



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:26 pm BST

PDB ID : 1GZV
Title : The crystal structure of phosphoglucose isomerase from pig muscle complexed with 5-phosphoarabinonate
Authors : Davies, C.; Muirhead, H.
Deposited on : 2002-06-06
Resolution : 3.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

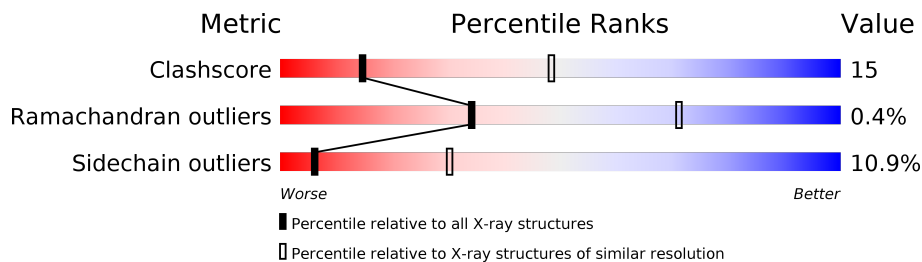
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)

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 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	557	

2 Entry composition [i](#)

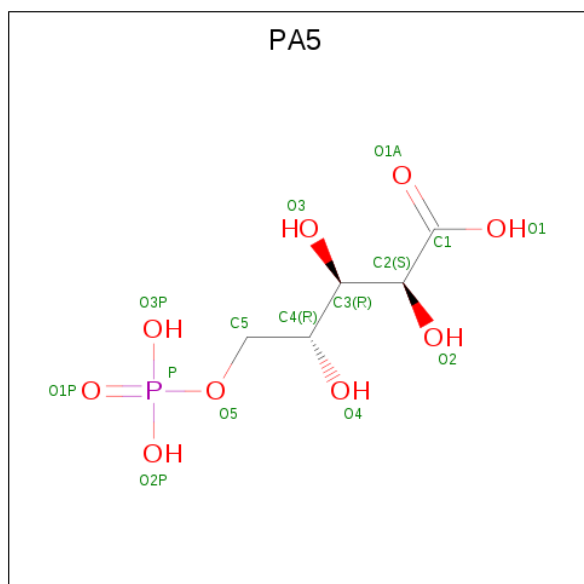
There are 2 unique types of molecules in this entry. The entry contains 4437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-6-PHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4422	2828	768	810	16	0	0	0

- Molecule 2 is 5-PHOSPHOARABINONIC ACID (three-letter code: PA5) (formula: C₅H₁₁O₉P).



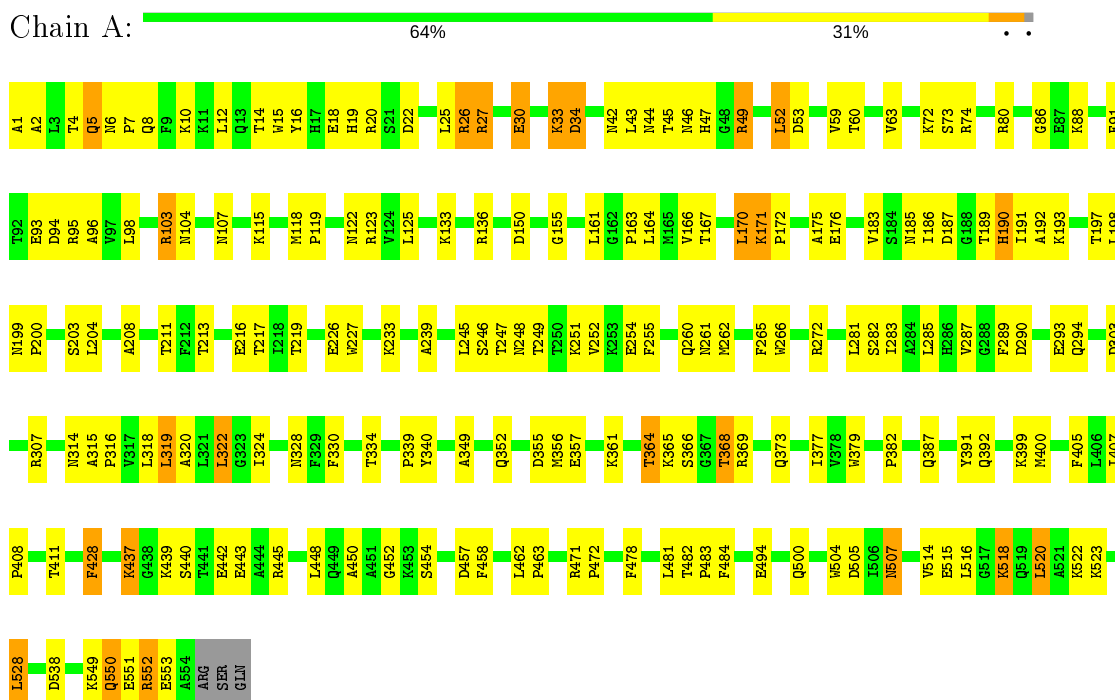
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	15	5	9	1	0	0

