



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DPG
Title : GLUCOSE 6-PHOSPHATE DEHYDROGENASE FROM LEUCONOSTOC
MESENTEROIDES
Authors : Adams, M.J.; Rowland, P.; Gover, S.
Deposited on : 1995-12-04
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

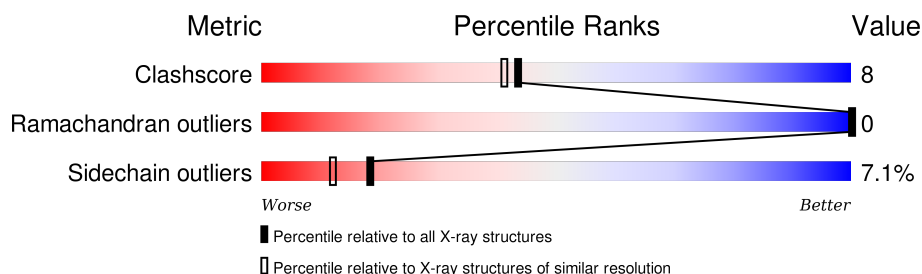
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 $\leq 5\%$. 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	485	 79% 18% •
1	B	485	 84% 14% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8305 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 DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3840	2449	635	746	10			
1	B	485	Total	C	N	O	S	0	0	0
			3840	2449	635	746	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	CYS	SER	ENGINEERED	UNP P11411
B	61	CYS	SER	ENGINEERED	UNP P11411

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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

- Molecule 3 is water.

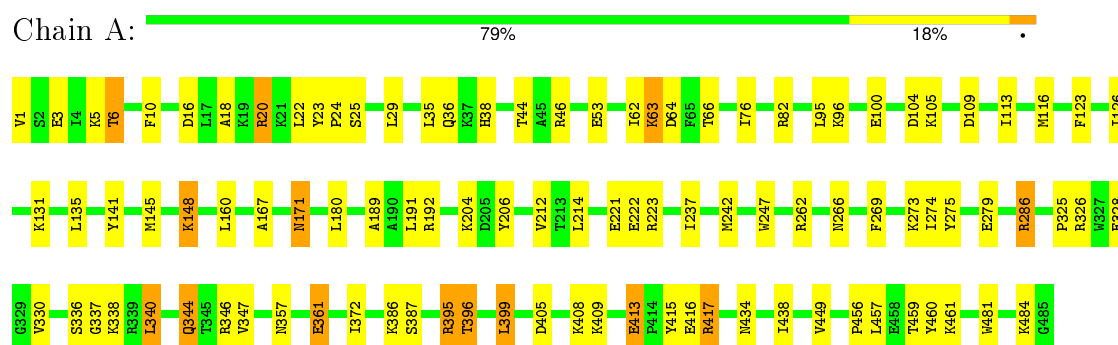
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		
3	B	300	Total	O	0	0
			300	300		

3 Residue-property plots [i](#)

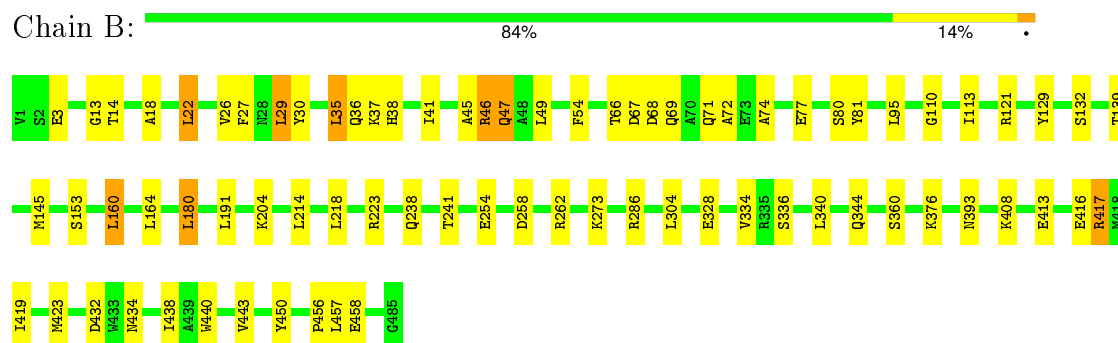
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GLUCOSE 6-PHOSPHATE DEHYDROGENASE



• Molecule 1: GLUCOSE 6-PHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.71Å 105.71Å 224.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.0 (27.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8305	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: PO4

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	0.51	0/3925	0.69	0/5309
1	B	0.48	0/3925	0.67	0/5309
All	All	0.50	0/7850	0.68	0/10618

