Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:08 PM GMT

PDB ID	:	1NOK
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

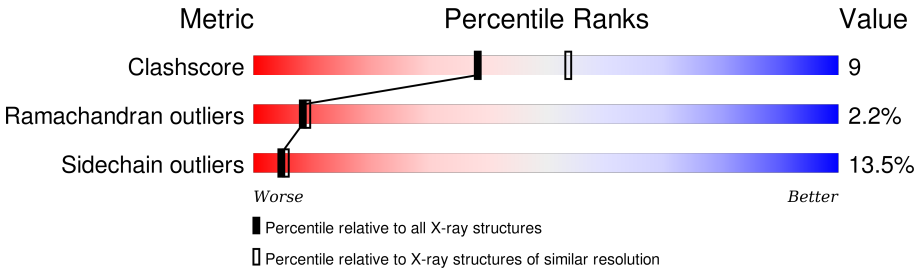
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 >=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 <=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	66% 22% 8%

2 Entry composition

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.

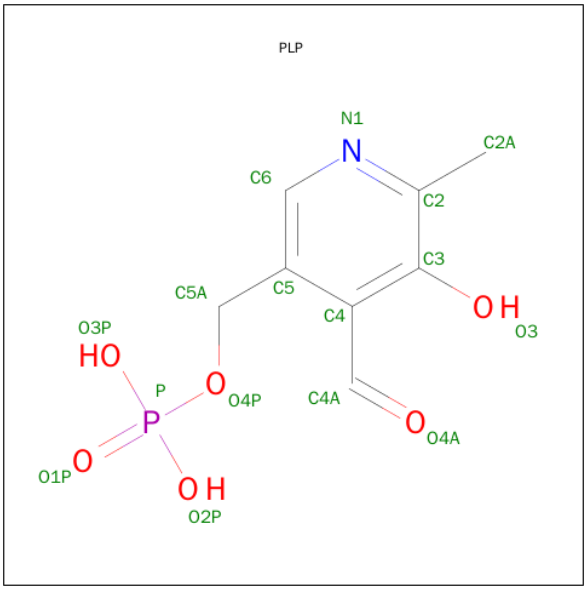
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

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

There are 2 discrepancies between the modelled and reference sequences:

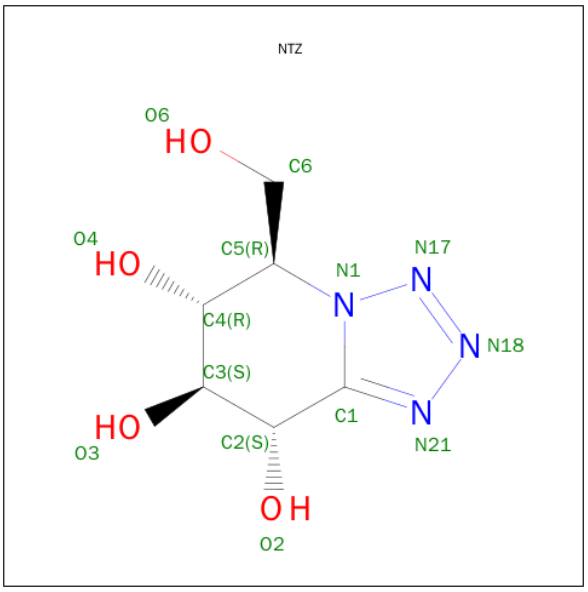
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
A	609	PRO	ALA	CONFLICT	UNP P00489

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



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

- Molecule 3 is NOJIRIMYCINE TETRAZOLE (three-letter code: NTZ) (formula: $C_6H_{10}N_4O_4$).



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

- Molecule 4 is water.

