



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:58 AM UTC

PDB ID : 6WBT / pdb_00006wbt
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

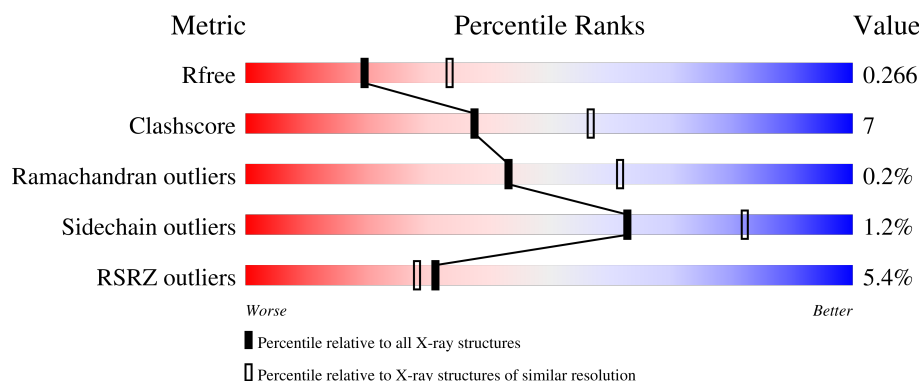
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	443	3% 81% 19% .
1	B	443	3% 84% 15% .
1	C	443	7% 81% 18% .
1	D	443	6% 76% 20% .

2 Entry composition

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.

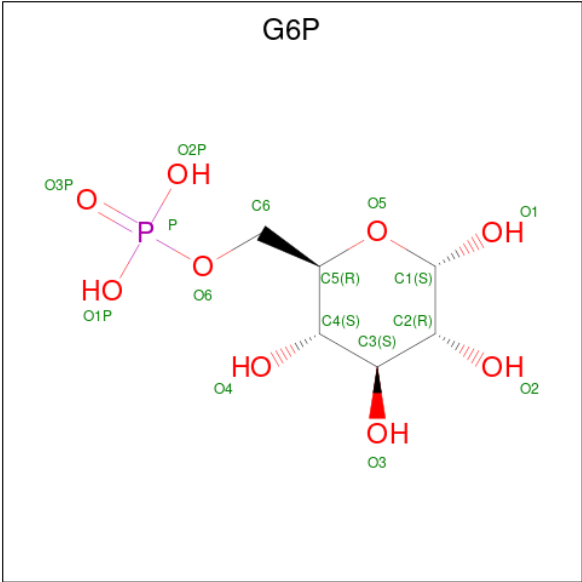
- Molecule 1 is a protein called cellulase IBT99.

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 (CCD ID: MN) (formula: Mn).

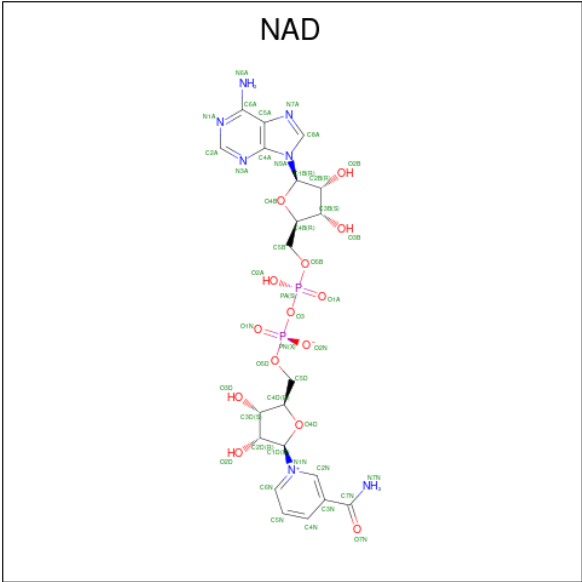
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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 (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

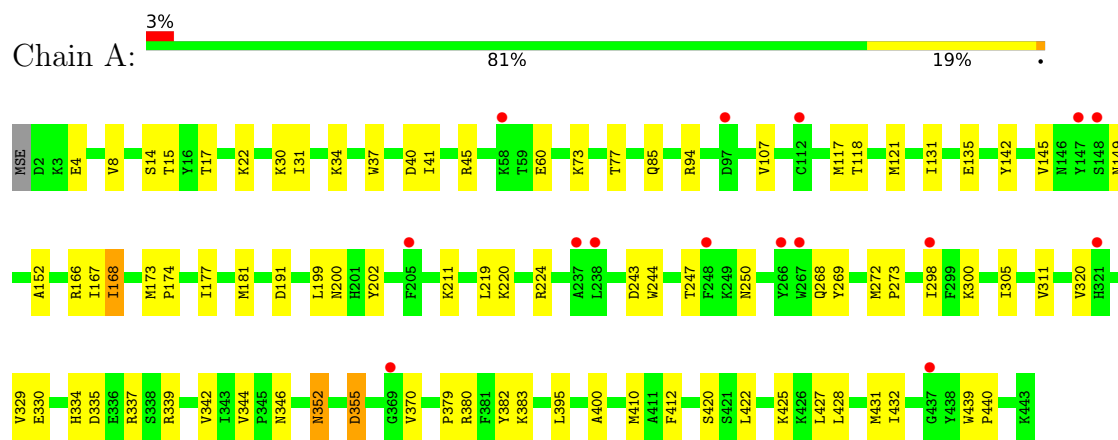
- Molecule 7 is water.

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

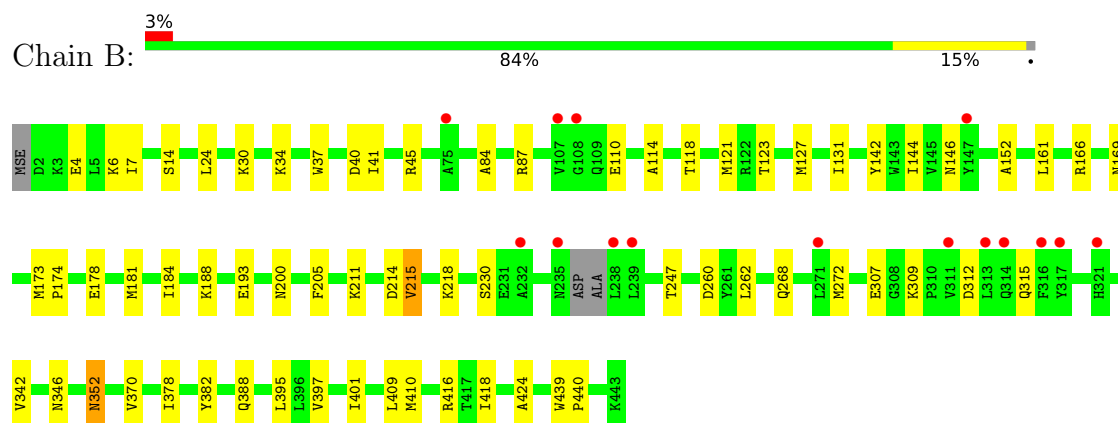
3 Residue-property plots [i](#)

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.

