Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 06:00 AM EST

PDB ID	:	6WBT
Title	:	2.52 Angstrom Resolution Crystal Structure of 6-phospho-alpha-glucosidase from Gut Microorganisms in Complex with NAD and Glucose-6-phosphate
Authors	:	Wu, R.; Kim, Y.; Endres, M.; Joachimiak, J.
Deposited on	:	2020-03-27
Resolution	:	2.52 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:

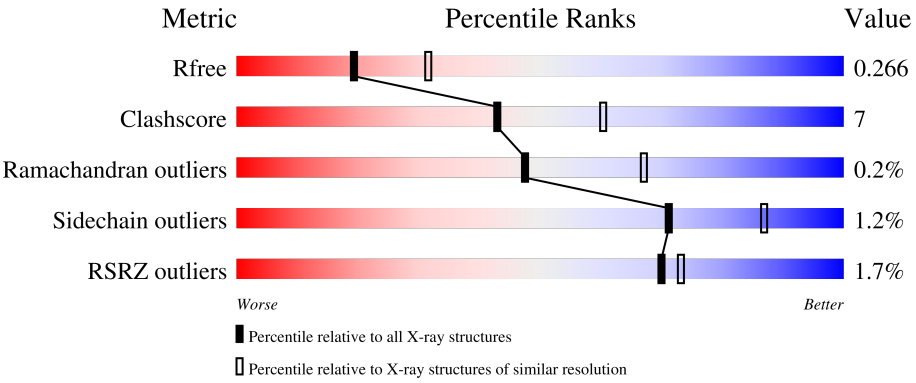
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.52 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))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	443	82% 17%
1	B	443	84% 15%
1	C	443	3% 81% 18%
1	D	443	2% 77% 19%

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
6	EDO	D	901	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14440 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.

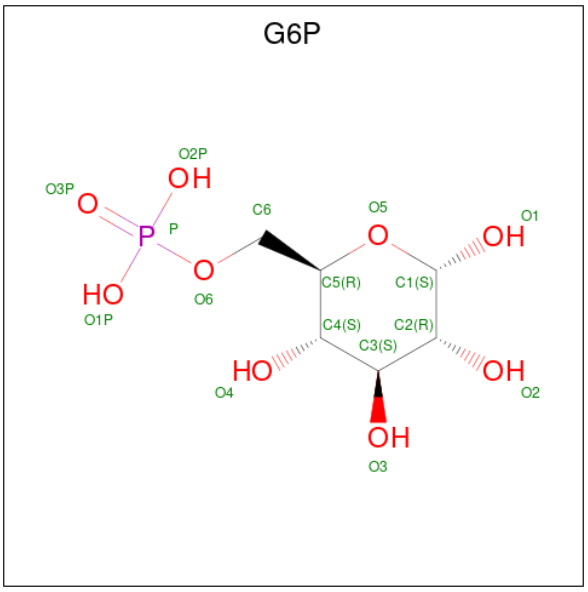
- Molecule 1 is a protein called cellulase IBT99.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	1	0
			3543	2258	594	666	9	16			
1	B	440	Total	C	N	O	S	Se	0	0	0
			3522	2247	590	660	9	16			
1	C	441	Total	C	N	O	S	Se	0	0	0
			3527	2250	591	661	9	16			
1	D	428	Total	C	N	O	S	Se	0	0	0
			3421	2182	573	642	9	15			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

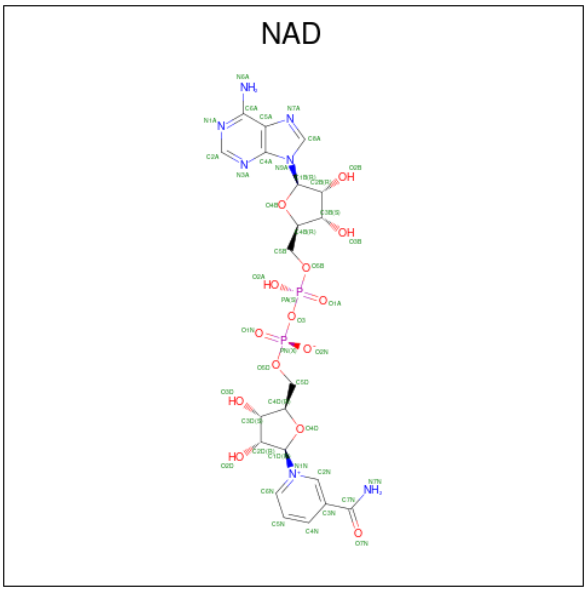
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $C_6H_{13}O_9P$) (labeled as "Ligand of Interest" by depositor).



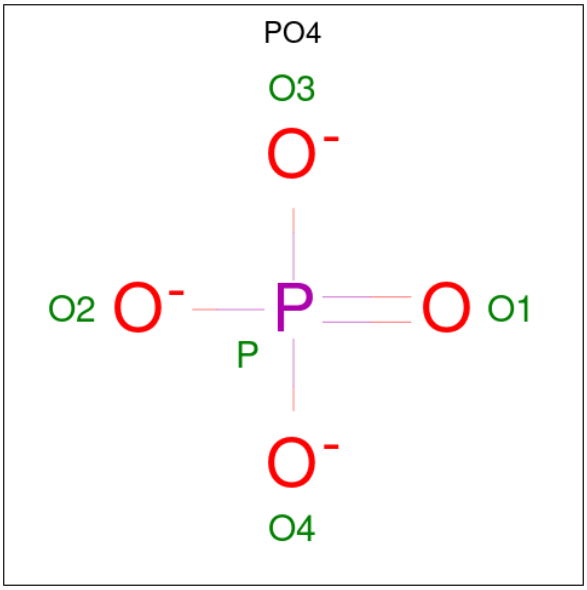
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 16 6 9 1	0	0
3	C	1	Total C O P 16 6 9 1	0	0
3	D	1	Total C O P 16 6 9 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



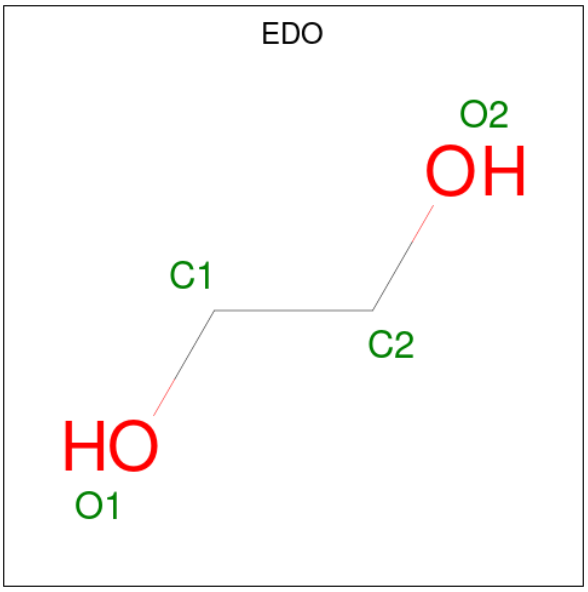
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

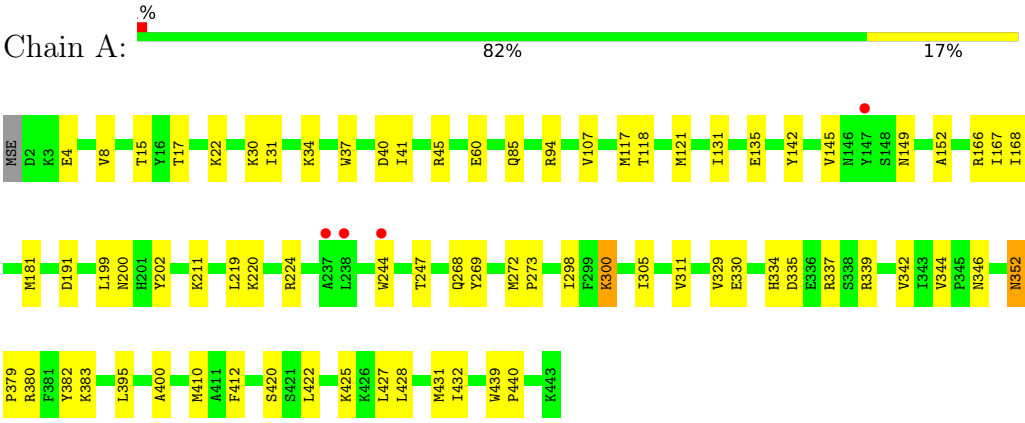
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	49	Total O 49 49	0	0
7	B	42	Total O 42 42	0	0
7	C	52	Total O 52 52	0	0
7	D	42	Total O 42 42	0	0

3 Residue-property plots (i)

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 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.

