



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 10:03 am GMT

PDB ID : 1AXR  
Title : COOPERATIVITY BETWEEN HYDROGEN-BONDING AND  
CHARGE-DIPOLE INTERACTIONS IN THE INHIBITION OF BETA-  
GLYCOSIDASES BY AZOLOPYRIDINES: EVIDENCE FROM A STUDY  
WITH GLYCOGEN PHOSPHORYLASE B  
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Deposited on : 1997-10-20  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

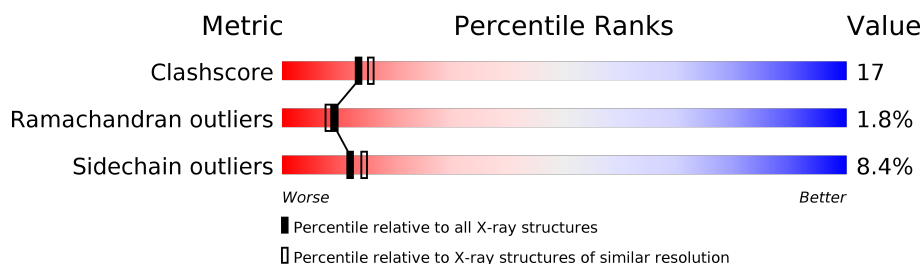
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (2.30-2.30)

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	

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 7281 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	829	Total	C	N	O	S	0	0	0
			6742	4297	1188	1227	30			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



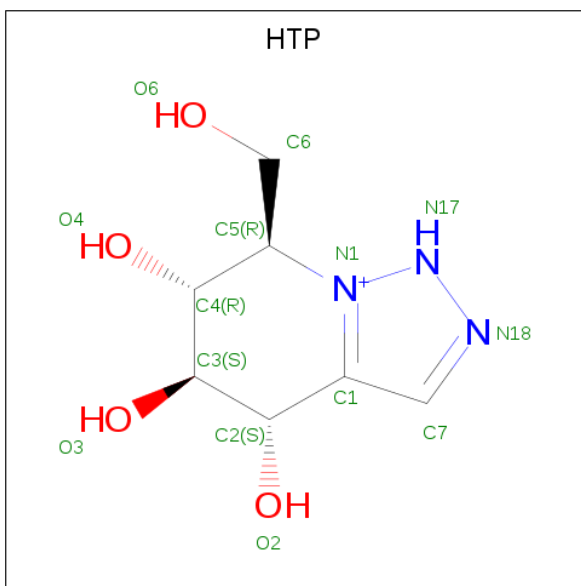
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- 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 4,5,6-TRIHIDROXY-7-HYDROXYMETHYL-4,5,6,7-TETRAHYDRO-1H-[1,2,3]TRIAZOLO[1,5-A]PYRIDIN-8-YLIUM (three-letter code: HTP) (formula:  $C_7H_{12}N_3O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	7	3	4		

- Molecule 5 is water.