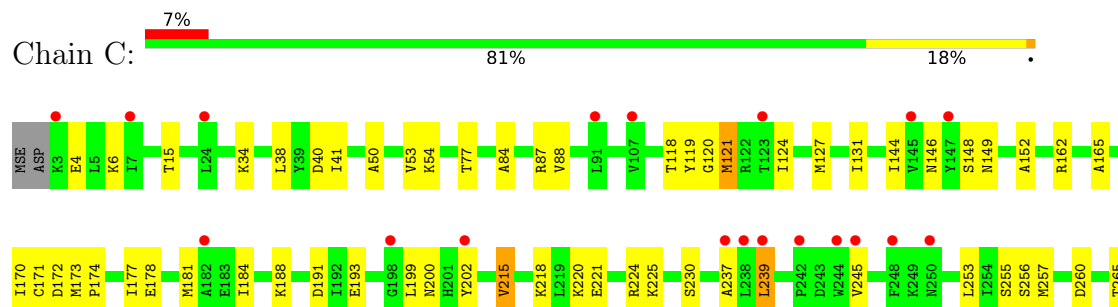
• Molecule 1: cellulase IBT99

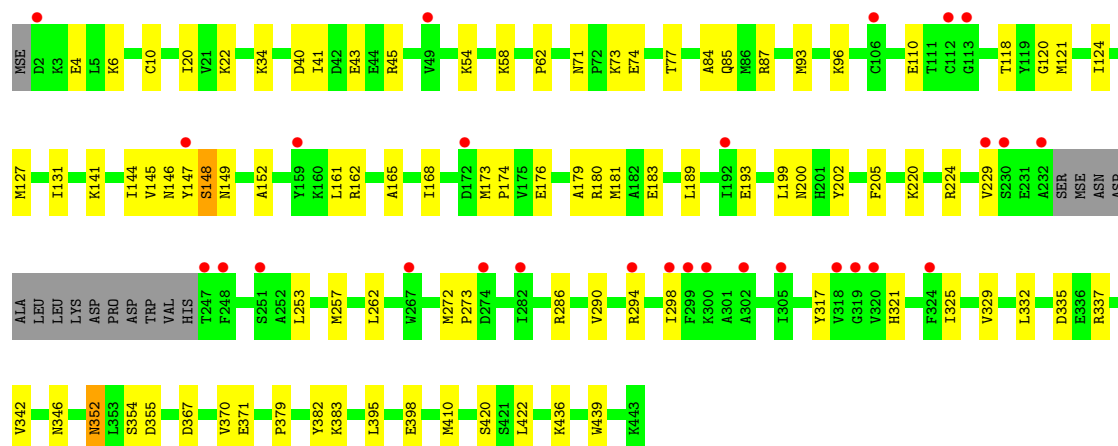


• Molecule 1: cellulase IBT99



• Molecule 1: cellulase IBT99





4 Data and refinement statistics

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 70.92 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.9 (70.92-2.52) 92.9 (70.92-2.52)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.227 , 0.266 0.228 , 0.266	Depositor DCC
R_{free} test set	3582 reflections (4.73%)	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)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MN, G6P, NAD, PO4, EDO

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	0.10	0/3597	0.27	0/4837
1	B	0.10	0/3575	0.27	0/4805
1	C	0.10	0/3581	0.28	0/4815
1	D	0.10	0/3471	0.27	0/4664
All	All	0.10	0/14224	0.27	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 [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	3543	0	3548	57	0
1	B	3522	0	3533	41	0
1	C	3527	0	3539	51	0
1	D	3421	0	3437	62	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	4	0
4	B	44	0	26	4	0
4	C	44	0	26	6	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	2	0
All	All	14440	0	14199	198	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 (198) 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: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:C:309:LYS:NZ	1:C:310:PRO:O	2.35	0.53
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:D:352:ASN:O	1:D:383:LYS:NZ	2.42	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:A:135:GLU:OE1	1:A:142:TYR:OH	2.24	0.51
1:D:173:MSE:HE3	1:D:176:GLU:HB2	1.92	0.51
1:B:40:ASP:OD1	1:B:41:ILE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PHE:HB2	1:B:262:LEU:HB2	1.92	0.50
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: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:6:LYS:NZ	1:C:77:THR:O	2.42	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:D:73:LYS:O	1:D:77:THR:OG1	2.20	0.47
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: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: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:A:14:SER:OG	4:A:503:NAD:O1N	2.31	0.45
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:A:243:ASP:O	1:A:247:THR:OG1	2.22	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:141:LYS:NZ	7:D:1001:HOH:O	2.50	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:73:LYS:O	1:A:77:THR:OG1	2.27	0.42
1:A:107:VAL:HG11	1:A:269:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:40:ASP:OD2	4:B:503:NAD:O3B	2.21	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: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:C:119:TYR:OH	4:C:503:NAD:O3D	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	43	62
1	B	436/443 (98%)	420 (96%)	15 (3%)	1 (0%)	43	62
1	C	439/443 (99%)	426 (97%)	12 (3%)	1 (0%)	43	62
1	D	424/443 (96%)	412 (97%)	11 (3%)	1 (0%)	43	62
All	All	1740/1772 (98%)	1687 (97%)	49 (3%)	4 (0%)	43	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	ASN

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

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	387/370 (105%)	382 (99%)	5 (1%)	61	81
1	B	385/370 (104%)	382 (99%)	3 (1%)	73	88
1	C	385/370 (104%)	382 (99%)	3 (1%)	73	88
1	D	373/370 (101%)	366 (98%)	7 (2%)	50	74
All	All	1530/1480 (103%)	1512 (99%)	18 (1%)	63	82

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

Mol	Chain	Res	Type
1	A	168	ILE
1	A	250	ASN
1	A	320	VAL
1	A	352	ASN
1	A	355	ASP
1	B	123	THR
1	B	215	VAL
1	B	352	ASN
1	C	121	MSE
1	C	215	VAL
1	C	239	LEU
1	D	43	GLU
1	D	93	MSE
1	D	121	MSE
1	D	148	SER
1	D	229	VAL
1	D	298	ILE
1	D	352	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	99	GLN
1	A	268	GLN
1	A	284	ASN
1	A	389	GLN
1	B	27	GLN
1	B	32	ASN
1	B	149	ASN
1	B	169	ASN
1	B	200	ASN
1	B	235	ASN
1	B	250	ASN
1	B	268	GLN
1	B	315	GLN
1	B	388	GLN
1	B	403	HIS
1	C	32	ASN
1	C	149	ASN
1	C	284	ASN
1	C	334	HIS
1	C	340	GLN
1	D	29	GLN
1	D	32	ASN
1	D	129	GLN
1	D	149	ASN
1	D	200	ASN
1	D	250	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 oligosaccharides 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$
3	G6P	A	502	2	16,16,16	0.54	0	23,24,24	0.74	0
6	EDO	D	901	-	3,3,3	0.43	0	2,2,2	0.38	0
4	NAD	B	503	2	46,48,48	0.55	1 (2%)	64,73,73	0.68	1 (1%)
4	NAD	C	503	2	46,48,48	0.58	1 (2%)	64,73,73	0.67	1 (1%)
3	G6P	C	502	2	16,16,16	0.61	0	23,24,24	1.57	4 (17%)
4	NAD	D	904	2	46,48,48	0.61	1 (2%)	64,73,73	0.64	1 (1%)
4	NAD	A	503	2	46,48,48	0.57	1 (2%)	64,73,73	0.65	1 (1%)
5	PO4	C	504	-	4,4,4	0.97	0	6,6,6	0.47	0
3	G6P	D	903	2	16,16,16	0.56	0	23,24,24	1.21	5 (21%)
5	PO4	B	502	-	4,4,4	0.97	0	6,6,6	0.45	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
3	G6P	A	502	2	-	5/6/26/26	0/1/1/1
6	EDO	D	901	-	-	0/1/1/1	-
4	NAD	B	503	2	-	1/30/62/62	0/5/5/5
4	NAD	C	503	2	-	4/30/62/62	0/5/5/5
3	G6P	C	502	2	-	0/6/26/26	0/1/1/1
4	NAD	D	904	2	-	7/30/62/62	0/5/5/5
4	NAD	A	503	2	-	2/30/62/62	0/5/5/5
3	G6P	D	903	2	-	5/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAD	C2N-N1N	2.44	1.37	1.35
4	A	503	NAD	C2N-N1N	2.17	1.37	1.35
4	D	904	NAD	C2N-N1N	2.07	1.37	1.35
4	B	503	NAD	C2N-N1N	2.03	1.37	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	G6P	O5-C1-C2	4.46	118.14	110.30
3	C	502	G6P	C1-O5-C5	3.63	120.68	113.65
4	D	904	NAD	C6N-N1N-C2N	-2.64	119.63	121.88
4	B	503	NAD	C6N-N1N-C2N	-2.59	119.67	121.88
4	A	503	NAD	C6N-N1N-C2N	-2.56	119.70	121.88
4	C	503	NAD	C6N-N1N-C2N	-2.45	119.79	121.88
3	C	502	G6P	C1-C2-C3	2.41	115.26	110.36
3	D	903	G6P	O5-C1-C2	2.36	114.44	110.30
3	D	903	G6P	O5-C5-C4	2.14	113.55	109.70
3	D	903	G6P	O2P-P-O1P	2.13	115.77	107.80
3	D	903	G6P	C6-C5-C4	-2.07	107.72	112.07
3	D	903	G6P	C1-O5-C5	2.03	117.57	113.65
3	C	502	G6P	C6-C5-C4	-2.00	107.87	112.07