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

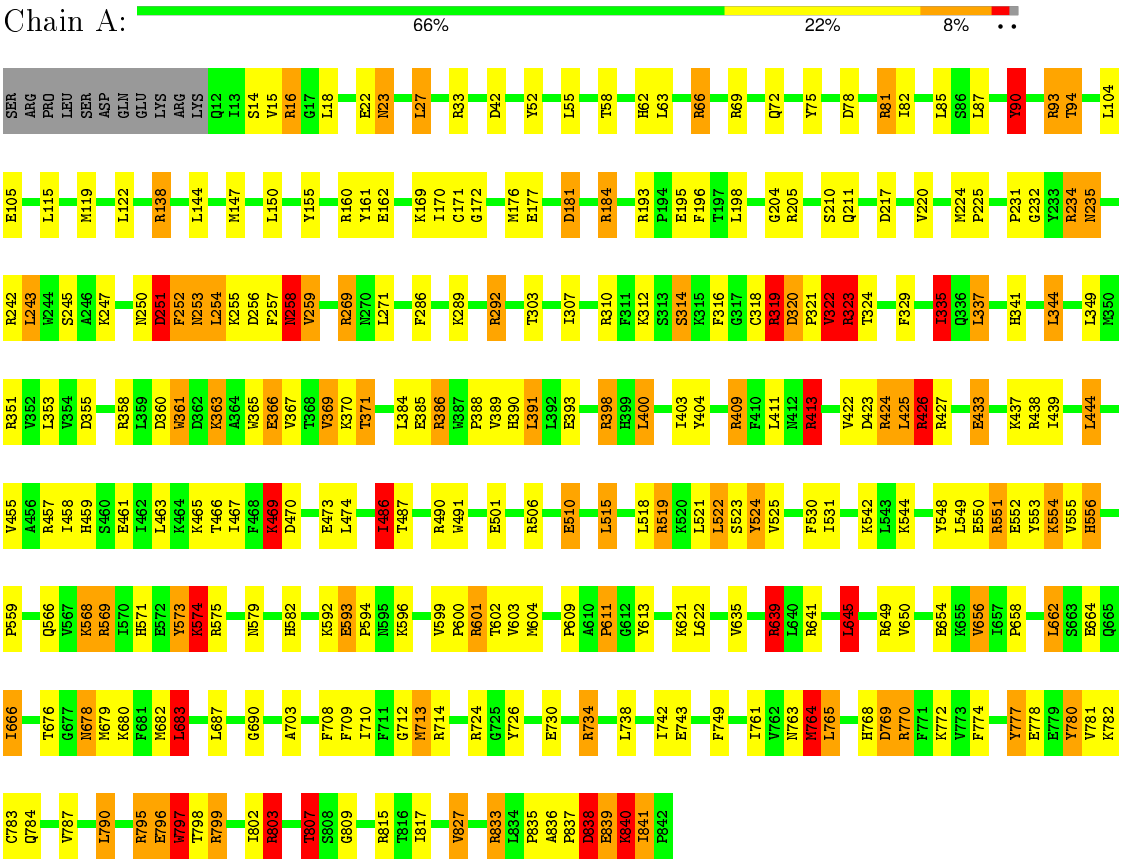
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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, 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	0.82	3/6913 (0.0%)	1.65	135/9356 (1.4%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	CA-CB	6.10	1.68	1.54
1	A	259	VAL	CB-CG2	5.85	1.65	1.52
1	A	259	VAL	CB-CG1	5.31	1.64	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	A	424	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	649	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	601	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	A	413	ARG	CB-CG-CD	-10.08	85.39	111.60
1	A	713	MET	CG-SD-CE	-9.95	84.29	100.20
1	A	457	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	A	138	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	734	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	81	ARG	NE-CZ-NH2	-9.05	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	724	ARG	CA-CB-CG	8.82	132.81	113.40
1	A	413	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	734	ARG	CA-CB-CG	8.51	132.13	113.40
1	A	90	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	A	770	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	426	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	63	LEU	CA-CB-CG	8.26	134.29	115.30
1	A	409	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	714	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	656	VAL	CB-CA-C	-7.90	96.38	111.40
1	A	413	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	486	ILE	CA-CB-CG1	-7.75	96.27	111.00
1	A	506	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	292	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	807	THR	N-CA-CB	-7.38	96.27	110.30
1	A	666	ILE	N-CA-CB	-7.36	93.89	110.80
1	A	639	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	319	ARG	CA-CB-CG	7.32	129.50	113.40
1	A	803	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	575	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	469	LYS	CA-CB-CG	7.22	129.29	113.40
1	A	457	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	256	ASP	N-CA-C	-7.20	91.57	111.00
1	A	649	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	575	ARG	CB-CG-CD	-7.17	92.96	111.60
1	A	490	ARG	CB-CA-C	-7.11	96.17	110.40
1	A	553	TYR	CA-CB-CG	7.01	126.71	113.40
1	A	78	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	486	ILE	CA-CB-CG2	6.96	124.81	110.90
1	A	682	MET	CG-SD-CE	6.86	111.17	100.20
1	A	712	GLY	CA-C-N	-6.83	102.18	117.20
1	A	764	MET	CG-SD-CE	-6.71	89.47	100.20
1	A	556	HIS	N-CA-C	6.63	128.91	111.00
1	A	569	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	310	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	170	ILE	CA-C-N	6.52	131.55	117.20
1	A	259	VAL	O-C-N	6.49	134.22	123.20
1	A	554	LYS	CA-C-N	-6.47	102.96	117.20
1	A	444	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	662	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	322	VAL	CA-CB-CG2	-6.42	101.27	110.90
1	A	90	TYR	CB-CG-CD1	6.37	124.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	840	LYS	CA-C-N	-6.36	103.21	117.20
1	A	242	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	184	ARG	CA-CB-CG	6.31	127.28	113.40
1	A	369	VAL	CG1-CB-CG2	-6.21	100.95	110.90
1	A	574	LYS	CA-CB-CG	6.16	126.96	113.40
1	A	16	ARG	CB-CG-CD	6.11	127.48	111.60
1	A	259	VAL	CG1-CB-CG2	-6.03	101.25	110.90
1	A	683	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	344	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	93	ARG	CG-CD-NE	5.96	124.33	111.80