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3840	0	3709	71	0
1	B	3840	0	3709	51	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
3	A	310	0	0	22	0
3	B	300	0	0	9	0
All	All	8305	0	7418	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (122) 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:B:45:ALA:HB2	3:B:2272:HOH:O	1.64	0.98
1:A:212:VAL:HG22	3:A:2187:HOH:O	1.71	0.89
1:A:417:ARG:HG3	1:A:417:ARG:HH11	1.45	0.82
1:A:222:GLU:H	1:A:223:ARG:HH11	1.28	0.81
1:A:266:ASN:HA	3:A:2252:HOH:O	1.80	0.81
1:A:481:TRP:HE3	3:A:2285:HOH:O	1.66	0.77
1:B:37:LYS:HG3	1:B:38:HIS:HD2	1.49	0.76
1:B:18:ALA:HA	1:B:22:LEU:HB2	1.66	0.76
1:B:47:GLN:HG3	1:B:49:LEU:HD13	1.69	0.75
1:B:417:ARG:HG2	1:B:417:ARG:HH11	1.51	0.74
1:A:223:ARG:N	1:A:223:ARG:HD2	2.05	0.71
1:A:387:SER:HA	1:A:395:ARG:HD2	1.72	0.71
1:B:74:ALA:O	1:B:77:GLU:HG2	1.91	0.71
1:A:116:MET:HE1	1:A:123:PHE:HA	1.76	0.68
1:A:6:THR:HG23	1:A:141:TYR:OH	1.95	0.67
1:A:192:ARG:HB3	3:A:2278:HOH:O	1.94	0.67
1:A:116:MET:HE3	1:A:126:ILE:HD12	1.76	0.67
1:A:347:VAL:HG22	3:A:2187:HOH:O	1.94	0.66
1:B:37:LYS:HG3	1:B:38:HIS:CD2	2.31	0.65
1:A:269:PHE:HB2	3:A:2252:HOH:O	1.97	0.65
1:A:417:ARG:CG	1:A:417:ARG:HH11	2.09	0.65
1:A:148:LYS:HE3	3:A:2126:HOH:O	1.97	0.64
1:B:241:THR:HG21	1:B:334:VAL:CG1	2.28	0.64
1:A:346:ARG:HG3	3:A:2261:HOH:O	1.98	0.64
1:A:18:ALA:HA	1:A:22:LEU:HB2	1.79	0.63
1:A:413:GLU:HG2	3:A:2200:HOH:O	1.99	0.63
1:B:286:ARG:HD2	1:B:450:TYR:CE1	2.35	0.62
1:A:116:MET:CE	1:A:123:PHE:HA	2.29	0.61
1:A:221:GLU:HB3	1:A:223:ARG:NH1	2.15	0.61
1:B:54:PHE:CD2	1:B:81:TYR:HB2	2.36	0.61
1:A:189:ALA:HA	3:A:2278:HOH:O	2.00	0.61
1:A:396:THR:HG23	3:A:2084:HOH:O	2.02	0.60
1:A:416:GLU:HA	3:A:2256:HOH:O	2.00	0.60
1:B:68:ASP:O	1:B:71:GLN:HG2	2.02	0.59
1:A:347:VAL:HG13	3:A:2187:HOH:O	2.03	0.59
1:B:29:LEU:HD13	1:B:416:GLU:HG3	1.85	0.59
1:A:171:ASN:HD22	1:A:171:ASN:H	1.52	0.57
1:A:286:ARG:HD3	1:A:456:PRO:O	2.05	0.57
1:B:238:GLN:HB2	1:B:443:VAL:HG21	1.87	0.56
1:B:129:TYR:HA	1:B:132:SER:HB3	1.86	0.56
1:B:262:ARG:HH11	1:B:262:ARG:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:HG21	1:B:72:ALA:HB2	1.89	0.55
1:A:25:SER:HB3	3:A:2256:HOH:O	2.05	0.55
1:A:273:LYS:HB2	3:A:2240:HOH:O	2.07	0.55
1:A:417:ARG:CG	1:A:417:ARG:NH1	2.69	0.55
1:A:413:GLU:OE2	1:A:415:TYR:HD1	1.90	0.55
1:B:241:THR:HG21	1:B:334:VAL:HG13	1.88	0.54
1:B:304:LEU:HD23	3:B:2133:HOH:O	2.07	0.54
1:A:96:LYS:O	1:A:100:GLU:HG3	2.08	0.54
1:B:241:THR:HG21	1:B:334:VAL:HG11	1.90	0.54
1:A:221:GLU:HB3	1:A:223:ARG:HH11	1.73	0.52
1:A:405:ASP:HA	1:A:408:LYS:HE3	1.91	0.52
1:A:116:MET:HE2	1:A:123:PHE:HD1	1.75	0.52
1:B:413:GLU:HB3	3:B:2282:HOH:O	2.12	0.50
1:B:46:ARG:HB3	1:B:46:ARG:HH11	1.77	0.50
1:A:131:LYS:HB2	1:A:167:ALA:HB2	1.94	0.49
1:A:344:GLN:OE1	1:A:346:ARG:HD2	2.12	0.49
1:A:82:ARG:NH1	3:A:2176:HOH:O	2.46	0.49
1:A:116:MET:CE	1:A:126:ILE:HD12	2.42	0.49
1:A:116:MET:HE2	1:A:123:PHE:CD1	2.47	0.49
1:B:3:GLU:HG3	1:B:36:GLN:HB2	1.94	0.49