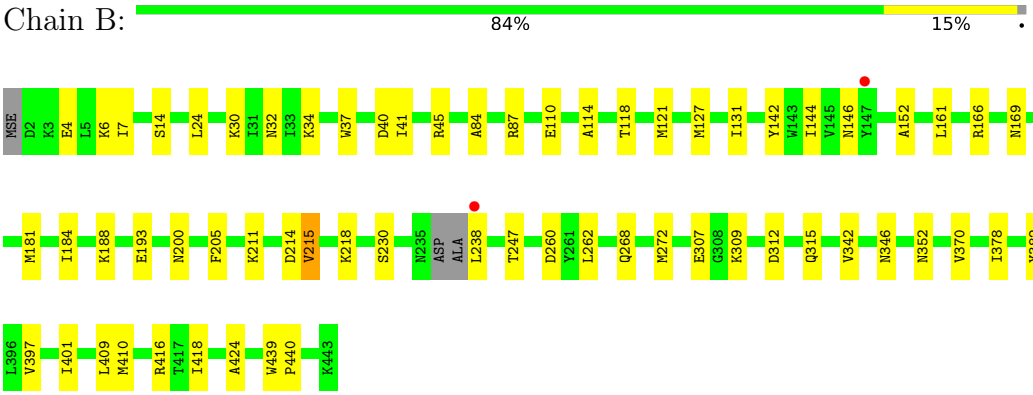
• Molecule 1: cellulase IBT99

Chain A:



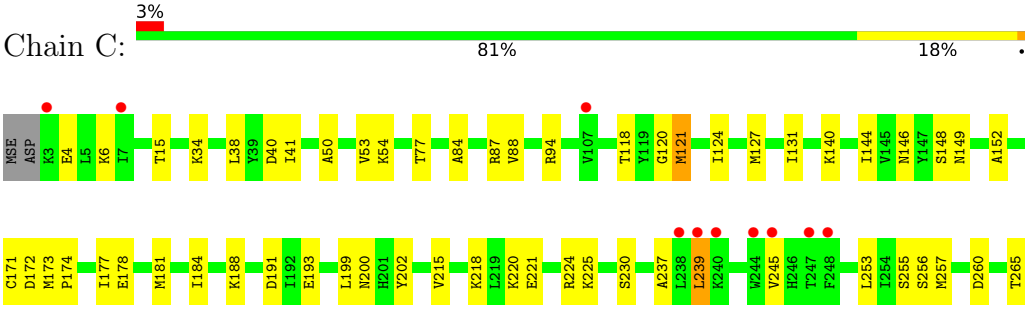
• Molecule 1: cellulase IBT99

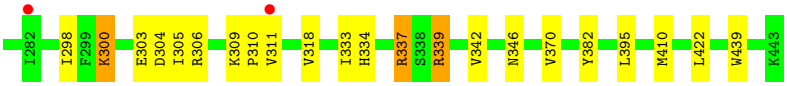
Chain B:



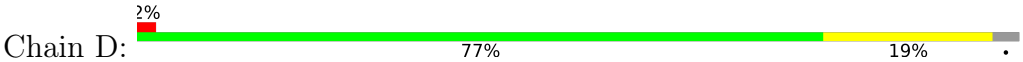
• Molecule 1: cellulase IBT99

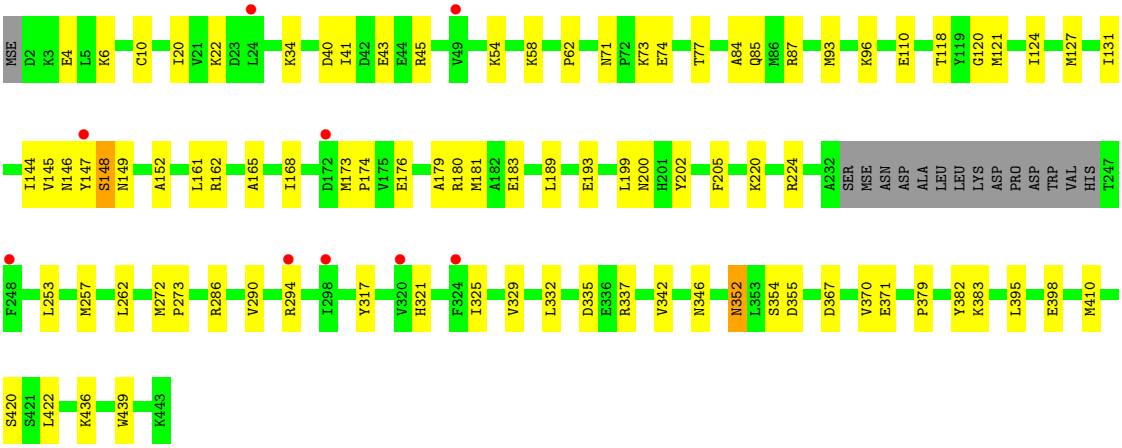
Chain C:





• Molecule 1: cellulase IBT99





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.80Å 219.72Å 97.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.92 – 2.52 75.06 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.9 (70.92-2.52) 92.9 (75.06-2.52)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.227 , 0.266 0.227 , 0.266	Depositor DCC
R_{free} test set	3582 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14440	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, EDO, G6P, PO4, NAD

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	0.23	0/3597	0.38	0/4837
1	B	0.23	0/3575	0.39	0/4805
1	C	0.23	0/3581	0.39	0/4815
1	D	0.23	0/3471	0.38	0/4664
All	All	0.23	0/14224	0.39	0/19121

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	3543	0	3548	54	0
1	B	3522	0	3533	41	0
1	C	3527	0	3539	50	0
1	D	3421	0	3437	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	16	0	10	2	0
3	D	16	0	11	2	0
4	A	44	0	26	3	0
4	B	44	0	26	4	0
4	C	44	0	26	5	0
4	D	44	0	26	4	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	D	4	0	6	2	0
7	A	49	0	0	1	0
7	B	42	0	0	0	0
7	C	52	0	0	0	0
7	D	42	0	0	1	0
All	All	14440	0	14199	193	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 7.