There are no chirality outliers.

All (24) 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
3	D	903	G6P	C6-O6-P-O3P
4	C	503	NAD	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	503	NAD	PN-O3-PA-O1A
4	A	503	NAD	PN-O3-PA-O2A
4	C	503	NAD	PN-O3-PA-O2A
4	D	904	NAD	C2B-C1B-N9A-C8A
4	C	503	NAD	C2B-C1B-N9A-C8A
4	B	503	NAD	PN-O3-PA-O2A
4	C	503	NAD	O4B-C4B-C5B-O5B
4	D	904	NAD	C4D-C5D-O5D-PN

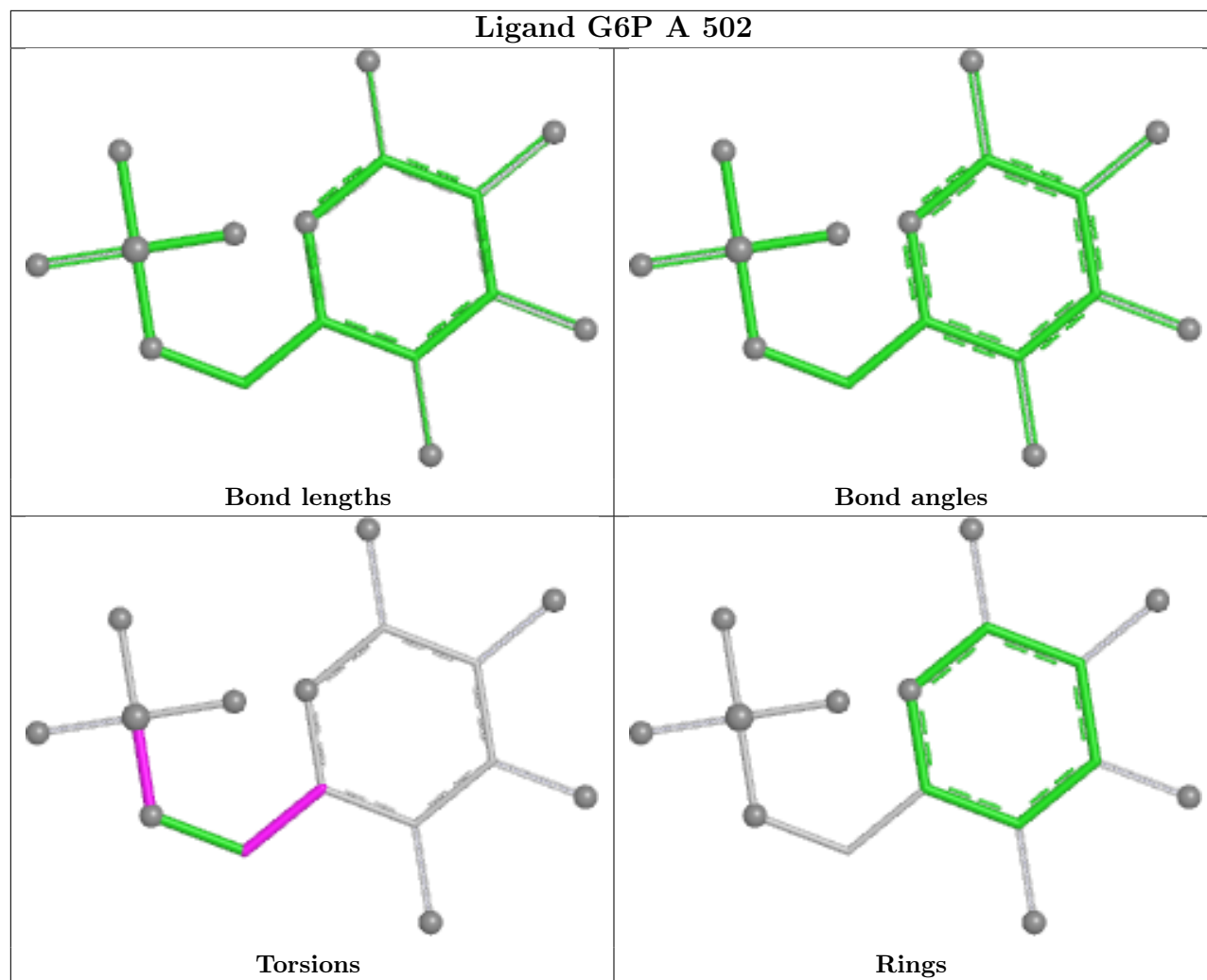
There are no ring outliers.