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. 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: GLUCOSE-6-PHOSPHATE ISOMERASE



4 Data and refinement statistics

Xtrriage (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	95.60Å 95.60Å 138.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.51	Depositor
% Data completeness (in resolution range)	92.8 (15.00-3.51)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0.32	Depositor
R, R_{free}	0.190 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4437	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: PA5

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	0.84	0/4533	1.05	12/6136 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	95	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	53	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	538	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	505	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	355	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	150	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	26	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	322	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	123	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	12	LEU	CA-CB-CG	-5.18	103.37	115.30
1	A	290	ASP	CB-CG-OD2	5.12	122.91	118.30

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	4422	0	4376	134	0
2	A	15	0	8	3	0
All	All	4437	0	4384	134	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 15.

All (134) 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:364:THR:HG22	1:A:366:SER:H	1.20	1.03
1:A:448:LEU:HD13	1:A:458:PHE:HB2	1.63	0.81
1:A:328:ASN:HD21	1:A:504:TRP:HE1	1.29	0.79
1:A:103:ARG:HD2	1:A:303:ASP:OD2	1.82	0.78
1:A:1:ALA:O	1:A:5:GLN:HB2	1.85	0.77
1:A:440:SER:OG	1:A:443:GLU:HG3	1.84	0.76
1:A:518:LYS:NZ	2:A:600:PA5:O4	2.19	0.75
1:A:364:THR:HG22	1:A:366:SER:N	2.01	0.73
1:A:185:ASN:H	1:A:190:HIS:HD2	1.39	0.71
1:A:330:PHE:HB3	1:A:400:MET:HE3	1.74	0.70
1:A:4:THR:O	1:A:10:LYS:HE2	1.93	0.69
1:A:528:LEU:O	1:A:552:ARG:NH1	2.27	0.68
1:A:166:VAL:CG1	1:A:170:LEU:HD22	2.24	0.68
1:A:516:LEU:O	1:A:520:LEU:HG	1.93	0.67
1:A:33:LYS:HD3	1:A:33:LYS:N	2.09	0.67
1:A:34:ASP:N	1:A:34:ASP:OD2	2.26	0.67
1:A:247:THR:HG22	1:A:265:PHE:O	1.95	0.66
1:A:163:PRO:HA	1:A:283:ILE:HD11	1.78	0.66
1:A:450:ALA:C	1:A:452:GLY:H	1.98	0.64
1:A:45:THR:O	1:A:46:ASN:HB2	1.96	0.64
1:A:175:ALA:HB3	1:A:176:GLU:OE1	1.98	0.64
1:A:252:VAL:HG21	1:A:262:MET:SD	2.37	0.63