All (193) 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:C:4:GLU:HB3	1:C:34:LYS:HB2	1.67	0.76
1:A:152:ALA:HB2	1:A:200:ASN:HB3	1.76	0.67
1:B:4:GLU:HB3	1:B:34:LYS:HB2	1.77	0.65
1:D:4:GLU:HB3	1:D:34:LYS:HB2	1.78	0.65
1:C:239:LEU:HD13	1:C:245:VAL:HG22	1.80	0.64
1:C:84:ALA:HB1	1:C:127:MSE:HE1	1.80	0.64
1:A:425:LYS:HD2	1:D:257:MSE:HE2	1.78	0.63
1:C:184:ILE:HG12	1:C:230:SER:HB2	1.81	0.62
1:B:84:ALA:HB1	1:B:127:MSE:HE1	1.81	0.61
1:B:152:ALA:HB2	1:B:200:ASN:HB3	1.82	0.61
1:D:352:ASN:OD1	1:D:352:ASN:N	2.24	0.61
1:B:247:THR:HG22	1:B:268:GLN:HE22	1.66	0.61
1:D:54:LYS:HD2	1:D:58:LYS:HE3	1.82	0.60
1:A:177:ILE:HG22	1:A:181:MSE:HE2	1.83	0.60
1:C:15:THR:HA	1:C:298:ILE:HD13	1.83	0.60
1:C:131:ILE:HD13	1:C:144:ILE:HD12	1.84	0.60
1:A:422:LEU:HD11	1:D:272:MSE:HE3	1.83	0.60
1:C:171:CYS:HA	4:C:503:NAD:H72N	1.67	0.59
1:C:84:ALA:HB3	1:C:146:ASN:HA	1.84	0.59
1:A:379:PRO:HG2	1:A:382:TYR:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLU:OE1	1:B:309:LYS:NZ	2.36	0.58
1:C:170:ILE:HG22	1:C:342:VAL:HG12	1.86	0.58
1:A:118:THR:HA	1:A:439:TRP:HZ2	1.69	0.58
1:C:178:GLU:HA	1:C:181:MSE:HE2	1.85	0.58
1:A:15:THR:HA	1:A:298:ILE:HD13	1.85	0.58
1:B:146:ASN:HD22	1:B:169:ASN:HD22	1.51	0.58
1:C:152:ALA:HB2	1:C:200:ASN:HB3	1.84	0.58
1:C:342:VAL:HG21	1:C:370:VAL:HG11	1.86	0.58
1:B:418:ILE:HG21	1:B:424:ALA:HB2	1.87	0.57
1:D:379:PRO:HG2	1:D:382:TYR:CD2	2.40	0.57
1:B:114:ALA:HB2	1:B:418:ILE:HD11	1.85	0.56
1:A:94:ARG:NH2	3:A:502:G6P:O1P	2.26	0.56
1:C:193:GLU:OE2	1:D:337:ARG:NH2	2.38	0.56
1:D:205:PHE:HB2	1:D:262:LEU:HB2	1.88	0.56
1:D:379:PRO:HG2	1:D:382:TYR:HD2	1.71	0.56
1:A:272:MSE:HE3	1:D:422:LEU:HD21	1.88	0.56
1:C:309:LYS:NZ	1:C:310:PRO:O	2.35	0.56
1:A:142:TYR:O	1:A:166:ARG:NH2	2.35	0.55
1:D:84:ALA:HB1	1:D:127:MSE:HE1	1.89	0.55
1:A:199:LEU:HB2	1:A:202:TYR:HB3	1.89	0.54
1:A:395:LEU:HD13	1:A:410:MSE:HB3	1.90	0.54
1:C:162:ARG:HB3	1:C:165:ALA:HB2	1.89	0.54
1:B:352:ASN:OD1	1:B:352:ASN:N	2.36	0.54
1:C:337:ARG:NH2	1:D:193:GLU:OE2	2.34	0.54
1:A:379:PRO:HG2	1:A:382:TYR:CD2	2.43	0.54
1:A:305:ILE:HG13	1:A:311:VAL:HG21	1.89	0.53
1:D:58:LYS:HA	1:D:62:PRO:HB3	1.90	0.53
1:B:388:GLN:HE22	1:B:416:ARG:HH11	1.58	0.52
1:B:45:ARG:NH2	4:B:503:NAD:O2A	2.42	0.52
1:C:40:ASP:OD1	1:C:41:ILE:N	2.42	0.52
1:B:14:SER:OG	4:B:503:NAD:O1N	2.21	0.52
1:B:215:VAL:O	1:B:218:LYS:N	2.43	0.52
1:C:224:ARG:HD3	1:C:256:SER:HA	1.92	0.52
1:C:395:LEU:HD13	1:C:410:MSE:HB3	1.92	0.52
1:D:10:CYS:HB3	1:D:84:ALA:HA	1.90	0.52
1:A:17:THR:OG1	1:A:85:GLN:NE2	2.43	0.52
1:D:152:ALA:HB2	1:D:200:ASN:HB3	1.91	0.52
1:D:173:MSE:HE3	1:D:176:GLU:HB2	1.92	0.51
1:B:40:ASP:OD2	4:B:503:NAD:O3B	2.21	0.51
1:B:40:ASP:OD1	1:B:41:ILE:N	2.43	0.51
1:B:205:PHE:HB2	1:B:262:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LEU:HB2	1:D:202:TYR:HB3	1.93	0.50
1:D:286:ARG:NE	3:D:903:G6P:O2P	2.33	0.50
1:D:352:ASN:O	1:D:383:LYS:NZ	2.42	0.50
1:A:4:GLU:HB3	1:A:34:LYS:HB2	1.93	0.50
1:D:149:ASN:ND2	3:D:903:G6P:O3	2.44	0.50
1:D:395:LEU:HD13	1:D:410:MSE:HB3	1.94	0.50
1:D:118:THR:HA	1:D:439:TRP:HZ2	1.75	0.49
1:A:380:ARG:NH1	1:D:398:GLU:OE1	2.45	0.49
1:D:40:ASP:OD1	1:D:41:ILE:N	2.42	0.49
1:D:290:VAL:HG23	1:D:294:ARG:HB3	1.95	0.49
1:D:110:GLU:OE2	4:D:904:NAD:O2D	2.31	0.49
1:A:300:LYS:HB3	1:A:300:LYS:HE3	1.61	0.49
1:B:142:TYR:O	1:B:166:ARG:NH2	2.38	0.49
1:A:337:ARG:NH2	1:B:193:GLU:OE2	2.33	0.49
1:C:148:SER:HA	4:C:503:NAD:H1D	1.94	0.48
1:D:40:ASP:OD2	4:D:904:NAD:O3B	2.27	0.48
1:D:145:VAL:HG21	1:D:329:VAL:HG22	1.94	0.48
1:C:215:VAL:HG12	1:C:218:LYS:HB3	1.94	0.48
1:B:161:LEU:HD21	1:B:401:ILE:HD12	1.95	0.48
1:C:172:ASP:OD1	3:C:502:G6P:O2	2.32	0.48
1:D:146:ASN:OD1	1:D:148:SER:OG	2.30	0.48
1:D:220:LYS:HE2	1:D:224:ARG:NH2	2.29	0.48
1:A:335:ASP:OD2	1:A:337:ARG:NH1	2.46	0.47
1:B:312:ASP:HB3	1:B:315:GLN:HE21	1.79	0.47
1:D:22:LYS:HD2	1:D:317:TYR:CG	2.49	0.47
1:B:184:ILE:HG12	1:B:230:SER:HB3	1.95	0.47
1:C:173:MSE:HB3	1:C:174:PRO:HD3	1.96	0.47
1:A:31:ILE:HD11	1:A:330:GLU:HB2	1.97	0.47
1:C:6:LYS:NZ	1:C:77:THR:O	2.42	0.47
1:D:45:ARG:NH2	4:D:904:NAD:O2A	2.49	0.46
1:B:121:MSE:HE2	1:B:440:PRO:HD2	1.97	0.46
1:B:397:VAL:O	1:B:401:ILE:HG12	2.15	0.46
1:D:73:LYS:O	1:D:77:THR:OG1	2.20	0.46
1:D:342:VAL:HG11	1:D:370:VAL:HG21	1.96	0.46
1:C:121:MSE:HE2	1:C:121:MSE:HB3	1.85	0.46
1:A:342:VAL:HG21	1:A:370:VAL:HG11	1.96	0.46
1:D:168:ILE:HD12	1:D:332:LEU:HD11	1.97	0.46
1:C:224:ARG:NH1	1:C:255:SER:O	2.39	0.45
1:B:7:ILE:HG21	1:B:24:LEU:HD11	1.98	0.45
1:D:85:GLN:HB3	1:D:147:TYR:CZ	2.51	0.45
1:D:162:ARG:HB3	1:D:165:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:NH1	1:D:371:GLU:OE2	2.48	0.45
1:D:335:ASP:OD1	1:D:337:ARG:NH1	2.50	0.45
1:A:342:VAL:HG23	1:A:344:VAL:HG13	1.99	0.45
1:A:173:MSE:HB3	1:A:174:PRO:HD3	1.99	0.45
1:C:118:THR:HA	1:C:439:TRP:HZ2	1.82	0.45
1:D:71:ASN:HB3	1:D:74:GLU:HB2	1.98	0.45
1:A:145:VAL:HG21	1:A:329:VAL:HG22	1.98	0.45
1:A:247:THR:HG23	1:A:268:GLN:HE22	1.81	0.45
1:A:420:SER:HB2	1:D:272:MSE:HA	1.99	0.45
1:B:214:ASP:OD1	1:B:215:VAL:N	2.50	0.45
1:D:20:ILE:HD11	1:D:321:HIS:CE1	2.52	0.45
1:A:40:ASP:OD2	4:A:503:NAD:O3B	2.34	0.45
1:C:149:ASN:ND2	3:C:502:G6P:O4	2.50	0.45
1:D:120:GLY:O	1:D:124:ILE:HG13	2.17	0.44
1:A:149:ASN:HB2	4:A:503:NAD:O2D	2.16	0.44
1:B:87:ARG:NH2	1:B:110:GLU:OE1	2.48	0.44
1:A:352:ASN:O	1:A:383:LYS:NZ	2.49	0.44
1:D:6:LYS:NZ	1:D:77:THR:O	2.39	0.44
1:D:335:ASP:HB2	1:D:367:ASP:HB3	1.98	0.44
1:C:120:GLY:O	1:C:124:ILE:HG13	2.18	0.44
1:B:342:VAL:HG21	1:B:370:VAL:HG21	1.99	0.44
1:C:199:LEU:HB2	1:C:202:TYR:HB3	2.00	0.44
1:C:188:LYS:HB2	1:C:191:ASP:OD1	2.18	0.44
1:A:220:LYS:HE2	1:A:224:ARG:NH2	2.32	0.44
1:B:260:ASP:HB2	1:B:382:TYR:OH	2.17	0.44
1:A:22:LYS:HG2	1:A:60:GLU:HG3	1.99	0.43
1:A:117:MSE:HE1	1:A:412:PHE:HA	2.00	0.43
1:D:173:MSE:HB3	1:D:174:PRO:HD3	2.00	0.43
1:A:8:VAL:HG22	1:A:37:TRP:HB2	2.01	0.43
1:C:87:ARG:HB3	4:C:503:NAD:H51A	2.00	0.43
1:C:172:ASP:H	4:C:503:NAD:H72N	1.66	0.43
1:C:260:ASP:HB2	1:C:382:TYR:OH	2.18	0.43
1:A:247:THR:HG23	1:A:268:GLN:NE2	2.34	0.43
1:C:38:LEU:HD21	1:C:53:VAL:HG21	2.01	0.43
1:C:303:GLU:OE1	1:C:306:ARG:NH1	2.47	0.43
1:D:200:ASN:ND2	7:D:1002:HOH:O	2.38	0.43
1:A:107:VAL:HG11	1:A:269:TYR:HB3	2.01	0.42
1:A:121:MSE:HE3	1:A:400:ALA:HB2	2.01	0.42
1:A:428:LEU:O	1:A:432:ILE:HG12	2.19	0.42
1:C:221:GLU:O	1:C:225:LYS:HD3	2.19	0.42
1:C:333:ILE:HG22	1:C:334:HIS:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LYS:HA	1:D:96:LYS:HD2	1.82	0.42
1:D:253:LEU:HD12	1:D:272:MSE:HE1	2.01	0.42
1:A:181:MSE:SE	1:A:219:LEU:HD13	2.69	0.42
1:A:355:ASP:N	1:A:355:ASP:OD1	2.51	0.42
1:B:178:GLU:HA	1:B:181:MSE:HB2	2.02	0.42
1:B:211:LYS:HA	1:B:211:LYS:HD2	1.86	0.42
1:A:40:ASP:OD1	1:A:41:ILE:N	2.52	0.42
1:D:131:ILE:HD13	1:D:144:ILE:HD12	2.01	0.42
1:A:135:GLU:OE1	1:A:142:TYR:OH	2.24	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB3	1.69	0.42
1:A:427:LEU:O	1:A:431:MSE:HG2	2.20	0.42
1:B:118:THR:HA	1:B:439:TRP:HZ2	1.84	0.42
1:B:131:ILE:HD13	1:B:144:ILE:HD12	2.01	0.42
1:B:188:LYS:HD3	1:B:188:LYS:HA	1.86	0.42
1:A:191:ASP:HB3	1:A:211:LYS:HG3	2.00	0.42
1:A:273:PRO:HD2	1:D:420:SER:HB3	2.01	0.42
1:B:272:MSE:HE3	1:C:422:LEU:HD21	2.01	0.42
1:B:6:LYS:HE3	1:B:37:TRP:CD1	2.55	0.42
1:B:87:ARG:HB3	4:B:503:NAD:H51A	2.02	0.42
1:C:15:THR:HG22	1:C:298:ILE:HG21	2.01	0.42
1:C:88:VAL:HG12	4:C:503:NAD:N7A	2.35	0.42
1:C:237:ALA:HB3	1:C:318:VAL:HG11	2.02	0.42
1:D:181:MSE:HE2	1:D:262:LEU:HD13	2.00	0.42
1:B:173:MSE:HB3	1:B:174:PRO:HD3	2.02	0.42
1:D:179:ALA:HA	1:D:189:LEU:HD13	2.02	0.42
1:D:180:ARG:NH1	1:D:183:GLU:OE2	2.52	0.42
1:C:305:ILE:HG13	1:C:311:VAL:HG21	2.01	0.41
1:C:50:ALA:O	1:C:54:LYS:HG3	2.20	0.41
1:A:420:SER:HB3	1:D:273:PRO:HD2	2.01	0.41
1:A:131:ILE:HD11	1:A:167:ILE:HD12	2.02	0.41
1:B:352:ASN:HD21	1:B:378:ILE:H	1.68	0.41
1:C:300:LYS:HE3	1:C:300:LYS:HB3	1.85	0.41
1:A:121:MSE:HE2	1:A:440:PRO:HD2	2.01	0.41
1:A:145:VAL:HA	1:A:168:ILE:HG23	2.01	0.41
1:A:339:ARG:NH1	7:A:612:HOH:O	2.54	0.41
1:B:395:LEU:HD13	1:B:410:MSE:HB3	2.03	0.41
1:D:354:SER:HA	6:D:901:EDO:H22	2.02	0.41
1:B:30:LYS:HE3	1:B:30:LYS:HB3	1.90	0.41
1:D:161:LEU:O	1:D:162:ARG:HD2	2.21	0.41
1:C:220:LYS:HD3	1:C:224:ARG:NH2	2.36	0.41
1:D:147:TYR:CE1	1:D:325:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HB3	4:D:904:NAD:H51A	2.03	0.40
1:A:45:ARG:NH2	4:A:503:NAD:O2A	2.54	0.40
1:D:355:ASP:H	6:D:901:EDO:H22	1.86	0.40
1:D:436:LYS:HA	1:D:436:LYS:HD2	1.88	0.40
1:A:244:TRP:HZ2	3:A:502:G6P:H62	1.85	0.40
1:A:30:LYS:HE2	1:A:334:HIS:CE1	2.56	0.40
1:B:409:LEU:HD21	1:C:257:MSE:HE2	2.03	0.40
1:C:177:ILE:HD11	1:C:265:THR:H	1.86	0.40
1:C:253:LEU:HB2	1:C:272:MSE:HE1	2.03	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	441/443 (100%)	429 (97%)	11 (2%)	1 (0%)	47	67
1	B	436/443 (98%)	420 (96%)	15 (3%)	1 (0%)	47	67
1	C	439/443 (99%)	426 (97%)	12 (3%)	1 (0%)	47	67
1	D	424/443 (96%)	412 (97%)	11 (3%)	1 (0%)	47	67
All	All	1740/1772 (98%)	1687 (97%)	49 (3%)	4 (0%)	47	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	ASN
1	D	346	ASN
1	C	346	ASN
1	A	346	ASN