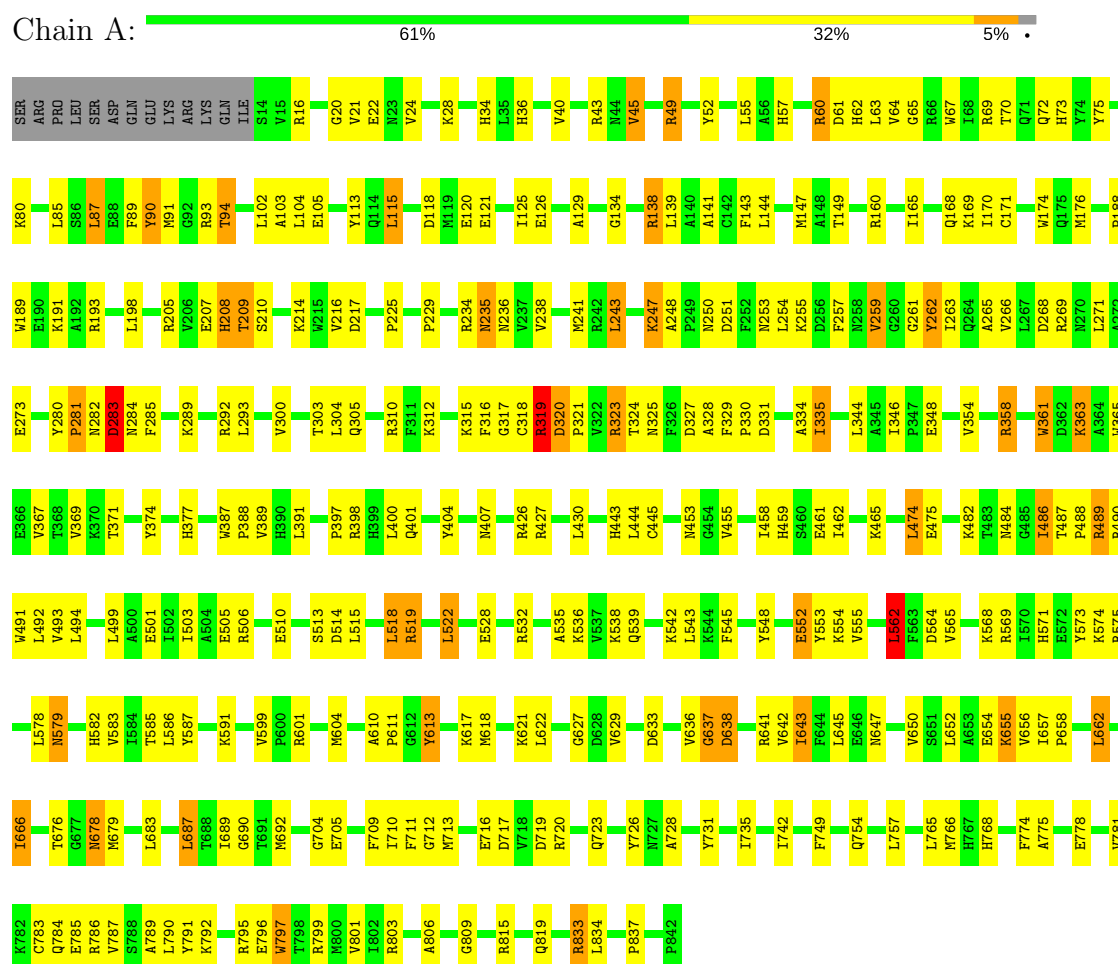
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	500	Total 500	O 500	0	0

### 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 the various outlier classes 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 is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.72Å 126.72Å 115.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	84.9 (8.00-2.30)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.203 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PLP, HTP

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	0.41	0/6896	0.66	1/9333 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	562	LEU	CA-CB-CG	6.71	130.73	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	6742	0	6684	232	0
2	A	10	0	0	2	0
3	A	15	0	7	0	0
4	A	14	0	12	0	0
5	A	500	0	0	23	0
All	All	7281	0	6703	232	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 17.



