



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:19 PM UTC

PDB ID : 1UP7 / pdb_00001up7
Title : Structure of the 6-phospho-beta glucosidase from *Thermotoga maritima* at 2.4 Angstrom resolution in the tetragonal form with NAD and glucose-6-phosphate
Authors : Varrot, A.; Yip, V.L.; Withers, S.G.; Davies, G.J.
Deposited on : 2003-09-29
Resolution : 2.40 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:

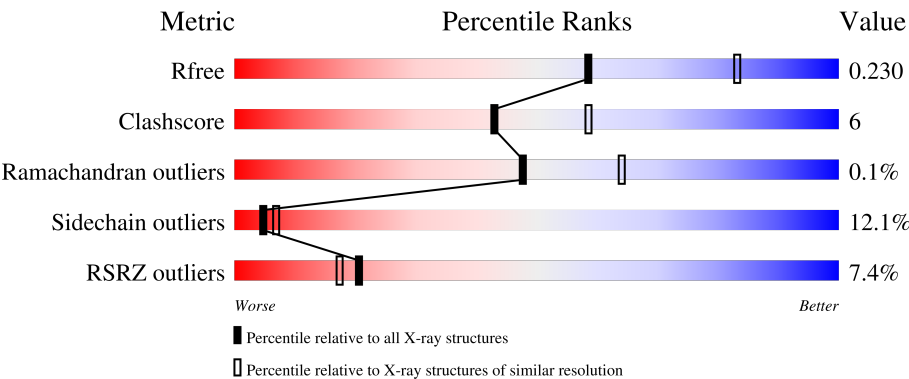
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	417	4% 77% 18% 5%
1	B	417	12% 78% 17%
1	C	417	5% 77% 19%
1	D	417	5% 75% 20%
1	E	417	15% 76% 19%

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Mol	Chain	Length	Quality of chain
1	F	417	
1	G	417	
1	H	417	

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
3	G6P	A	1417	X	-	-	-
3	G6P	B	1417	X	-	-	-
3	G6P	C	1417	X	-	-	-
3	G6P	D	1417	X	-	-	-
3	G6P	E	1417	X	-	-	-
3	G6P	F	1417	X	-	-	-
3	G6P	G	1417	X	-	-	-
3	G6P	H	1417	X	-	-	-

2 Entry composition

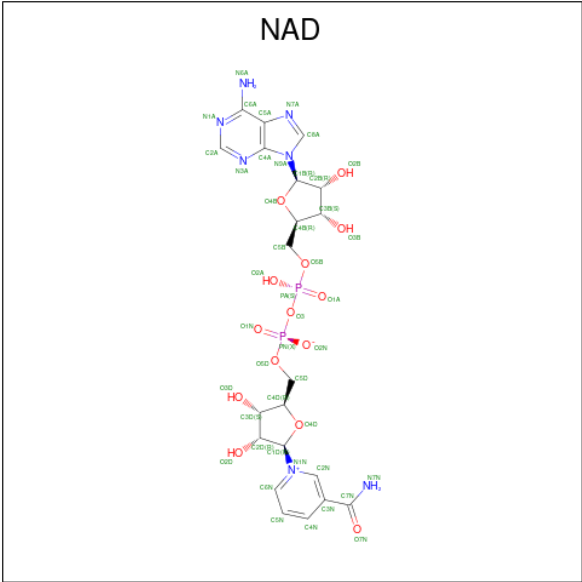
There are 5 unique types of molecules in this entry. The entry contains 27816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-PHOSPHO-BETA-GLUCOSIDASE.

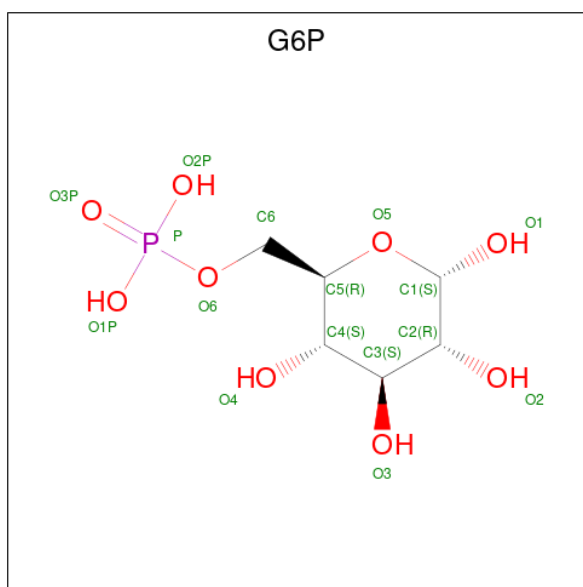
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	10	0	0
			3362	2166	563	624	9			
1	B	409	Total	C	N	O	S	74	0	0
			3318	2139	553	617	9			
1	C	409	Total	C	N	O	S	26	1	0
			3325	2144	553	618	10			
1	D	409	Total	C	N	O	S	51	0	0
			3317	2137	552	619	9			
1	E	406	Total	C	N	O	S	154	0	0
			3294	2124	548	613	9			
1	F	411	Total	C	N	O	S	116	0	0
			3333	2148	555	621	9			
1	G	409	Total	C	N	O	S	77	0	0
			3318	2139	553	617	9			
1	H	407	Total	C	N	O	S	86	0	0
			3300	2127	549	615	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



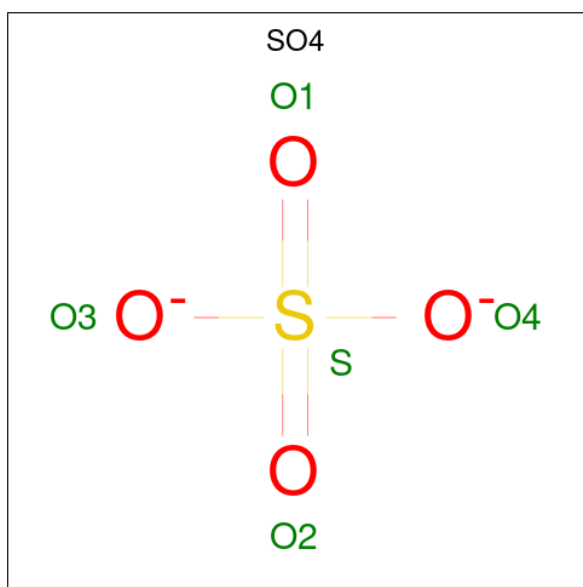
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G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

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	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		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

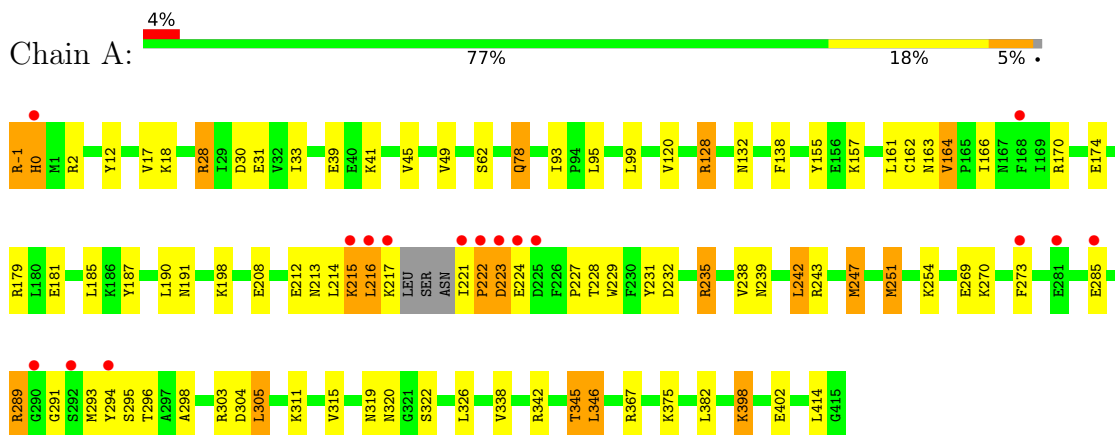
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total	O	0	0
			149	149		
5	B	103	Total	O	0	0
			103	103		
5	C	108	Total	O	0	0
			108	108		
5	D	91	Total	O	0	0
			91	91		
5	E	78	Total	O	0	0
			78	78		
5	F	83	Total	O	0	0
			83	83		
5	G	81	Total	O	0	0
			81	81		
5	H	66	Total	O	0	0
			66	66		

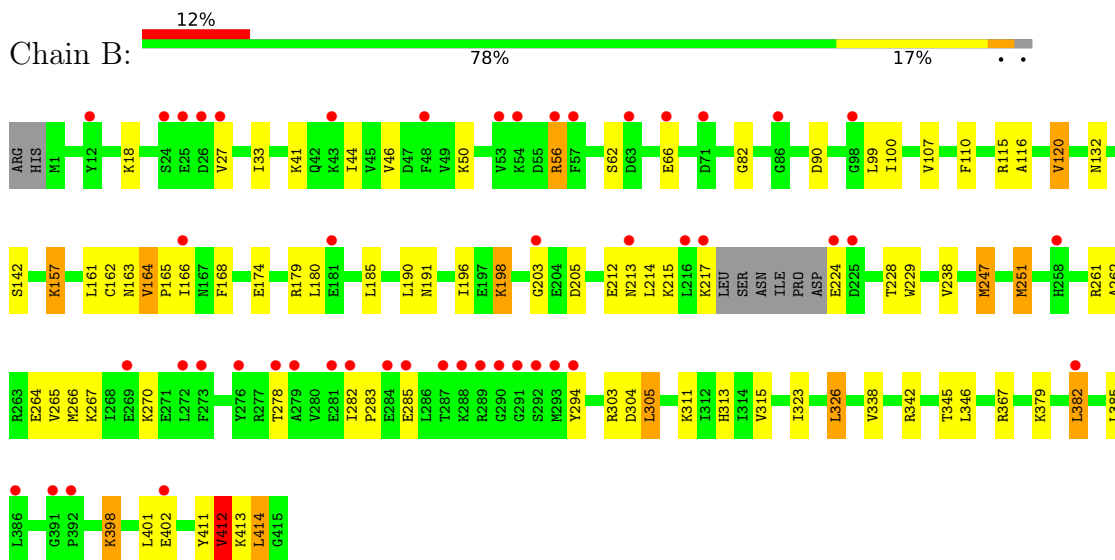
3 Residue-property plots

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.

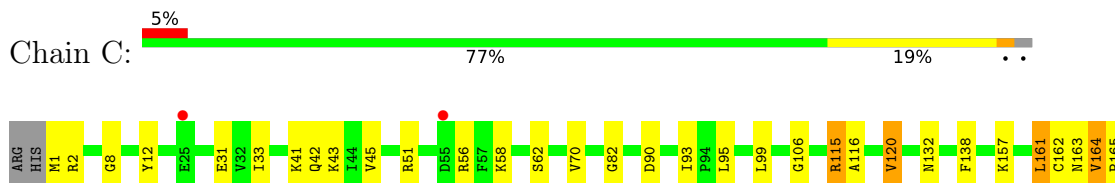
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

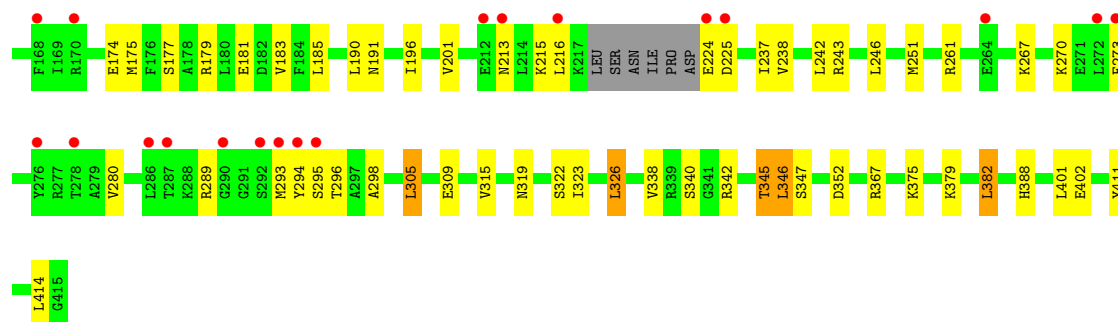


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

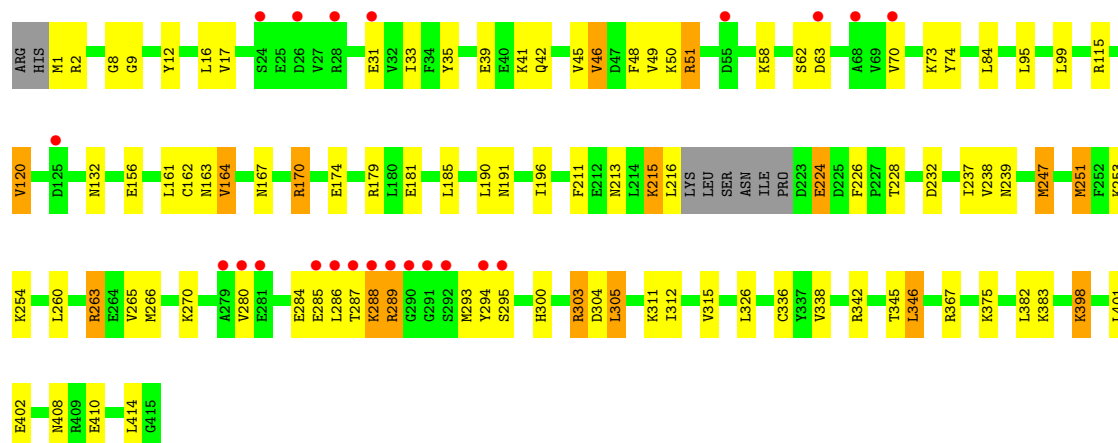
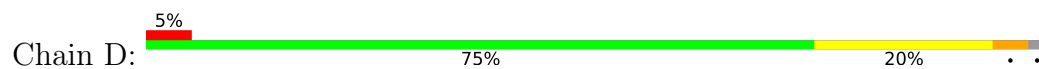


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

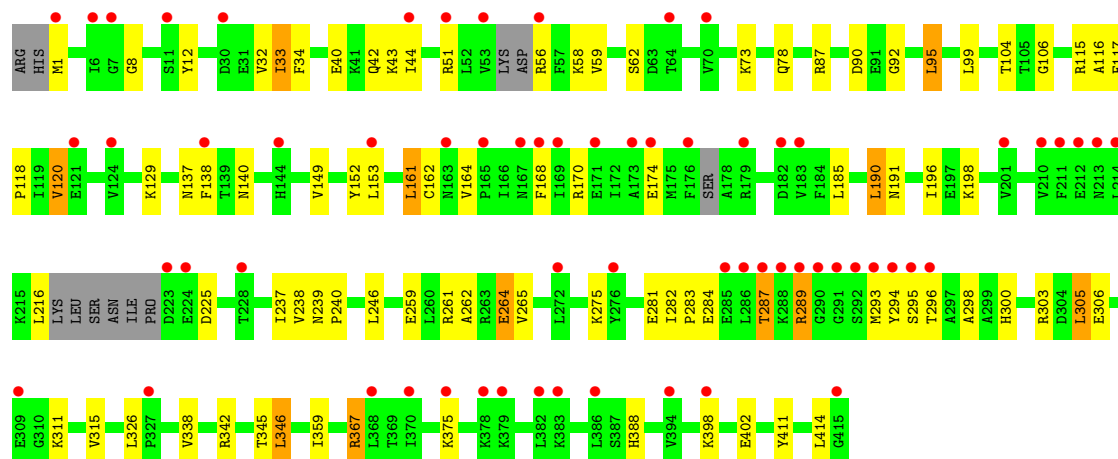
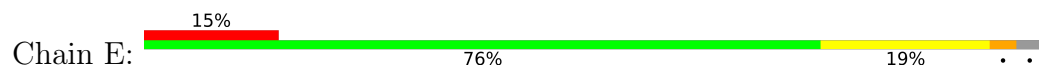




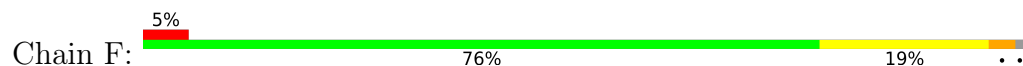
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

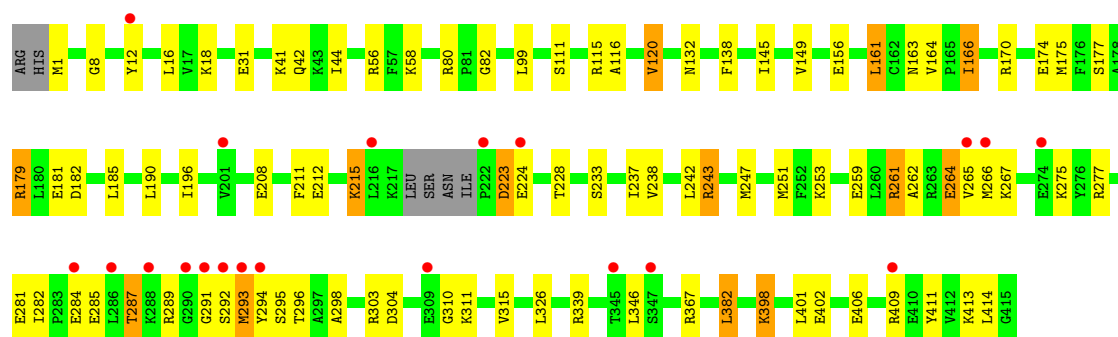


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

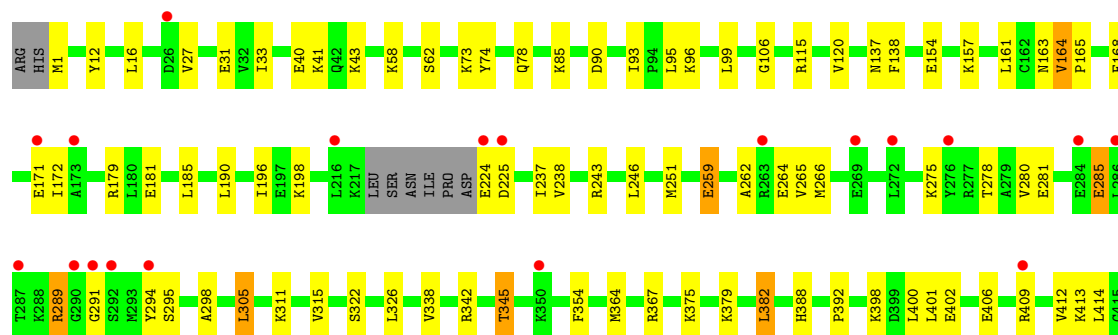
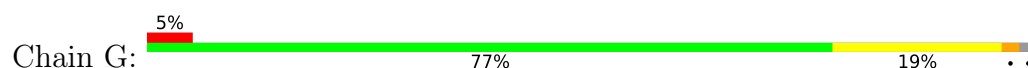


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

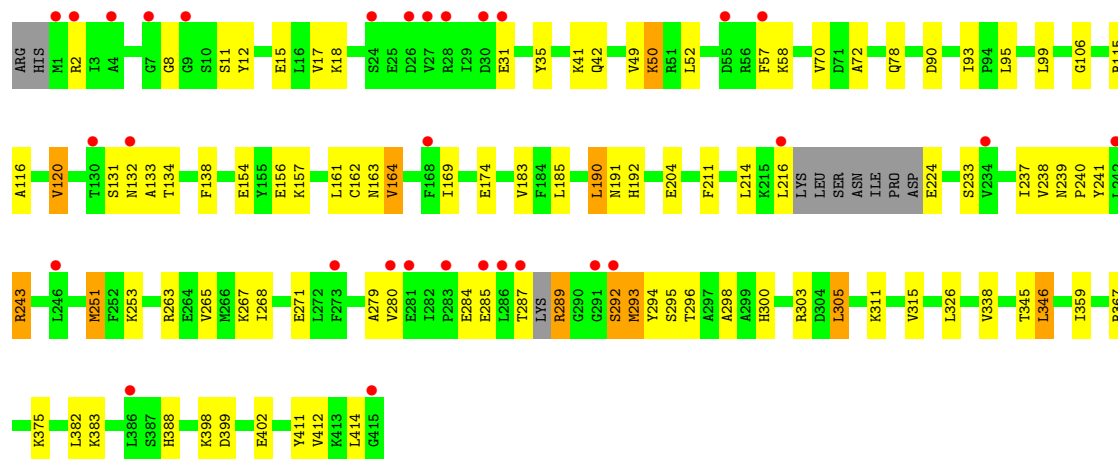
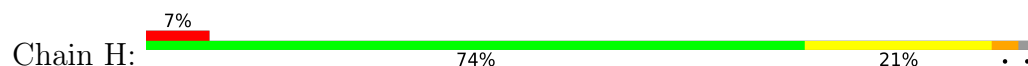




• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.13Å 178.13Å 278.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.96-2.40) 98.1 (19.96-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.240 0.193 , 0.230	Depositor DCC
R_{free} test set	16459 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27816	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.65% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD, G6P