1:A:405:PHE:HB3	1:A:428:PHE:CE1	2.34	0.63
1:A:44:ASN:HB2	1:A:49:ARG:HH11	1.64	0.63
1:A:91:PHE:CE1	1:A:365:LYS:HD2	2.34	0.63
1:A:448:LEU:HD13	1:A:458:PHE:CB	2.28	0.63
1:A:364:THR:CG2	1:A:365:LYS:N	2.61	0.62
1:A:364:THR:CG2	1:A:366:SER:H	2.03	0.62
1:A:445:ARG:HH11	1:A:445:ARG:HB3	1.65	0.62
1:A:328:ASN:ND2	1:A:504:TRP:HE1	1.98	0.61
1:A:442:GLU:OE1	1:A:445:ARG:NH1	2.34	0.60
1:A:49:ARG:HG2	1:A:49:ARG:NH1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ALA:HB1	1:A:500:GLN:HG3	1.83	0.60
1:A:248:ASN:OD1	1:A:251:LYS:HG2	2.02	0.59
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.67	0.59
1:A:352:GLN:O	1:A:356:MET:HB2	2.02	0.58
1:A:44:ASN:HB2	1:A:49:ARG:NH1	2.18	0.58
1:A:550:GLN:NE2	1:A:551:GLU:HG2	2.19	0.58
1:A:185:ASN:H	1:A:190:HIS:CD2	2.21	0.58
1:A:340:TYR:OH	1:A:387:GLN:NE2	2.30	0.58
1:A:166:VAL:HG13	1:A:170:LEU:HD22	1.87	0.57
1:A:44:ASN:OD1	1:A:46:ASN:N	2.34	0.57
1:A:199:ASN:OD1	1:A:200:PRO:HD2	2.05	0.57
1:A:294:GLN:HE21	1:A:484:PHE:HB2	1.69	0.57
1:A:314:ASN:OD1	1:A:316:PRO:HD2	2.04	0.57
1:A:364:THR:HG23	1:A:365:LYS:N	2.21	0.56
1:A:189:THR:HG22	1:A:193:LYS:HE3	1.87	0.56
1:A:482:THR:HB	1:A:483:PRO:HD2	1.87	0.56
1:A:166:VAL:CG1	1:A:170:LEU:CD2	2.84	0.55
1:A:27:ARG:HA	1:A:30:GLU:HG2	1.88	0.55
1:A:166:VAL:HG12	1:A:170:LEU:HD22	1.88	0.55
1:A:387:GLN:HA	1:A:391:TYR:CG	2.43	0.54
1:A:6:ASN:OD1	1:A:8:GLN:N	2.40	0.54
1:A:183:VAL:HG11	1:A:191:ILE:HD13	1.90	0.53
1:A:349:ALA:O	1:A:352:GLN:HB2	2.08	0.53
1:A:368:THR:CG2	1:A:369:ARG:N	2.71	0.53
1:A:450:ALA:C	1:A:452:GLY:N	2.62	0.53
1:A:442:GLU:CD	1:A:445:ARG:NH1	2.62	0.53
1:A:49:ARG:CG	1:A:49:ARG:HH11	2.22	0.52
1:A:364:THR:HG23	1:A:365:LYS:H	1.75	0.52
1:A:93:GLU:O	1:A:94:ASP:HB3	2.09	0.52
1:A:52:LEU:HD11	1:A:319:LEU:HD13	1.92	0.52
1:A:19:HIS:O	1:A:22:ASP:N	2.44	0.50
1:A:60:THR:OG1	1:A:63:VAL:HG23	2.11	0.50
1:A:330:PHE:HB3	1:A:400:MET:CE	2.42	0.50
1:A:445:ARG:HB3	1:A:445:ARG:NH1	2.27	0.50
1:A:171:LYS:HB3	1:A:172:PRO:HD3	1.94	0.50
1:A:379:TRP:N	1:A:379:TRP:CD1	2.78	0.50
1:A:281:LEU:O	1:A:285:LEU:HB2	2.11	0.49
1:A:428:PHE:CD2	1:A:428:PHE:C	2.85	0.49
1:A:361:LYS:NZ	1:A:507:ASN:O	2.45	0.49
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.93	0.49
1:A:103:ARG:NH1	1:A:303:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:O	1:A:213:THR:HG23	2.13	0.49
1:A:7:PRO:HG2	1:A:8:GLN:NE2	2.28	0.49
1:A:439:LYS:HG3	1:A:443:GLU:HB2	1.93	0.49
1:A:334:THR:HG22	1:A:377:ILE:HB	1.95	0.49
1:A:2:ALA:HB1	1:A:74:ARG:NH2	2.28	0.49
1:A:330:PHE:CB	1:A:400:MET:HE3	2.40	0.48