1	A	827	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	A	666	ILE	CA-CB-CG1	-5.94	99.71	111.00
1	A	554	LYS	N-CA-C	5.93	127.03	111.00
1	A	66	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	650	VAL	CG1-CB-CG2	-5.89	101.47	110.90
1	A	666	ILE	CA-CB-CG2	5.89	122.68	110.90
1	A	66	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	119	MET	CB-CA-C	-5.87	98.67	110.40
1	A	838	ASP	O-C-N	5.85	132.06	122.70
1	A	386	ARG	CB-CG-CD	-5.84	96.42	111.60
1	A	490	ARG	N-CA-CB	5.83	121.10	110.60
1	A	510	GLU	CA-CB-CG	5.76	126.07	113.40
1	A	613	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	A	171	CYS	CA-CB-SG	5.76	124.36	114.00
1	A	795	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	251	ASP	CA-C-N	5.74	129.84	117.20
1	A	734	ARG	CB-CG-CD	5.74	126.53	111.60
1	A	501	GLU	CA-CB-CG	5.74	126.02	113.40
1	A	609	PRO	N-CA-CB	5.73	110.18	103.30
1	A	93	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	833	ARG	CA-CB-CG	5.72	125.98	113.40
1	A	519	ARG	CG-CD-NE	-5.71	99.82	111.80
1	A	322	VAL	CA-CB-CG1	5.70	119.45	110.90
1	A	269	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	524	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	553	TYR	CA-C-N	5.58	129.48	117.20
1	A	772	LYS	CA-CB-CG	5.56	125.64	113.40
1	A	524	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	840	LYS	O-C-N	5.54	131.57	122.70
1	A	838	ASP	CA-C-N	-5.52	105.05	117.20
1	A	224	MET	CG-SD-CE	-5.51	91.39	100.20
1	A	770	ARG	CD-NE-CZ	5.50	131.31	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	777	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	797	TRP	NE1-CE2-CZ2	-5.49	124.36	130.40
1	A	573	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	256	ASP	CA-C-N	-5.47	105.17	117.20
1	A	253	ASN	O-C-N	5.46	131.44	122.70
1	A	393	GLU	CA-CB-CG	5.46	125.41	113.40
1	A	438	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	554	LYS	O-C-N	5.42	131.37	122.70
1	A	601	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	569	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	433	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	799	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	A	777	TYR	CB-CG-CD1	5.40	124.24	121.00
1	A	838	ASP	CA-CB-CG	-5.38	101.56	113.40
1	A	713	MET	CA-CB-CG	5.37	122.43	113.30
1	A	635	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	A	769	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	469	LYS	CB-CG-CD	5.36	125.53	111.60
1	A	666	ILE	CB-CA-C	5.33	122.25	111.60
1	A	712	GLY	O-C-N	5.33	131.22	122.70
1	A	770	ARG	CG-CD-NE	5.31	122.95	111.80
1	A	780	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	602	THR	CA-CB-CG2	-5.27	105.02	112.40
1	A	18	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	271	LEU	N-CA-C	-5.26	96.80	111.00
1	A	772	LYS	N-CA-CB	-5.26	101.13	110.60
1	A	138	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	234	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	205	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	815	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	162	GLU	CA-CB-CG	5.14	124.70	113.40
1	A	645	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	A	253	ASN	CA-C-N	-5.13	105.91	117.20
1	A	796	GLU	N-CA-CB	-5.12	101.38	110.60
1	A	181	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	259	VAL	CA-C-N	-5.10	106.00	116.20
1	A	573	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	458	ILE	CB-CG1-CD1	-5.07	99.70	113.90
1	A	366	GLU	CA-CB-CG	5.04	124.50	113.40
1	A	654	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	220	VAL	CA-CB-CG2	-5.03	103.36	110.90