All (232) 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:565:VAL:HG12	1:A:604:MET:HB2	1.48	0.93
1:A:320:ASP:HB3	1:A:321:PRO:HD2	1.54	0.90
1:A:320:ASP:HB3	1:A:321:PRO:CD	2.01	0.89
1:A:283:ASP:HB2	1:A:569:ARG:HD2	1.59	0.83
1:A:666:ILE:HG23	1:A:711:PHE:HZ	1.47	0.79
1:A:321:PRO:HB2	1:A:323:ARG:NH2	1.97	0.79
1:A:678:ASN:HD22	1:A:679:MET:H	1.31	0.78
1:A:704:GLY:HA2	5:A:1078:HOH:O	1.83	0.77
1:A:571:HIS:HB2	1:A:574:LYS:HD3	1.65	0.77
1:A:742:ILE:HG21	1:A:766:MET:HE1	1.69	0.74
1:A:637:GLY:O	1:A:638:ASP:HB2	1.87	0.74
1:A:545:PHE:CZ	1:A:656:VAL:HG22	2.22	0.73
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.52	0.72
1:A:578:LEU:HD23	1:A:666:ILE:HG21	1.71	0.72
1:A:815:ARG:HH11	1:A:819:GLN:NE2	1.88	0.71
1:A:323:ARG:NH1	1:A:323:ARG:HB2	2.08	0.68
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.75	0.68
1:A:474:LEU:HD13	1:A:475:GLU:HG3	1.75	0.68
1:A:458:ILE:O	1:A:462:ILE:HG13	1.94	0.68
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.76	0.67
1:A:514:ASP:HB2	5:A:1433:HOH:O	1.93	0.67
1:A:250:ASN:HB3	1:A:269:ARG:NH2	2.10	0.67
1:A:235:ASN:H	1:A:235:ASN:HD22	1.44	0.66
1:A:610:ALA:HB3	1:A:613:TYR:HB2	1.78	0.66
1:A:236:ASN:HB2	1:A:834:LEU:O	1.95	0.66
1:A:678:ASN:ND2	1:A:679:MET:H	1.94	0.66
1:A:293:LEU:HD23	1:A:391:LEU:HD22	1.76	0.66
1:A:165:ILE:HD11	1:A:281:PRO:HA	1.78	0.66
1:A:578:LEU:HD23	1:A:666:ILE:CG2	2.27	0.65
1:A:455:VAL:H	1:A:459:HIS:HD2	1.43	0.65
1:A:315:LYS:O	1:A:319:ARG:HD3	1.97	0.65
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.79	0.65
1:A:569:ARG:HG2	1:A:574:LYS:HE3	1.80	0.63
1:A:426:ARG:HH21	1:A:427:ARG:HG2	1.63	0.63
1:A:247:LYS:HA	1:A:273:GLU:HG2	1.81	0.63
1:A:312:LYS:O	1:A:317:GLY:HA3	1.99	0.62
1:A:599:VAL:HG23	1:A:792:LYS:HE3	1.80	0.62
1:A:89:PHE:HB3	1:A:91:MET:HE3	1.81	0.62
1:A:692:MET:HG2	1:A:710:ILE:HG21	1.80	0.61
1:A:87:LEU:HD22	1:A:292:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:ARG:O	1:A:799:ARG:HG3	2.01	0.61
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.82	0.61
1:A:316:PHE:CZ	1:A:328:ALA:HB3	2.35	0.61
1:A:323:ARG:HH11	1:A:323:ARG:HB2	1.66	0.61
1:A:170:ILE:HA	1:A:174:TRP:O	2.01	0.61
1:A:69:ARG:NH2	1:A:837:PRO:HA	2.16	0.61
1:A:552:GLU:HB3	1:A:553:TYR:CD1	2.36	0.60
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.01	0.60
1:A:43:ARG:HH21	1:A:115:LEU:HG	1.66	0.59
1:A:678:ASN:HD22	1:A:678:ASN:N	1.99	0.59
1:A:335:ILE:HG23	1:A:371:THR:HG22	1.84	0.59
1:A:118:ASP:O	1:A:121:GLU:HG2	2.03	0.58
1:A:61:ASP:O	1:A:64:VAL:HG22	2.02	0.58
1:A:728:ALA:HB1	1:A:774:PHE:CD2	2.39	0.58
1:A:545:PHE:CE1	1:A:656:VAL:HG22	2.39	0.58
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.86	0.57
1:A:487:THR:O	1:A:491:TRP:HB2	2.04	0.57
1:A:784:GLN:O	1:A:787:VAL:HG22	2.05	0.57
1:A:510:GLU:HB2	5:A:1390:HOH:O	2.04	0.56
1:A:69:ARG:CZ	1:A:837:PRO:HA	2.34	0.56
1:A:89:PHE:HB3	1:A:91:MET:CE	2.36	0.56
1:A:361:TRP:HZ3	5:A:1354:HOH:O	1.88	0.56
1:A:316:PHE:HZ	1:A:328:ALA:HB3	1.71	0.55
1:A:329:PHE:N	1:A:330:PRO:HD2	2.21	0.55
1:A:666:ILE:HG23	1:A:711:PHE:CZ	2.34	0.55
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.89	0.55
1:A:768:HIS:HE1	5:A:1365:HOH:O	1.90	0.55
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.88	0.54
1:A:506:ARG:HH11	1:A:506:ARG:HG2	1.73	0.54
1:A:315:LYS:HD2	1:A:319:ARG:HH11	1.71	0.54
1:A:248:ALA:HB3	1:A:269:ARG:HG3	1.90	0.54
1:A:62:HIS:HD2	5:A:1422:HOH:O	1.89	0.54
1:A:62:HIS:CD2	5:A:1422:HOH:O	2.60	0.54
1:A:678:ASN:ND2	1:A:678:ASN:N	2.55	0.54
1:A:499:LEU:O	1:A:503:ILE:HG13	2.07	0.54
1:A:548:TYR:CE1	1:A:655:LYS:HE2	2.44	0.53
1:A:687:LEU:HD13	1:A:801:VAL:HG22	1.90	0.53