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	387/370 (105%)	385 (100%)	2 (0%)	88 95
1	B	385/370 (104%)	382 (99%)	3 (1%)	81 92
1	C	385/370 (104%)	377 (98%)	8 (2%)	53 76
1	D	373/370 (101%)	368 (99%)	5 (1%)	69 86
All	All	1530/1480 (103%)	1512 (99%)	18 (1%)	71 87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	LYS
1	A	352	ASN
1	B	32	ASN
1	B	215	VAL
1	B	238	LEU
1	C	94	ARG
1	C	121	MSE
1	C	140	LYS
1	C	239	LEU
1	C	300	LYS
1	C	304	ASP
1	C	337	ARG
1	C	339	ARG
1	D	43	GLU
1	D	93	MSE
1	D	121	MSE
1	D	148	SER
1	D	352	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN

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Mol	Chain	Res	Type
1	A	85	GLN
1	A	149	ASN
1	A	268	GLN
1	A	334	HIS
1	B	27	GLN
1	B	32	ASN
1	B	149	ASN
1	B	169	ASN
1	B	235	ASN
1	B	250	ASN
1	B	268	GLN
1	B	315	GLN
1	B	388	GLN
1	C	149	ASN
1	C	334	HIS
1	D	29	GLN
1	D	32	ASN
1	D	149	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAD	A	503	2	42,48,48	0.63	0	50,73,73	1.11	4 (8%)
6	EDO	D	901	-	3,3,3	0.46	0	2,2,2	0.33	0
4	NAD	C	503	2	42,48,48	0.65	1 (2%)	50,73,73	1.10	4 (8%)
5	PO4	B	502	-	4,4,4	0.92	0	6,6,6	0.42	0
3	G6P	C	502	2	16,16,16	0.60	0	24,24,24	1.55	4 (16%)
3	G6P	A	502	2	16,16,16	0.53	0	24,24,24	0.74	0
3	G6P	D	903	2	16,16,16	0.55	0	24,24,24	1.20	5 (20%)
4	NAD	B	503	2	42,48,48	0.62	0	50,73,73	1.09	4 (8%)
5	PO4	C	504	-	4,4,4	0.92	0	6,6,6	0.43	0
4	NAD	D	904	2	42,48,48	0.66	0	50,73,73	0.89	4 (8%)

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
4	NAD	A	503	2	-	3/26/62/62	0/5/5/5
6	EDO	D	901	-	-	0/1/1/1	-
4	NAD	C	503	2	-	3/26/62/62	0/5/5/5
3	G6P	C	502	2	-	1/6/26/26	0/1/1/1
3	G6P	A	502	2	-	5/6/26/26	0/1/1/1
3	G6P	D	903	2	-	5/6/26/26	0/1/1/1
4	NAD	B	503	2	-	2/26/62/62	0/5/5/5
4	NAD	D	904	2	-	8/26/62/62	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAD	C2N-N1N	2.22	1.37	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	NAD	O4D-C1D-C2D	-5.36	99.09	106.93
4	B	503	NAD	O4D-C1D-C2D	-5.20	99.33	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	NAD	O4D-C1D-C2D	-5.03	99.57	106.93
3	C	502	G6P	O5-C1-C2	4.40	118.14	110.28
3	C	502	G6P	C1-O5-C5	3.72	120.68	113.66
4	C	503	NAD	O4B-C1B-C2B	-3.14	102.34	106.93
4	D	904	NAD	O4B-C1B-C2B	-2.95	102.62	106.93
4	A	503	NAD	O4B-C1B-C2B	-2.85	102.76	106.93
4	B	503	NAD	O4B-C1B-C2B	-2.73	102.94	106.93
4	D	904	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
4	B	503	NAD	C6N-N1N-C2N	-2.53	119.67	121.97
4	A	503	NAD	C6N-N1N-C2N	-2.49	119.70	121.97
4	C	503	NAD	C6N-N1N-C2N	-2.39	119.79	121.97
3	C	502	G6P	C1-C2-C3	2.38	115.26	110.31
3	D	903	G6P	O5-C1-C2	2.33	114.44	110.28
4	B	503	NAD	C5A-C6A-N6A	2.27	123.80	120.35
4	D	904	NAD	C5A-C6A-N6A	2.27	123.80	120.35
4	C	503	NAD	C5A-C6A-N6A	2.23	123.74	120.35
4	A	503	NAD	C5A-C6A-N6A	2.22	123.73	120.35
3	D	903	G6P	O2P-P-O1P	2.13	115.77	107.64
3	D	903	G6P	O5-C5-C4	2.13	113.55	109.69
4	D	904	NAD	O4D-C1D-C2D	-2.11	103.84	106.93
3	D	903	G6P	C6-C5-C4	-2.09	107.72	112.09
3	D	903	G6P	C1-O5-C5	2.07	117.57	113.66
3	C	502	G6P	C6-C5-C4	-2.02	107.87	112.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	G6P	C4-C5-C6-O6
3	A	502	G6P	O5-C5-C6-O6
3	A	502	G6P	C6-O6-P-O1P
3	A	502	G6P	C6-O6-P-O2P
3	A	502	G6P	C6-O6-P-O3P
3	D	903	G6P	C4-C5-C6-O6
3	D	903	G6P	O5-C5-C6-O6
3	D	903	G6P	C6-O6-P-O1P
3	D	903	G6P	C6-O6-P-O2P
4	D	904	NAD	C5D-O5D-PN-O1N
4	D	904	NAD	O4D-C1D-N1N-C2N
4	D	904	NAD	O4D-C1D-N1N-C6N
4	D	904	NAD	C2D-C1D-N1N-C2N
4	D	904	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	D	903	G6P	C6-O6-P-O3P
4	C	503	NAD	PN-O3-PA-O1A
4	A	503	NAD	PN-O3-PA-O1A
4	A	503	NAD	PN-O3-PA-O2A
4	C	503	NAD	PN-O3-PA-O2A
3	C	502	G6P	C4-C5-C6-O6
4	C	503	NAD	O4B-C4B-C5B-O5B
4	A	503	NAD	O4B-C4B-C5B-O5B
4	B	503	NAD	O4B-C4B-C5B-O5B
4	D	904	NAD	O4B-C4B-C5B-O5B
4	B	503	NAD	PN-O3-PA-O2A
4	D	904	NAD	C4D-C5D-O5D-PN
4	D	904	NAD	O4D-C4D-C5D-O5D

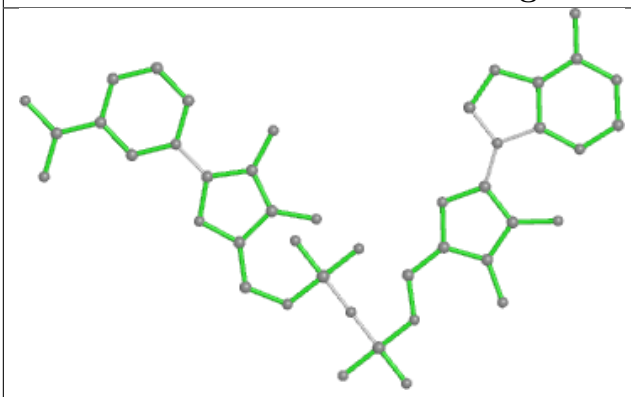
There are no ring outliers.