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 (i)

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	123	0
2	A	15	0	7	0	0
3	A	14	0	10	0	0
4	A	442	0	0	11	0
All	All	7230	0	6716	123	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 9.

All (123) 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:764:MET:HE2	1:A:769:ASP:HA	1.61	0.83
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:764:MET:CE	1:A:769:ASP:HA	2.20	0.70
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.37	0.58
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.68	0.58
1:A:550:GLU:HA	1:A:554:LYS:HB2	1.85	0.58
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:795:ARG:O	1:A:799:ARG:HG3	2.09	0.53
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.48	0.53
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.89	0.53
1:A:568:LYS:HG3	1:A:574:LYS:HE3	1.89	0.53
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.73	0.53
1:A:94:THR:HG22	4:A:1424:HOH:O	2.10	0.52
1:A:548:TYR:HA	1:A:551:ARG:HD3	1.91	0.52
1:A:181:ASP:HB3	1:A:184:ARG:HH11	1.75	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:144:LEU:HD12	1:A:147:MET:HE3	1.91	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:251:ASP:CG	1:A:252:PHE:H	2.17	0.47
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.95	0.47
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.14	0.47
1:A:515:LEU:HD13	1:A:809:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:749:PHE:HB2	4:A:1538:HOH:O	2.16	0.46
1:A:15:VAL:HG13	1:A:15:VAL:O	2.16	0.46
1:A:390:HIS:HD2	4:A:1265:HOH:O	1.98	0.46
1:A:81:ARG:HG3	1:A:155:TYR:HE1	1.81	0.46
1:A:58:THR:O	1:A:62:HIS:HD2	1.99	0.46
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.98	0.45
1:A:548:TYR:HA	1:A:551:ARG:HH11	1.81	0.45
1:A:69:ARG:HD3	1:A:837:PRO:HA	1.98	0.45
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.51	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:388:PRO:HG2	1:A:391:LEU:HD12	1.98	0.45
1:A:85:LEU:HD11	1:A:303:THR:HG21	1.97	0.45
1:A:335:ILE:O	1:A:335:ILE:HG13	2.16	0.45
1:A:554:LYS:HD3	1:A:555:VAL:H	1.80	0.45
1:A:455:VAL:H	1:A:459:HIS:HD2	1.62	0.45
1:A:809:GLY:HA3	4:A:1060:HOH:O	2.17	0.45
1:A:738:LEU:HD12	1:A:777:TYR:CD2	2.52	0.45
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.50	0.45
1:A:335:ILE:HD11	1:A:337:LEU:HD11	1.98	0.45
1:A:764:MET:HE2	1:A:769:ASP:CA	2.39	0.45
1:A:798:THR:O	1:A:802:ILE:HG13	2.16	0.45
1:A:329:PHE:CD2	1:A:371:THR:HG21	2.51	0.44
1:A:322:VAL:O	1:A:323:ARG:NH1	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:469:LYS:HD3	4:A:1171:HOH:O	2.17	0.44
1:A:423:ASP:O	1:A:426:ARG:HG3	2.18	0.44
1:A:316:PHE:HA	1:A:320:ASP:HB2	2.00	0.44
1:A:519:ARG:NH1	1:A:807:THR:HA	2.32	0.43
1:A:16:ARG:HD2	4:A:1430:HOH:O	2.18	0.43
1:A:72:GLN:O	1:A:75:TYR:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:303:THR:O	1:A:307:ILE:HG13	2.18	0.42
1:A:16:ARG:HB3	1:A:105:GLU:HB3	2.02	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:424:ARG:HH22	1:A:473:GLU:CD	2.23	0.42
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.50	0.42
1:A:542:LYS:HE2	1:A:559:PRO:O	2.20	0.42
1:A:366:GLU:O	1:A:370:LYS:HB2	2.18	0.42
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.55	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:803:ARG:HB2	1:A:803:ARG:HH11	1.84	0.42
1:A:599:VAL:HA	1:A:600:PRO:HD3	1.92	0.42
1:A:423:ASP:O	1:A:427:ARG:HB2	2.19	0.42
1:A:204:GLY:HA2	1:A:217:ASP:O	2.20	0.42
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.02	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.18	0.41
1:A:403:ILE:HG21	1:A:403:ILE:HD13	1.87	0.41
1:A:466:THR:O	1:A:469:LYS:HE2	2.20	0.41
1:A:23:ASN:O	1:A:27:LEU:HD22	2.20	0.41
1:A:319:ARG:HE	1:A:320:ASP:H	1.68	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: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 (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%)	770 (93%)	41 (5%)	18 (2%)	8 9