1:A:573:TYR:CZ	1:A:574:LYS:HD2	2.44	0.53
1:A:93:ARG:CG	1:A:93:ARG:HH11	2.21	0.53
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.73	0.53
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:HD13	1:A:778:GLU:HG3	1.90	0.53
1:A:486:ILE:HD11	1:A:676:THR:HB	1.91	0.52
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.44	0.52
1:A:731:TYR:CE2	1:A:775:ALA:HA	2.43	0.52
1:A:138:ARG:O	1:A:138:ARG:HD3	2.10	0.52
1:A:216:VAL:HG22	1:A:217:ASP:H	1.75	0.52
1:A:67:TRP:HA	1:A:238:VAL:HB	1.92	0.52
1:A:216:VAL:HG22	1:A:217:ASP:N	2.25	0.51
1:A:575:ARG:HD3	1:A:666:ILE:O	2.10	0.51
1:A:678:ASN:HD22	1:A:679:MET:N	2.03	0.51
1:A:461:GLU:HB3	1:A:465:LYS:HE2	1.91	0.51
1:A:650:VAL:O	1:A:654:GLU:HG3	2.10	0.51
1:A:235:ASN:N	1:A:235:ASN:HD22	2.04	0.51
1:A:254:LEU:HD11	1:A:266:VAL:CG2	2.41	0.50
1:A:346:ILE:CD1	1:A:445:CYS:HA	2.41	0.50
1:A:93:ARG:HD2	5:A:1007:HOH:O	2.11	0.50
1:A:205:ARG:HH12	1:A:207:GLU:HG3	1.78	0.49
1:A:282:ASN:O	1:A:284:ASN:N	2.46	0.49
1:A:304:LEU:HD22	1:A:348:GLU:HG3	1.94	0.49
1:A:102:LEU:O	1:A:103:ALA:HB3	2.12	0.49
1:A:253:ASN:O	1:A:254:LEU:HB2	2.13	0.49
1:A:815:ARG:HH11	1:A:819:GLN:HE21	1.59	0.49
1:A:60:ARG:HG3	1:A:188:PRO:O	2.12	0.49
1:A:783:CYS:O	1:A:787:VAL:HG13	2.13	0.49
1:A:254:LEU:HD12	1:A:262:TYR:CD1	2.48	0.49
1:A:149:THR:HG21	1:A:489:ARG:NH1	2.28	0.49
1:A:662:LEU:HD22	1:A:689:ILE:HG22	1.95	0.49
1:A:781:VAL:O	1:A:785:GLU:HG3	2.13	0.49
1:A:709:PHE:CD1	1:A:787:VAL:HG12	2.49	0.48
1:A:266:VAL:O	1:A:269:ARG:HB3	2.13	0.48
1:A:490:ARG:HA	1:A:494:LEU:HD22	1.96	0.48
1:A:538:LYS:O	1:A:542:LYS:HG3	2.13	0.48
1:A:171:CYS:SG	1:A:176:MET:HG3	2.54	0.48
1:A:28:LYS:HD2	1:A:115:LEU:HD13	1.94	0.48
1:A:582:HIS:O	1:A:585:THR:HB	2.13	0.48
1:A:65:GLY:CA	1:A:837:PRO:HG3	2.44	0.48
1:A:129:ALA:HB2	5:A:1009:HOH:O	2.12	0.48
1:A:569:ARG:HG3	1:A:571:HIS:CD2	2.48	0.48
1:A:501:GLU:O	1:A:505:GLU:HG3	2.14	0.48
1:A:143:PHE:O	1:A:147:MET:HG3	2.14	0.47
1:A:389:VAL:HG21	1:A:404:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:O	1:A:40:VAL:HA	2.13	0.47
1:A:70:THR:O	1:A:73:HIS:HB3	2.14	0.47
1:A:321:PRO:HG3	1:A:325:ASN:HB3	1.96	0.47
1:A:407:ASN:OD1	1:A:430:LEU:HG	2.14	0.47
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.29	0.47
1:A:254:LEU:HD13	1:A:265:ALA:HB3	1.95	0.47
1:A:742:ILE:HG21	1:A:766:MET:CE	2.42	0.47
1:A:214:LYS:HA	5:A:1154:HOH:O	2.13	0.47
1:A:139:LEU:CD2	1:A:377:HIS:HE1	2.27	0.47
1:A:198:LEU:HD23	1:A:305:GLN:HB2	1.95	0.47
1:A:293:LEU:CD2	1:A:391:LEU:HD22	2.44	0.47
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.97	0.46
1:A:690:GLY:O	1:A:710:ILE:HA	2.15	0.46
1:A:268:ASP:O	1:A:271:LEU:HB3	2.16	0.46
1:A:562:LEU:HB3	1:A:601:ARG:HG3	1.97	0.46
1:A:536:LYS:HB3	1:A:536:LYS:NZ	2.31	0.46
1:A:719:ASP:O	1:A:723:GLN:HG3	2.15	0.46
1:A:455:VAL:H	1:A:459:HIS:CD2	2.28	0.46
1:A:282:ASN:HB3	1:A:285:PHE:HB3	1.97	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.97	0.46
1:A:711:PHE:HA	5:A:1453:HOH:O	2.14	0.46
1:A:20:GLY:O	1:A:24:VAL:HG23	2.16	0.46
1:A:453:ASN:ND2	1:A:482:LYS:HB2	2.31	0.46
1:A:569:ARG:NH1	2:A:997:PO4:P	2.88	0.46
1:A:208:HIS:HD2	5:A:1471:HOH:O	1.97	0.46
1:A:259:VAL:HB	5:A:1149:HOH:O	2.15	0.46
1:A:535:ALA:HA	5:A:1052:HOH:O	2.14	0.46
1:A:539:GLN:NE2	1:A:542:LYS:HD3	2.31	0.46
1:A:799:ARG:O	1:A:803:ARG:HG3	2.16	0.46
1:A:300:VAL:O	1:A:304:LEU:HD13	2.15	0.45
1:A:72:GLN:HA	1:A:75:TYR:CD2	2.51	0.45
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.52	0.45
1:A:795:ARG:HG3	1:A:795:ARG:HH11	1.82	0.45
1:A:354:VAL:O	1:A:358:ARG:HA	2.17	0.45
1:A:587:TYR:O	1:A:591:LYS:HG2	2.16	0.45
1:A:712:GLY:HA2	5:A:1164:HOH:O	2.16	0.45
1:A:488:PRO:O	1:A:492:LEU:HB3	2.16	0.45