1:A:206:TYR:HB2	3:A:2247:HOH:O	2.11	0.49
1:B:27:PHE:CE2	1:B:66:THR:HG22	2.48	0.49
1:B:417:ARG:CG	1:B:417:ARG:HH11	2.24	0.48
1:A:16:ASP:O	1:A:20:ARG:HG3	2.13	0.48
1:A:274:ILE:N	1:A:274:ILE:HD12	2.28	0.48
1:A:10:PHE:O	1:A:44:THR:HG22	2.14	0.48
1:A:372:ILE:HD12	1:A:372:ILE:N	2.29	0.47
1:B:121:ARG:HB3	3:B:2265:HOH:O	2.14	0.47
1:A:337:GLY:O	1:A:340:LEU:HD22	2.15	0.47
1:B:77:GLU:HB2	3:B:2218:HOH:O	2.13	0.47
1:B:27:PHE:CZ	1:B:66:THR:HG22	2.50	0.47
1:B:160:LEU:HD22	1:B:164:LEU:HG	1.97	0.47
1:A:459:THR:HG22	1:A:460:TYR:N	2.29	0.46
1:A:116:MET:HE3	1:A:126:ILE:CD1	2.44	0.46
1:B:286:ARG:HD3	1:B:456:PRO:O	2.15	0.46
1:B:328:GLU:HG2	3:B:2095:HOH:O	2.14	0.46
1:B:258:ASP:O	1:B:262:ARG:HG3	2.15	0.46
1:B:22:LEU:O	1:B:26:VAL:HG23	2.16	0.46
1:B:14:THR:N	3:B:2272:HOH:O	2.49	0.46
1:B:113:ILE:HG21	1:B:145:MET:HE2	1.98	0.46
1:A:481:TRP:CE3	3:A:2285:HOH:O	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HG21	1:A:145:MET:CE	2.47	0.45
1:A:1:VAL:N	3:A:2091:HOH:O	2.47	0.44
1:A:62:ILE:O	1:A:66:THR:HG23	2.16	0.44
1:B:223:ARG:HG3	3:B:2288:HOH:O	2.16	0.44
1:A:481:TRP:O	1:A:484:LYS:HD3	2.18	0.44
1:A:247:TRP:HZ2	3:A:2288:HOH:O	2.01	0.44
1:B:434:ASN:O	1:B:438:ILE:HG12	2.17	0.44
1:A:361:GLU:HB2	3:A:2295:HOH:O	2.17	0.44
1:A:148:LYS:HB3	2:A:2000:PO4:O1	2.18	0.43
1:A:434:ASN:O	1:A:438:ILE:HG12	2.18	0.43
1:B:153:SER:HA	1:B:440:TRP:CH2	2.53	0.43
1:A:5:LYS:HG2	1:A:38:HIS:HB2	1.99	0.43
1:B:30:TYR:HA	1:B:35:LEU:HB2	2.01	0.43
1:B:262:ARG:NH1	1:B:432:ASP:HB3	2.34	0.43
1:B:69:GLN:O	1:B:72:ALA:HB3	2.19	0.43
1:A:63:LYS:HG3	1:A:64:ASP:N	2.34	0.42
1:B:180:LEU:HD12	1:B:180:LEU:HA	1.93	0.42
1:A:399:LEU:HD23	1:A:399:LEU:N	2.34	0.42
1:A:275:TYR:HB3	1:A:279:GLU:HB2	2.01	0.42
1:B:417:ARG:HG2	1:B:417:ARG:NH1	2.27	0.42
1:A:113:ILE:HG21	1:A:145:MET:HE2	2.02	0.42
1:A:23:TYR:N	1:A:24:PRO:CD	2.83	0.42
1:B:45:ALA:HB3	1:B:81:TYR:OH	2.19	0.42
1:B:408:LYS:HE2	1:B:408:LYS:HB3	1.86	0.41
1:A:214:LEU:O	1:A:336:SER:HA	2.20	0.41
1:B:13:GLY:N	3:B:2272:HOH:O	2.52	0.41
1:A:325:PRO:HA	1:A:328:GLU:HG3	2.03	0.41
1:A:3:GLU:HB2	1:A:36:GLN:NE2	2.34	0.41
1:B:419:ILE:O	1:B:423:MET:HG3	2.20	0.41
1:B:113:ILE:HG21	1:B:145:MET:CE	2.51	0.41
1:A:237:ILE:O	1:A:242:MET:HG2	2.21	0.41
1:B:214:LEU:O	1:B:336:SER:HA	2.21	0.41
1:B:360:SER:HB2	1:B:393:ASN:OD1	2.21	0.41
1:B:110:GLY:HA3	1:B:139:THR:O	2.21	0.41
1:A:461:LYS:HB2	1:A:461:LYS:HE3	1.90	0.41
1:A:481:TRP:HB3	3:A:2285:HOH:O	2.21	0.41
1:A:386:LYS:HG2	1:A:387:SER:O	2.21	0.40
1:A:286:ARG:HG2	1:A:286:ARG:O	2.22	0.40
1:B:41:ILE:N	1:B:41:ILE:HD12	2.36	0.40
1:A:53:GLU:OE1	1:A:53:GLU:HA	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	483/485 (100%)	472 (98%)	11 (2%)	0	100	100
1	B	483/485 (100%)	459 (95%)	24 (5%)	0	100	100
All	All	966/970 (100%)	931 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	396/396 (100%)	361 (91%)	35 (9%)	12	7
1	B	396/396 (100%)	375 (95%)	21 (5%)	28	22
All	All	792/792 (100%)	736 (93%)	56 (7%)	18	12