1:A:260:GLN:O	1:A:260:GLN:HG3	2.13	0.48
1:A:482:THR:HB	1:A:483:PRO:CD	2.43	0.48
1:A:407:ILE:HG13	1:A:408:PRO:HD2	1.94	0.47
1:A:255:PHE:O	1:A:255:PHE:CD1	2.67	0.47
1:A:387:GLN:HG2	1:A:391:TYR:CE2	2.49	0.47
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.48	0.47
1:A:448:LEU:HD13	1:A:458:PHE:CG	2.50	0.46
1:A:281:LEU:HA	1:A:281:LEU:HD12	1.62	0.46
1:A:186:ILE:HB	1:A:216:GLU:HB3	1.98	0.46
1:A:86:GLY:HA2	1:A:98:LEU:HD21	1.98	0.46
1:A:107:ASN:ND2	1:A:122:ASN:OD1	2.49	0.46
1:A:163:PRO:O	1:A:167:THR:HG23	2.16	0.46
1:A:454:SER:O	1:A:457:ASP:N	2.46	0.45
1:A:211:THR:HG23	2:A:600:PA5:O1P	2.16	0.45
1:A:239:ALA:O	1:A:261:ASN:ND2	2.50	0.45
1:A:334:THR:HB	1:A:377:ILE:O	2.16	0.45
1:A:7:PRO:HG2	1:A:8:GLN:HE21	1.81	0.45
1:A:19:HIS:O	1:A:20:ARG:C	2.54	0.45
1:A:199:ASN:O	1:A:203:SER:OG	2.22	0.44
1:A:471:ARG:HA	1:A:472:PRO:HD3	1.70	0.44
1:A:103:ARG:NH2	1:A:494:GLU:OE1	2.51	0.44
1:A:549:LYS:HG2	1:A:552:ARG:NH1	2.31	0.44
1:A:88:LYS:HA	1:A:96:ALA:HA	1.99	0.44
1:A:200:PRO:HG3	1:A:227:TRP:CH2	2.53	0.44
1:A:439:LYS:HA	1:A:443:GLU:OE2	2.17	0.43
1:A:16:TYR:C	1:A:18:GLU:N	2.68	0.43
1:A:16:TYR:OH	1:A:20:ARG:NH1	2.52	0.43
1:A:185:ASN:N	1:A:190:HIS:HD2	2.11	0.43
1:A:287:VAL:O	1:A:287:VAL:HG13	2.18	0.43
1:A:166:VAL:HG12	1:A:170:LEU:CD2	2.46	0.43
1:A:528:LEU:HA	1:A:528:LEU:HD12	1.83	0.43
1:A:357:GLU:OE1	2:A:600:PA5:O1A	2.37	0.42
1:A:164:LEU:C	1:A:164:LEU:HD23	2.40	0.42
1:A:26:ARG:CZ	1:A:437:LYS:HG3	2.49	0.42
1:A:118:MET:N	1:A:119:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HB2	1:A:245:LEU:HD12	2.02	0.42
1:A:104:ASN:HD22	1:A:118:MET:CE	2.32	0.42
1:A:45:THR:O	1:A:47:HIS:HD2	2.03	0.42
1:A:93:GLU:O	1:A:94:ASP:CB	2.67	0.42
1:A:15:TRP:O	1:A:19:HIS:HD2	2.02	0.42
1:A:289:PHE:CE2	1:A:293:GLU:CG	3.03	0.42
1:A:289:PHE:CD2	1:A:293:GLU:HG3	2.55	0.41
1:A:104:ASN:HB3	1:A:118:MET:HE1	2.02	0.41
1:A:391:TYR:O	1:A:392:GLN:C	2.59	0.41
1:A:191:ILE:CG2	1:A:192:ALA:N	2.83	0.41
1:A:266:TRP:N	1:A:266:TRP:CD2	2.87	0.41
1:A:339:PRO:O	1:A:382:PRO:HA	2.20	0.41
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.86	0.41
1:A:189:THR:HG22	1:A:193:LYS:CE	2.49	0.41
1:A:155:GLY:HA2	1:A:217:THR:HG23	2.03	0.41
1:A:251:LYS:HE3	1:A:251:LYS:HB3	1.93	0.41
1:A:80:ARG:HD3	1:A:307:ARG:HA	2.03	0.41
1:A:272:ARG:NH2	1:A:357:GLU:OE1	2.52	0.40
1:A:462:LEU:HB3	1:A:463:PRO:HD3	2.02	0.40
1:A:246:SER:OG	1:A:247:THR:N	2.54	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	552/557 (99%)	516 (94%)	34 (6%)	2 (0%)	34 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	LEU