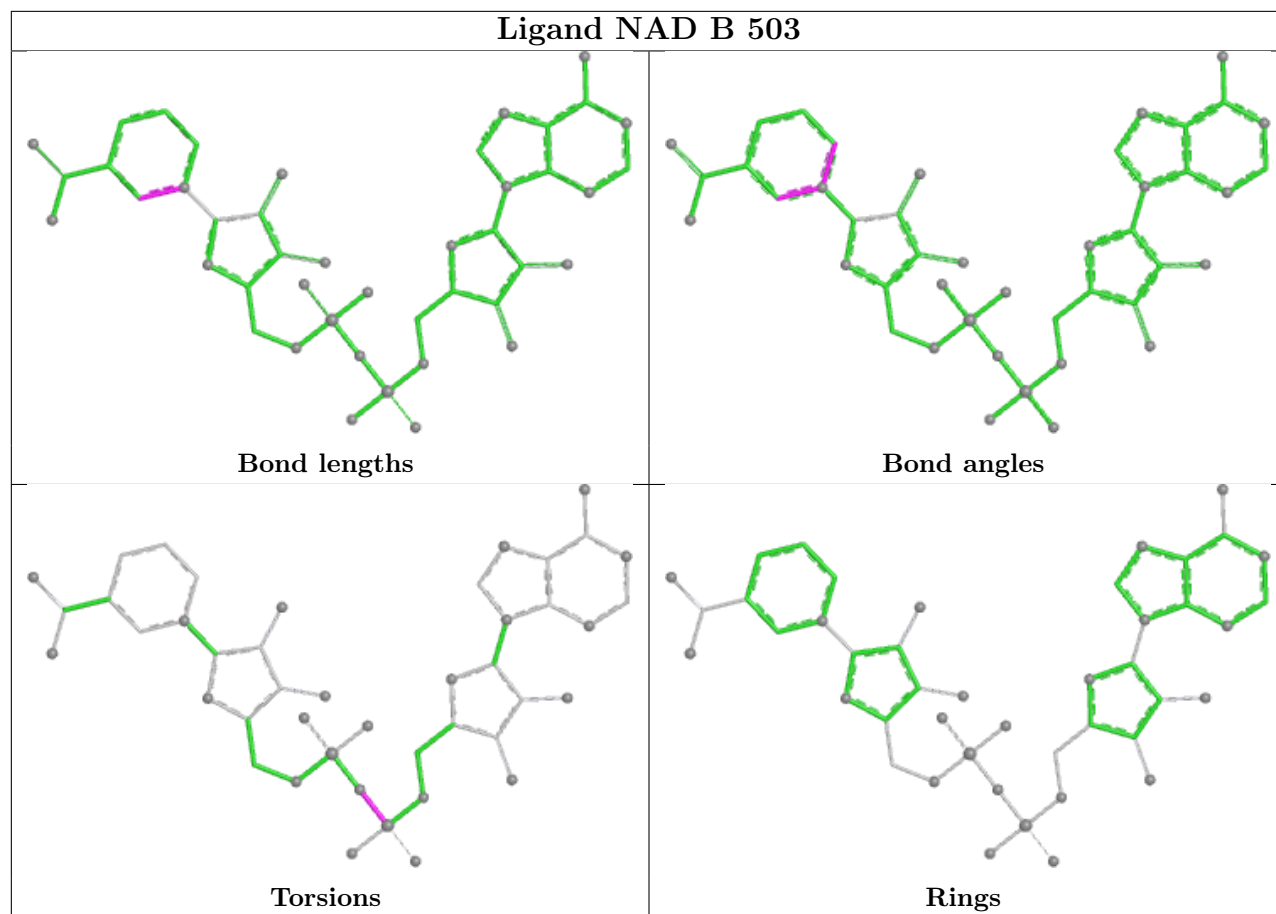
8 monomers are involved in 26 short contacts:

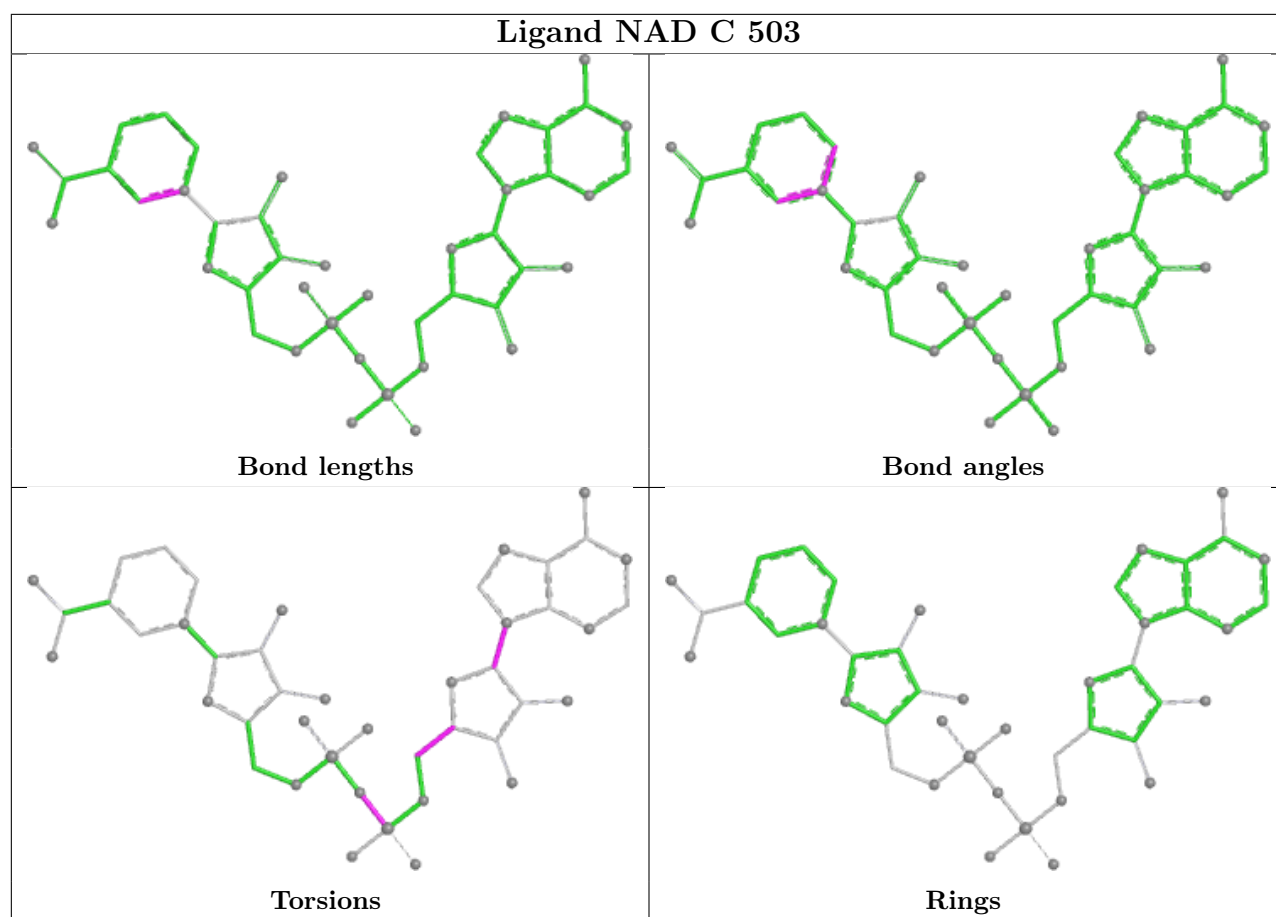
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	G6P	2	0
6	D	901	EDO	2	0
4	B	503	NAD	4	0
4	C	503	NAD	6	0
3	C	502	G6P	2	0
4	D	904	NAD	4	0
4	A	503	NAD	4	0
3	D	903	G6P	2	0

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 than 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.