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	0.87	3/3429 (0.1%)	0.99	0/4620
1	B	0.77	3/3383 (0.1%)	0.99	1/4557 (0.0%)
1	C	0.81	4/3391 (0.1%)	0.98	1/4567 (0.0%)
1	D	0.91	7/3382 (0.2%)	1.00	1/4557 (0.0%)
1	E	0.74	4/3357 (0.1%)	0.88	3/4521 (0.1%)
1	F	0.64	0/3399	0.90	1/4579 (0.0%)
1	G	0.71	1/3383 (0.0%)	0.95	1/4557 (0.0%)
1	H	0.70	4/3364 (0.1%)	0.91	0/4532
All	All	0.77	26/27088 (0.1%)	0.95	8/36490 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	ARG	CZ-NH1	21.79	1.63	1.32
1	A	93	ILE	CA-CB	10.91	1.60	1.54
1	D	251	MET	SD-CE	-10.33	1.53	1.79
1	D	51	ARG	NE-CZ	9.48	1.43	1.33
1	E	51	ARG	NE-CZ	9.43	1.43	1.33
1	C	93	ILE	CA-CB	8.98	1.59	1.54
1	E	59	VAL	CA-CB	7.73	1.64	1.54
1	A	247	MET	SD-CE	-7.70	1.60	1.79
1	B	251	MET	SD-CE	-7.43	1.60	1.79
1	D	58	LYS	N-CA	7.15	1.54	1.46
1	A	251	MET	SD-CE	-7.06	1.61	1.79
1	D	46	VAL	N-CA	6.53	1.54	1.46
1	B	100	ILE	CA-CB	6.32	1.61	1.54
1	H	279	ALA	C-O	5.73	1.30	1.23
1	C	70	VAL	CA-CB	5.45	1.60	1.54
1	E	51	ARG	CZ-NH2	5.41	1.40	1.33
1	D	120	VAL	CA-CB	5.38	1.61	1.54
1	B	412	VAL	CA-CB	5.36	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	VAL	CA-CB	5.36	1.57	1.54
1	D	247	MET	SD-CE	-5.28	1.66	1.79
1	D	51	ARG	CD-NE	5.28	1.53	1.46
1	G	93	ILE	CA-CB	5.28	1.57	1.54
1	H	50	LYS	CB-CG	5.25	1.68	1.52
1	H	93	ILE	CA-CB	5.13	1.57	1.54
1	H	251	MET	SD-CE	-5.13	1.66	1.79
1	C	293	MET	SD-CE	5.12	1.92	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ARG	NE-CZ-NH2	-10.92	109.37	119.20
1	E	51	ARG	CD-NE-CZ	-6.73	114.97	124.40
1	B	142	SER	N-CA-C	5.90	117.39	111.07
1	D	70	VAL	N-CA-C	5.87	116.53	110.36
1	C	115	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	F	223	ASP	N-CA-C	-5.25	106.55	113.17
1	E	137	ASN	N-CA-C	5.08	116.80	108.52
1	G	137	ASN	N-CA-C	5.07	116.78	108.52

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	3362	0	3397	56	0
1	B	3318	0	3355	39	0
1	C	3325	0	3363	41	0
1	D	3317	0	3346	54	0
1	E	3294	0	3322	43	0
1	F	3333	0	3367	36	0
1	G	3318	0	3355	32	0
1	H	3300	0	3328	49	0
2	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	1	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	2	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	2	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	149	0	0	2	0
5	B	103	0	0	1	0
5	C	108	0	0	0	0
5	D	91	0	0	1	0
5	E	78	0	0	0	0
5	F	83	0	0	1	0
5	G	81	0	0	1	0
5	H	66	0	0	0	0
All	All	27816	0	27129	326	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 6.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HG2	1:A:235:ARG:HH11	0.97	1.07
1:H:162:CYS:HB2	1:H:191:ASN:ND2	1.80	0.96
1:A:235:ARG:HG2	1:A:235:ARG:NH1	1.76	0.92
1:E:162:CYS:HB2	1:E:191:ASN:HD21	1.34	0.91
1:F:224:GLU:HG2	1:F:251:MET:HE1	1.54	0.91
1:B:398:LYS:O	1:B:402:GLU:HG3	1.72	0.87
1:H:162:CYS:HB2	1:H:191:ASN:HD21	1.34	0.87
1:A:224:GLU:HG2	1:A:251:MET:HE1	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:HD13	1:B:338:VAL:HG13	1.58	0.83
1:A:346:LEU:HD12	1:D:346:LEU:CD1	2.08	0.82
1:D:48:PHE:HA	1:D:51:ARG:CZ	2.10	0.81
1:A:346:LEU:CD1	1:D:346:LEU:CD1	2.59	0.80
1:D:162:CYS:CB	1:D:191:ASN:HD21	1.97	0.77
1:E:346:LEU:HD12	1:H:346:LEU:HD12	1.66	0.77
1:H:162:CYS:CB	1:H:191:ASN:ND2	2.48	0.76
1:H:162:CYS:CB	1:H:191:ASN:HD21	1.99	0.75
1:A:345:THR:HG22	5:A:2106:HOH:O	1.85	0.75
1:C:8:GLY:HA3	1:C:42:GLN:HE21	1.51	0.75
1:B:224:GLU:HG2	1:B:251:MET:HE1	1.69	0.74
1:A:162:CYS:CB	1:A:191:ASN:HD21	2.01	0.74
1:A:235:ARG:HH11	1:A:235:ARG:CG	1.89	0.73
1:A:162:CYS:HB2	1:A:191:ASN:HD21	1.54	0.73
1:G:90:ASP:OD1	1:G:115:ARG:NH2	2.22	0.72
1:E:162:CYS:HB2	1:E:191:ASN:ND2	2.05	0.72
1:D:2:ARG:HG3	1:D:31:GLU:HG3	1.70	0.71
1:G:90:ASP:CG	1:G:115:ARG:HH22	1.98	0.71
1:C:90:ASP:CG	1:C:115:ARG:HH22	1.98	0.71
1:E:33:ILE:HD11	1:E:62:SER:HB2	1.73	0.71
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.54	0.70
1:B:346:LEU:HD23	1:C:346:LEU:HD12	1.73	0.70
1:D:162:CYS:HB2	1:D:191:ASN:HD21	1.56	0.70
1:H:224:GLU:CG	1:H:251:MET:HE1	2.21	0.70
1:F:138:PHE:HZ	1:F:298:ALA:HB2	1.57	0.70
1:H:224:GLU:HG2	1:H:251:MET:HE1	1.73	0.70
1:E:162:CYS:CB	1:E:191:ASN:HD21	2.05	0.69
1:G:224:GLU:HG3	1:G:251:MET:HE1	1.73	0.69
1:C:2:ARG:HG3	1:C:31:GLU:HG3	1.75	0.69
1:D:224:GLU:HG2	1:D:251:MET:HE1	1.72	0.69
1:F:8:GLY:HA3	1:F:42:GLN:HE21	1.58	0.68
1:A:212:GLU:HA	1:A:215:LYS:HD3	1.77	0.67
1:A:295:SER:OG	1:A:296:THR:N	2.26	0.67
1:G:179:ARG:NH1	1:G:181:GLU:OE2	2.28	0.67
1:D:8:GLY:HA3	1:D:42:GLN:HE21	1.60	0.67
1:D:163:ASN:HB3	1:D:294:TYR:CD1	2.30	0.66
1:A:166:ILE:HG12	1:A:293:MET:HE3	1.77	0.66
1:C:90:ASP:OD1	1:C:115:ARG:NH2	2.24	0.66
1:E:346:LEU:CD1	1:H:346:LEU:HD12	2.26	0.66
1:D:48:PHE:HA	1:D:51:ARG:NH2	2.11	0.65
1:E:259:GLU:OE1	1:E:264:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:VAL:O	1:H:131:SER:HB3	1.97	0.64
1:B:247:MET:HE2	1:B:251:MET:HE3	1.78	0.64
1:A:346:LEU:HD12	1:D:346:LEU:HD13	1.78	0.64
1:F:289:ARG:NH2	2:F:1416:NAD:O1N	2.29	0.64
1:D:16:LEU:HA	1:D:295:SER:HB3	1.78	0.64
1:H:138:PHE:HZ	1:H:298:ALA:HB2	1.64	0.63
1:A:179:ARG:NH1	1:A:181:GLU:OE2	2.33	0.62
1:B:90:ASP:OD1	1:B:115:ARG:NH2	2.33	0.61
1:H:90:ASP:OD1	1:H:115:ARG:NH2	2.33	0.61
1:D:162:CYS:CB	1:D:191:ASN:ND2	2.64	0.61
1:E:87:ARG:NH1	1:E:265:VAL:HG21	2.16	0.61
1:H:163:ASN:HB3	1:H:294:TYR:CD1	2.36	0.61
1:A:269:GLU:O	1:A:273:PHE:HD2	1.84	0.60
1:H:296:THR:HG22	1:H:300:HIS:CE1	2.36	0.60
1:E:90:ASP:OD1	1:E:115:ARG:NH2	2.34	0.60
1:B:262:ALA:O	1:B:266:MET:HG3	2.01	0.60
1:E:90:ASP:CG	1:E:115:ARG:HH22	2.10	0.60
1:F:138:PHE:CZ	1:F:298:ALA:HB2	2.35	0.60
1:H:138:PHE:CZ	1:H:298:ALA:HB2	2.36	0.60
1:E:296:THR:HG23	1:E:300:HIS:CE1	2.36	0.60
1:A:215:LYS:HG2	1:A:228:THR:HG23	1.83	0.59
1:E:87:ARG:HD3	1:E:262:ALA:CB	2.32	0.59
1:D:12:TYR:OH	1:D:289:ARG:HB3	2.02	0.59
1:B:164:VAL:HG22	1:B:165:PRO:HD3	1.84	0.59
1:H:17:VAL:HG11	1:H:49:VAL:HG13	1.85	0.59
1:E:87:ARG:HD3	1:E:262:ALA:HB2	1.84	0.59
1:C:163:ASN:HB3	1:C:294:TYR:CD1	2.38	0.59
1:F:12:TYR:OH	1:F:289:ARG:HB3	2.03	0.59
1:D:263:ARG:HD3	5:D:2049:HOH:O	2.01	0.59
1:A:162:CYS:CB	1:A:191:ASN:ND2	2.66	0.59
1:B:162:CYS:HB2	1:B:191:ASN:ND2	2.17	0.59
1:G:259:GLU:OE1	1:G:264:GLU:HG2	2.03	0.59
1:D:33:ILE:HD11	1:D:62:SER:HB2	1.86	0.58
1:E:346:LEU:CD1	1:H:346:LEU:CD1	2.82	0.58
1:B:82:GLY:HA2	1:B:411:TYR:CZ	2.39	0.58
1:B:90:ASP:CG	1:B:115:ARG:HH22	2.11	0.57
1:H:305:LEU:HD13	1:H:338:VAL:HG13	1.86	0.57
1:H:292:SER:O	1:H:293:MET:HB2	2.03	0.57
1:C:305:LEU:HD13	1:C:338:VAL:HG13	1.86	0.57
1:D:48:PHE:HA	1:D:51:ARG:NH1	2.19	0.57
1:D:300:HIS:HD2	1:D:303:ARG:NH2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD13	1:A:338:VAL:HG13	1.85	0.57
1:D:46:VAL:HG12	1:D:50:LYS:HE3	1.87	0.57
1:D:303:ARG:HD2	1:D:304:ASP:OD1	2.05	0.57
1:H:90:ASP:CG	1:H:115:ARG:HH22	2.12	0.56
1:B:56:ARG:HG2	1:B:56:ARG:NH1	2.18	0.56
1:C:319:ASN:O	1:C:345:THR:HG21	2.06	0.56
1:G:33:ILE:HD11	1:G:62:SER:HB2	1.87	0.56
1:A:45:VAL:CG2	1:A:273:PHE:HE1	2.18	0.56
1:C:322:SER:HB2	1:C:345:THR:HG23	1.87	0.56
1:H:240:PRO:O	1:H:243:ARG:HG2	2.06	0.55
1:D:164:VAL:HG21	1:D:239:ASN:ND2	2.22	0.55
1:E:170:ARG:O	1:E:174:GLU:HG3	2.06	0.55
1:C:382:LEU:HD13	1:C:401:LEU:HD22	1.89	0.55
1:E:116:ALA:O	1:E:120:VAL:HG13	2.07	0.55
1:F:82:GLY:HA3	1:F:115:ARG:HD3	1.89	0.55
1:B:305:LEU:HD13	1:B:338:VAL:CG1	2.35	0.54
1:C:179:ARG:NH1	1:C:181:GLU:OE2	2.39	0.54
1:F:262:ALA:O	1:F:266:MET:HG3	2.07	0.54
1:D:305:LEU:HD13	1:D:338:VAL:HG13	1.90	0.54
1:C:224:GLU:HG3	1:C:251:MET:HE1	1.89	0.54
1:C:295:SER:OG	1:C:296:THR:N	2.40	0.54
1:B:132:ASN:O	1:B:157:LYS:NZ	2.42	0.53
1:H:12:TYR:OH	1:H:289:ARG:HB3	2.07	0.53
1:C:175:MET:HE2	1:C:213:ASN:HD22	1.73	0.53
1:A:17:VAL:HG11	1:A:49:VAL:HG13	1.91	0.53
1:F:382:LEU:HD13	1:F:401:LEU:HD22	1.90	0.53
1:C:382:LEU:HD13	1:C:401:LEU:CD2	2.38	0.53
1:D:224:GLU:OE2	1:D:254:LYS:HE3	2.09	0.53
1:D:35:TYR:C	1:D:42:GLN:HE22	2.17	0.53
1:G:305:LEU:HD13	1:G:338:VAL:HG13	1.91	0.53
1:D:294:TYR:HE1	3:D:1417:G6P:H3	1.73	0.53
1:D:382:LEU:HD21	1:D:398:LYS:HA	1.90	0.53
1:E:8:GLY:HA3	1:E:42:GLN:HE21	1.73	0.53
1:F:224:GLU:HB3	1:F:243:ARG:HH11	1.74	0.52
1:F:80:ARG:NH2	2:F:1416:NAD:O1N	2.40	0.52
1:F:292:SER:O	1:F:293:MET:HB2	2.09	0.52
1:F:163:ASN:HB3	1:F:294:TYR:CD1	2.45	0.52
1:H:240:PRO:O	1:H:243:ARG:CG	2.58	0.52
1:H:268:ILE:HG21	1:H:289:ARG:HG2	1.92	0.52
1:F:82:GLY:HA2	1:F:411:TYR:CZ	2.45	0.52
1:G:73:LYS:HG2	1:G:74:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	1:A:304:ASP:OD1	2.10	0.51
1:F:211:PHE:O	1:F:215:LYS:HD2	2.09	0.51
1:A:398:LYS:HD2	1:B:229:TRP:CD1	2.45	0.51
1:E:78:GLN:HG2	1:E:78:GLN:O	2.10	0.51
1:F:179:ARG:NH2	1:F:181:GLU:OE2	2.44	0.51
1:H:78:GLN:O	1:H:78:GLN:HG2	2.11	0.51
1:D:179:ARG:HH12	1:D:181:GLU:CD	2.19	0.51
1:G:1:MET:N	5:G:2001:HOH:O	2.43	0.51
1:A:319:ASN:O	1:A:345:THR:HG21	2.10	0.51
1:E:115:ARG:HG2	1:E:411:TYR:CB	2.41	0.51
1:G:168:PHE:CZ	1:G:172:ILE:HD11	2.46	0.50
1:G:16:LEU:HD22	1:G:78:GLN:OE1	2.11	0.50
1:A:162:CYS:HB2	1:A:191:ASN:ND2	2.24	0.50
1:C:12:TYR:OH	1:C:289:ARG:HB3	2.12	0.50
1:G:16:LEU:HA	1:G:295:SER:HB2	1.93	0.50
1:C:162:CYS:HB2	1:C:191:ASN:ND2	2.27	0.50
1:E:12:TYR:OH	1:E:289:ARG:HB3	2.12	0.50
1:A:346:LEU:HD12	1:D:346:LEU:HD12	1.92	0.50
1:A:346:LEU:CD1	1:D:346:LEU:HD11	2.40	0.49
1:B:323:ILE:HG21	1:B:326:LEU:HD22	1.94	0.49
1:F:196:ILE:HB	1:F:237:ILE:HB	1.94	0.49
1:F:262:ALA:O	1:F:265:VAL:HG22	2.13	0.49
1:F:303:ARG:HD2	1:F:304:ASP:OD1	2.13	0.49
1:E:346:LEU:HD12	1:H:346:LEU:CD1	2.41	0.49
1:F:224:GLU:OE1	1:F:243:ARG:NH1	2.45	0.49
1:H:72:ALA:O	1:H:133:ALA:HB2	2.12	0.49
1:B:412:VAL:HG23	1:B:414:LEU:HD13	1.94	0.49
1:C:305:LEU:HD13	1:C:338:VAL:CG1	2.42	0.49
1:E:190:LEU:HD13	1:E:359:ILE:HG23	1.93	0.49
1:A:2:ARG:HG3	1:A:31:GLU:HG3	1.94	0.49
1:A:208:GLU:OE2	1:A:235:ARG:NH2	2.45	0.49
1:E:305:LEU:HD13	1:E:338:VAL:HG13	1.94	0.49
1:F:224:GLU:O	1:F:243:ARG:HD2	2.12	0.49
1:H:294:TYR:HE1	3:H:1417:G6P:H3	1.77	0.49
1:A:45:VAL:CG2	1:A:273:PHE:CE1	2.96	0.48
1:B:198:LYS:NZ	1:B:205:ASP:OD2	2.46	0.48
1:B:46:VAL:O	1:B:50:LYS:HG3	2.13	0.48
1:E:117:PHE:N	1:E:118:PRO:HD2	2.28	0.48
1:A:224:GLU:OE2	1:A:254:LYS:HE3	2.13	0.48
1:C:183:VAL:HG22	1:C:201:VAL:HG22	1.95	0.48
1:G:406:GLU:OE1	1:G:406:GLU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:GLU:O	1:F:287:THR:OG1	2.31	0.48
1:D:287:THR:C	1:D:289:ARG:H	2.20	0.48
1:A:322:SER:HB2	1:A:345:THR:HG23	1.96	0.48
1:B:66:GLU:HB2	5:B:2008:HOH:O	2.13	0.48
1:A:138:PHE:CZ	1:A:298:ALA:HB2	2.48	0.48
1:F:243:ARG:HG2	1:F:247:MET:HE2	1.95	0.48
1:F:295:SER:OG	1:F:296:THR:N	2.45	0.48
1:H:164:VAL:HG11	1:H:239:ASN:HD21	1.79	0.48
1:C:164:VAL:HB	1:C:165:PRO:HD3	1.96	0.48
1:B:168:PHE:CE2	1:B:196:ILE:HD13	2.49	0.48
1:A:291:GLY:O	1:A:294:TYR:HD1	1.96	0.47
1:H:190:LEU:HD13	1:H:359:ILE:HG23	1.95	0.47
1:C:33:ILE:HD11	1:C:62:SER:HB2	1.96	0.47
1:D:287:THR:C	1:D:289:ARG:N	2.72	0.47
1:G:291:GLY:O	1:G:294:TYR:HD2	1.97	0.47
1:F:310:GLY:HA2	1:F:339:ARG:HB2	1.96	0.47
1:C:41:LYS:HE2	1:C:273:PHE:CZ	2.49	0.47
1:E:162:CYS:CB	1:E:191:ASN:ND2	2.73	0.47
1:E:346:LEU:HD11	1:H:346:LEU:CD1	2.45	0.47
1:H:8:GLY:HA3	1:H:42:GLN:HE21	1.80	0.47
1:C:116:ALA:O	1:C:120:VAL:HG13	2.15	0.47
1:C:31:GLU:HB3	1:C:58:LYS:HB2	1.97	0.46
1:G:382:LEU:HD13	1:G:401:LEU:HD22	1.97	0.46
1:G:379:LYS:HB3	1:H:233:SER:HA	1.97	0.46
1:H:35:TYR:C	1:H:42:GLN:HE22	2.23	0.46
1:E:104:THR:HG22	1:E:140:ASN:HB3	1.96	0.46
1:A:164:VAL:HG21	1:A:239:ASN:ND2	2.31	0.46
1:D:162:CYS:HB2	1:D:191:ASN:ND2	2.25	0.46
1:A:320:ASN:ND2	5:A:2107:HOH:O	2.49	0.46
1:E:152:TYR:OH	1:E:367:ARG:HD2	2.14	0.46
1:A:78:GLN:CG	1:A:78:GLN:O	2.64	0.46
1:C:224:GLU:OE2	1:C:243:ARG:NH1	2.48	0.46
1:F:145:ILE:O	1:F:149:VAL:HG23	2.15	0.46
1:D:115:ARG:HD3	1:D:408:ASN:OD1	2.16	0.46
1:E:73:LYS:NZ	1:E:306:GLU:OE2	2.38	0.46
1:F:295:SER:HB3	5:F:2041:HOH:O	2.15	0.46
1:G:196:ILE:HB	1:G:237:ILE:HB	1.98	0.45
1:G:224:GLU:OE2	1:G:243:ARG:NH1	2.49	0.45
1:B:304:ASP:OD2	1:B:313:HIS:NE2	2.42	0.45
1:B:162:CYS:SG	1:B:191:ASN:ND2	2.90	0.45
1:D:398:LYS:HE3	1:D:398:LYS:HB2	1.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:LEU:HD12	1:F:161:LEU:HA	1.74	0.45
1:H:116:ALA:O	1:H:120:VAL:HG13	2.17	0.45
1:E:168:PHE:CE2	1:E:196:ILE:HD13	2.52	0.45
1:B:163:ASN:HB3	1:B:294:TYR:CD2	2.52	0.45
1:D:16:LEU:CA	1:D:295:SER:HB3	2.46	0.45
1:A:33:ILE:HD11	1:A:62:SER:HB2	1.99	0.45
1:B:285:GLU:O	1:B:285:GLU:HG3	2.16	0.45
1:F:382:LEU:HD21	1:F:398:LYS:HG3	1.99	0.45
1:G:12:TYR:OH	1:G:289:ARG:HB3	2.16	0.45
1:G:224:GLU:CG	1:G:251:MET:HE1	2.42	0.45
1:A:346:LEU:HD11	1:D:346:LEU:HD11	1.97	0.45
1:B:346:LEU:CD2	1:C:346:LEU:HD12	2.46	0.45
1:D:294:TYR:CE1	3:D:1417:G6P:H3	2.52	0.45
1:E:32:VAL:HG12	1:E:34:PHE:CE1	2.51	0.45
1:A:216:LEU:O	1:A:217:LYS:O	2.34	0.44
1:C:106:GLY:HA2	1:C:388:HIS:CE1	2.52	0.44
1:G:285:GLU:O	1:G:285:GLU:HG3	2.17	0.44
1:C:138:PHE:CZ	1:C:298:ALA:HB2	2.53	0.44
1:A:0:HIS:HA	1:A:30:ASP:OD2	2.18	0.44
1:H:57:PHE:CD1	1:H:57:PHE:C	2.95	0.44
1:A:238:VAL:HG22	1:A:242:LEU:HD23	2.00	0.44
1:B:346:LEU:HD23	1:C:346:LEU:CD1	2.46	0.44
1:D:73:LYS:HG2	1:D:74:TYR:CE2	2.52	0.44
1:B:116:ALA:O	1:B:120:VAL:HG13	2.18	0.44
1:D:226:PHE:CD1	1:D:247:MET:HE3	2.53	0.44
1:A:222:PRO:C	1:A:224:GLU:H	2.26	0.44
1:A:285:GLU:O	1:A:285:GLU:CG	2.65	0.44
1:D:284:GLU:C	1:D:286:LEU:H	2.26	0.44
1:B:346:LEU:CD2	1:C:346:LEU:CD1	2.95	0.43
1:H:106:GLY:HA2	1:H:388:HIS:CE1	2.53	0.43
1:A:-1:ARG:HD3	1:A:28:ARG:HD3	1.99	0.43
1:B:33:ILE:HD11	1:B:62:SER:HB2	2.01	0.43
1:G:164:VAL:N	1:G:165:PRO:CD	2.81	0.43
1:H:115:ARG:HG2	1:H:411:TYR:HB3	2.00	0.43
1:H:211:PHE:CE1	1:H:237:ILE:HG13	2.53	0.43
1:C:352:ASP:OD2	1:D:383:LYS:NZ	2.45	0.43
1:E:282:ILE:HA	1:E:283:PRO:HD3	1.89	0.43
1:D:211:PHE:O	1:D:215:LYS:HD2	2.19	0.43
1:D:84:LEU:HB2	1:D:266:MET:HE2	2.00	0.43
1:H:11:SER:OG	1:H:289:ARG:NH1	2.51	0.43
1:E:138:PHE:CZ	1:E:298:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:CYS:SG	1:H:164:VAL:HG12	2.59	0.43
1:D:196:ILE:HB	1:D:237:ILE:HB	2.01	0.43
1:F:179:ARG:HG2	1:F:182:ASP:OD2	2.18	0.43
1:A:138:PHE:HZ	1:A:298:ALA:HB2	1.84	0.43
1:D:17:VAL:HG11	1:D:49:VAL:HG13	2.01	0.43
1:E:284:GLU:O	1:E:287:THR:OG1	2.34	0.43
1:G:392:PRO:HG3	1:G:400:LEU:HD23	2.00	0.43
1:C:196:ILE:HB	1:C:237:ILE:HB	1.99	0.43
1:B:107:VAL:O	1:B:110:PHE:HB3	2.19	0.42
1:E:261:ARG:HA	1:E:264:GLU:HG3	2.01	0.42
1:G:163:ASN:HB3	1:G:294:TYR:CD2	2.53	0.42
1:H:169:ILE:HG23	1:H:183:VAL:HB	2.01	0.42
1:A:163:ASN:HB3	1:A:294:TYR:CD1	2.54	0.42
1:E:296:THR:CG2	1:E:300:HIS:CE1	3.02	0.42
1:F:116:ALA:O	1:F:120:VAL:HG13	2.20	0.42
1:E:149:VAL:HG22	1:E:153:LEU:HD12	2.02	0.42
1:B:382:LEU:HD13	1:B:401:LEU:HD22	2.02	0.42
1:B:215:LYS:HD3	1:B:228:THR:HG23	2.00	0.42
1:A:214:LEU:HD23	1:A:231:TYR:CZ	2.55	0.42
1:A:285:GLU:O	1:A:285:GLU:HG3	2.20	0.42
1:D:167:ASN:OD1	1:D:170:ARG:NH2	2.53	0.42
1:G:364:MET:HE2	1:G:364:MET:HA	2.02	0.42
1:H:305:LEU:HD13	1:H:338:VAL:CG1	2.49	0.42
1:B:282:ILE:HA	1:B:283:PRO:HD3	1.86	0.42
1:E:78:GLN:HG3	2:E:1416:NAD:N7N	2.35	0.42
1:H:192:HIS:CD2	1:H:241:TYR:CE2	3.07	0.42
1:A:346:LEU:CD1	1:D:346:LEU:HD12	2.48	0.42
1:A:224:GLU:OE1	1:A:243:ARG:NH1	2.53	0.42
1:D:48:PHE:HB2	1:D:51:ARG:HH22	1.85	0.42
1:E:161:LEU:HD12	1:E:161:LEU:HA	1.90	0.42
1:A:128:ARG:HB2	1:A:155:TYR:CE1	2.55	0.42
1:C:379:LYS:HE3	1:D:232:ASP:HB3	2.02	0.41
1:B:215:LYS:HG2	1:B:228:THR:HG23	2.01	0.41
1:E:92:GLY:HA2	1:E:95:LEU:HD22	2.01	0.41
1:G:31:GLU:HB3	1:G:58:LYS:HB2	2.02	0.41
1:H:162:CYS:SG	1:H:163:ASN:N	2.93	0.41
1:B:203:GLY:HA3	1:C:340:SER:HB3	2.02	0.41
1:E:239:ASN:OD1	1:E:240:PRO:HD2	2.20	0.41
1:A:12:TYR:OH	1:A:289:ARG:HB3	2.21	0.41
1:A:187:TYR:CD1	1:A:187:TYR:C	2.98	0.41
1:C:323:ILE:HG21	1:C:326:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:GLY:HA2	1:E:388:HIS:CE1	2.55	0.41
1:F:291:GLY:O	1:F:294:TYR:HD1	2.02	0.41
1:G:106:GLY:HA2	1:G:388:HIS:CE1	2.55	0.41
1:B:261:ARG:HA	1:B:264:GLU:HG3	2.03	0.41
1:C:45:VAL:CG2	1:C:273:PHE:CE1	3.03	0.41
1:H:2:ARG:HG3	1:H:31:GLU:HG3	2.02	0.41
1:G:354:PHE:HB2	1:H:383:LYS:HE2	2.02	0.41
1:A:232:ASP:HB3	1:B:379:LYS:HE2	2.03	0.41
1:D:305:LEU:HD13	1:D:338:VAL:CG1	2.51	0.41
1:E:196:ILE:HB	1:E:237:ILE:HB	2.02	0.41
1:F:166:ILE:HD13	1:F:293:MET:SD	2.61	0.41
1:G:322:SER:HB2	1:G:345:THR:HG23	2.02	0.41
1:D:9:GLY:HA2	1:D:45:VAL:HG21	2.03	0.41
1:F:409:ARG:HE	1:F:409:ARG:HB2	1.56	0.41
1:G:138:PHE:CZ	1:G:298:ALA:HB2	2.56	0.41
1:H:134:THR:HA	1:H:157:LYS:HB3	2.01	0.41
1:H:294:TYR:CE1	3:H:1417:G6P:H3	2.55	0.41
1:A:227:PRO:HG2	1:A:229:TRP:CE2	2.56	0.40
1:C:162:CYS:HB2	1:C:191:ASN:HD21	1.86	0.40
1:C:224:GLU:CG	1:C:251:MET:HE1	2.51	0.40
1:A:224:GLU:HA	1:A:247:MET:HE1	2.04	0.40
1:C:82:GLY:HA2	1:C:411:TYR:CZ	2.56	0.40
1:D:312:ILE:HA	1:D:336:CYS:O	2.21	0.40
1:G:262:ALA:O	1:G:266:MET:HG3	2.21	0.40
1:C:82:GLY:HA3	1:C:115:ARG:HD3	2.04	0.40
1:D:260:LEU:O	1:D:263:ARG:HB2	2.22	0.40
1:F:16:LEU:HA	1:F:295:SER:HB2	2.02	0.40
1:G:379:LYS:O	1:H:233:SER:HB3	2.22	0.40
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.96	0.40
1:D:382:LEU:HG	1:D:401:LEU:HD22	2.04	0.40
1:F:261:ARG:HA	1:F:264:GLU:HG3	2.01	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	410/417 (98%)	402 (98%)	6 (2%)	2 (0%)	24	37
1	B	405/417 (97%)	400 (99%)	5 (1%)	0	100	100
1	C	406/417 (97%)	399 (98%)	7 (2%)	0	100	100
1	D	405/417 (97%)	397 (98%)	6 (2%)	2 (0%)	24	37
1	E	398/417 (95%)	392 (98%)	6 (2%)	0	100	100
1	F	407/417 (98%)	399 (98%)	8 (2%)	0	100	100
1	G	405/417 (97%)	397 (98%)	8 (2%)	0	100	100
1	H	401/417 (96%)	391 (98%)	10 (2%)	0	100	100
All	All	3237/3336 (97%)	3177 (98%)	56 (2%)	4 (0%)	48	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO
1	A	223	ASP
1	D	288	LYS
1	D	285	GLU