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	20	ARG
1	A	29	LEU
1	A	35	LEU
1	A	46	ARG
1	A	63	LYS
1	A	76	ILE
1	A	95	LEU

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Mol	Chain	Res	Type
1	A	104	ASP
1	A	105	LYS
1	A	109	ASP
1	A	135	LEU
1	A	148	LYS
1	A	160	LEU
1	A	171	ASN
1	A	180	LEU
1	A	191	LEU
1	A	204	LYS
1	A	262	ARG
1	A	286	ARG
1	A	326	ARG
1	A	330	VAL
1	A	338	LYS
1	A	340	LEU
1	A	344	GLN
1	A	357	ASN
1	A	361	GLU
1	A	395	ARG
1	A	396	THR
1	A	399	LEU
1	A	409	LYS
1	A	413	GLU
1	A	417	ARG
1	A	449	VAL
1	A	457	LEU
1	B	22	LEU
1	B	29	LEU
1	B	35	LEU
1	B	46	ARG
1	B	47	GLN
1	B	67	ASP
1	B	80	SER
1	B	95	LEU
1	B	160	LEU
1	B	180	LEU
1	B	191	LEU
1	B	204	LYS
1	B	218	LEU
1	B	254	GLU
1	B	273	LYS

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Mol	Chain	Res	Type
1	B	340	LEU
1	B	344	GLN
1	B	376	LYS
1	B	417	ARG
1	B	457	LEU
1	B	458	GLU

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	36	GLN
1	A	47	GLN
1	A	84	HIS
1	A	171	ASN
1	A	238	GLN
1	A	266	ASN
1	A	357	ASN
1	A	424	ASN
1	B	38	HIS
1	B	78	HIS
1	B	270	ASN
1	B	312	ASN
1	B	420	HIS
1	B	434	ASN

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

3 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	2000	-	4,4,4	2.35	2 (50%)	6,6,6	0.32	0
2	PO4	A	2002	-	4,4,4	2.04	2 (50%)	6,6,6	0.39	0
2	PO4	B	2001	-	4,4,4	1.98	1 (25%)	6,6,6	0.31	0

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	2000	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2001	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	PO4	P-O3	-3.53	1.40	1.53
2	A	2000	PO4	P-O1	-3.37	1.37	1.52
2	A	2002	PO4	P-O4	-2.76	1.43	1.53
2	A	2000	PO4	P-O4	-2.54	1.44	1.53
2	A	2002	PO4	P-O3	-2.36	1.44	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	PO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.