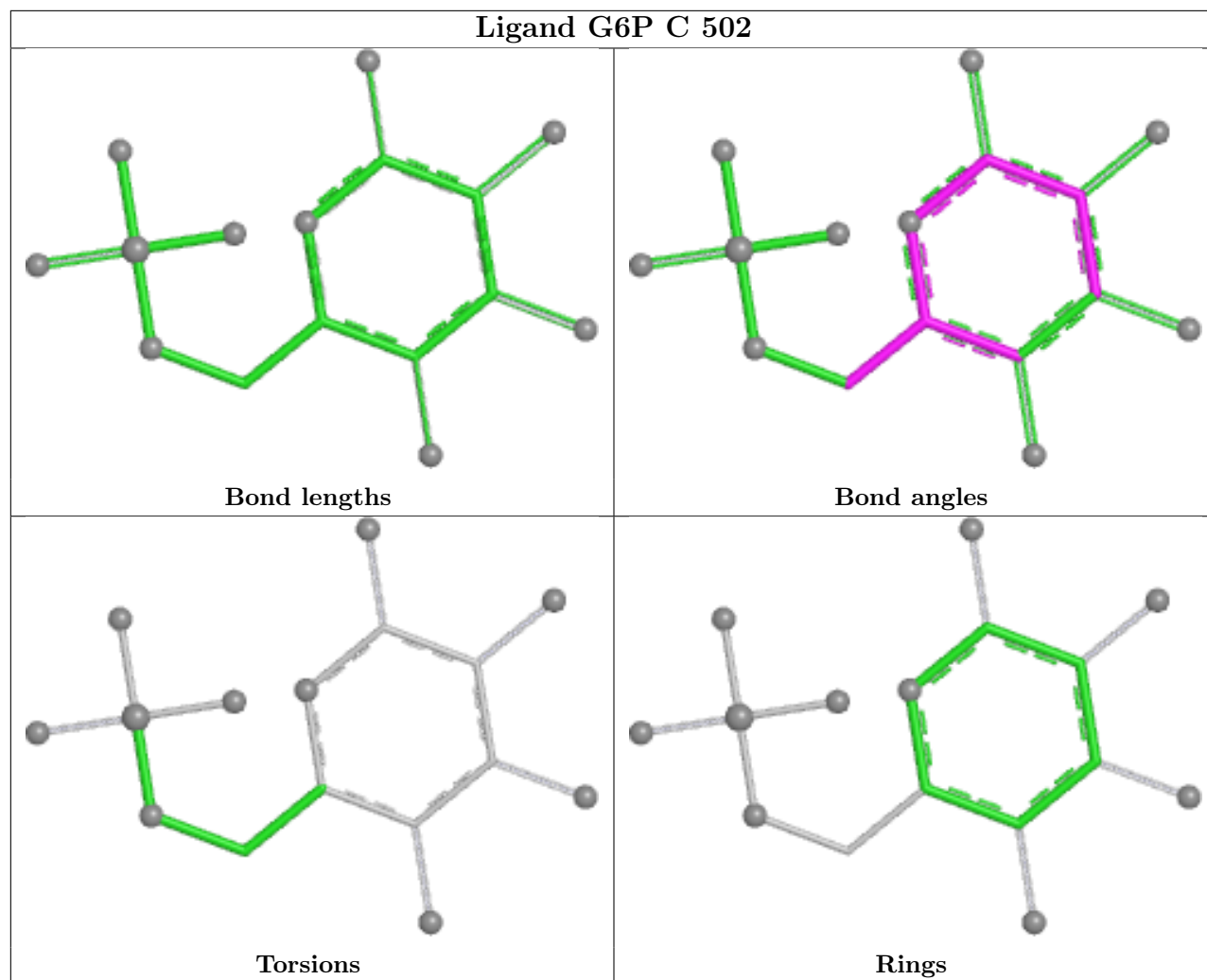
Ligand G6P A 502

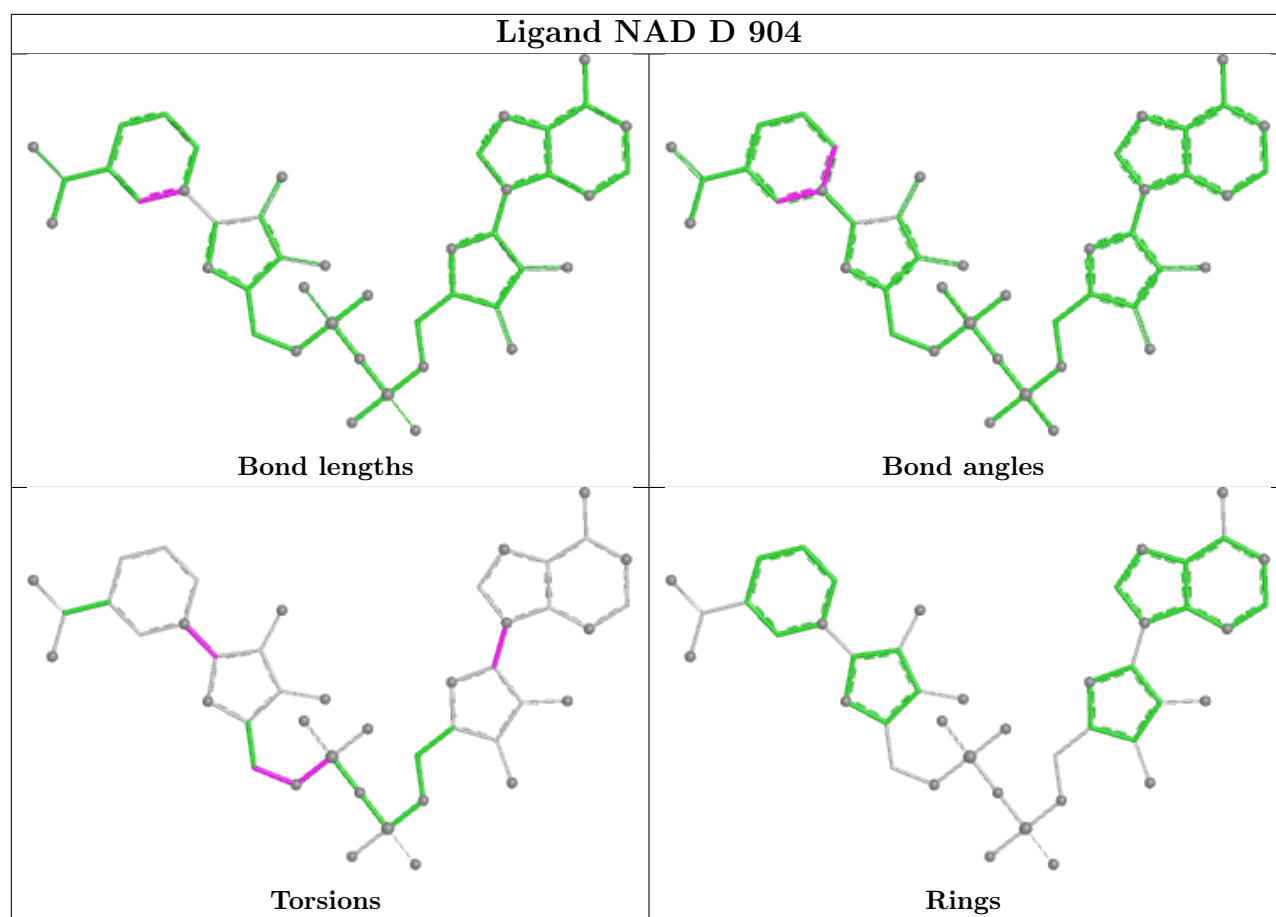


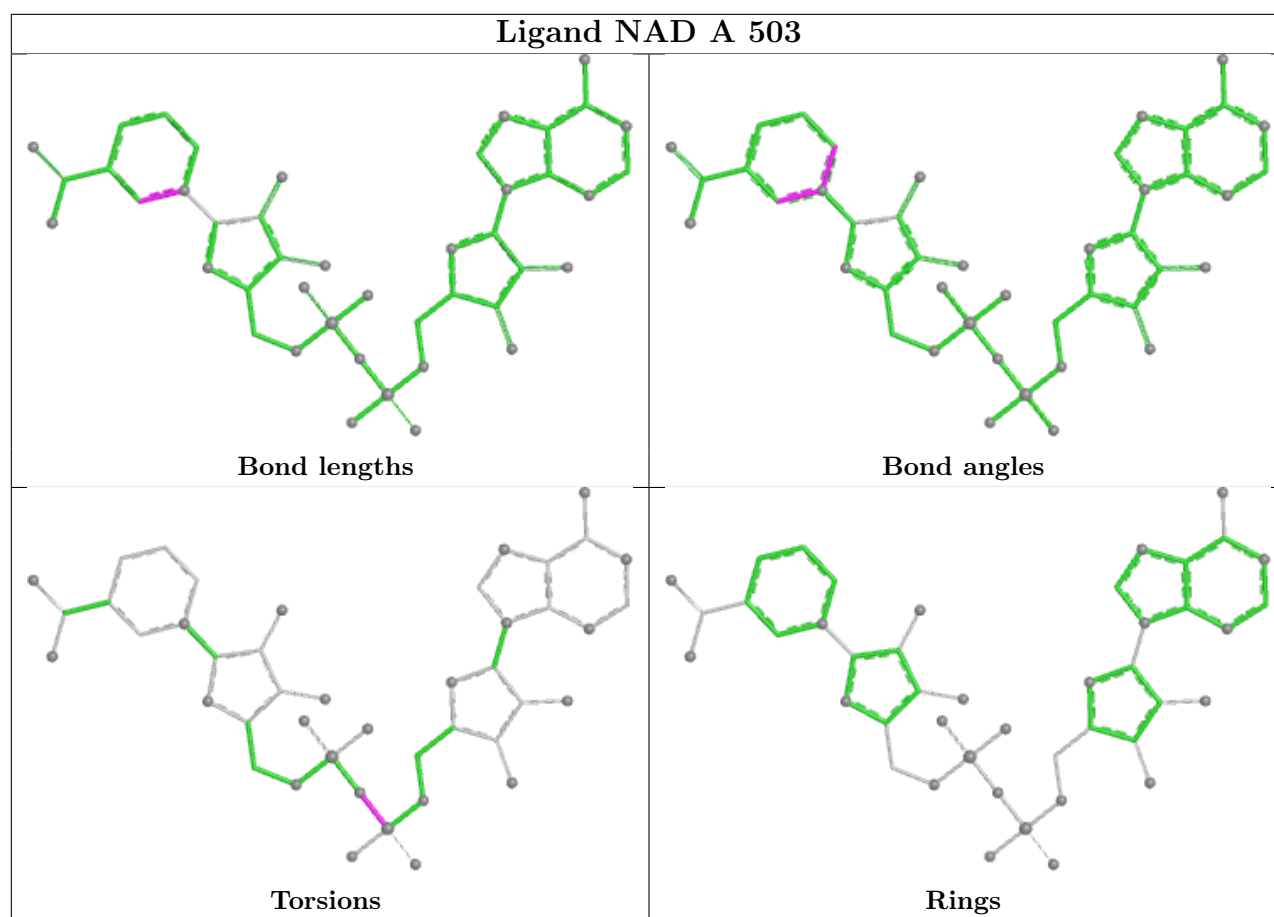


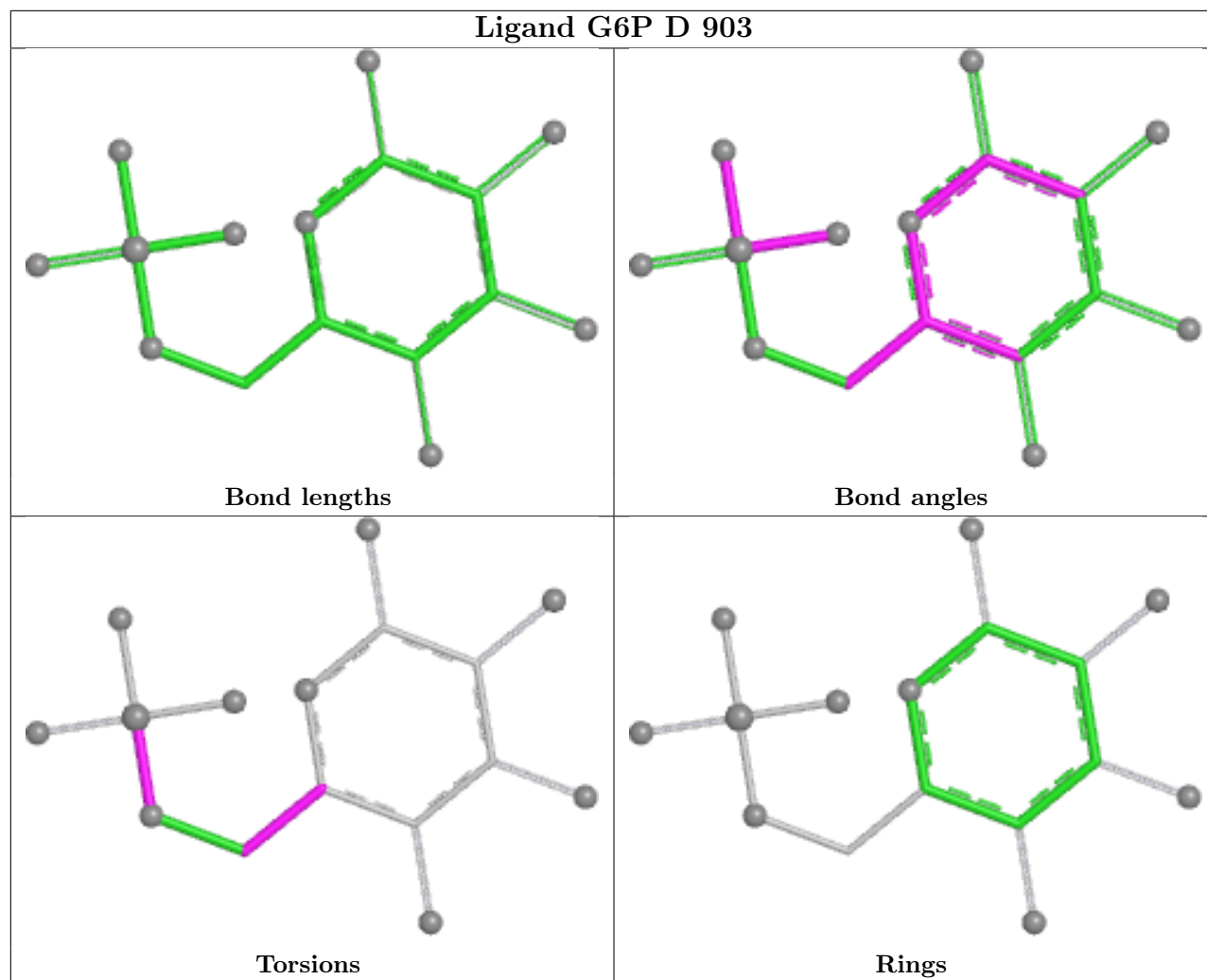


Ligand G6P C 502









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, 95th 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%)	0.51	15 (3%) 47 43	25, 57, 86, 124	1 (0%)
1	B	424/443 (95%)	0.53	15 (3%) 47 43	31, 58, 89, 118	0
1	C	425/443 (95%)	0.69	33 (7%) 19 17	34, 63, 109, 145	0
1	D	413/443 (93%)	0.68	28 (6%) 23 21	33, 65, 101, 126	0
All	All	1688/1772 (95%)	0.60	91 (5%) 31 28	25, 60, 99, 145	1 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	TYR	4.5
1	C	145	VAL	4.3
1	A	147	TYR	4.2
1	C	244	TRP	4.2
1	A	112	CYS	3.9
1	D	232	ALA	3.6
1	D	302	ALA	3.6
1	D	282	ILE	3.5
1	C	238	LEU	3.3
1	A	237	ALA	3.2
1	C	248	PHE	3.1
1	C	273	PRO	3.1
1	D	320	VAL	3.1
1	C	282	ILE	3.1
1	C	182	ALA	3.1
1	D	49	VAL	3.1
1	C	147	TYR	3.0
1	D	251	SER	3.0
1	C	311	VAL	3.0
1	C	237	ALA	3.0
1	B	238	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	298	ILE	2.8
1	D	112	CYS	2.8
1	C	239	LEU	2.8
1	B	321	HIS	2.8