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	366/369 (99%)	324 (88%)	42 (12%)	5	8
1	B	361/369 (98%)	320 (89%)	41 (11%)	5	8
1	C	362/369 (98%)	325 (90%)	37 (10%)	7	11
1	D	361/369 (98%)	318 (88%)	43 (12%)	5	7
1	E	358/369 (97%)	317 (88%)	41 (12%)	5	8
1	F	363/369 (98%)	309 (85%)	54 (15%)	3	3
1	G	361/369 (98%)	318 (88%)	43 (12%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	359/369 (97%)	309 (86%)	50 (14%)	3	4
All	All	2891/2952 (98%)	2540 (88%)	351 (12%)	5	7

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	0	HIS
1	A	18	LYS
1	A	28	ARG
1	A	39	GLU
1	A	41	LYS
1	A	78	GLN
1	A	95	LEU
1	A	99	LEU
1	A	120	VAL
1	A	128	ARG
1	A	132	ASN
1	A	157	LYS
1	A	161	LEU
1	A	164	VAL
1	A	170	ARG
1	A	174	GLU
1	A	185	LEU
1	A	190	LEU
1	A	198	LYS
1	A	213	ASN
1	A	215	LYS
1	A	216	LEU
1	A	221	ILE
1	A	223	ASP
1	A	235	ARG
1	A	242	LEU
1	A	270	LYS
1	A	289	ARG
1	A	305	LEU
1	A	311	LYS
1	A	315	VAL
1	A	326	LEU
1	A	342	ARG
1	A	345	THR
1	A	346	LEU

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Mol	Chain	Res	Type
1	A	367	ARG
1	A	375	LYS
1	A	382	LEU
1	A	398	LYS
1	A	402	GLU
1	A	414	LEU
1	B	18	LYS
1	B	27	VAL
1	B	41	LYS
1	B	44	ILE
1	B	56	ARG
1	B	99	LEU
1	B	120	VAL
1	B	157	LYS
1	B	161	LEU
1	B	164	VAL
1	B	166	ILE
1	B	174	GLU
1	B	179	ARG
1	B	180	LEU
1	B	185	LEU
1	B	190	LEU
1	B	198	LYS
1	B	212	GLU
1	B	213	ASN
1	B	214	LEU
1	B	217	LYS
1	B	238	VAL
1	B	247	MET
1	B	265	VAL
1	B	267	LYS
1	B	270	LYS
1	B	278	THR
1	B	303	ARG
1	B	305	LEU
1	B	311	LYS
1	B	315	VAL
1	B	326	LEU
1	B	342	ARG
1	B	345	THR
1	B	367	ARG
1	B	382	LEU

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Mol	Chain	Res	Type
1	B	385	LEU
1	B	398	LYS
1	B	412	VAL
1	B	413	LYS
1	B	414	LEU
1	C	1	MET
1	C	43	LYS
1	C	51	ARG
1	C	56	ARG
1	C	95	LEU
1	C	99	LEU
1	C	120	VAL
1	C	132	ASN
1	C	157	LYS
1	C	161	LEU
1	C	174	GLU
1	C	177	SER
1	C	185	LEU
1	C	190	LEU
1	C	215	LYS
1	C	216	LEU
1	C	225	ASP
1	C	238	VAL
1	C	242	LEU
1	C	246	LEU
1	C	261	ARG
1	C	267	LYS
1	C	270	LYS
1	C	280	VAL
1	C	305	LEU
1	C	309	GLU
1	C	315	VAL
1	C	326	LEU
1	C	342	ARG
1	C	345	THR
1	C	346	LEU
1	C	347	SER
1	C	367	ARG
1	C	375	LYS
1	C	382	LEU
1	C	402	GLU
1	C	414	LEU

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Mol	Chain	Res	Type
1	D	1	MET
1	D	39	GLU
1	D	41	LYS
1	D	63	ASP
1	D	95	LEU
1	D	99	LEU
1	D	120	VAL
1	D	132	ASN
1	D	156	GLU
1	D	161	LEU
1	D	164	VAL
1	D	170	ARG
1	D	174	GLU
1	D	185	LEU
1	D	190	LEU
1	D	213	ASN
1	D	215	LYS
1	D	216	LEU
1	D	224	GLU
1	D	228	THR
1	D	238	VAL
1	D	253	LYS
1	D	263	ARG
1	D	265	VAL
1	D	270	LYS
1	D	280	VAL
1	D	288	LYS
1	D	289	ARG
1	D	293	MET
1	D	303	ARG
1	D	305	LEU
1	D	311	LYS
1	D	315	VAL
1	D	326	LEU
1	D	342	ARG
1	D	345	THR
1	D	346	LEU
1	D	367	ARG
1	D	375	LYS
1	D	398	LYS
1	D	402	GLU
1	D	410	GLU

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Mol	Chain	Res	Type
1	D	414	LEU
1	E	1	MET
1	E	33	ILE
1	E	40	GLU
1	E	43	LYS
1	E	44	ILE
1	E	56	ARG
1	E	58	LYS
1	E	95	LEU
1	E	99	LEU
1	E	120	VAL
1	E	129	LYS
1	E	161	LEU
1	E	164	VAL
1	E	185	LEU
1	E	190	LEU
1	E	198	LYS
1	E	216	LEU
1	E	225	ASP
1	E	238	VAL
1	E	246	LEU
1	E	264	GLU
1	E	275	LYS
1	E	281	GLU
1	E	287	THR
1	E	289	ARG
1	E	293	MET
1	E	294	TYR
1	E	295	SER
1	E	303	ARG
1	E	305	LEU
1	E	311	LYS
1	E	315	VAL
1	E	326	LEU
1	E	342	ARG
1	E	345	THR
1	E	346	LEU
1	E	367	ARG
1	E	375	LYS
1	E	398	LYS
1	E	402	GLU
1	E	414	LEU

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Mol	Chain	Res	Type
1	F	1	MET
1	F	18	LYS
1	F	31	GLU
1	F	41	LYS
1	F	44	ILE
1	F	56	ARG
1	F	58	LYS
1	F	99	LEU
1	F	111	SER
1	F	120	VAL
1	F	132	ASN
1	F	156	GLU
1	F	161	LEU
1	F	164	VAL
1	F	166	ILE
1	F	170	ARG
1	F	174	GLU
1	F	175	MET
1	F	177	SER
1	F	179	ARG
1	F	185	LEU
1	F	190	LEU
1	F	208	GLU
1	F	212	GLU
1	F	215	LYS
1	F	223	ASP
1	F	228	THR
1	F	233	SER
1	F	238	VAL
1	F	242	LEU
1	F	243	ARG
1	F	253	LYS
1	F	259	GLU
1	F	261	ARG
1	F	264	GLU
1	F	267	LYS
1	F	275	LYS
1	F	277	ARG
1	F	281	GLU
1	F	282	ILE
1	F	285	GLU
1	F	287	THR

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Mol	Chain	Res	Type
1	F	293	MET
1	F	311	LYS
1	F	315	VAL
1	F	326	LEU
1	F	346	LEU
1	F	367	ARG
1	F	382	LEU
1	F	398	LYS
1	F	402	GLU
1	F	406	GLU
1	F	413	LYS
1	F	414	LEU
1	G	27	VAL
1	G	40	GLU
1	G	41	LYS
1	G	43	LYS
1	G	85	LYS
1	G	95	LEU
1	G	96	LYS
1	G	99	LEU
1	G	120	VAL
1	G	154	GLU
1	G	157	LYS
1	G	161	LEU
1	G	164	VAL
1	G	171	GLU
1	G	185	LEU
1	G	190	LEU
1	G	198	LYS
1	G	225	ASP
1	G	238	VAL
1	G	246	LEU
1	G	259	GLU
1	G	265	VAL
1	G	275	LYS
1	G	278	THR
1	G	280	VAL
1	G	281	GLU
1	G	285	GLU
1	G	289	ARG
1	G	305	LEU
1	G	311	LYS

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Mol	Chain	Res	Type
1	G	315	VAL
1	G	326	LEU
1	G	342	ARG
1	G	345	THR
1	G	367	ARG
1	G	375	LYS
1	G	382	LEU
1	G	398	LYS
1	G	402	GLU
1	G	409	ARG
1	G	412	VAL
1	G	413	LYS
1	G	414	LEU
1	H	15	GLU
1	H	18	LYS
1	H	41	LYS
1	H	50	LYS
1	H	52	LEU
1	H	58	LYS
1	H	95	LEU
1	H	99	LEU
1	H	120	VAL
1	H	132	ASN
1	H	154	GLU
1	H	156	GLU
1	H	161	LEU
1	H	164	VAL
1	H	174	GLU
1	H	185	LEU
1	H	190	LEU
1	H	204	GLU
1	H	214	LEU
1	H	216	LEU
1	H	238	VAL
1	H	243	ARG
1	H	253	LYS
1	H	263	ARG
1	H	265	VAL
1	H	267	LYS
1	H	271	GLU
1	H	280	VAL
1	H	284	GLU

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Mol	Chain	Res	Type
1	H	285	GLU
1	H	287	THR
1	H	289	ARG
1	H	292	SER
1	H	293	MET
1	H	295	SER
1	H	303	ARG
1	H	305	LEU
1	H	311	LYS
1	H	315	VAL
1	H	326	LEU
1	H	345	THR
1	H	346	LEU
1	H	367	ARG
1	H	375	LYS
1	H	382	LEU
1	H	398	LYS
1	H	399	ASP
1	H	402	GLU
1	H	412	VAL
1	H	414	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	191	ASN
1	A	320	ASN
1	B	132	ASN
1	B	213	ASN
1	B	320	ASN
1	C	42	GLN
1	C	191	ASN
1	C	213	ASN
1	C	320	ASN
1	D	42	GLN
1	D	191	ASN
1	D	300	HIS
1	D	320	ASN
1	E	42	GLN
1	E	78	GLN
1	E	191	ASN

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Mol	Chain	Res	Type
1	E	300	HIS
1	E	320	ASN
1	F	42	GLN
1	F	213	ASN
1	F	320	ASN
1	G	132	ASN
1	G	320	ASN
1	H	42	GLN
1	H	213	ASN
1	H	300	HIS
1	H	320	ASN
1	H	344	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
3	G6P	F	1417	-	16,16,16	0.51	0	23,24,24	1.01	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	1416	-	46,48,48	1.82	5 (10%)	64,73,73	1.61	9 (14%)
2	NAD	H	1416	-	46,48,48	1.65	3 (6%)	64,73,73	1.49	7 (10%)
3	G6P	G	1417	-	16,16,16	0.64	0	23,24,24	0.94	1 (4%)
3	G6P	A	1417	-	16,16,16	0.72	0	23,24,24	1.21	2 (8%)
3	G6P	C	1417	-	16,16,16	0.70	0	23,24,24	1.11	1 (4%)
4	SO4	A	1418	-	4,4,4	0.47	0	6,6,6	0.56	0
2	NAD	A	1416	-	46,48,48	1.82	8 (17%)	64,73,73	1.80	13 (20%)
2	NAD	F	1416	-	46,48,48	1.75	5 (10%)	64,73,73	1.56	8 (12%)
2	NAD	G	1416	-	46,48,48	1.80	4 (8%)	64,73,73	1.61	12 (18%)
4	SO4	C	1418	-	4,4,4	0.69	0	6,6,6	0.36	0
3	G6P	D	1417	-	16,16,16	0.45	0	23,24,24	0.94	1 (4%)
2	NAD	C	1416	-	46,48,48	1.74	4 (8%)	64,73,73	1.70	11 (17%)
3	G6P	H	1417	-	16,16,16	0.46	0	23,24,24	1.02	1 (4%)
3	G6P	E	1417	-	16,16,16	0.56	0	23,24,24	0.81	0
2	NAD	B	1416	-	46,48,48	1.87	7 (15%)	64,73,73	1.59	9 (14%)
2	NAD	E	1416	-	46,48,48	1.72	4 (8%)	64,73,73	1.65	10 (15%)
3	G6P	B	1417	-	16,16,16	0.46	0	23,24,24	0.72	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	F	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	G	1417	-	1/1/6/6	5/6/26/26	0/1/1/1
2	NAD	D	1416	-	-	11/30/62/62	0/5/5/5
2	NAD	H	1416	-	-	6/30/62/62	0/5/5/5
3	G6P	A	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	C	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
2	NAD	A	1416	-	-	6/30/62/62	0/5/5/5
2	NAD	F	1416	-	-	9/30/62/62	0/5/5/5
2	NAD	G	1416	-	-	9/30/62/62	0/5/5/5
3	G6P	D	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
2	NAD	C	1416	-	-	11/30/62/62	0/5/5/5
3	G6P	H	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	E	1417	-	1/1/6/6	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1416	-	-	4/30/62/62	0/5/5/5
2	NAD	E	1416	-	-	7/30/62/62	0/5/5/5
3	G6P	B	1417	-	1/1/6/6	2/6/26/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1416	NAD	O7N-C7N	9.98	1.42	1.24
2	G	1416	NAD	O7N-C7N	9.77	1.42	1.24
2	D	1416	NAD	O7N-C7N	9.77	1.42	1.24
2	A	1416	NAD	O7N-C7N	9.57	1.42	1.24
2	C	1416	NAD	O7N-C7N	9.44	1.41	1.24
2	E	1416	NAD	O7N-C7N	9.37	1.41	1.24
2	F	1416	NAD	O7N-C7N	9.35	1.41	1.24
2	H	1416	NAD	O7N-C7N	9.15	1.41	1.24
2	G	1416	NAD	PA-O3	3.20	1.63	1.59
2	B	1416	NAD	C2A-N1A	3.11	1.39	1.33
2	E	1416	NAD	C2A-N1A	2.99	1.39	1.33
2	D	1416	NAD	C8A-N7A	2.95	1.37	1.31
2	A	1416	NAD	C2N-N1N	2.87	1.38	1.35
2	C	1416	NAD	C2A-N1A	2.86	1.39	1.33
2	A	1416	NAD	C2A-N1A	2.80	1.38	1.33
2	D	1416	NAD	C2A-N1A	2.79	1.38	1.33
2	C	1416	NAD	C2A-N3A	2.74	1.38	1.33
2	F	1416	NAD	C2A-N1A	2.68	1.38	1.33
2	G	1416	NAD	C2A-N1A	2.56	1.38	1.33
2	E	1416	NAD	C2A-N3A	2.53	1.38	1.33
2	B	1416	NAD	PN-O3	2.51	1.62	1.59
2	B	1416	NAD	C2A-N3A	2.51	1.38	1.33
2	C	1416	NAD	C8A-N7A	2.45	1.36	1.31
2	G	1416	NAD	C2A-N3A	2.39	1.38	1.33
2	H	1416	NAD	C2A-N1A	2.37	1.38	1.33
2	D	1416	NAD	C2A-N3A	2.36	1.38	1.33
2	F	1416	NAD	PN-O3	2.35	1.62	1.59
2	H	1416	NAD	C8A-N7A	2.33	1.36	1.31
2	E	1416	NAD	C8A-N7A	2.32	1.36	1.31
2	A	1416	NAD	C5A-N7A	-2.24	1.35	1.39
2	B	1416	NAD	C8A-N7A	2.21	1.35	1.31
2	A	1416	NAD	C2A-N3A	2.21	1.37	1.33
2	A	1416	NAD	PN-O2N	-2.20	1.45	1.55
2	F	1416	NAD	C2A-N3A	2.19	1.37	1.33
2	D	1416	NAD	PN-O3	2.18	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1416	NAD	C8A-N7A	2.16	1.35	1.31
2	B	1416	NAD	PA-O3	2.12	1.61	1.59
2	B	1416	NAD	C2N-N1N	2.12	1.37	1.35
2	A	1416	NAD	O4D-C1D	2.05	1.43	1.40
2	A	1416	NAD	C8A-N7A	2.02	1.35	1.31