1:A:365:TRP:O	1:A:369:VAL:HG22	2.17	0.44
1:A:430:LEU:CD2	1:A:443:HIS:HB3	2.45	0.44
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.99	0.44
1:A:486:ILE:CD1	1:A:676:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:HA	1:A:320:ASP:HB2	1.99	0.44
1:A:692:MET:HG2	1:A:710:ILE:CG2	2.45	0.44
1:A:63:LEU:HD13	1:A:229:PRO:HG3	1.99	0.44
1:A:801:VAL:HG11	5:A:1286:HOH:O	2.15	0.44
1:A:786:ARG:O	1:A:789:ALA:HB3	2.17	0.44
1:A:289:LYS:HE2	1:A:289:LYS:HA	2.00	0.44
1:A:374:TYR:HB2	1:A:445:CYS:HB3	2.00	0.44
1:A:284:ASN:HB3	5:A:1437:HOH:O	2.17	0.44
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.98	0.44
1:A:613:TYR:O	1:A:617:LYS:HG2	2.18	0.44
1:A:754:GLN:O	1:A:757:LEU:HB2	2.18	0.44
1:A:235:ASN:H	1:A:235:ASN:ND2	2.12	0.43
1:A:678:ASN:ND2	1:A:678:ASN:H	2.16	0.43
1:A:139:LEU:HD11	1:A:143:PHE:CZ	2.53	0.43
1:A:579:ASN:O	1:A:583:VAL:HG23	2.18	0.43
1:A:716:GLU:O	1:A:720:ARG:HG3	2.18	0.43
1:A:465:LYS:HD3	5:A:1394:HOH:O	2.18	0.43
1:A:21:VAL:HG13	1:A:22:GLU:N	2.33	0.43
1:A:678:ASN:ND2	1:A:679:MET:N	2.64	0.43
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.48	0.43
1:A:618:MET:O	1:A:621:LYS:HB3	2.18	0.43
1:A:652:LEU:HD12	1:A:655:LYS:HZ3	1.84	0.43
1:A:726:TYR:HE1	1:A:775:ALA:HB2	1.84	0.43
1:A:91:MET:HE1	1:A:141:ALA:HA	2.01	0.43
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.90	0.43
1:A:90:TYR:HE2	1:A:134:GLY:HA2	1.83	0.43
1:A:205:ARG:NH1	1:A:207:GLU:HG3	2.34	0.42
1:A:254:LEU:HD11	1:A:266:VAL:HG23	2.01	0.42
1:A:455:VAL:HB	1:A:484:ASN:ND2	2.34	0.42
1:A:488:PRO:O	1:A:493:VAL:HG23	2.20	0.42
1:A:310:ARG:HH11	2:A:996:PO4:P	2.42	0.42
1:A:165:ILE:HD12	1:A:165:ILE:HA	1.88	0.42
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.00	0.42
1:A:519:ARG:O	1:A:522:LEU:HB2	2.19	0.42
1:A:397:PRO:O	1:A:401:GLN:HG3	2.20	0.42
1:A:636:VAL:HG12	1:A:641:ARG:HH21	1.84	0.42
1:A:754:GLN:HG3	1:A:757:LEU:HD22	2.01	0.42
1:A:169:LYS:O	1:A:176:MET:N	2.53	0.42
1:A:168:GLN:HB3	1:A:647:ASN:HA	2.01	0.41
1:A:627:GLY:HA2	1:A:642:VAL:HB	2.01	0.41
1:A:63:LEU:HD13	1:A:229:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HE3	5:A:1467:HOH:O	2.19	0.41
1:A:94:THR:HG23	1:A:189:TRP:NE1	2.35	0.41
1:A:165:ILE:HD12	5:A:1352:HOH:O	2.19	0.41
1:A:139:LEU:HD23	1:A:377:HIS:HE1	1.85	0.41
1:A:633:ASP:HB3	1:A:636:VAL:HG23	2.02	0.41
1:A:261:GLY:O	1:A:263:ILE:N	2.54	0.41
1:A:319:ARG:HB2	1:A:320:ASP:H	1.68	0.41
1:A:510:GLU:HG2	5:A:1376:HOH:O	2.21	0.41
1:A:552:GLU:HB3	1:A:553:TYR:CE1	2.55	0.41
1:A:655:LYS:HB2	1:A:655:LYS:NZ	2.36	0.41
1:A:280:TYR:HA	1:A:281:PRO:HD2	1.86	0.41
1:A:778:GLU:O	1:A:781:VAL:HG22	2.20	0.41
1:A:304:LEU:HD22	1:A:348:GLU:CG	2.51	0.41
1:A:209:THR:OG1	1:A:210:SER:N	2.53	0.41
1:A:241:MET:HG2	1:A:243:LEU:HD13	2.03	0.41
1:A:458:ILE:HG23	1:A:459:HIS:N	2.36	0.40
1:A:52:TYR:CZ	1:A:126:GLU:HB2	2.56	0.40
1:A:586:LEU:HD21	5:A:1472:HOH:O	2.20	0.40
1:A:629:VAL:HG11	1:A:749:PHE:CE2	2.55	0.40
1:A:250:ASN:CA	1:A:269:ARG:HH12	2.33	0.40
1:A:363:LYS:HZ1	1:A:367:VAL:CG2	2.33	0.40
1:A:562:LEU:HD12	1:A:564:ASP:HB2	2.04	0.40
1:A:321:PRO:HB2	1:A:323:ARG:HH22	1.80	0.40
1:A:331:ASP:HA	5:A:1439:HOH:O	2.21	0.40
1:A:528:GLU:HB3	1:A:532:ARG:NH1	2.37	0.40
1:A:16:ARG:HB3	1:A:105:GLU:HB3	2.04	0.40
1:A:387:TRP:HA	1:A:388:PRO:HD3	1.92	0.40
1:A:642:VAL:O	1:A:643:ILE:HD12	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	827/842 (98%)	741 (90%)	71 (9%)	15 (2%)	9 8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	A	320	ASP
1	A	555	VAL
1	A	637	GLY
1	A	259	VAL
1	A	262	TYR
1	A	283	ASP
1	A	638	ASP
1	A	318	CYS
1	A	324	THR
1	A	45	VAL
1	A	251	ASP
1	A	319	ARG
1	A	281	PRO
1	A	666	ILE