1	C	319	GLY	2.8
1	A	238	LEU	2.8
1	A	267	TRP	2.8
1	C	198	GLY	2.7
1	D	147	TYR	2.7
1	D	318	VAL	2.7
1	B	316	PHE	2.7
1	D	324	PHE	2.7
1	A	205	PHE	2.6
1	C	321	HIS	2.6
1	A	148	SER	2.6
1	A	58	LYS	2.6
1	C	242	PRO	2.6
1	D	172	ASP	2.6
1	D	305	ILE	2.6
1	B	107	VAL	2.6
1	C	107	VAL	2.6
1	C	287	GLY	2.5
1	A	298	ILE	2.5
1	D	247	THR	2.5
1	C	267	TRP	2.5
1	C	3	LYS	2.5
1	C	250	ASN	2.5
1	D	300	LYS	2.4
1	D	299	PHE	2.4
1	D	267	TRP	2.4
1	A	437	GLY	2.4
1	C	269	TYR	2.4
1	D	229	VAL	2.4
1	C	245	VAL	2.4
1	C	7	ILE	2.4
1	B	235	ASN	2.4
1	B	313	LEU	2.3
1	A	248	PHE	2.3
1	B	75	ALA	2.3
1	C	123	THR	2.3
1	B	108	GLY	2.3
1	C	290	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	192	ILE	2.2
1	B	232	ALA	2.2
1	A	321	HIS	2.2
1	A	369	GLY	2.2
1	C	91	LEU	2.2
1	C	299	PHE	2.2
1	B	311	VAL	2.2
1	C	24	LEU	2.2
1	A	266	TYR	2.2
1	D	2	ASP	2.2
1	B	271	LEU	2.1
1	D	294	ARG	2.1
1	A	97	ASP	2.1
1	D	248	PHE	2.1
1	B	317	TYR	2.1
1	D	274	ASP	2.1
1	C	439	TRP	2.1
1	D	319	GLY	2.1
1	C	281	ASP	2.1
1	D	106	CYS	2.1
1	B	314	GLN	2.1
1	C	301	ALA	2.1
1	C	308	GLY	2.1
1	C	202	TYR	2.1
1	D	159	TYR	2.0
1	B	239	LEU	2.0
1	D	113	GLY	2.0