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1416	NAD	N3A-C2A-N1A	-6.28	119.07	128.58
2	F	1416	NAD	N3A-C2A-N1A	-6.08	119.37	128.58
2	G	1416	NAD	N3A-C2A-N1A	-6.04	119.44	128.58
2	H	1416	NAD	N3A-C2A-N1A	-5.89	119.66	128.58
2	E	1416	NAD	N3A-C2A-N1A	-5.84	119.74	128.58
2	A	1416	NAD	N3A-C2A-N1A	-5.83	119.76	128.58
2	B	1416	NAD	N3A-C2A-N1A	-5.77	119.86	128.58
2	D	1416	NAD	N3A-C2A-N1A	-5.42	120.38	128.58
2	A	1416	NAD	N9A-C8A-N7A	-5.18	106.58	113.94
2	E	1416	NAD	C5A-C4A-N3A	-4.84	120.06	126.72
2	B	1416	NAD	N9A-C8A-N7A	-4.59	107.42	113.94
2	A	1416	NAD	C5A-N7A-C8A	4.41	110.38	103.45
2	C	1416	NAD	C5A-C4A-N3A	-4.31	120.78	126.72
2	C	1416	NAD	N9A-C8A-N7A	-4.22	107.94	113.94
2	G	1416	NAD	C5A-C4A-N3A	-4.17	120.98	126.72
2	D	1416	NAD	C5A-C4A-N3A	-4.16	120.98	126.72
2	B	1416	NAD	C5A-C4A-N3A	-4.13	121.04	126.72
2	D	1416	NAD	N9A-C8A-N7A	-4.10	108.12	113.94
2	F	1416	NAD	C5A-C4A-N3A	-4.06	121.12	126.72
2	G	1416	NAD	N9A-C8A-N7A	-4.01	108.25	113.94
2	F	1416	NAD	N9A-C8A-N7A	-3.97	108.31	113.94
2	H	1416	NAD	C5A-C4A-N3A	-3.78	121.51	126.72
2	D	1416	NAD	C5A-N7A-C8A	3.66	109.21	103.45
2	E	1416	NAD	C2A-N3A-C4A	3.63	120.71	111.83
2	H	1416	NAD	N9A-C8A-N7A	-3.61	108.81	113.94
2	B	1416	NAD	C5A-N7A-C8A	3.60	109.11	103.45
2	C	1416	NAD	C2A-N3A-C4A	3.57	120.56	111.83
2	C	1416	NAD	C5A-N7A-C8A	3.57	109.06	103.45
2	E	1416	NAD	O4B-C1B-N9A	3.57	114.94	108.09
2	G	1416	NAD	C2A-N3A-C4A	3.46	120.28	111.83
2	A	1416	NAD	C5A-C4A-N3A	-3.43	122.00	126.72
2	B	1416	NAD	C2A-N3A-C4A	3.40	120.14	111.83
2	G	1416	NAD	C5A-N7A-C8A	3.37	108.74	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1416	NAD	C2A-N3A-C4A	3.34	119.98	111.83
2	A	1416	NAD	C2A-N3A-C4A	3.26	119.79	111.83
2	F	1416	NAD	C5A-N7A-C8A	3.24	108.54	103.45
3	A	1417	G6P	O2P-P-O6	3.23	115.09	106.67
2	D	1416	NAD	C2A-N3A-C4A	3.18	119.59	111.83
2	H	1416	NAD	C2A-N3A-C4A	3.15	119.53	111.83
2	E	1416	NAD	N9A-C8A-N7A	-3.08	109.56	113.94
2	C	1416	NAD	O2A-PA-O3	-3.06	98.99	107.27
2	D	1416	NAD	C4A-C5A-N7A	-3.06	107.08	110.58
2	A	1416	NAD	C4D-O4D-C1D	3.06	112.73	109.92
2	E	1416	NAD	N3A-C4A-N9A	3.02	132.31	127.17
2	A	1416	NAD	C4A-C5A-N7A	-3.01	107.14	110.58
2	E	1416	NAD	C5A-N7A-C8A	2.99	108.15	103.45
2	B	1416	NAD	N3A-C4A-N9A	2.94	132.17	127.17
2	F	1416	NAD	N3A-C4A-N9A	2.89	132.08	127.17
2	H	1416	NAD	C5A-N7A-C8A	2.83	107.89	103.45
2	E	1416	NAD	C4D-O4D-C1D	2.75	112.44	109.92
2	G	1416	NAD	N3A-C4A-N9A	2.69	131.74	127.17
2	C	1416	NAD	C4A-C5A-N7A	-2.66	107.54	110.58
3	H	1417	G6P	O5-C5-C4	2.65	114.48	109.70
2	A	1416	NAD	O7N-C7N-C3N	2.50	122.66	119.60
2	A	1416	NAD	C4A-N9A-C8A	2.50	108.36	105.74
2	G	1416	NAD	O7N-C7N-C3N	2.48	122.64	119.60
2	B	1416	NAD	C4A-N9A-C8A	2.48	108.34	105.74
2	G	1416	NAD	C4A-C5A-N7A	-2.47	107.76	110.58
2	A	1416	NAD	O2N-PN-O3	2.46	113.93	107.27
2	A	1416	NAD	O3-PN-O1N	-2.44	103.37	110.70
2	C	1416	NAD	N3A-C4A-N9A	2.41	131.27	127.17
2	E	1416	NAD	C4A-C5A-N7A	-2.33	107.91	110.58
2	H	1416	NAD	O5D-C5D-C4D	2.28	116.74	108.99
2	C	1416	NAD	O2N-PN-O3	-2.27	101.13	107.27
3	C	1417	G6P	O2-C2-C1	2.27	114.48	109.25
2	H	1416	NAD	N3A-C4A-N9A	2.23	130.96	127.17
2	D	1416	NAD	O3-PN-O1N	-2.20	104.09	110.70
2	D	1416	NAD	N3A-C4A-N9A	2.20	130.90	127.17
2	A	1416	NAD	O7N-C7N-N7N	-2.19	119.45	122.62
2	F	1416	NAD	C4A-N9A-C8A	2.19	108.04	105.74
2	A	1416	NAD	C4A-N9A-C1B	-2.17	121.56	126.63
2	C	1416	NAD	C3N-C7N-N7N	2.17	120.41	117.74
2	G	1416	NAD	O3B-C3B-C4B	-2.14	104.93	111.08
2	G	1416	NAD	C4D-O4D-C1D	2.13	111.88	109.92
2	G	1416	NAD	C4A-N9A-C8A	2.12	107.96	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1417	G6P	O2P-P-O6	2.10	112.15	106.67
2	F	1416	NAD	O2N-PN-O1N	2.10	122.20	112.44
3	F	1417	G6P	O5-C5-C4	2.09	113.47	109.70
2	G	1416	NAD	O2N-PN-O1N	2.09	122.16	112.44
2	B	1416	NAD	O7N-C7N-C3N	2.09	122.15	119.60
2	C	1416	NAD	O2N-PN-O1N	2.08	122.14	112.44
2	D	1416	NAD	C5A-C4A-N9A	2.08	108.08	105.81
2	E	1416	NAD	C6N-N1N-C2N	-2.07	120.12	121.88
2	B	1416	NAD	O2N-PN-O1N	2.02	121.84	112.44
3	D	1417	G6P	C1-C2-C3	-2.01	106.25	110.36
3	A	1417	G6P	C4-C3-C2	-2.01	107.31	110.83

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1417	G6P	C1
3	B	1417	G6P	C1
3	C	1417	G6P	C1
3	D	1417	G6P	C1
3	E	1417	G6P	C1
3	F	1417	G6P	C1
3	G	1417	G6P	C1
3	H	1417	G6P	C1

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1416	NAD	PA-O3-PN-O5D
2	C	1416	NAD	C5D-O5D-PN-O2N
2	D	1416	NAD	C5B-O5B-PA-O1A
2	D	1416	NAD	C5B-O5B-PA-O2A
2	D	1416	NAD	C5B-O5B-PA-O3
2	D	1416	NAD	PN-O3-PA-O5B
2	D	1416	NAD	C5D-O5D-PN-O2N
2	F	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	PA-O3-PN-O5D
2	H	1416	NAD	C5D-O5D-PN-O2N
3	A	1417	G6P	C4-C5-C6-O6
3	A	1417	G6P	O5-C5-C6-O6
3	B	1417	G6P	C4-C5-C6-O6
3	B	1417	G6P	O5-C5-C6-O6
3	C	1417	G6P	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1417	G6P	O5-C5-C6-O6
3	D	1417	G6P	C4-C5-C6-O6
3	D	1417	G6P	O5-C5-C6-O6
3	E	1417	G6P	C4-C5-C6-O6
3	E	1417	G6P	O5-C5-C6-O6
3	F	1417	G6P	C4-C5-C6-O6
3	F	1417	G6P	O5-C5-C6-O6
3	G	1417	G6P	C4-C5-C6-O6
3	G	1417	G6P	O5-C5-C6-O6
3	G	1417	G6P	C6-O6-P-O1P
3	G	1417	G6P	C6-O6-P-O2P
3	H	1417	G6P	C4-C5-C6-O6
3	H	1417	G6P	O5-C5-C6-O6
2	E	1416	NAD	C3D-C4D-C5D-O5D
2	F	1416	NAD	C3D-C4D-C5D-O5D
2	C	1416	NAD	C2N-C3N-C7N-O7N
2	C	1416	NAD	O4D-C4D-C5D-O5D
2	C	1416	NAD	C3D-C4D-C5D-O5D
2	E	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	C3D-C4D-C5D-O5D
2	C	1416	NAD	C4N-C3N-C7N-O7N
2	C	1416	NAD	C2N-C3N-C7N-N7N
2	C	1416	NAD	C4N-C3N-C7N-N7N
2	H	1416	NAD	C3D-C4D-C5D-O5D
2	H	1416	NAD	O4D-C4D-C5D-O5D
3	G	1417	G6P	C6-O6-P-O3P
2	B	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	C4N-C3N-C7N-O7N
2	E	1416	NAD	PA-O3-PN-O5D
2	F	1416	NAD	PA-O3-PN-O5D
2	H	1416	NAD	PA-O3-PN-O5D
2	G	1416	NAD	C4N-C3N-C7N-N7N
2	B	1416	NAD	C3D-C4D-C5D-O5D
2	A	1416	NAD	C4N-C3N-C7N-O7N
2	E	1416	NAD	C2B-C1B-N9A-C8A
2	G	1416	NAD	C2N-C3N-C7N-O7N
2	F	1416	NAD	C2B-C1B-N9A-C8A
2	A	1416	NAD	C4N-C3N-C7N-N7N
2	F	1416	NAD	O4B-C4B-C5B-O5B
2	C	1416	NAD	C5B-O5B-PA-O3
2	D	1416	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	E	1416	NAD	C5B-O5B-PA-O3
2	F	1416	NAD	C5B-O5B-PA-O3
2	A	1416	NAD	PA-O3-PN-O2N
2	B	1416	NAD	PA-O3-PN-O2N
2	C	1416	NAD	C2B-C1B-N9A-C8A
2	G	1416	NAD	C2B-C1B-N9A-C8A
2	G	1416	NAD	C2N-C3N-C7N-N7N
2	G	1416	NAD	C2D-C1D-N1N-C2N
2	D	1416	NAD	O4D-C4D-C5D-O5D
2	D	1416	NAD	PA-O3-PN-O2N
2	D	1416	NAD	C3D-C4D-C5D-O5D
2	B	1416	NAD	C2B-C1B-N9A-C8A
2	D	1416	NAD	C2B-C1B-N9A-C8A
2	A	1416	NAD	C2N-C3N-C7N-O7N
2	A	1416	NAD	C2N-C3N-C7N-N7N
2	F	1416	NAD	O4B-C1B-N9A-C8A
2	H	1416	NAD	C2B-C1B-N9A-C8A
2	E	1416	NAD	PN-O3-PA-O2A
2	H	1416	NAD	PA-O3-PN-O2N
2	A	1416	NAD	C2B-C1B-N9A-C8A
2	C	1416	NAD	O4B-C1B-N9A-C8A
2	E	1416	NAD	O4B-C1B-N9A-C8A
2	D	1416	NAD	C4B-C5B-O5B-PA
2	F	1416	NAD	C3B-C4B-C5B-O5B
2	F	1416	NAD	PN-O3-PA-O2A

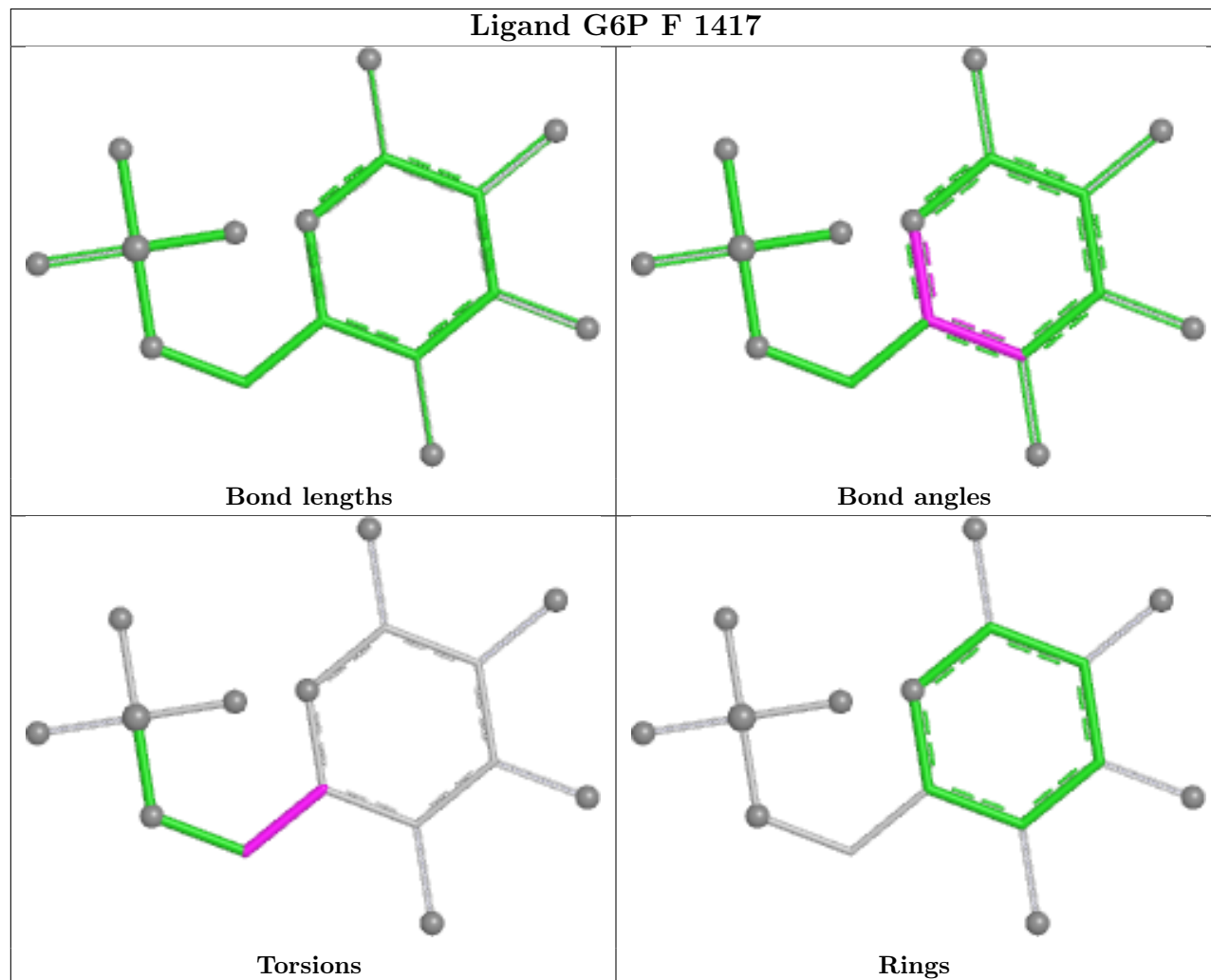
There are no ring outliers.