8 monomers are involved in 24 short contacts:

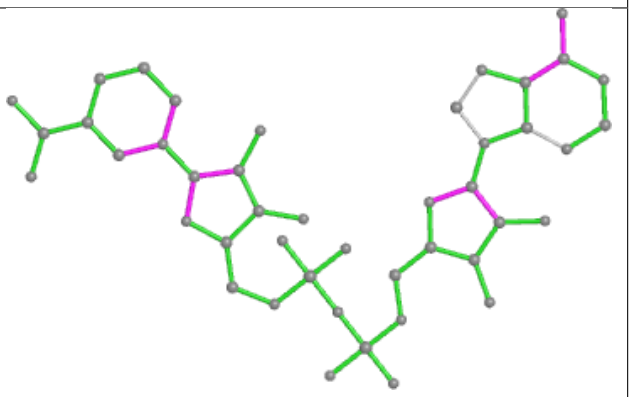
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	NAD	3	0
6	D	901	EDO	2	0
4	C	503	NAD	5	0
3	C	502	G6P	2	0
3	A	502	G6P	2	0
3	D	903	G6P	2	0
4	B	503	NAD	4	0
4	D	904	NAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

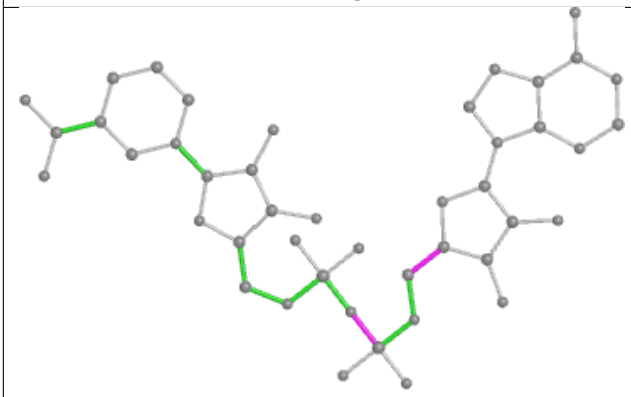
Ligand NAD A 503



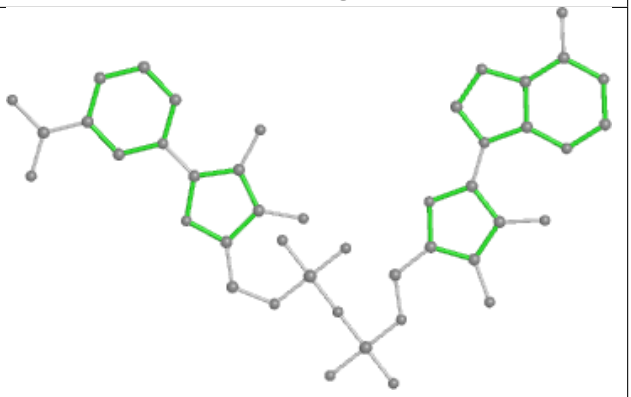
Bond lengths



Bond angles

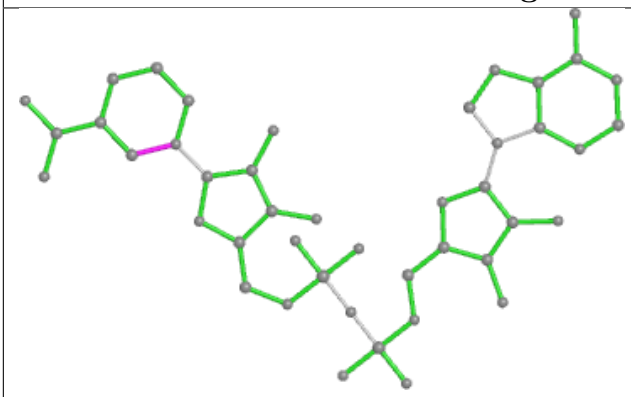


Torsions

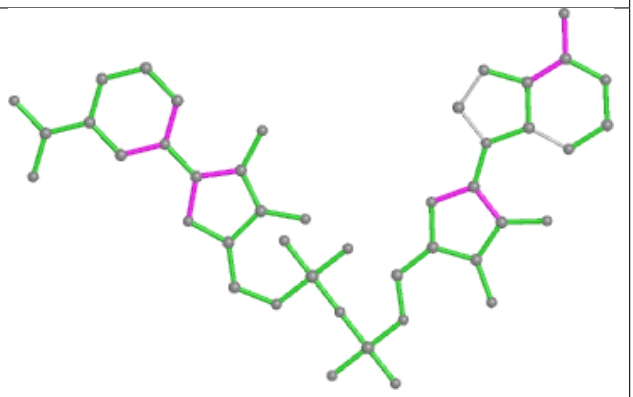


Rings

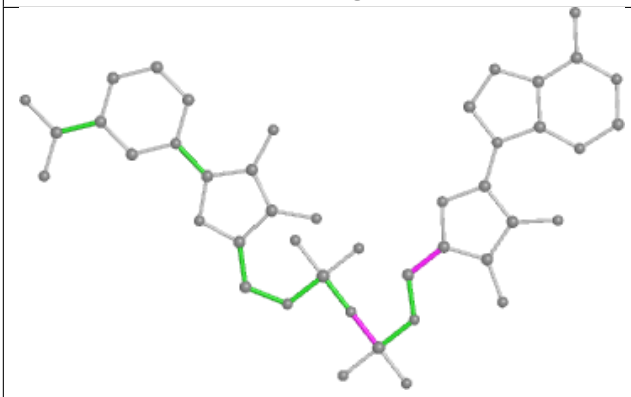
Ligand NAD C 503



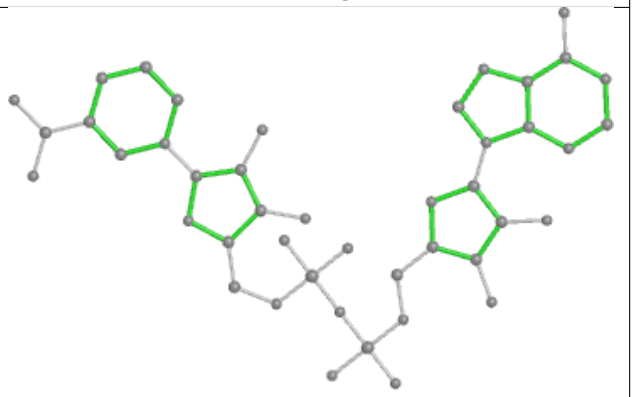
Bond lengths



Bond angles

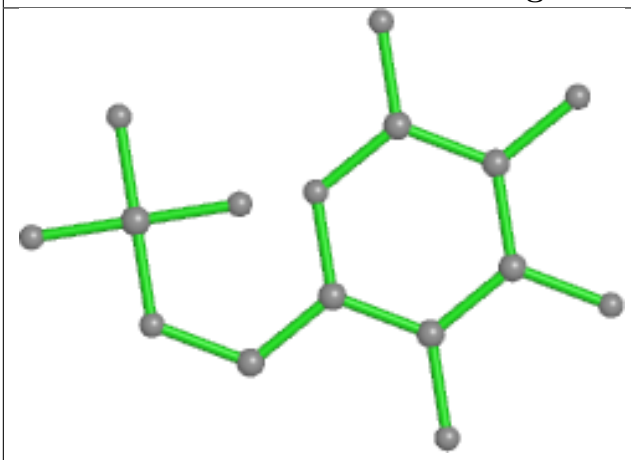


Torsions

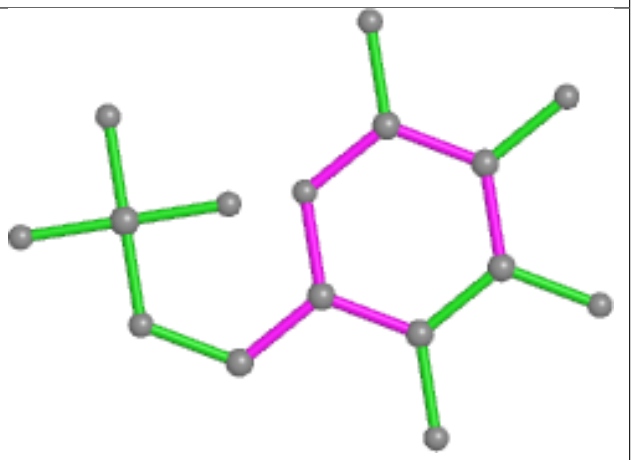


Rings

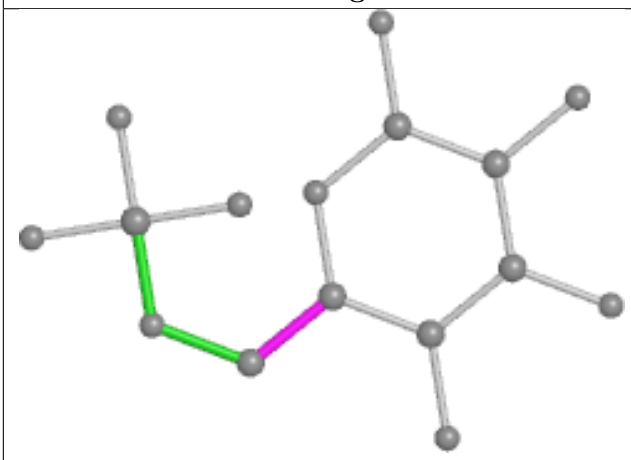
Ligand G6P C 502



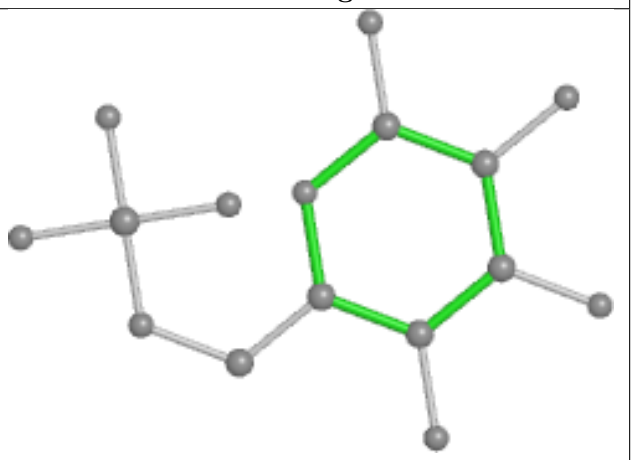
Bond lengths



Bond angles

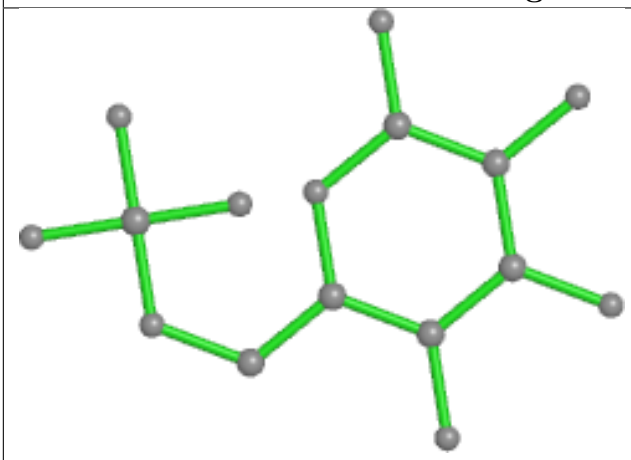


Torsions

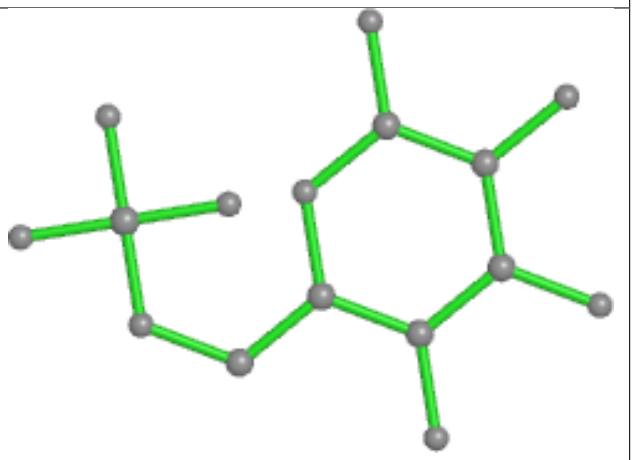


Rings

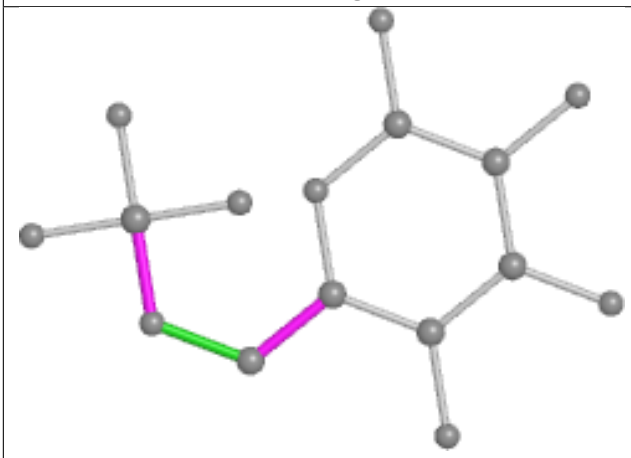
Ligand G6P A 502



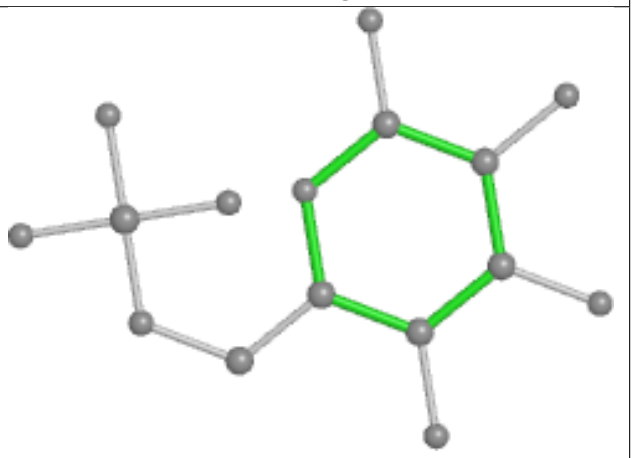
Bond lengths



Bond angles

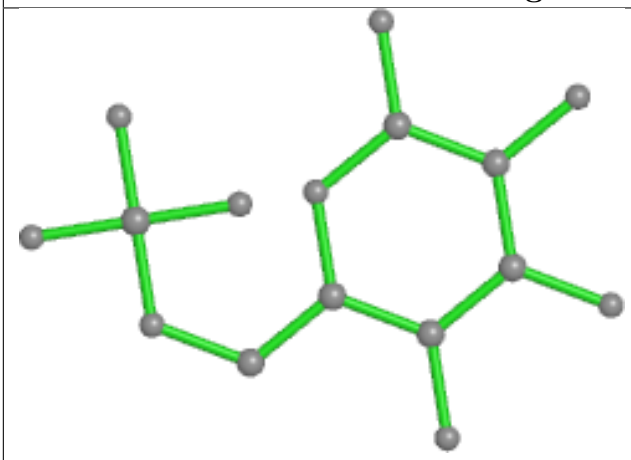


Torsions

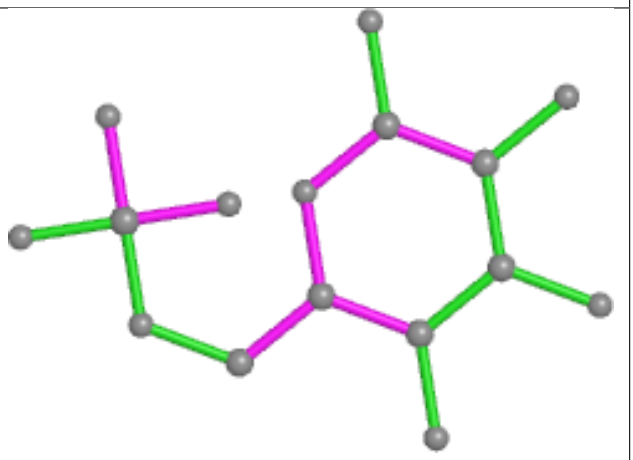