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Mol	Chain	Res	Type
1	A	233	LYS

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	476/479 (99%)	424 (89%)	52 (11%)	6 30

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	14	THR
1	A	25	LEU
1	A	27	ARG
1	A	30	GLU
1	A	33	LYS
1	A	34	ASP
1	A	42	ASN
1	A	43	LEU
1	A	49	ARG
1	A	52	LEU
1	A	59	VAL
1	A	72	LYS
1	A	73	SER
1	A	103	ARG
1	A	115	LYS
1	A	125	LEU
1	A	133	LYS
1	A	136	ARG
1	A	161	LEU
1	A	170	LEU
1	A	171	LYS
1	A	190	HIS
1	A	197	THR
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	219	THR
1	A	226	GLU
1	A	249	THR
1	A	254	GLU
1	A	282	SER
1	A	319	LEU
1	A	322	LEU
1	A	324	ILE
1	A	364	THR
1	A	368	THR
1	A	373	GLN
1	A	399	LYS
1	A	411	THR
1	A	428	PHE
1	A	437	LYS
1	A	478	PHE
1	A	507	ASN
1	A	514	VAL
1	A	515	GLU
1	A	518	LYS
1	A	522	LYS
1	A	523	LYS
1	A	528	LEU
1	A	550	GLN
1	A	552	ARG
1	A	553	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	13	GLN
1	A	42	ASN
1	A	46	ASN
1	A	47	HIS
1	A	57	ASN
1	A	107	ASN
1	A	122	ASN
1	A	190	HIS
1	A	230	GLN
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	294	GLN
1	A	300	HIS
1	A	328	ASN
1	A	359	ASN
1	A	387	GLN
1	A	474	ASN
1	A	500	GLN
1	A	507	ASN
1	A	550	GLN

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](#)

1 ligand is 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	PA5	A	600	1	11,14,14	0.82	0	16,20,20	1.35	2 (12%)

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	PA5	A	600	1	-	1/14/18/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	600	PA5	O3P-P-O2P	3.59	121.37	107.64
2	A	600	PA5	O2-C2-C1	-2.37	105.41	111.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	PA5	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PA5	3	0

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.