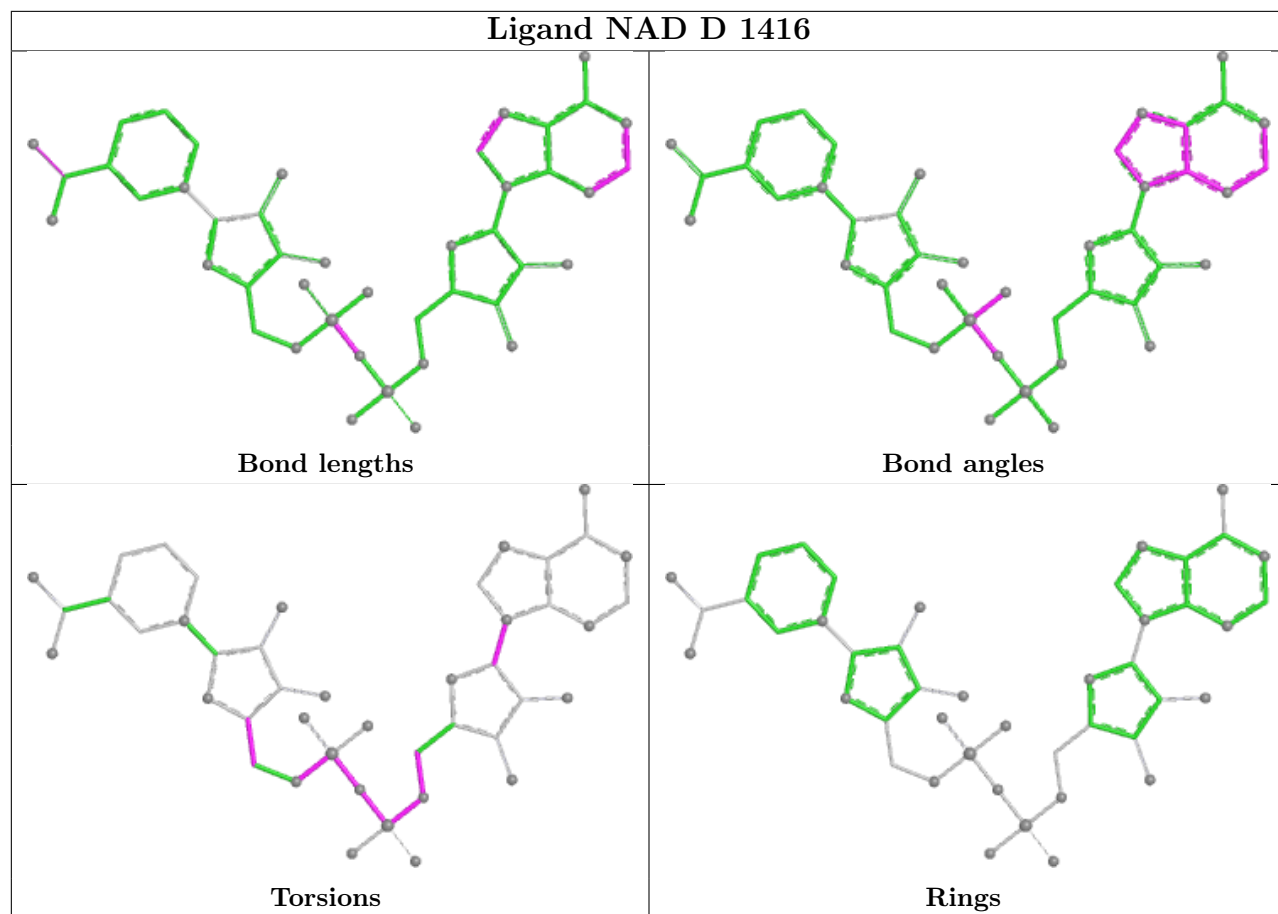
4 monomers are involved in 7 short contacts:

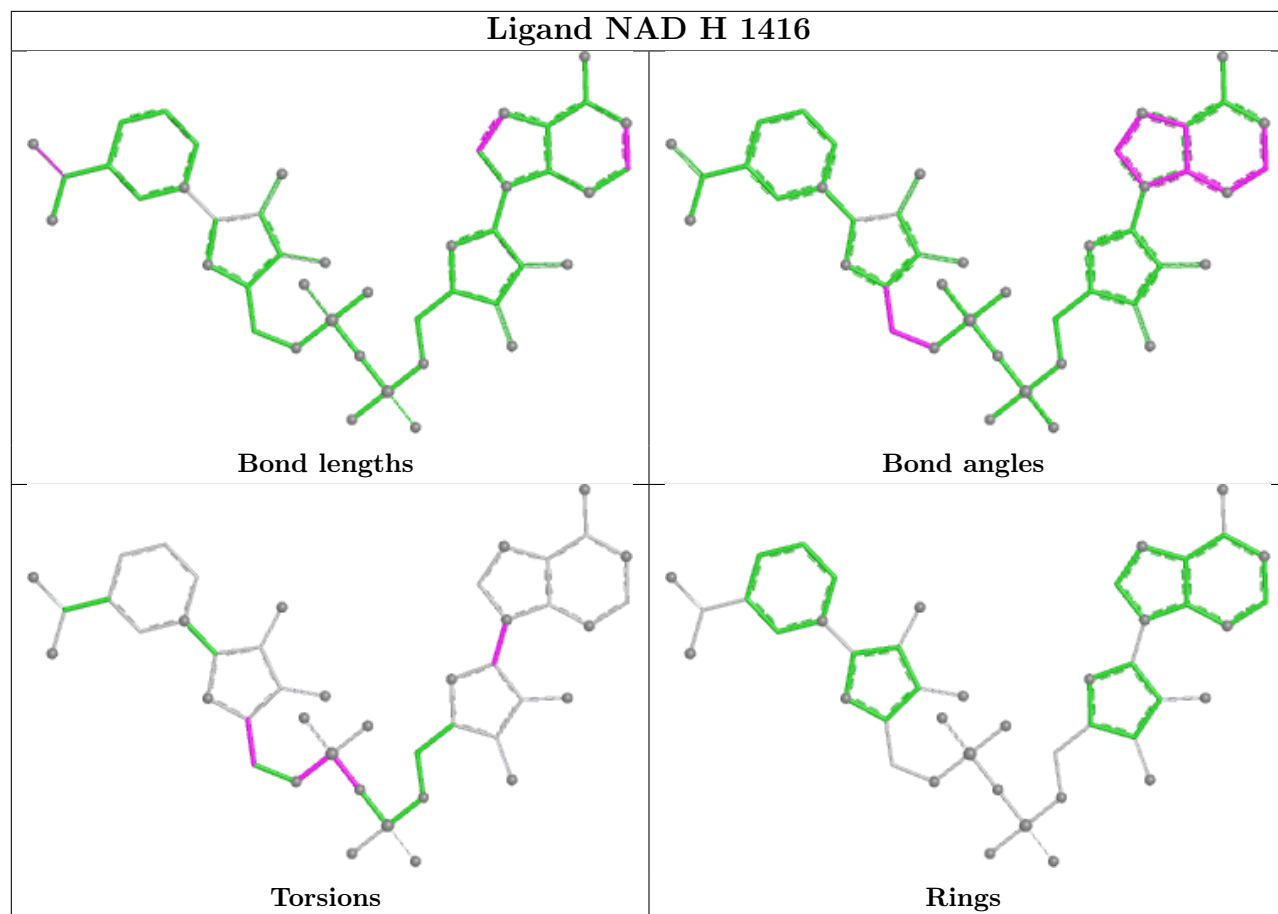
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1416	NAD	2	0
3	D	1417	G6P	2	0
3	H	1417	G6P	2	0
2	E	1416	NAD	1	0

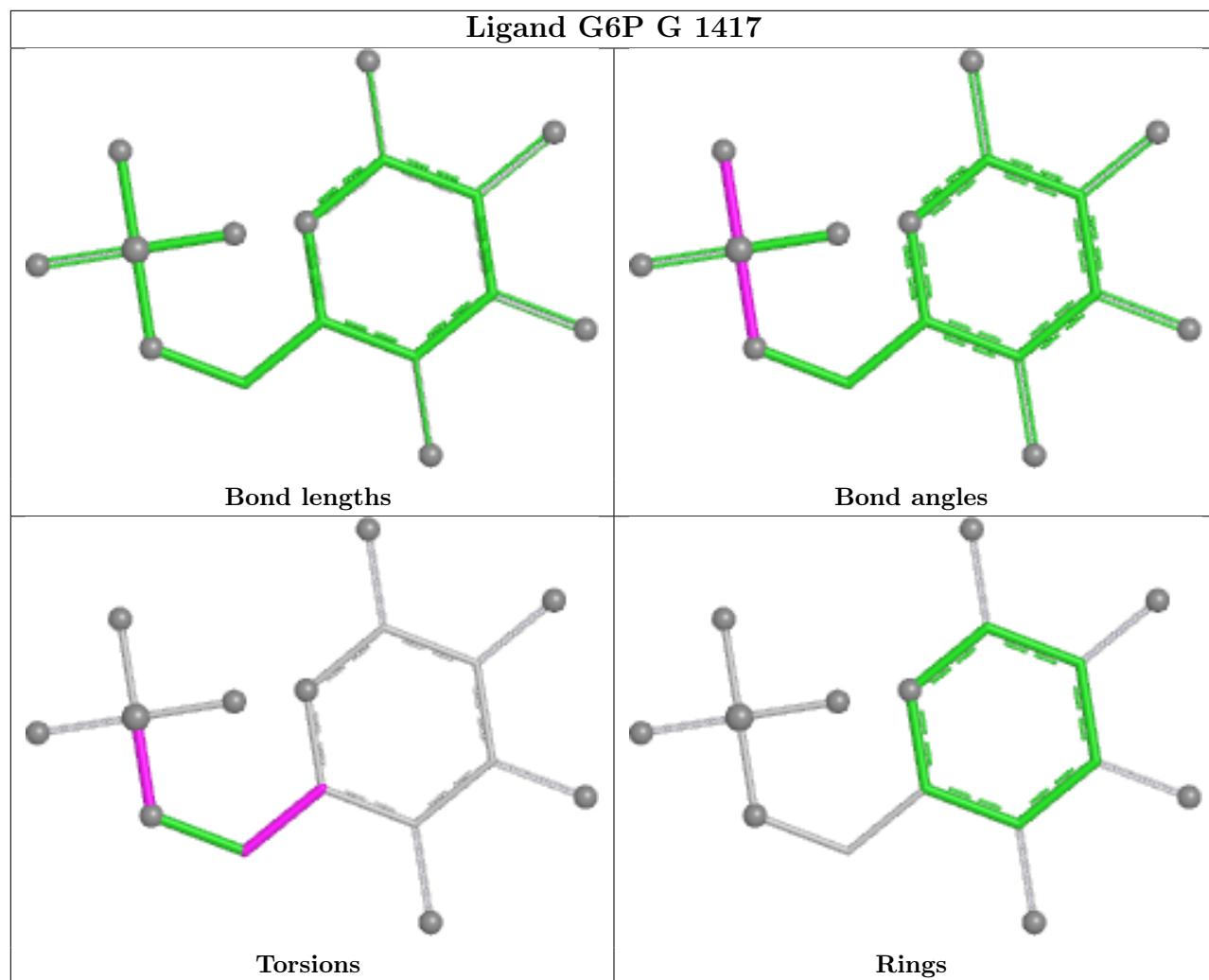
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

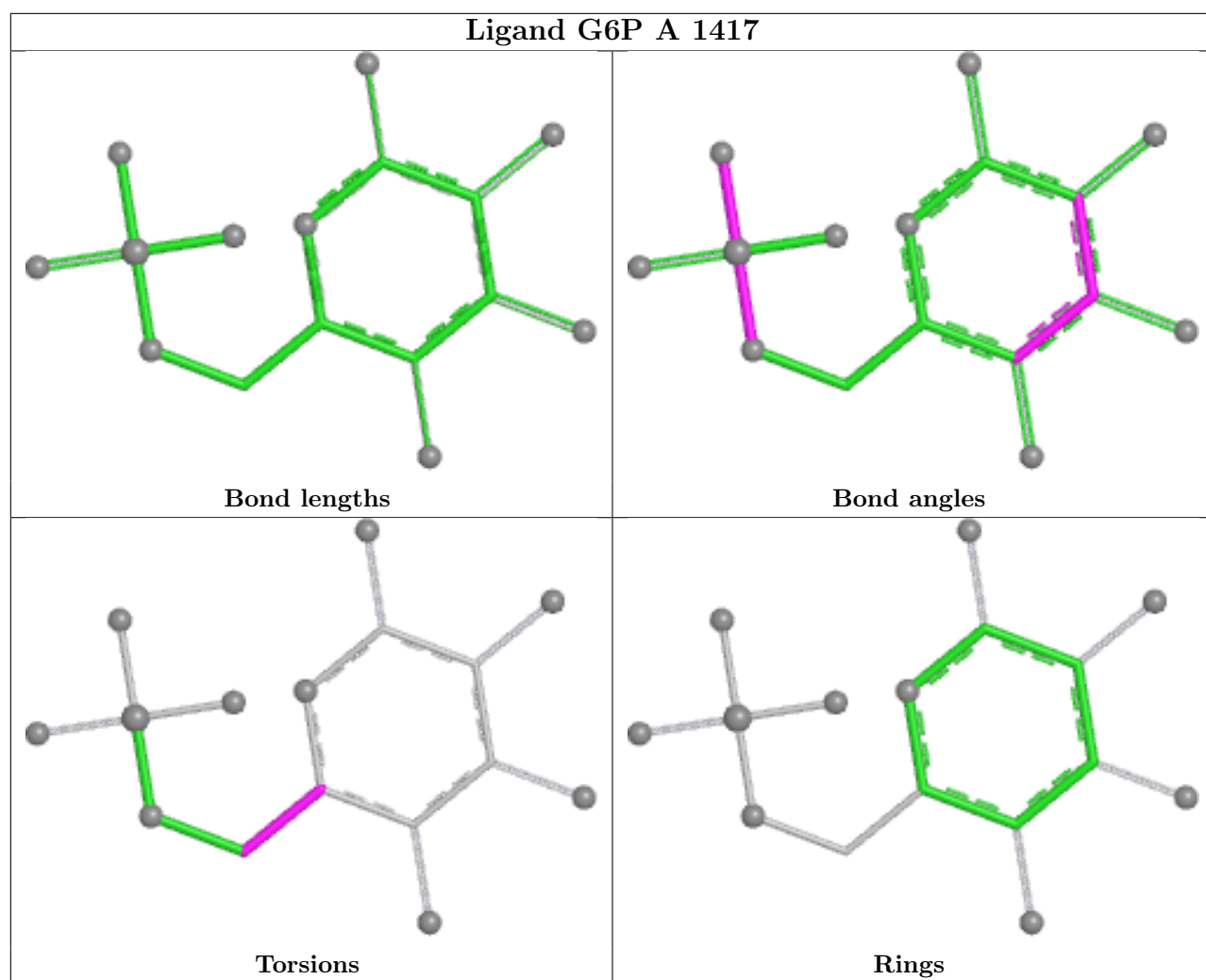
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