1	D	230	SER	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 oligosaccharides 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,

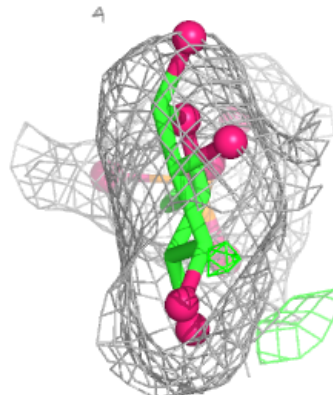
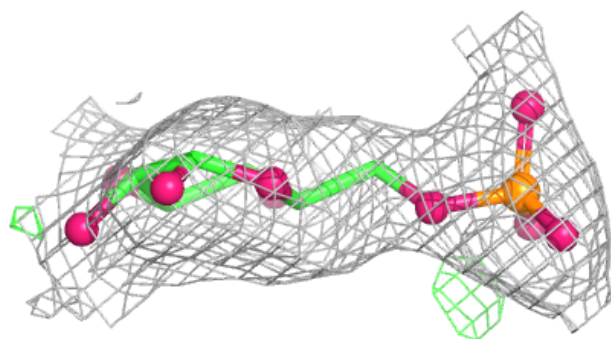
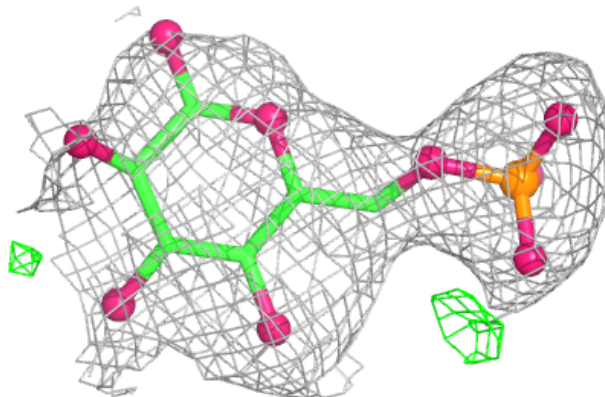
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	C	504	5/5	0.72	0.17	126,126,126,126	0
3	G6P	C	502	16/16	0.75	0.12	92,93,96,96	0
3	G6P	D	903	16/16	0.79	0.15	60,75,75,75	16
3	G6P	A	502	16/16	0.85	0.13	76,88,91,92	0
6	EDO	D	901	4/4	0.85	0.21	67,67,67,68	0
2	MN	C	501	1/1	0.89	0.10	86,86,86,86	1
4	NAD	D	904	44/44	0.89	0.12	44,60,78,80	44
4	NAD	C	503	44/44	0.90	0.11	63,73,88,88	0
4	NAD	B	503	44/44	0.91	0.10	60,65,77,80	0
5	PO4	B	502	5/5	0.91	0.17	65,65,66,67	0
4	NAD	A	503	44/44	0.93	0.09	58,62,71,75	0
2	MN	B	501	1/1	0.95	0.07	102,102,102,102	0
2	MN	D	902	1/1	0.97	0.04	41,41,41,41	1
2	MN	A	501	1/1	0.98	0.14	59,59,59,59	0

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.

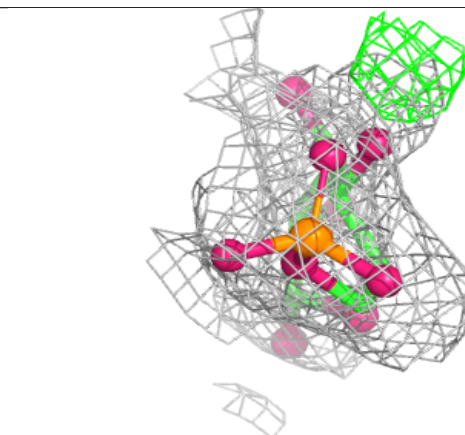
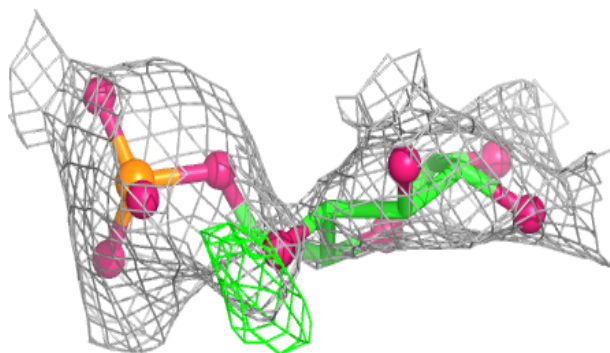
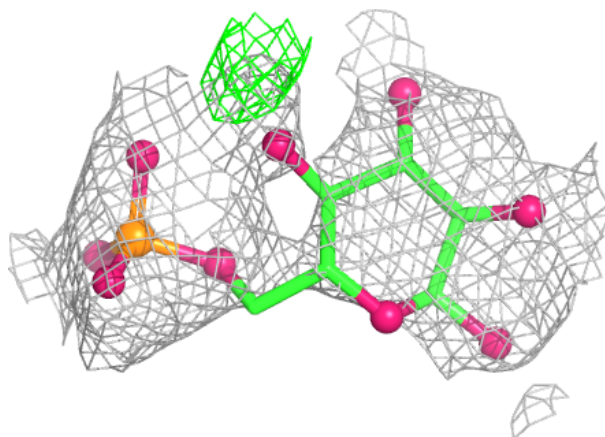
Electron density around G6P C 502:

