	HIS
1	A	453	ASN
1	A	566	GLN
1	A	579	ASN
1	A	614	HIS
1	A	678	ASN
1	A	767	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NTZ	A	998	-	13,15,15	3.39	6 (46%)	14,22,22	2.50	5 (35%)
2	PLP	A	999	1	15,15,16	1.63	3 (20%)	21,22,23	1.24	3 (14%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	NTZ	C1-N1	7.78	1.41	1.34
3	A	998	NTZ	C1-N21	6.76	1.39	1.32
3	A	998	NTZ	N17-N18	4.39	1.39	1.30
2	A	999	PLP	C3-C2	-3.83	1.37	1.41
3	A	998	NTZ	N21-N18	2.77	1.40	1.36
3	A	998	NTZ	N1-N17	2.68	1.39	1.35
2	A	999	PLP	P-O1P	-2.40	1.43	1.50
2	A	999	PLP	P-O3P	-2.39	1.45	1.54
3	A	998	NTZ	C4-C5	2.11	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	NTZ	N1-C1-N21	6.65	111.67	108.45
3	A	998	NTZ	C1-N1-N17	-4.24	105.65	108.47
3	A	998	NTZ	N1-N17-N18	2.71	108.08	106.00
2	A	999	PLP	O4P-C5A-C5	2.57	114.17	109.36
3	A	998	NTZ	C1-N21-N18	-2.30	104.26	105.81
2	A	999	PLP	C5-C6-N1	-2.23	120.21	123.83
3	A	998	NTZ	C6-C5-C4	2.16	116.18	112.93
2	A	999	PLP	C6-C5-C4	2.11	119.83	118.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	PLP	C6-C5-C5A-O4P

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

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.