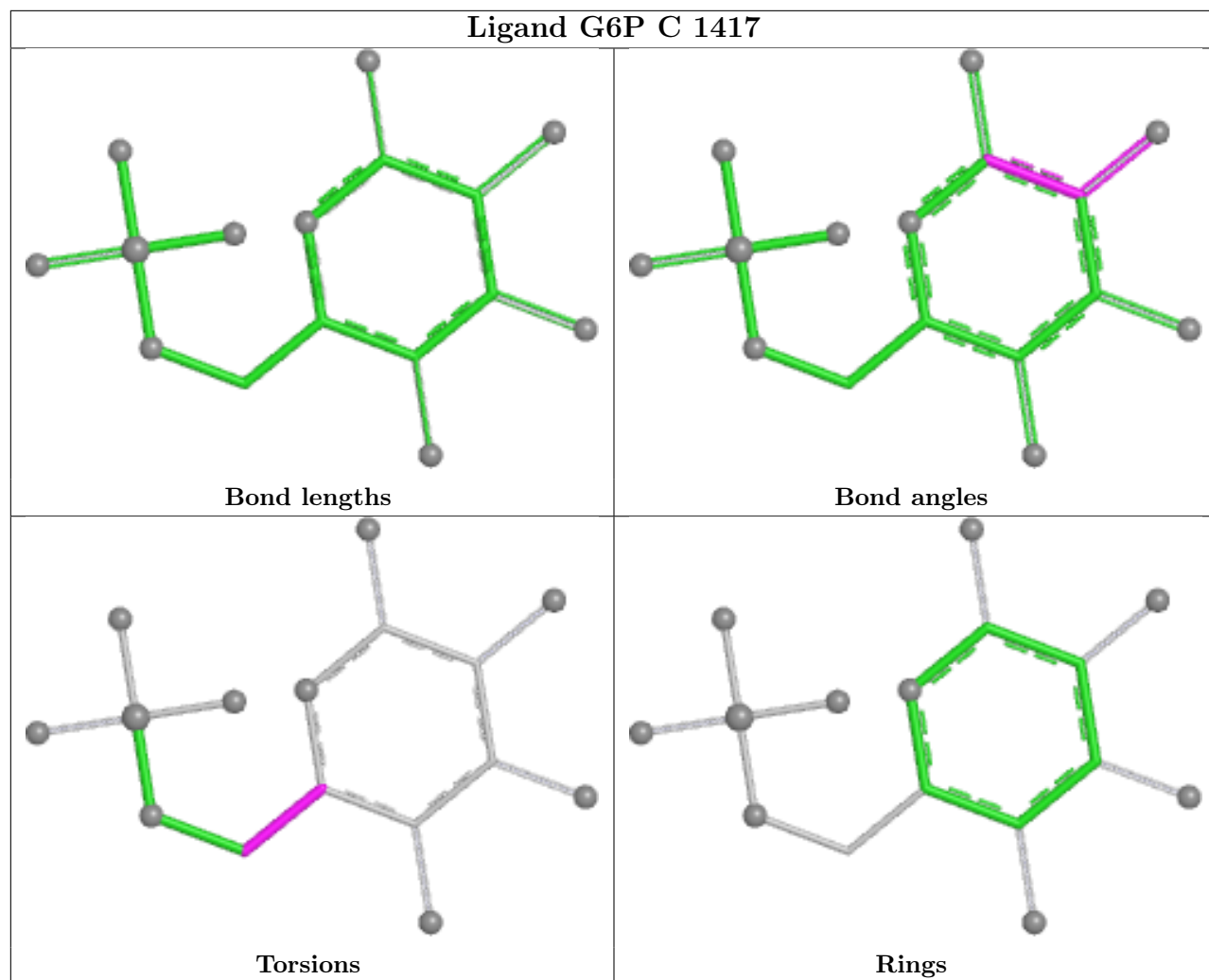


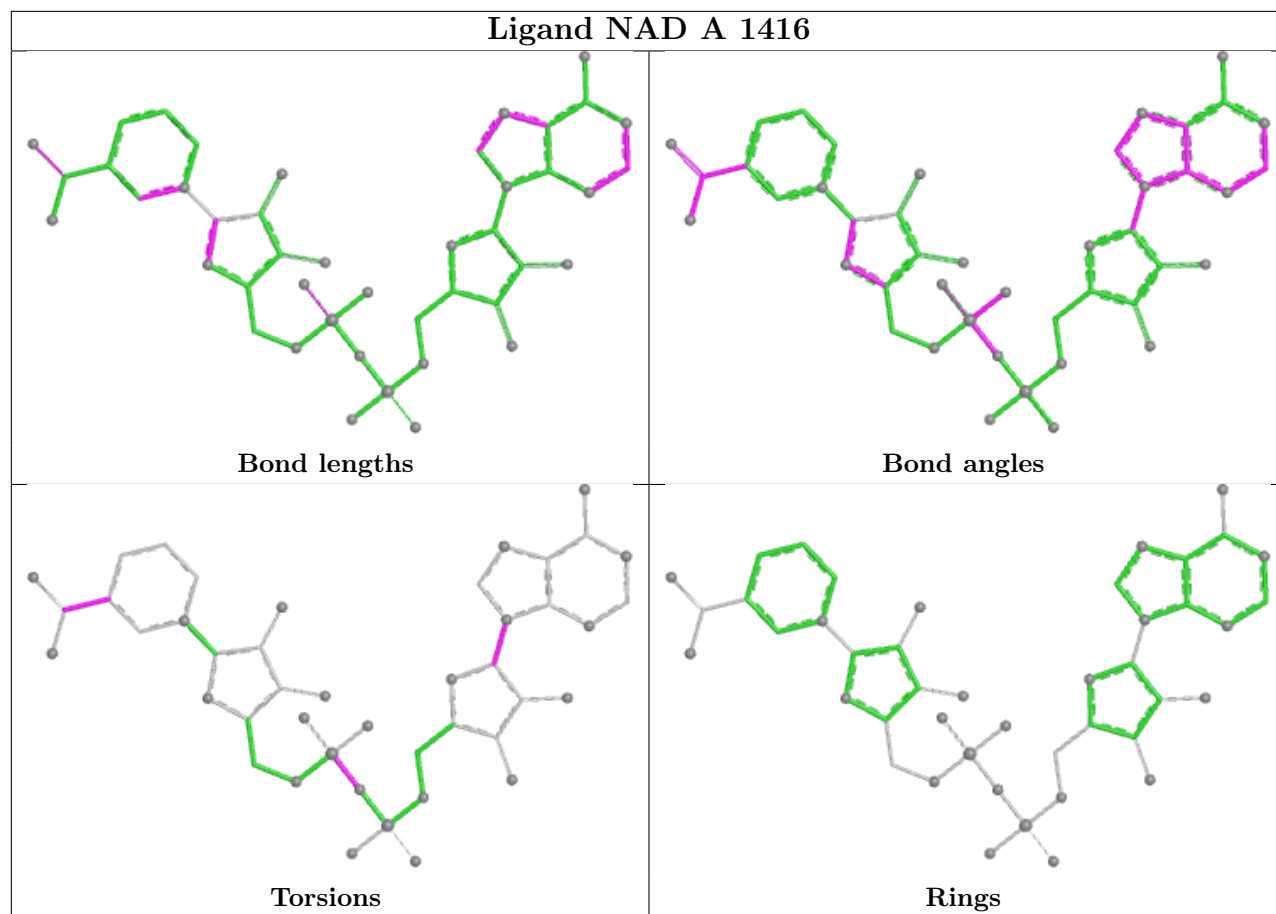


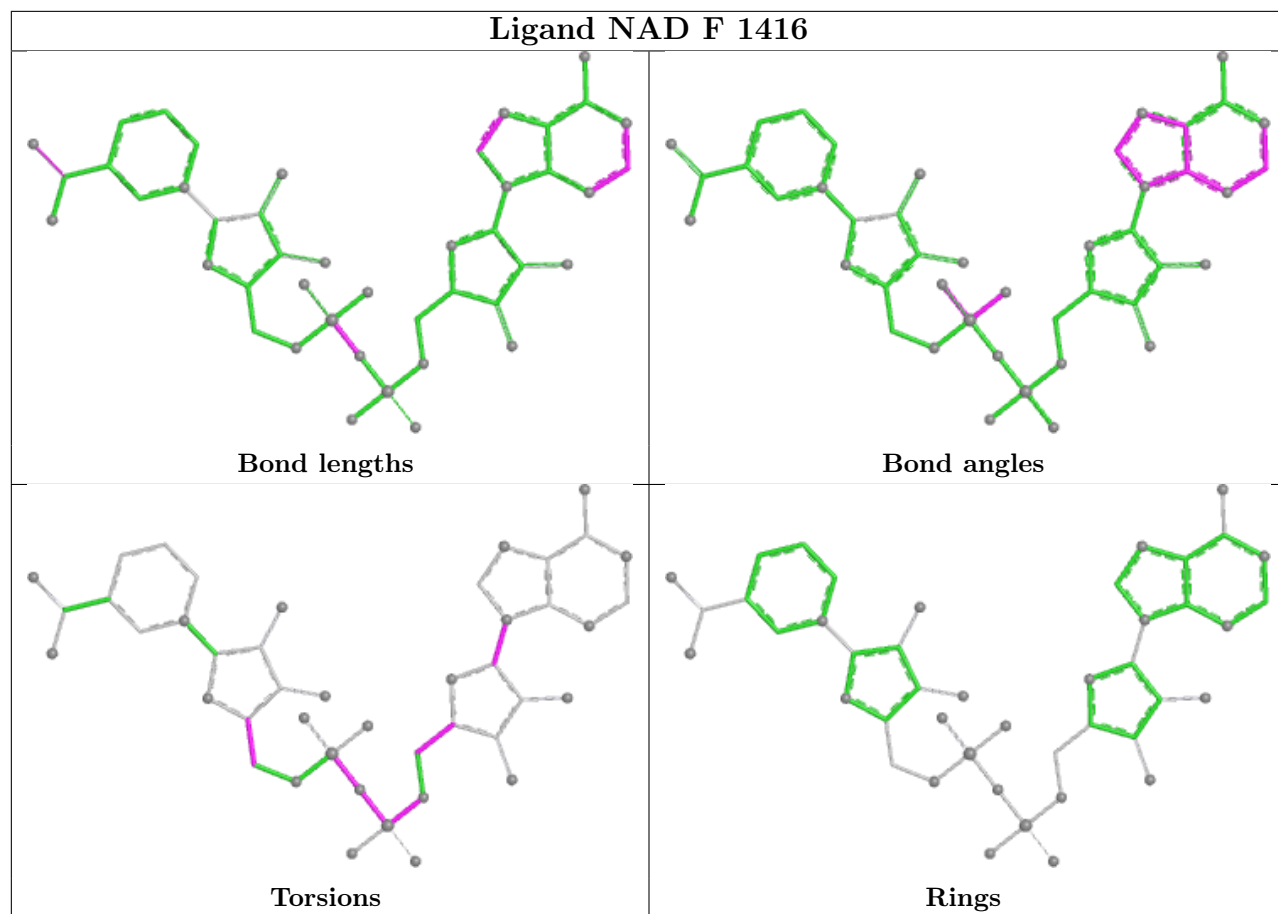


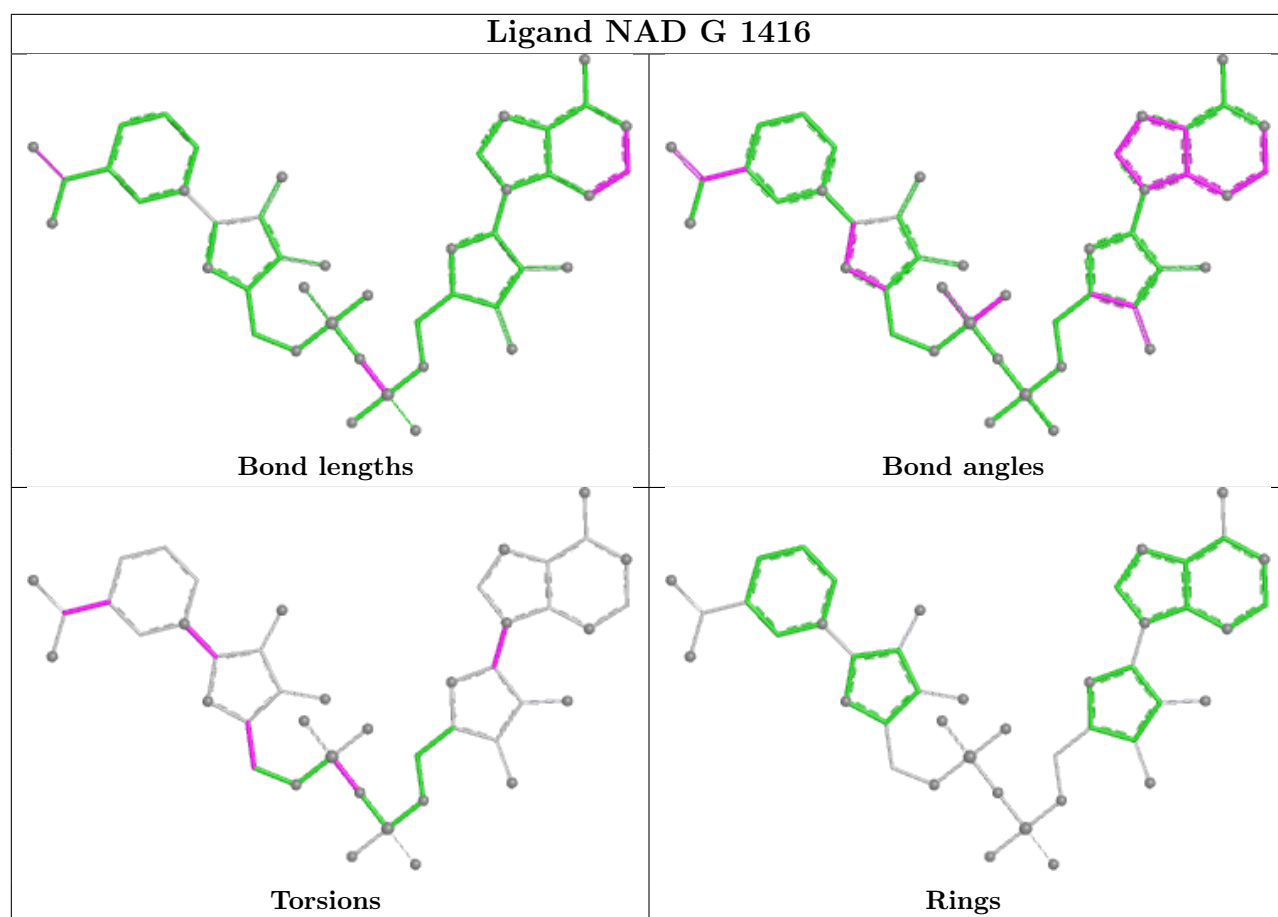


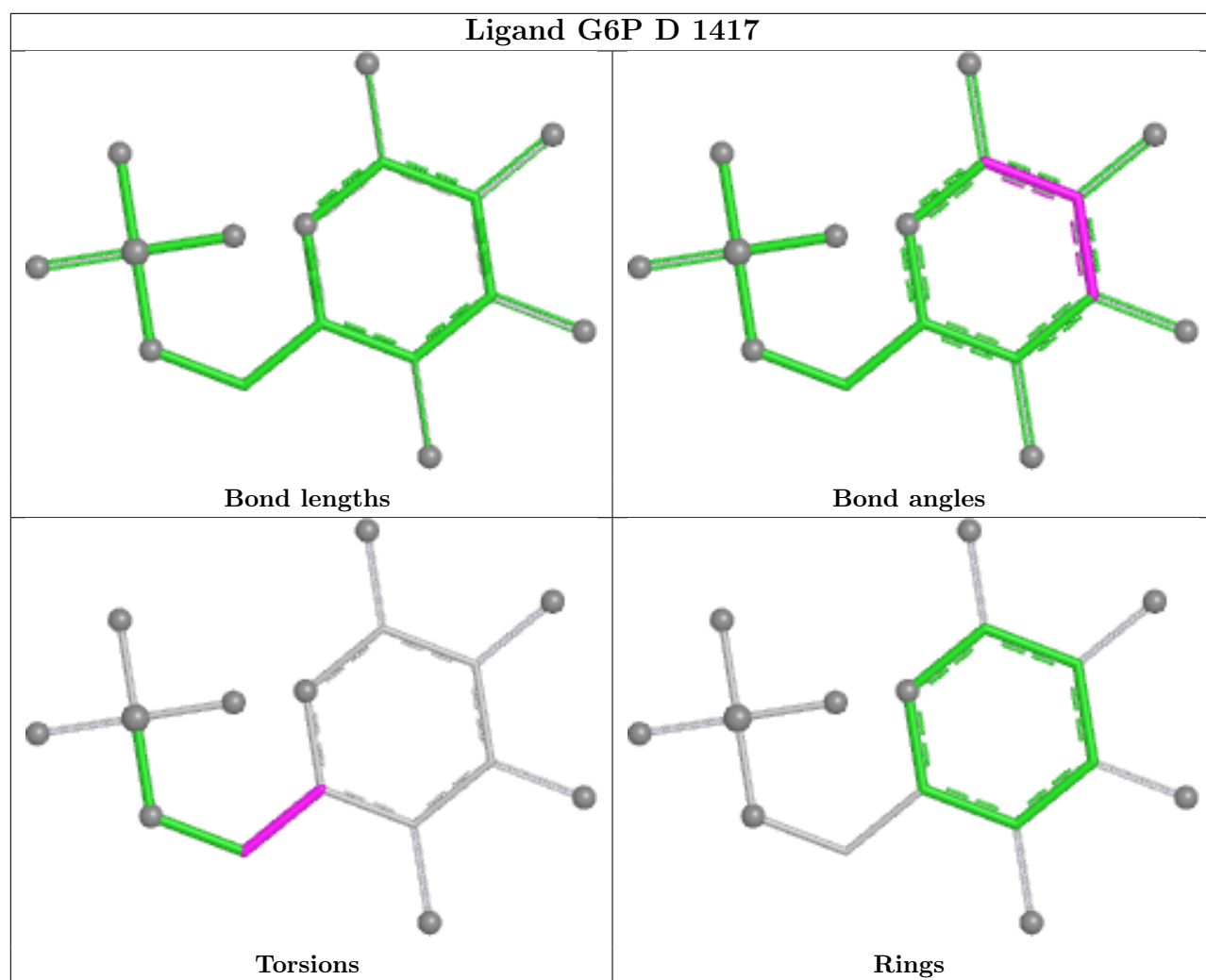


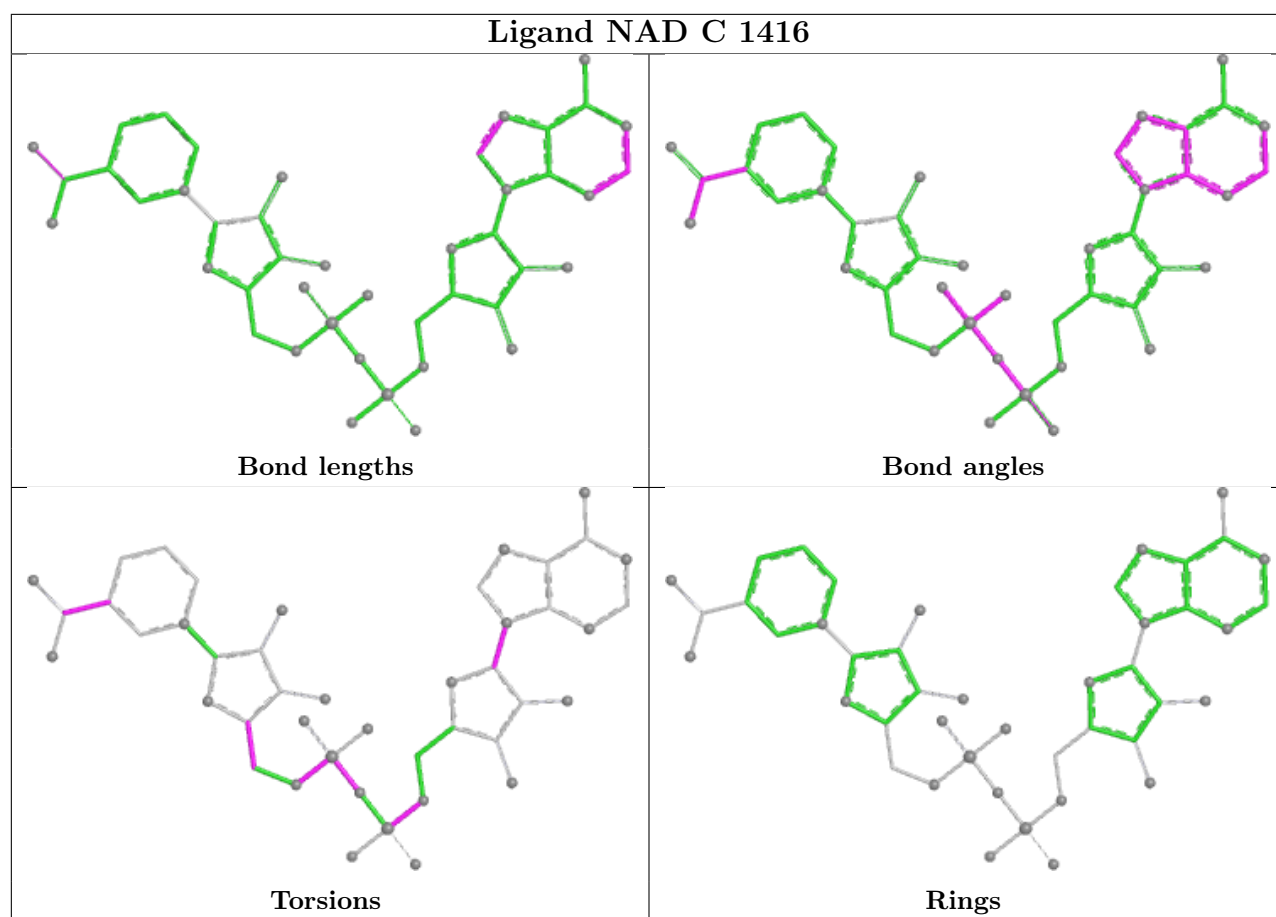


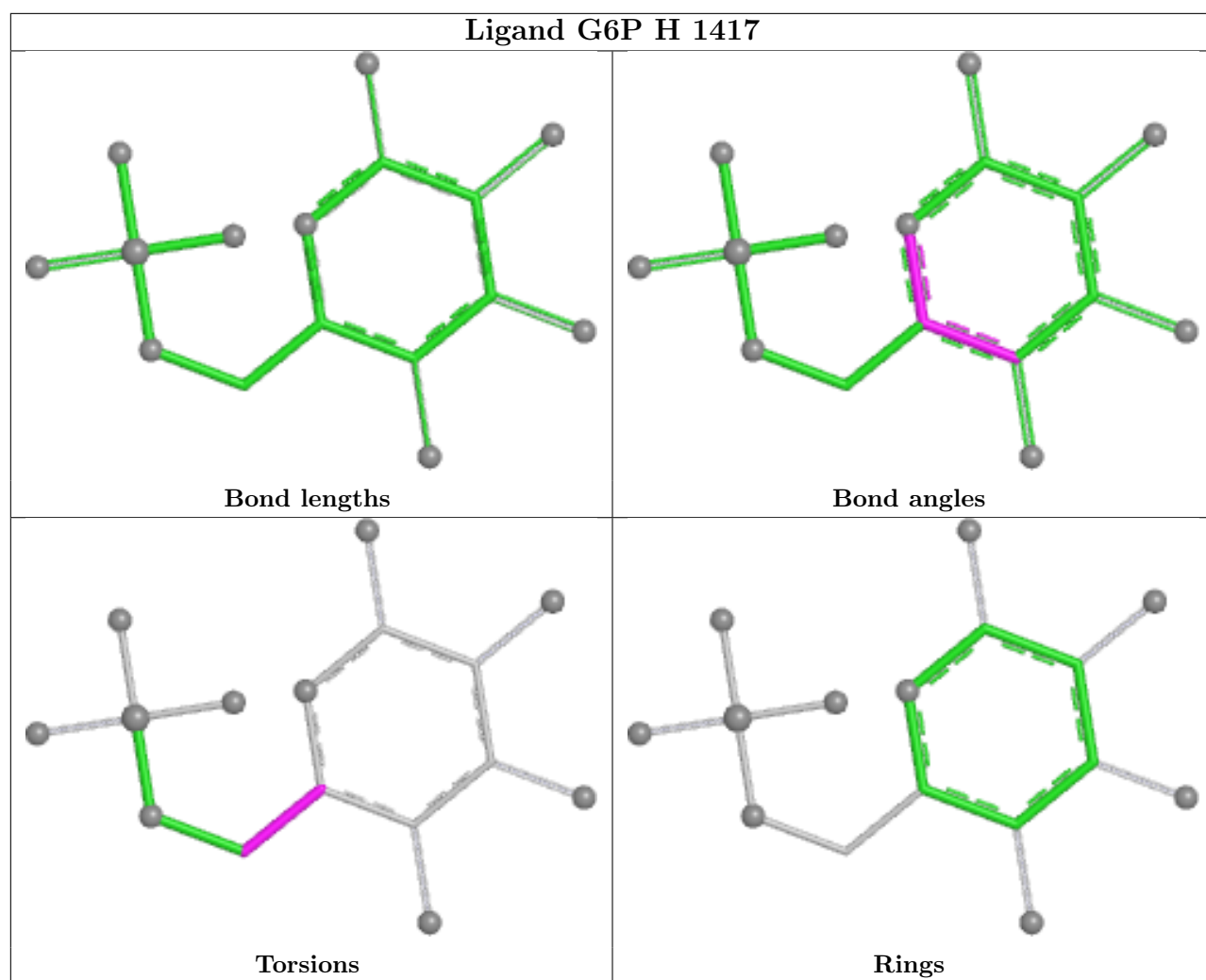


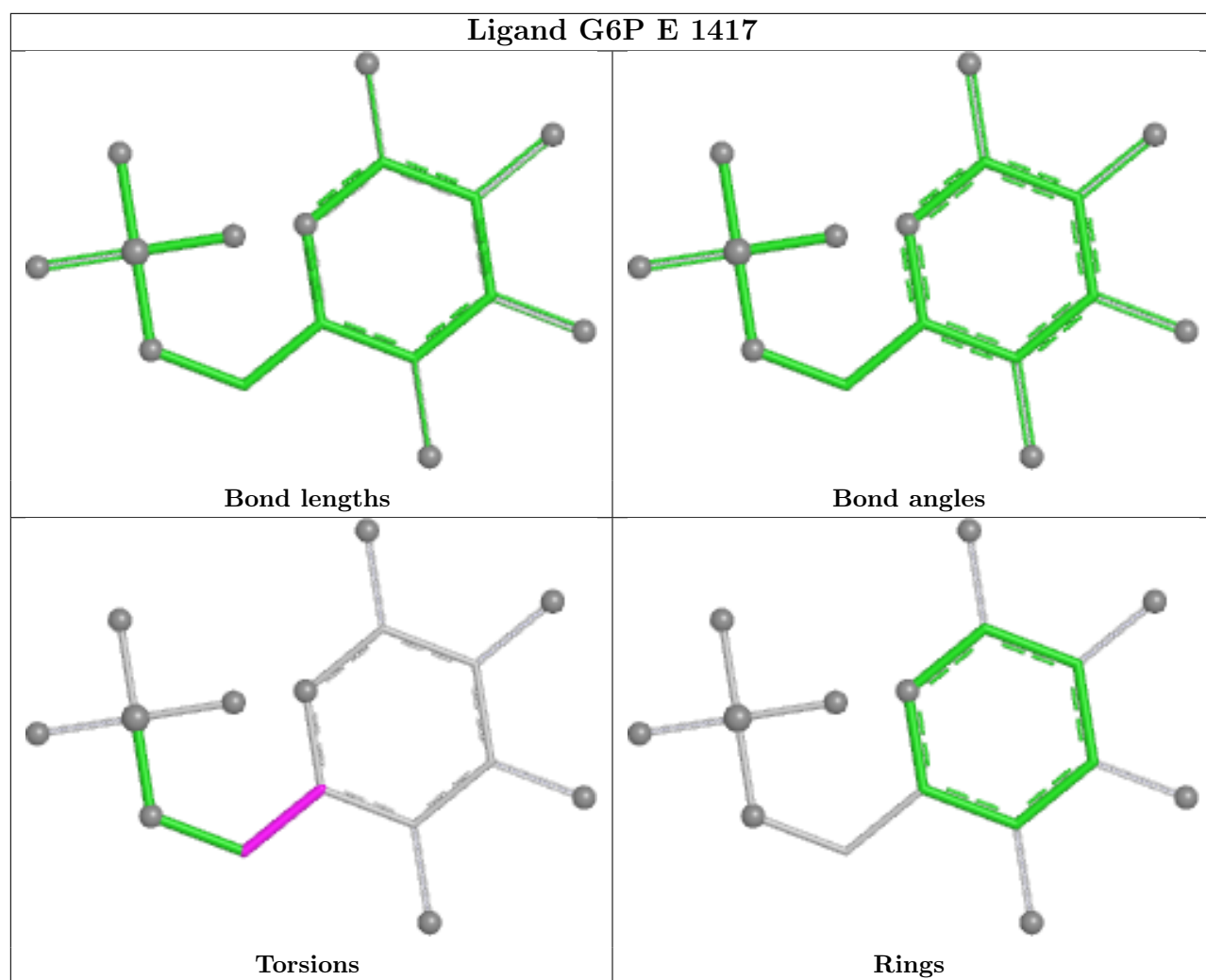


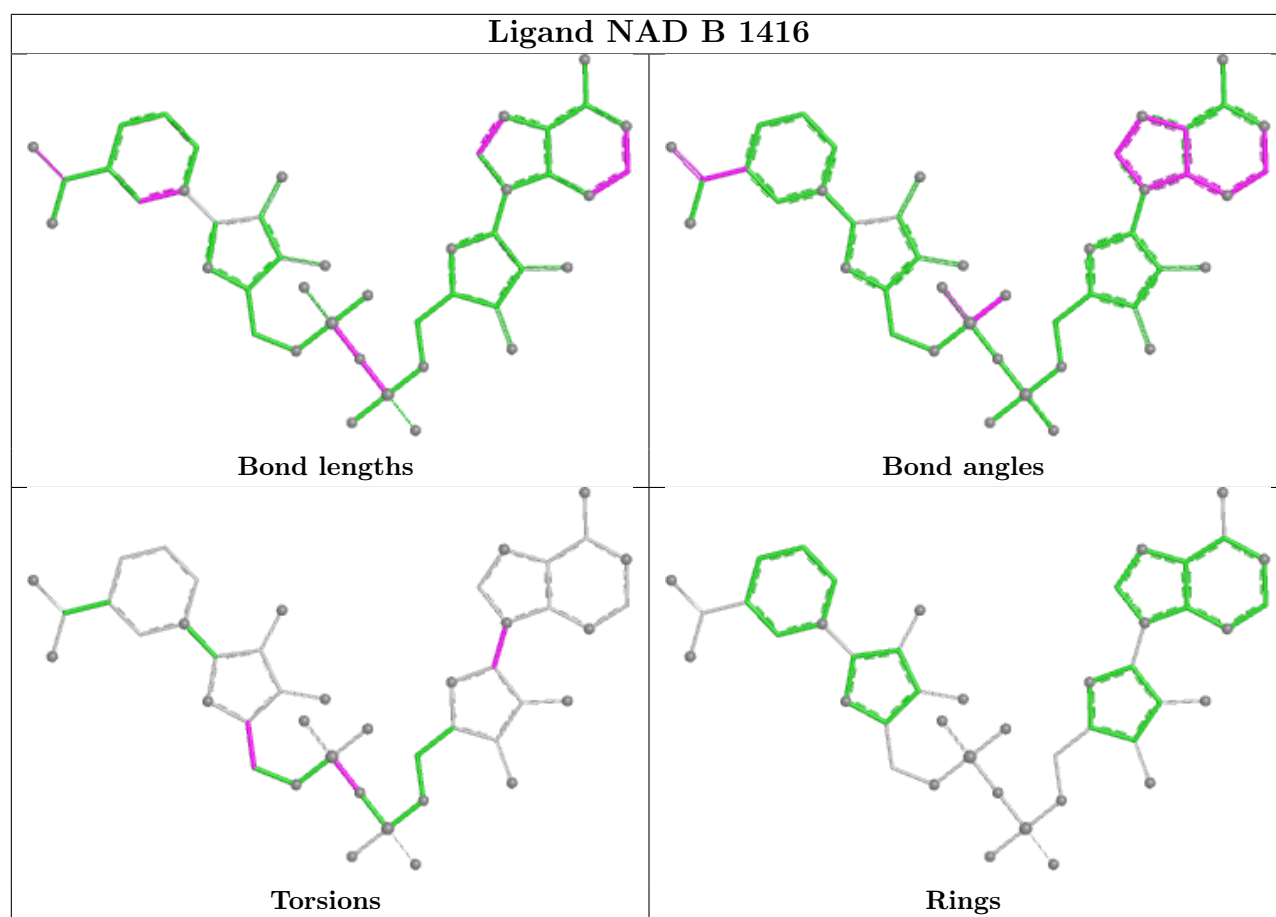


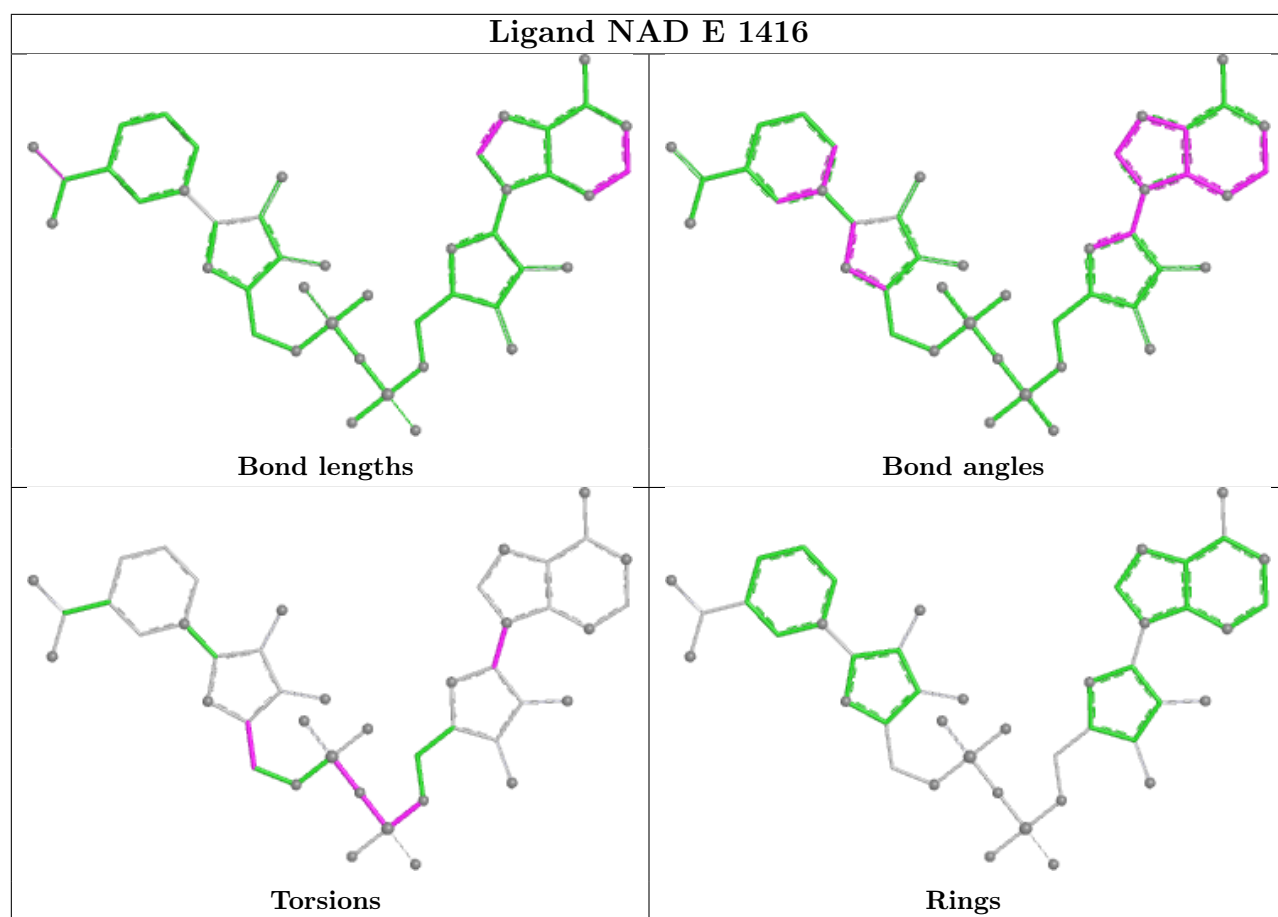


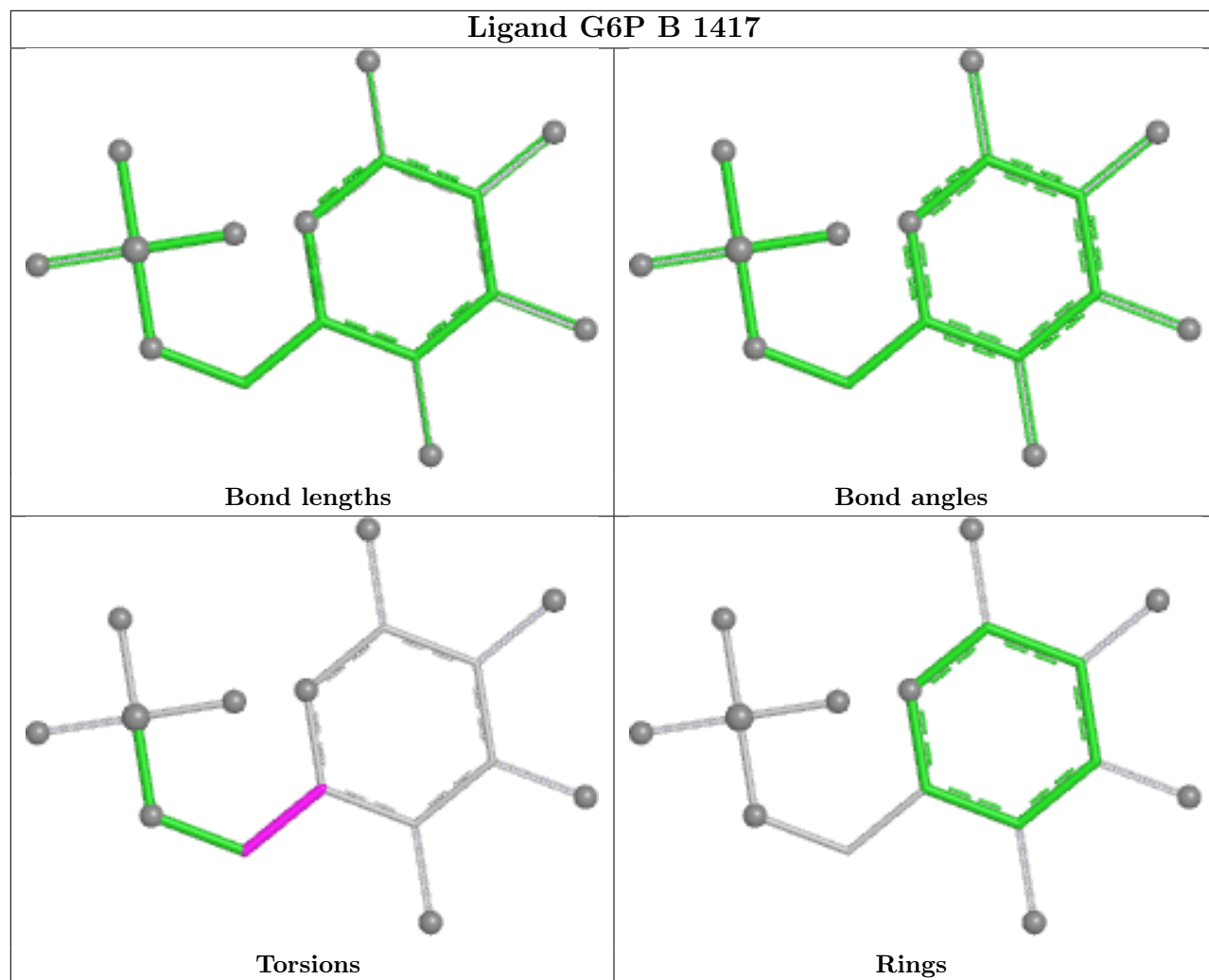












5.7 Other polymers [i](#)

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	414/417 (99%)	0.01	16 (3%) 43 39	12, 19, 26, 58	3 (0%)
1	B	409/417 (98%)	0.75	48 (11%) 9 7	9, 19, 25, 31	22 (5%)
1	C	409/417 (98%)	0.29	21 (5%) 33 30	9, 19, 25, 31	14 (3%)
1	D	409/417 (98%)	0.37	22 (5%) 31 28	10, 19, 27, 39	18 (4%)
1	E	406/417 (97%)	1.06	64 (15%) 5 4	7, 19, 24, 30	41 (10%)
1	F	411/417 (98%)	0.50	20 (4%) 35 31	9, 19, 25, 36	31 (7%)
1	G	409/417 (98%)	0.36	19 (4%) 37 33	9, 19, 25, 30	22 (5%)
1	H	407/417 (97%)	0.71	31 (7%) 20 16	9, 19, 25, 36	25 (6%)
All	All	3274/3336 (98%)	0.51	241 (7%) 20 17	7, 19, 25, 58	176 (5%)

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	276	TYR	4.8
1	E	272	LEU	4.8
1	A	223	ASP	4.7
1	E	294	TYR	4.5
1	B	216	LEU	4.5
1	E	169	ILE	4.5
1	B	63	ASP	4.3
1	A	294	TYR	4.3
1	G	286	LEU	4.2
1	B	213	ASN	4.2
1	B	24	SER	4.1
1	E	224	GLU	4.1
1	E	167	ASN	4.0
1	G	290	GLY	4.0
1	H	57	PHE	4.0
1	B	272	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	11	SER	4.0
1	E	286	LEU	4.0
1	E	292	SER	3.9
1	A	292	SER	3.9
1	B	292	SER	3.8
1	D	294	TYR	3.8
1	E	168	PHE	3.8
1	E	291	GLY	3.8
1	C	273	PHE	3.8
1	B	294	TYR	3.7
1	A	222	PRO	3.7
1	F	292	SER	3.7
1	B	269	GLU	3.7
1	D	290	GLY	3.6
1	G	294	TYR	3.5
1	E	293	MET	3.5
1	G	291	GLY	3.5
1	G	292	SER	3.5
1	D	291	GLY	3.5
1	H	24	SER	3.5
1	A	168	PHE	3.5
1	H	55	ASP	3.5
1	G	276	TYR	3.5
1	D	286	LEU	3.4
1	F	224	GLU	3.4
1	C	216	LEU	3.4
1	B	273	PHE	3.4
1	G	284	GLU	3.4
1	C	290	GLY	3.4
1	D	26	ASP	3.4
1	E	210	VAL	3.4
1	A	0	HIS	3.4
1	F	286	LEU	3.3
1	E	211	PHE	3.3
1	H	286	LEU	3.3
1	E	174	GLU	3.3
1	E	287	THR	3.3
1	G	224	GLU	3.3
1	H	31	GLU	3.3
1	E	1	MET	3.3
1	E	290	GLY	3.3
1	H	285	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	3.2
1	F	222	PRO	3.2
1	F	274	GLU	3.2
1	A	221	ILE	3.2
1	A	216	LEU	3.2
1	B	25	GLU	3.2
1	H	26	ASP	3.2
1	D	288	LYS	3.2
1	E	165	PRO	3.2
1	F	293	MET	3.1
1	E	223	ASP	3.1
1	H	287	THR	3.1
1	A	285	GLU	3.1
1	G	269	GLU	3.1
1	B	282	ILE	3.1
1	B	12	TYR	3.1
1	F	291	GLY	3.1
1	E	379	LYS	3.0
1	H	234	VAL	3.0
1	D	287	THR	3.0
1	B	181	GLU	3.0
1	E	179	ARG	3.0
1	B	287	THR	3.0
1	D	279	ALA	3.0
1	E	171	GLU	3.0
1	B	56	ARG	3.0
1	B	26	ASP	3.0
1	E	289	ARG	3.0
1	E	288	LYS	3.0
1	C	168	PHE	3.0
1	C	225	ASP	2.9
1	E	64	THR	2.9
1	C	55	ASP	2.9
1	A	273	PHE	2.9
1	B	285	GLU	2.9
1	E	378	LYS	2.9
1	E	173	ALA	2.9
1	E	214	LEU	2.9
1	F	216	LEU	2.9
1	G	216	LEU	2.9
1	B	224	GLU	2.9
1	D	70	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	276	TYR	2.8
1	E	370	ILE	2.8
1	E	382	LEU	2.8
1	H	1	MET	2.8
1	C	224	GLU	2.8
1	D	285	GLU	2.8
1	B	291	GLY	2.7
1	C	276	TYR	2.7
1	E	394	VAL	2.7
1	B	386	LEU	2.7
1	H	216	LEU	2.7
1	E	383	LYS	2.7
1	B	225	ASP	2.7
1	H	7	GLY	2.7
1	E	213	ASN	2.7
1	H	2	ARG	2.7
1	E	30	ASP	2.7
1	B	48	PHE	2.7
1	E	138	PHE	2.7
1	C	294	TYR	2.7
1	E	56	ARG	2.7
1	F	284	GLU	2.7