Rings

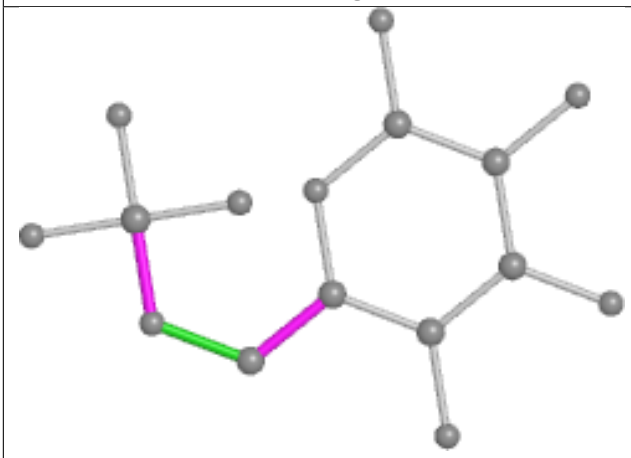
Ligand G6P D 903



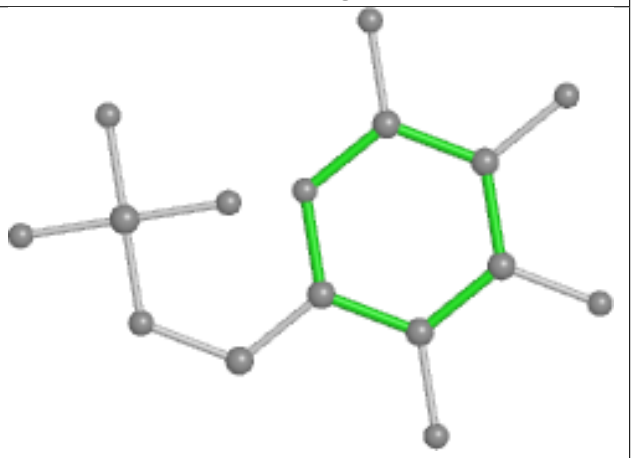
Bond lengths



Bond angles

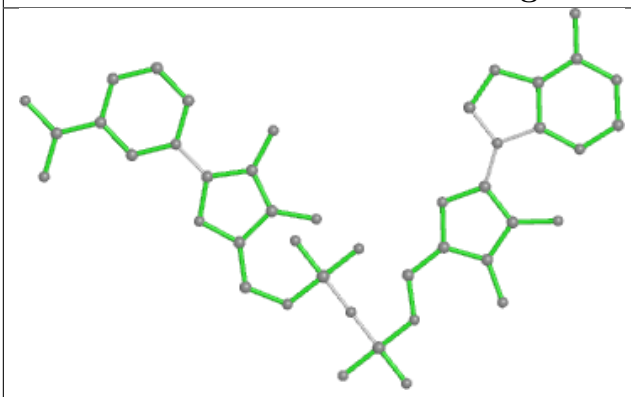


Torsions

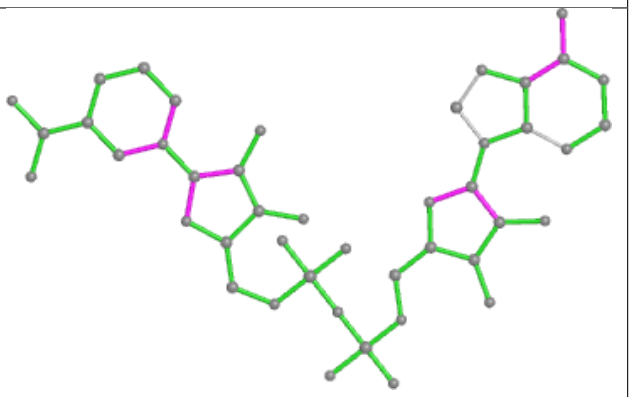


Rings

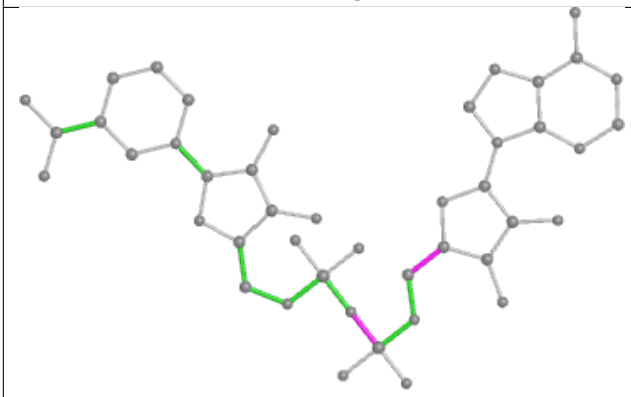
Ligand NAD B 503



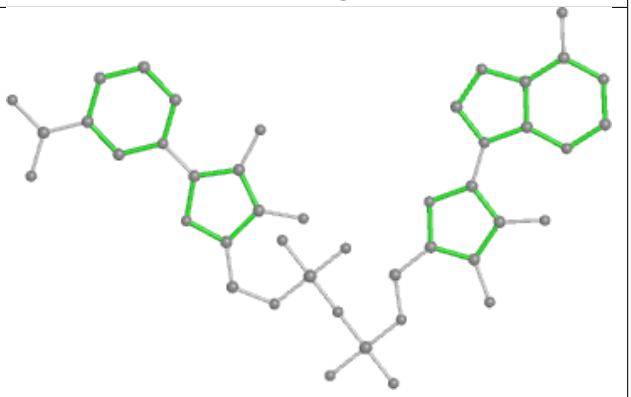
Bond lengths



Bond angles

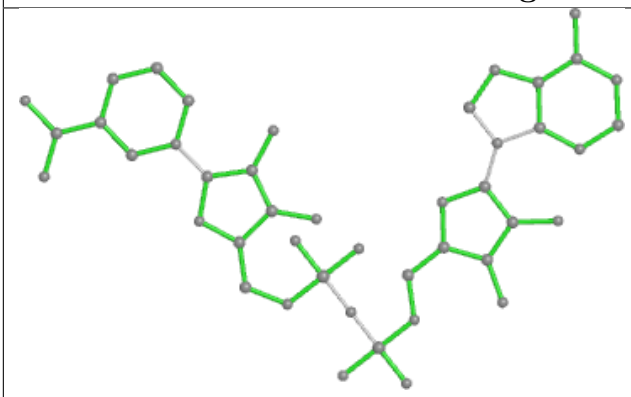


Torsions

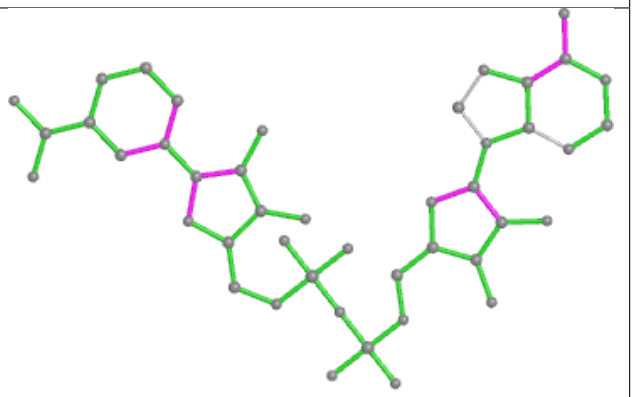


Rings

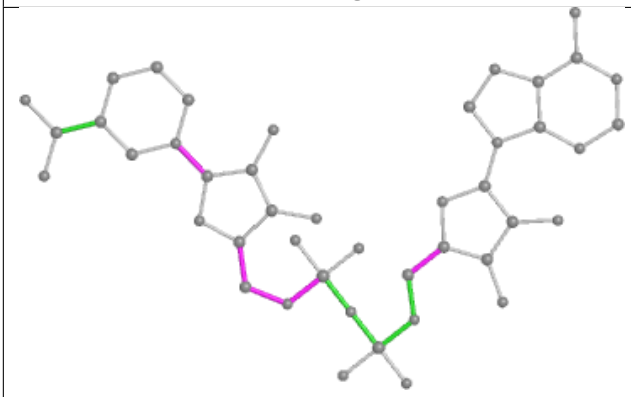
Ligand NAD D 904



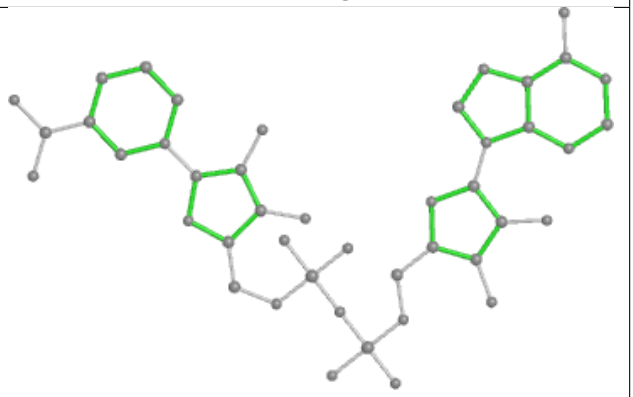
Bond lengths



Bond angles



Torsions



Rings

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	426/443 (96%)	0.03	4 (0%)	84	86	31, 57, 86, 124	0
1	B	424/443 (95%)	0.04	2 (0%)	91	92	31, 58, 89, 118	0
1	C	425/443 (95%)	0.19	14 (3%)	46	50	34, 63, 109, 145	0
1	D	413/443 (93%)	0.16	9 (2%)	62	65	33, 65, 101, 126	0
All	All	1688/1772 (95%)	0.11	29 (1%)	70	73	31, 60, 99, 145	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	TYR	4.5
1	C	282	ILE	4.4
1	C	248	PHE	4.2
1	C	239	LEU	3.9
1	C	245	VAL	3.9
1	D	248	PHE	3.7
1	C	3	LYS	3.6
1	A	238	LEU	3.4
1	C	311	VAL	3.1
1	B	238	LEU	3.1
1	C	244	TRP	3.0
1	C	273	PRO	2.7
1	C	247	THR	2.7
1	A	147	TYR	2.6