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
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 (i)

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%)	623 (86%)	97 (14%)	5 5

All (97) 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

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	42	ASP
1	A	55	LEU
1	A	90	TYR
1	A	93	ARG
1	A	94	THR
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	138	ARG
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	245	SER
1	A	251	ASP
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	258	ASN
1	A	289	LYS
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	371	THR
1	A	384	LEU
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	413	ARG
1	A	422	VAL

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	426	ARG
1	A	433	GLU
1	A	437	LYS
1	A	444	LEU
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	510	GLU
1	A	515	LEU
1	A	522	LEU
1	A	523	SER
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	568	LYS
1	A	569	ARG
1	A	574	LYS
1	A	579	ASN
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	641	ARG
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	708	PHE
1	A	713	MET
1	A	743	GLU
1	A	763	ASN
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	770	ARG

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Mol	Chain	Res	Type
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

Some 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	97	ASN
1	A	235	ASN
1	A	390	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	566	GLN
1	A	579	ASN
1	A	614	HIS
1	A	678	ASN
1	A	767	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates 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	-	12,15,15	2.13	6 (50%)	12,22,22	2.00	3 (25%)
2	PLP	A	999	1	15,15,16	1.88	3 (20%)	21,22,23	1.28	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	0/1/2/2
2	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-5.46	1.37	1.40
3	A	998	NTZ	C5-N1	-2.87	1.41	1.47
2	A	999	PLP	P-O1P	-2.48	1.43	1.51
2	A	999	PLP	P-O3P	-2.45	1.45	1.54
3	A	998	NTZ	C4-C5	2.01	1.57	1.53
3	A	998	NTZ	N17-N1	2.36	1.39	1.34
3	A	998	NTZ	C1-N1	2.66	1.41	1.34
3	A	998	NTZ	N21-N18	3.51	1.40	1.34
3	A	998	NTZ	N17-N18	3.87	1.39	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	998	NTZ	C1-C2-C3	-3.18	106.87	113.17
2	A	999	PLP	C5-C6-N1	-2.10	120.21	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	PLP	O3P-P-O1P	2.23	117.75	110.58
2	A	999	PLP	O4P-C5A-C5	3.13	114.17	108.99
3	A	998	NTZ	O2-C2-C1	3.36	114.84	109.97
3	A	998	NTZ	N18-N17-N1	3.66	108.08	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

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.