1	E	182	ASP	2.6
1	B	86	GLY	2.6
1	B	293	MET	2.6
1	C	212	GLU	2.6
1	B	288	LYS	2.6
1	F	288	LYS	2.6
1	B	289	ARG	2.6
1	B	392	PRO	2.6
1	H	28	ARG	2.6
1	B	284	GLU	2.5
1	C	278	THR	2.5
1	B	278	THR	2.5
1	B	402	GLU	2.5
1	C	25	GLU	2.5
1	C	213	ASN	2.5
1	D	24	SER	2.5
1	C	264	GLU	2.5
1	E	7	GLY	2.5
1	D	68	ALA	2.5
1	D	281	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	30	ASP	2.4
1	C	295	SER	2.4
1	H	291	GLY	2.4
1	F	345	THR	2.4
1	G	287	THR	2.4
1	F	347	SER	2.4
1	E	375	LYS	2.4
1	E	398	LYS	2.4
1	B	53	VAL	2.4
1	E	53	VAL	2.4
1	F	266	MET	2.4
1	A	224	GLU	2.4
1	H	281	GLU	2.4
1	C	292	SER	2.4
1	E	386	LEU	2.4
1	E	124	VAL	2.4
1	G	350	LYS	2.4
1	E	295	SER	2.3
1	E	201	VAL	2.3
1	G	173	ALA	2.3
1	C	287	THR	2.3
1	F	290	GLY	2.3
1	C	272	LEU	2.3
1	H	242	LEU	2.3
1	B	54	LYS	2.3
1	E	176	PHE	2.3
1	G	263	ARG	2.3
1	D	295	SER	2.3
1	B	71	ASP	2.3
1	G	409	ARG	2.3
1	H	4	ALA	2.2
1	B	203	GLY	2.2
1	B	43	LYS	2.2
1	E	44	ILE	2.2
1	E	212	GLU	2.2
1	E	285	GLU	2.2
1	E	183	VAL	2.2
1	F	201	VAL	2.2
1	F	294	TYR	2.2
1	E	296	THR	2.2
1	B	290	GLY	2.2
1	D	55	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	51	ARG	2.2
1	B	279	ALA	2.2
1	H	130	THR	2.2
1	C	286	LEU	2.2
1	E	153	LEU	2.2
1	D	63	ASP	2.2
1	D	289	ARG	2.2
1	B	27	VAL	2.2
1	F	265	VAL	2.2
1	H	292	SER	2.2
1	E	121	GLU	2.2
1	G	225	ASP	2.2
1	A	215	LYS	2.2
1	A	217	LYS	2.2
1	H	27	VAL	2.1
1	H	280	VAL	2.1
1	E	163	ASN	2.1
1	H	132	ASN	2.1
1	D	31	GLU	2.1
1	D	292	SER	2.1
1	B	217	LYS	2.1
1	A	290	GLY	2.1
1	B	382	LEU	2.1
1	G	272	LEU	2.1
1	H	415	GLY	2.1
1	D	28	ARG	2.1
1	E	309	GLU	2.1
1	F	12	TYR	2.1
1	H	168	PHE	2.1
1	B	391	GLY	2.1
1	C	170	ARG	2.1
1	F	309	GLU	2.1
1	E	327	PRO	2.1
1	H	283	PRO	2.1
1	E	70	VAL	2.1
1	F	409	ARG	2.1
1	A	281	GLU	2.1
1	B	66	GLU	2.1
1	A	225	ASP	2.1
1	D	125	ASP	2.1
1	C	293	MET	2.1
1	E	368	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	386	LEU	2.0
1	B	281	GLU	2.0
1	G	171	GLU	2.0
1	E	144	HIS	2.0
1	B	57	PHE	2.0
1	D	280	VAL	2.0
1	H	273	PHE	2.0
1	H	246	LEU	2.0
1	B	98	GLY	2.0
1	E	415	GLY	2.0
1	H	9	GLY	2.0
1	E	6	ILE	2.0
1	E	228	THR	2.0
1	G	26	ASP	2.0
1	B	258	HIS	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.

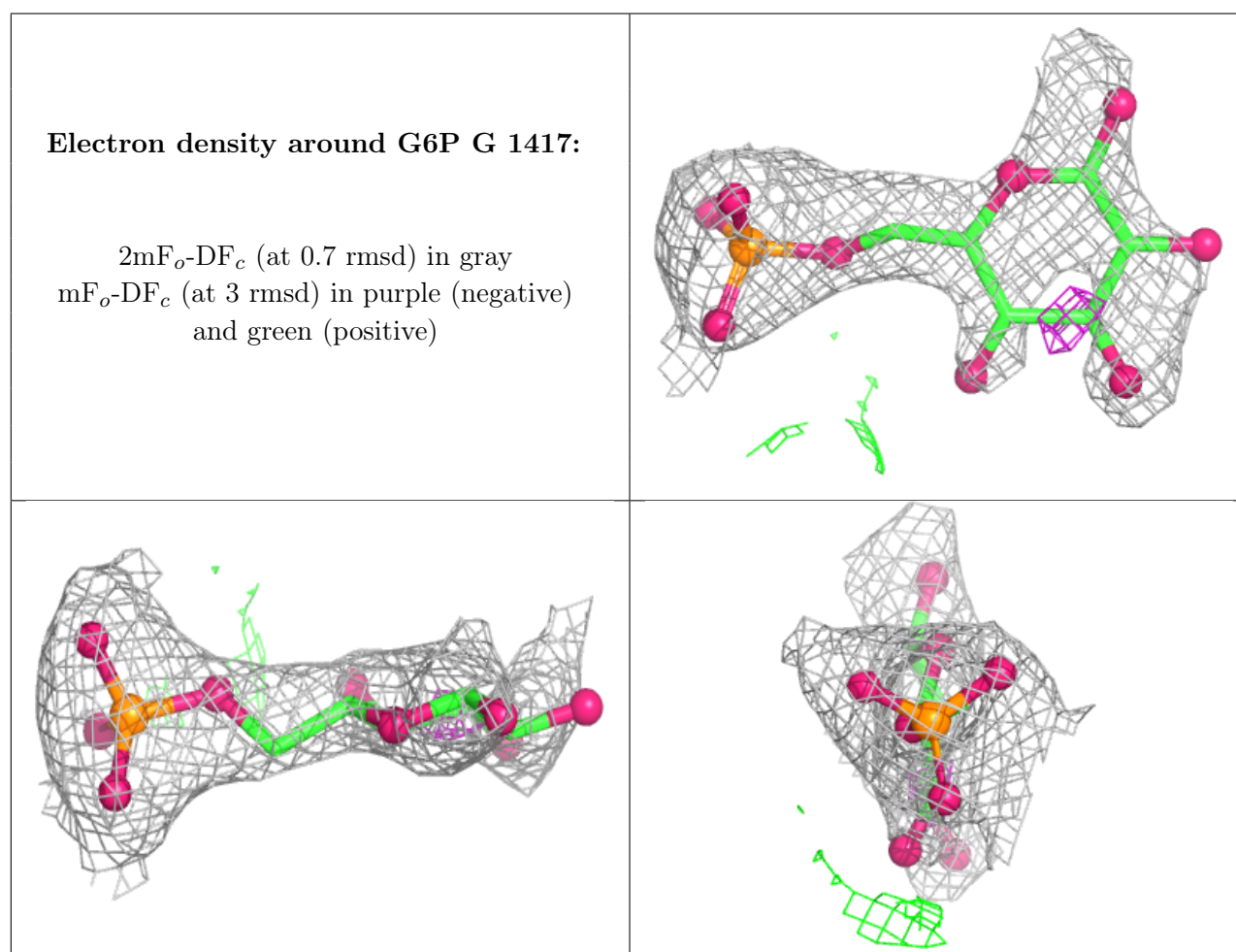
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	1418	5/5	0.67	0.18	53,54,61,63	0
4	SO4	A	1418	5/5	0.75	0.17	57,59,61,62	0
3	G6P	G	1417	16/16	0.80	0.17	62,70,71,71	0
3	G6P	D	1417	16/16	0.82	0.22	43,47,48,49	16
2	NAD	E	1416	44/44	0.84	0.22	31,33,39,41	44
3	G6P	C	1417	16/16	0.85	0.15	58,69,71,71	0
3	G6P	H	1417	16/16	0.87	0.20	43,48,49,51	16
3	G6P	F	1417	16/16	0.87	0.21	47,52,54,55	16

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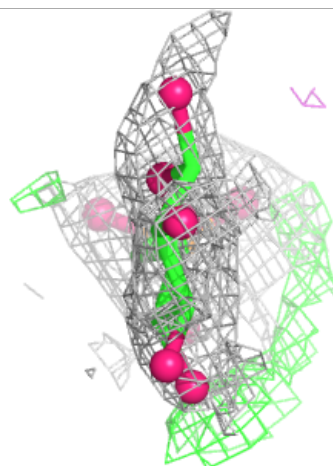
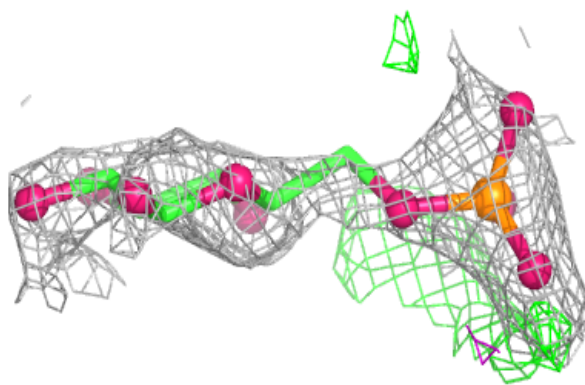
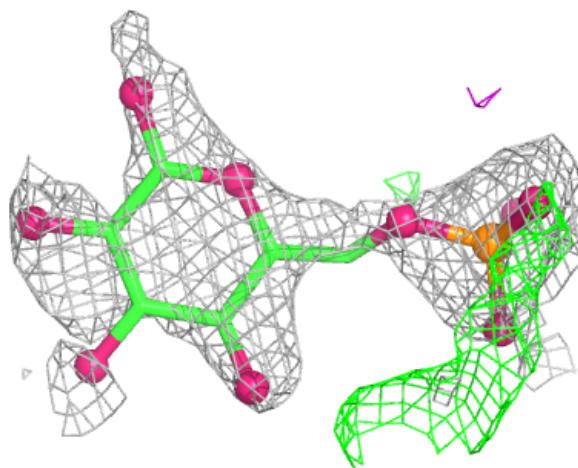
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	G6P	A	1417	16/16	0.87	0.15	46,58,60,60	0
2	NAD	H	1416	44/44	0.88	0.21	24,28,35,39	44
3	G6P	E	1417	16/16	0.89	0.15	36,39,40,40	16
2	NAD	F	1416	44/44	0.89	0.20	21,35,41,45	44
3	G6P	B	1417	16/16	0.90	0.20	37,42,45,45	16
2	NAD	B	1416	44/44	0.92	0.10	34,52,64,69	0
2	NAD	G	1416	44/44	0.94	0.10	30,48,59,62	0
2	NAD	D	1416	44/44	0.94	0.09	31,44,54,55	0
2	NAD	C	1416	44/44	0.95	0.08	24,41,53,59	0
2	NAD	A	1416	44/44	0.95	0.08	21,35,49,52	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.