### 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	718/731 (98%)	658 (92%)	60 (8%)	12 14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	49	ARG
1	A	55	LEU
1	A	60	ARG
1	A	87	LEU
1	A	90	TYR

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Mol	Chain	Res	Type
1	A	94	THR
1	A	104	LEU
1	A	113	TYR
1	A	115	LEU
1	A	120	GLU
1	A	138	ARG
1	A	144	LEU
1	A	191	LYS
1	A	208	HIS
1	A	209	THR
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	257	PHE
1	A	283	ASP
1	A	319	ARG
1	A	323	ARG
1	A	335	ILE
1	A	344	LEU
1	A	358	ARG
1	A	361	TRP
1	A	363	LYS
1	A	398	ARG
1	A	400	LEU
1	A	444	LEU
1	A	474	LEU
1	A	486	ILE
1	A	489	ARG
1	A	513	SER
1	A	518	LEU
1	A	519	ARG
1	A	522	LEU
1	A	543	LEU
1	A	552	GLU
1	A	554	LYS
1	A	562	LEU
1	A	568	LYS
1	A	579	ASN
1	A	611	PRO
1	A	613	TYR
1	A	622	LEU
1	A	643	ILE

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Mol	Chain	Res	Type
1	A	645	LEU
1	A	655	LYS
1	A	662	LEU
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	705	GLU
1	A	765	LEU
1	A	790	LEU
1	A	796	GLU
1	A	797	TRP
1	A	833	ARG