1	C	107	VAL	2.5
1	C	7	ILE	2.5
1	D	324	PHE	2.4
1	A	237	ALA	2.3
1	C	269	TYR	2.3
1	A	244	TRP	2.3
1	D	294	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	298	ILE	2.2
1	D	49	VAL	2.2
1	D	147	TYR	2.2
1	D	24	LEU	2.2
1	C	240	LYS	2.1
1	D	172	ASP	2.1
1	D	320	VAL	2.1
1	C	238	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

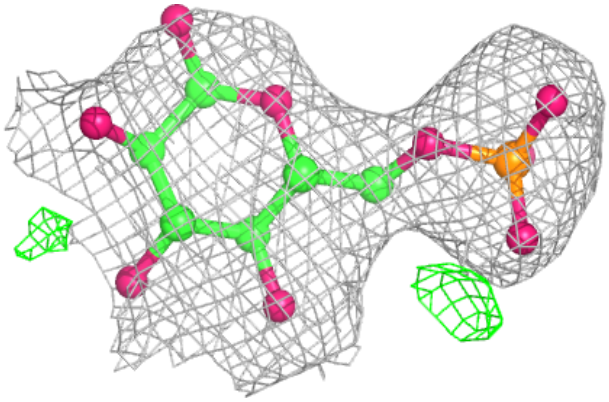
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

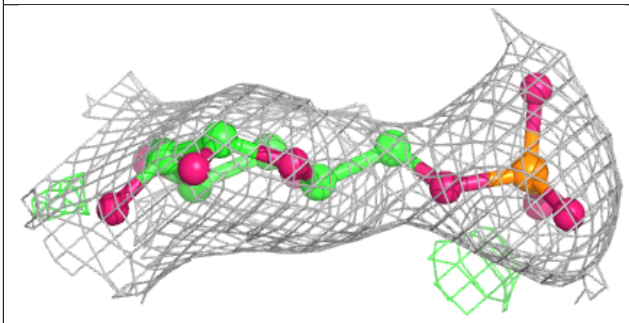
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	901	4/4	0.79	0.42	67,67,67,68	0
2	MN	C	501	1/1	0.82	0.11	86,86,86,86	1
5	PO4	C	504	5/5	0.85	0.20	126,126,126,126	0
3	G6P	C	502	16/16	0.87	0.15	92,93,96,96	0
3	G6P	A	502	16/16	0.91	0.17	76,88,91,92	0
3	G6P	D	903	16/16	0.92	0.20	60,75,75,75	16
4	NAD	D	904	44/44	0.93	0.17	44,60,78,80	44
4	NAD	C	503	44/44	0.94	0.15	63,73,88,88	0
4	NAD	B	503	44/44	0.95	0.16	60,65,77,80	0
4	NAD	A	503	44/44	0.96	0.13	58,62,71,75	0
2	MN	B	501	1/1	0.98	0.10	102,102,102,102	0
5	PO4	B	502	5/5	0.98	0.17	65,65,66,67	0
2	MN	A	501	1/1	0.98	0.03	59,59,59,59	0
2	MN	D	902	1/1	0.98	0.09	41,41,41,41	1

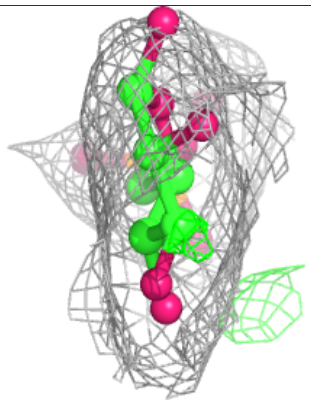
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G6P C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