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

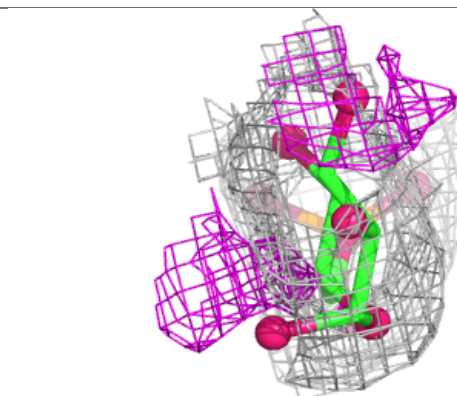
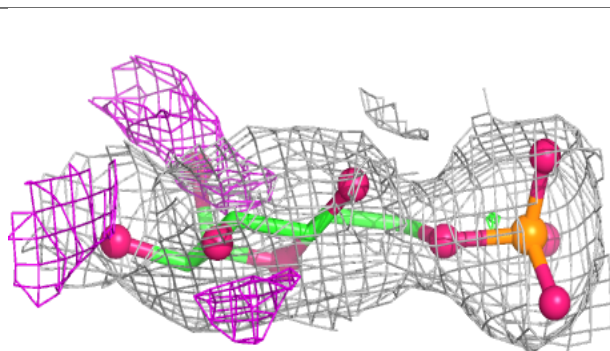


Electron density around G6P D 903:

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

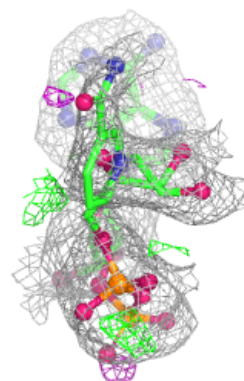
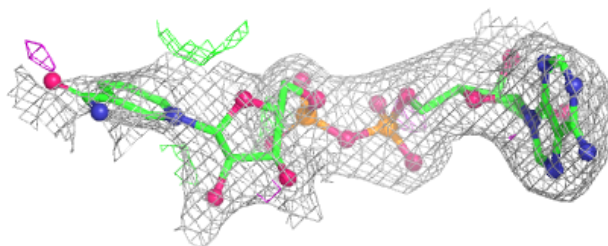
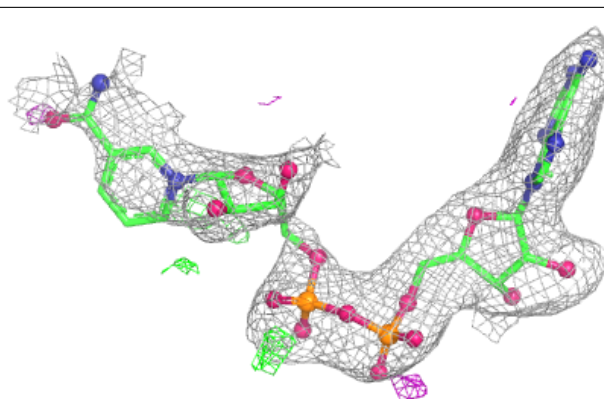
**Electron density around G6P A 502:**

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

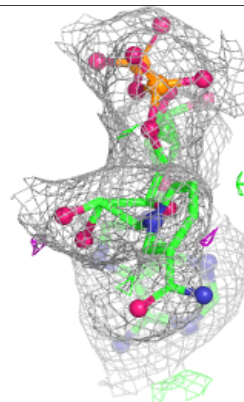
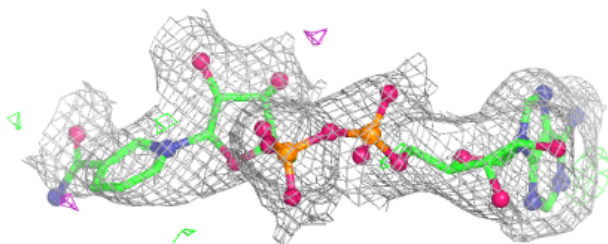
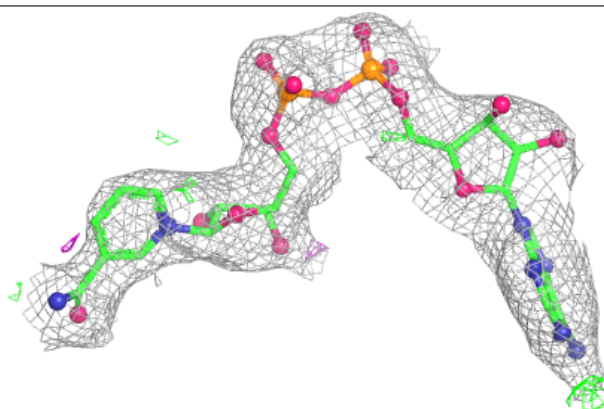


Electron density around NAD D 904:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

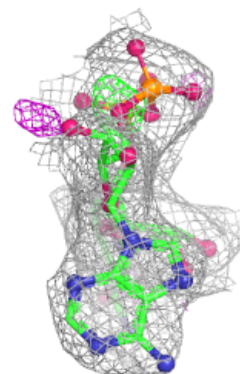
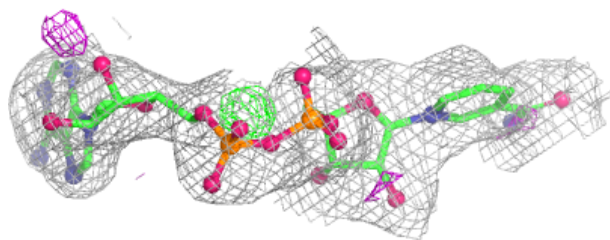
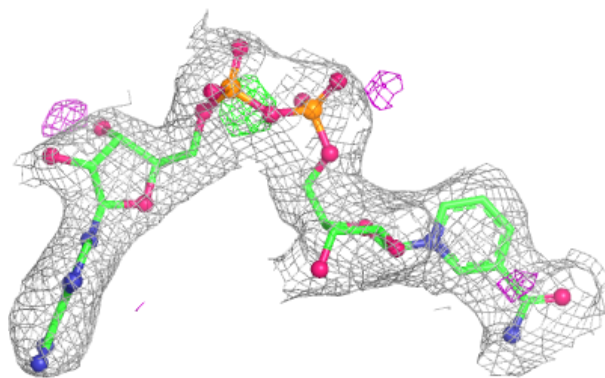
**Electron density around NAD C 503:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

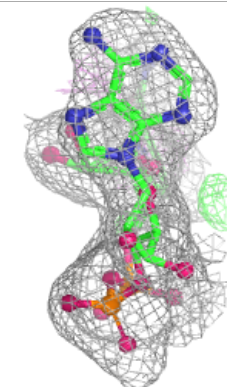
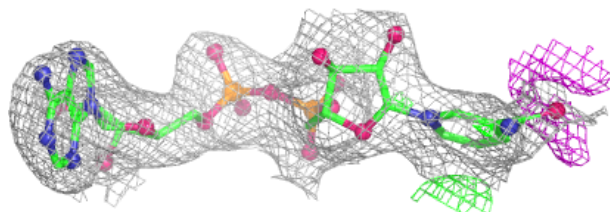
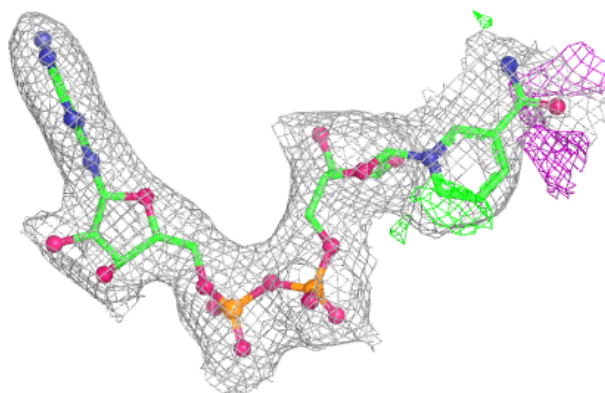


Electron density around NAD B 503:

$2mF_o-DF_c$ (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.