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	62	HIS
1	A	97	ASN
1	A	106	ASN
1	A	114	GLN
1	A	208	HIS
1	A	235	ASN
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	768	HIS
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 [i](#)

There are no carbohydrates 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
2	PO4	A	996	-	4,4,4	4.21	4 (100%)	6,6,6	1.92	3 (50%)
2	PO4	A	997	-	4,4,4	3.70	4 (100%)	6,6,6	1.82	2 (33%)
4	HTP	A	998	-	13,15,15	1.72	4 (30%)	12,22,22	4.36	1 (8%)
3	PLP	A	999	1	15,15,16	1.52	4 (26%)	20,22,23	2.31	6 (30%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	PO4	P-O3	-3.92	1.40	1.54
2	A	996	PO4	P-O3	-3.53	1.42	1.54
3	A	999	PLP	P-O3P	-3.44	1.41	1.54
2	A	996	PO4	P-O4	-3.20	1.43	1.54
2	A	997	PO4	P-O4	-2.79	1.44	1.54
2	A	996	PO4	P-O2	-2.44	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	PO4	P-O2	-2.20	1.46	1.54
4	A	998	HTP	C5-N1	-2.07	1.43	1.48
3	A	999	PLP	C3-C2	-2.02	1.39	1.40
3	A	999	PLP	C4A-C4	2.25	1.56	1.51
3	A	999	PLP	C5A-C5	2.37	1.57	1.50
4	A	998	HTP	N17-N1	2.43	1.39	1.34
4	A	998	HTP	N18-N17	2.78	1.39	1.34
4	A	998	HTP	C1-N1	3.89	1.43	1.37
2	A	997	PO4	P-O1	5.17	1.62	1.50
2	A	996	PO4	P-O1	6.50	1.65	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	HTP	C1-N1-N17	-14.64	107.19	113.08
3	A	999	PLP	O2P-P-O4P	-5.27	92.72	106.73
3	A	999	PLP	O2P-P-O1P	-4.66	92.42	110.60
2	A	997	PO4	O2-P-O1	-2.51	100.22	110.93
2	A	996	PO4	O2-P-O1	-2.37	100.81	110.93
2	A	996	PO4	O4-P-O2	2.22	116.03	107.94
3	A	999	PLP	O3P-P-O4P	2.60	113.66	106.73
2	A	996	PO4	O4-P-O3	2.62	117.49	107.94
2	A	997	PO4	O4-P-O3	3.12	119.34	107.94
3	A	999	PLP	O4P-C5A-C5	3.15	115.45	109.39
3	A	999	PLP	O3P-P-O1P	3.51	124.29	110.60
3	A	999	PLP	O4P-P-O1P	4.16	118.15	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	996	PO4	1	0
2	A	997	PO4	1	0

## 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.