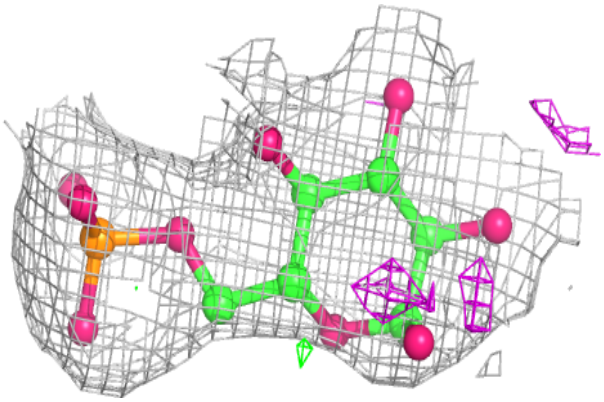


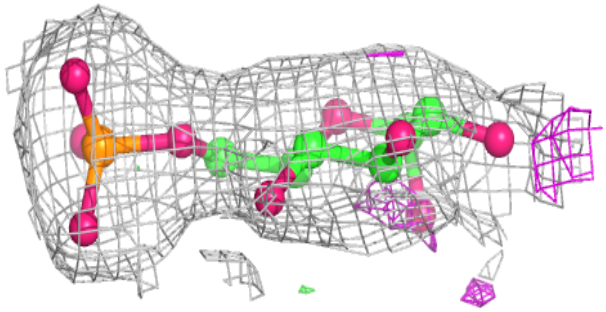


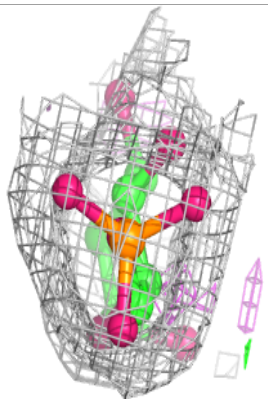


Electron density around G6P A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

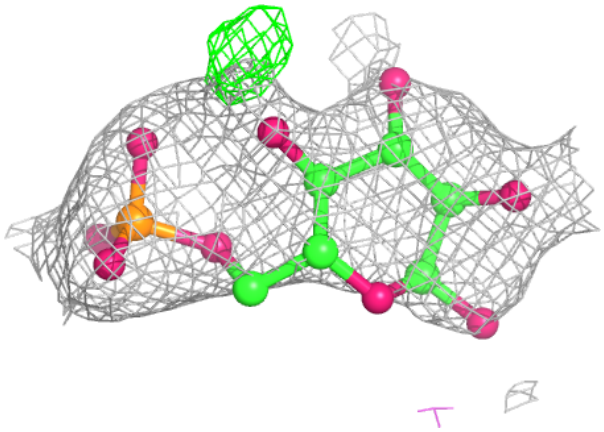


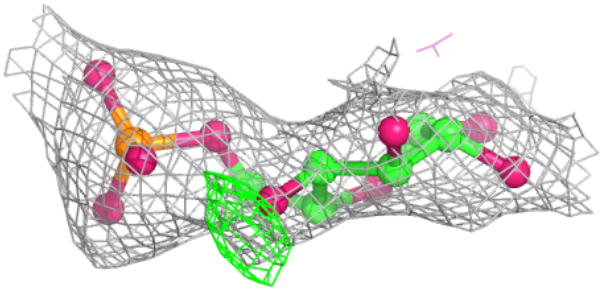


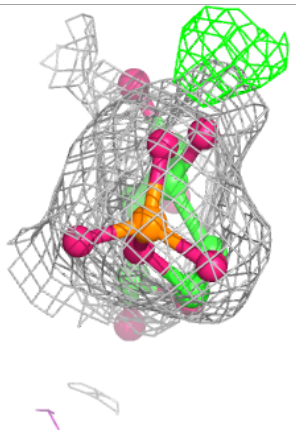


Electron density around G6P D 903:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

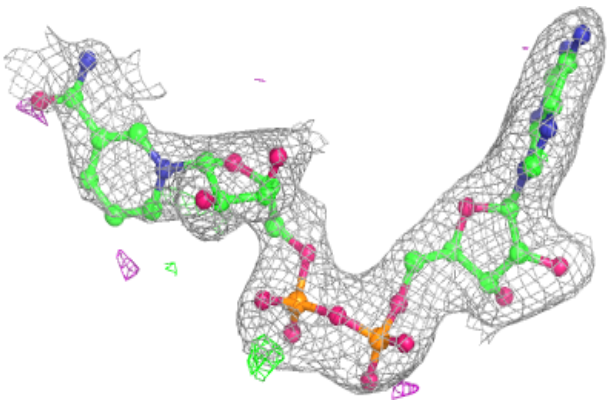


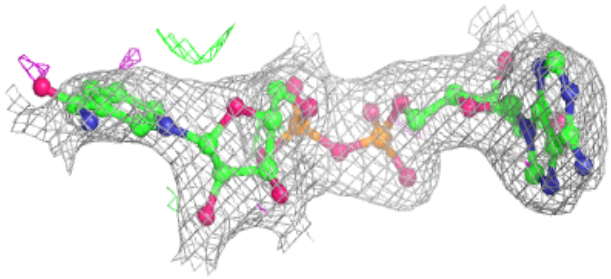


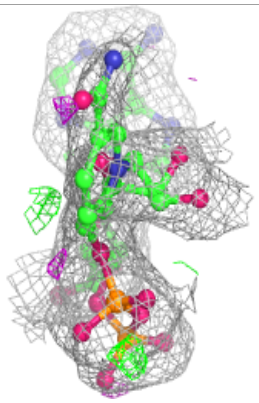


Electron density around NAD D 904:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

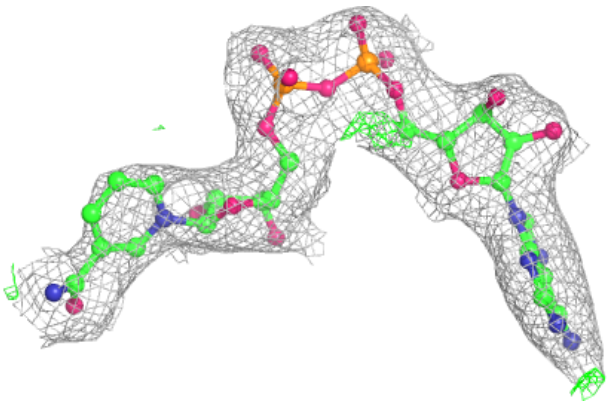


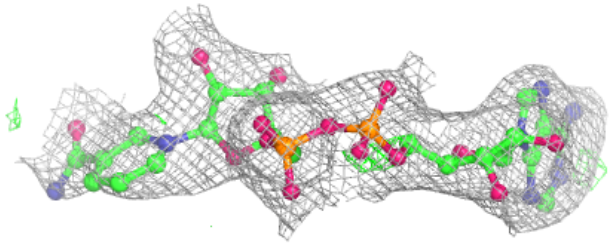


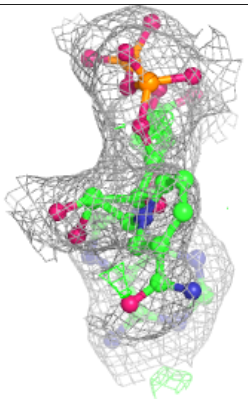


Electron density around NAD C 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

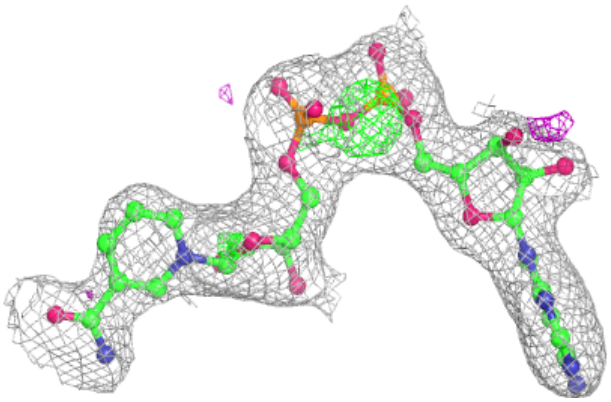


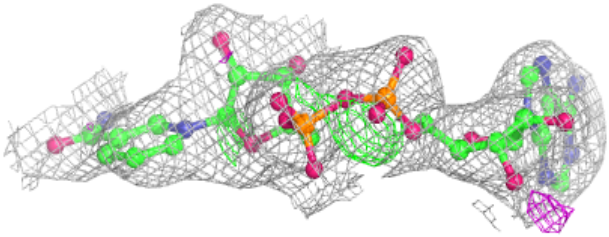


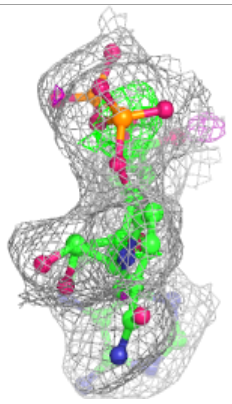


Electron density around NAD B 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

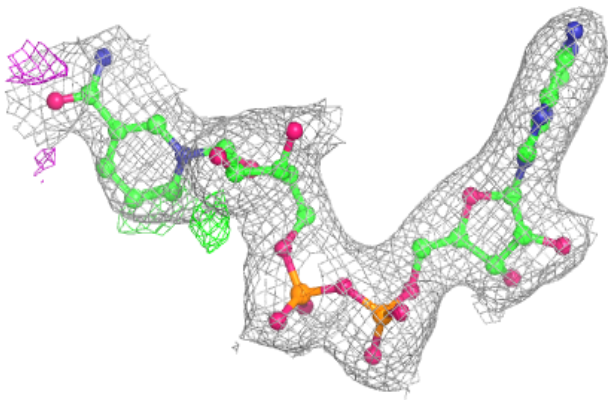


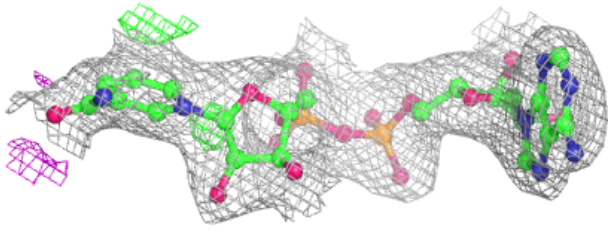


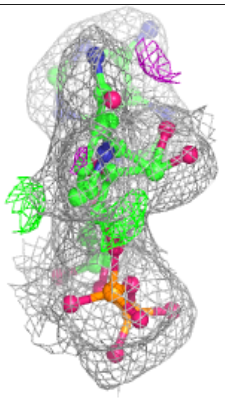


Electron density around NAD A 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.