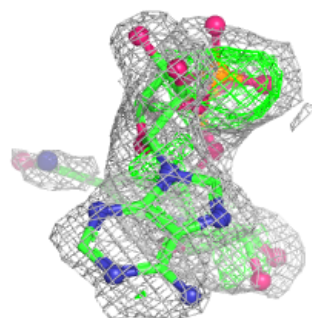
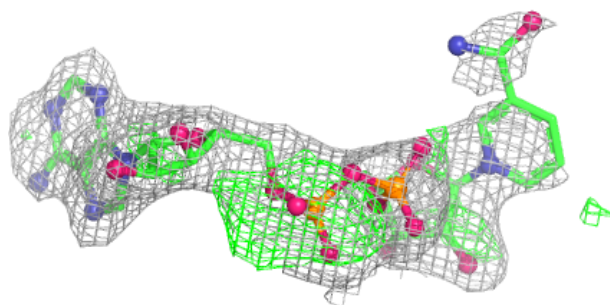
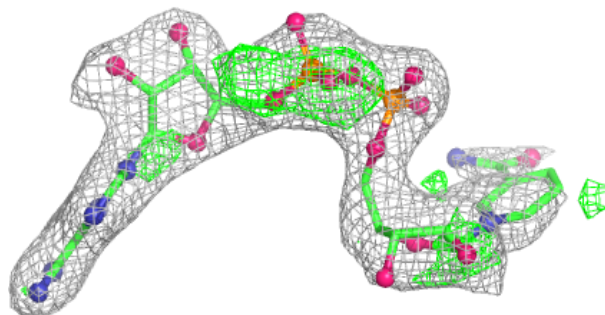
Electron density around G6P D 1417:

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

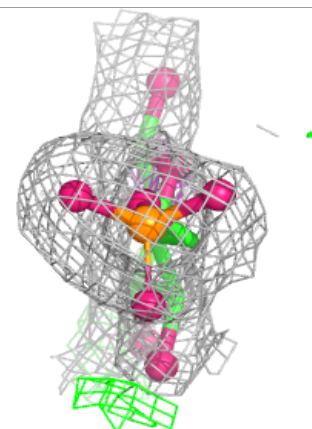
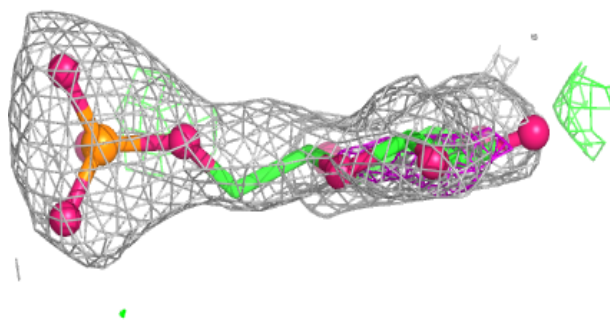
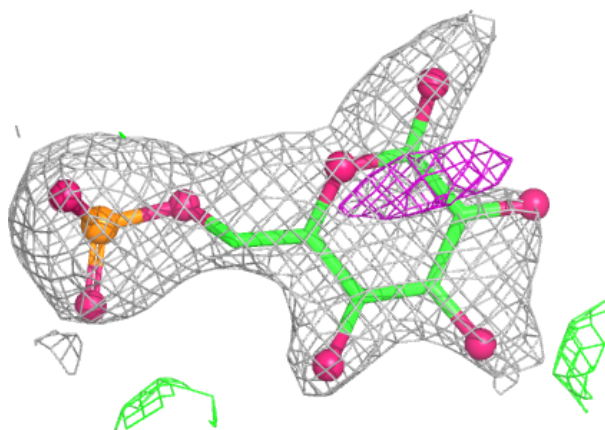


Electron density around NAD E 1416:

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

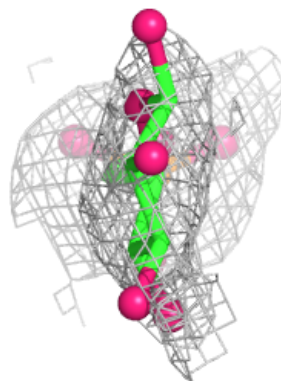
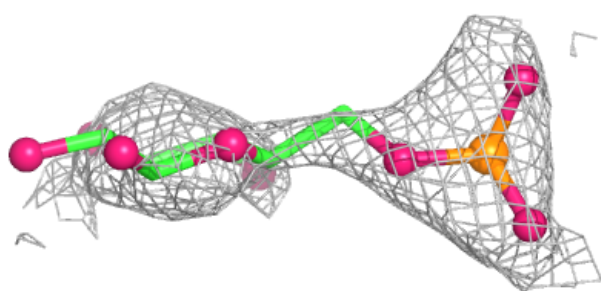
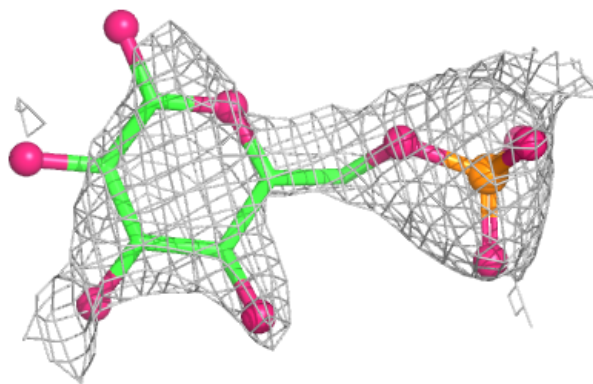
**Electron density around G6P C 1417:**

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

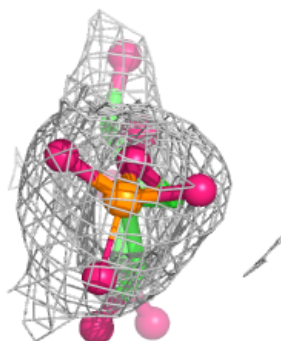
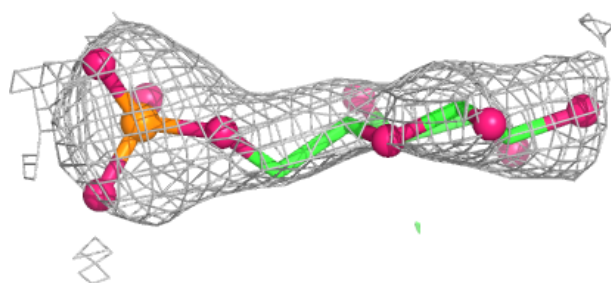
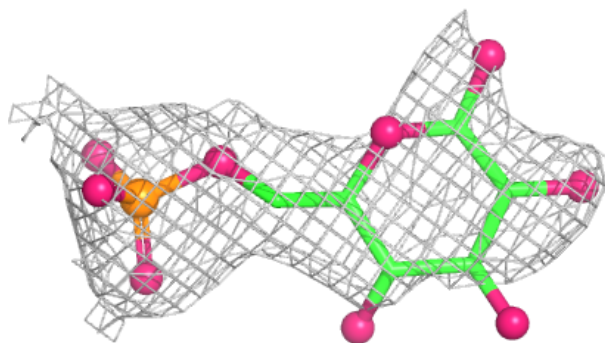


Electron density around G6P H 1417:

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

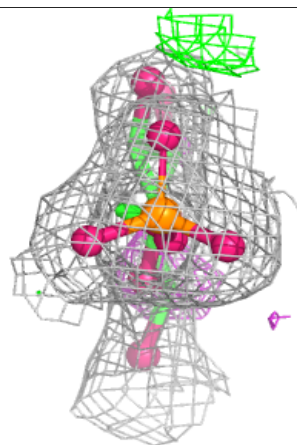
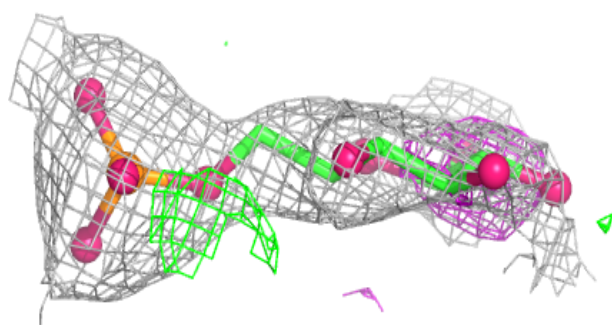
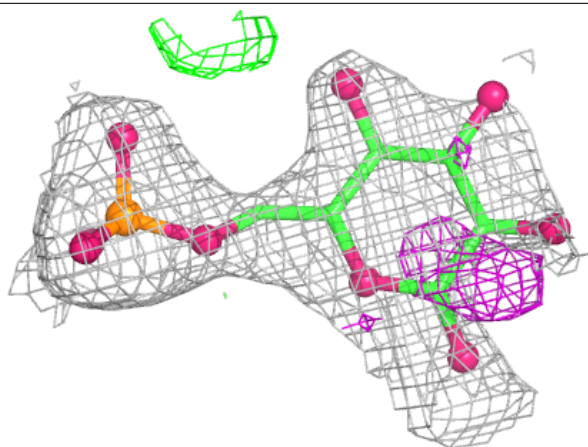
**Electron density around G6P F 1417:**

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

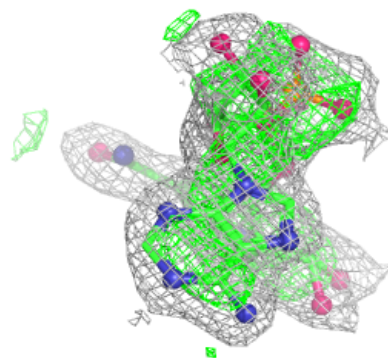
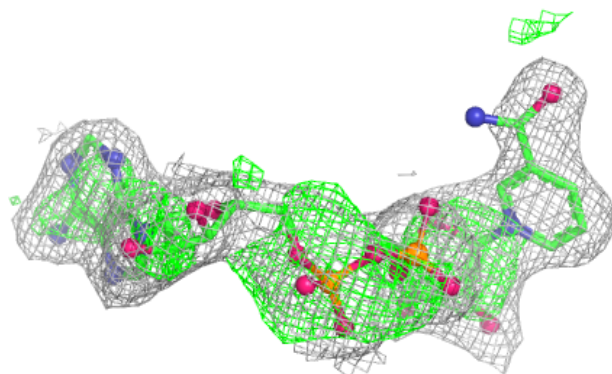
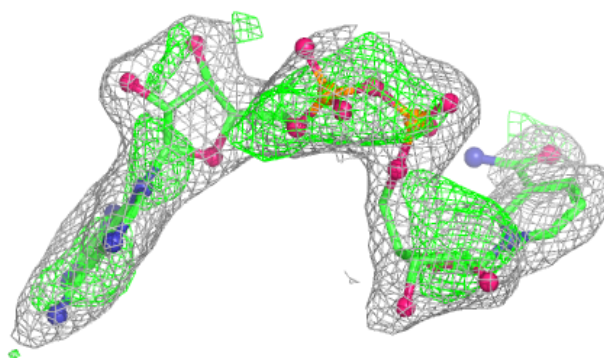


Electron density around G6P A 1417:

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

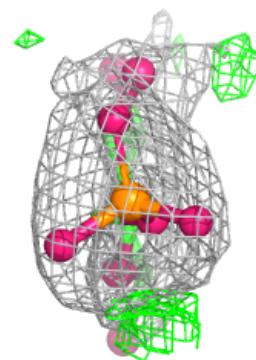
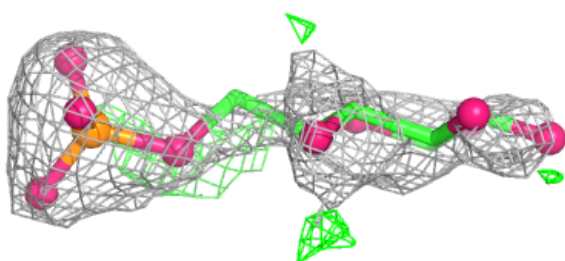
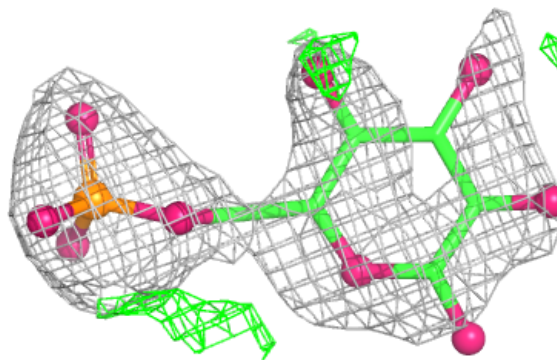
**Electron density around NAD H 1416:**

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

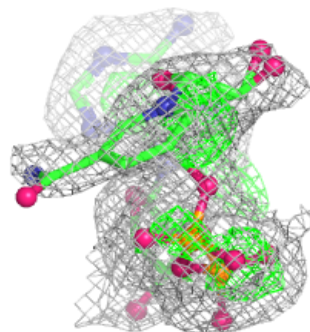
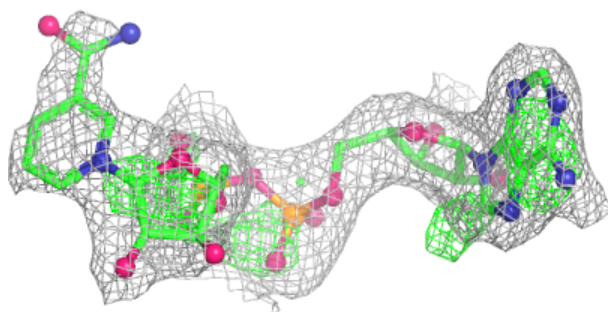
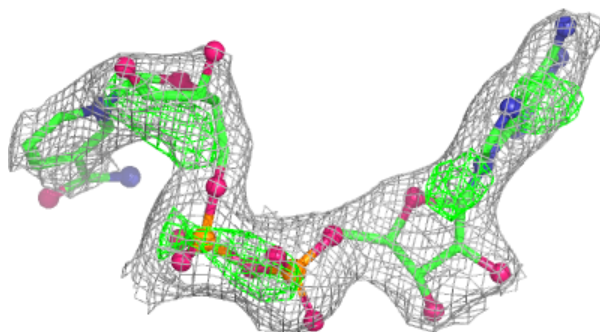


Electron density around G6P E 1417:

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

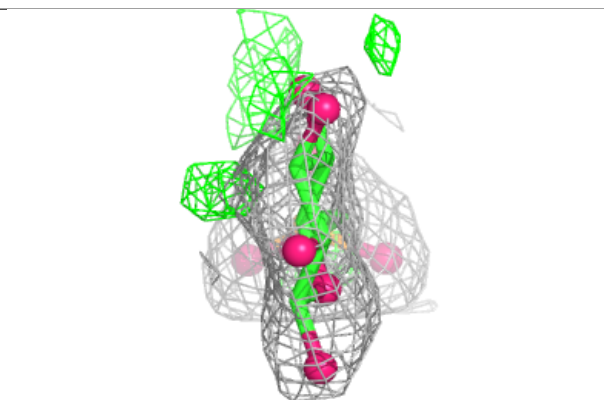
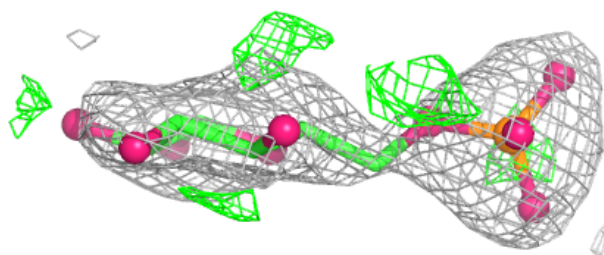
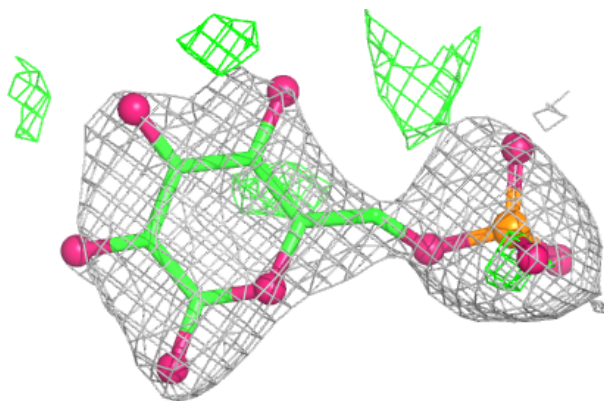
**Electron density around NAD F 1416:**

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

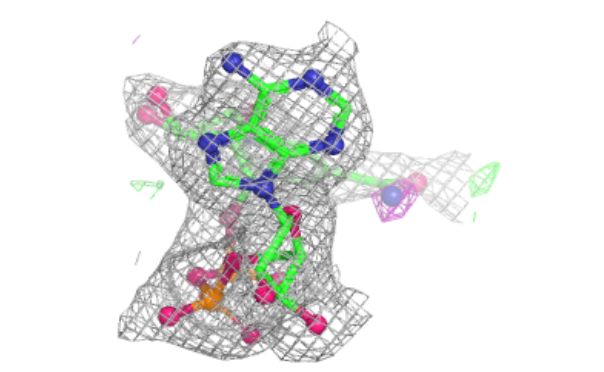
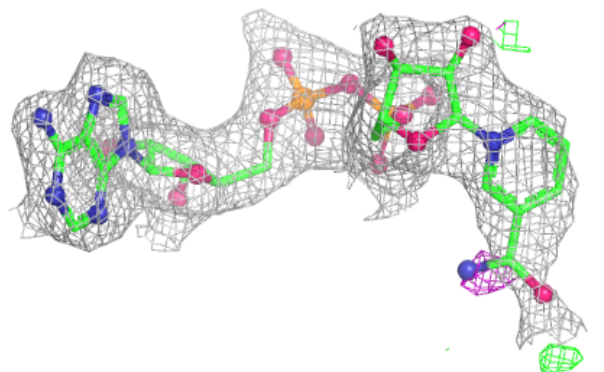
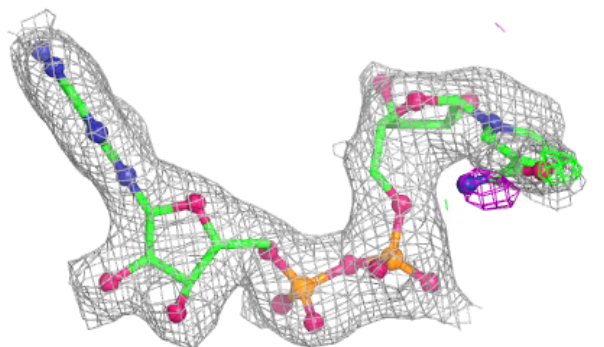


Electron density around G6P B 1417:

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

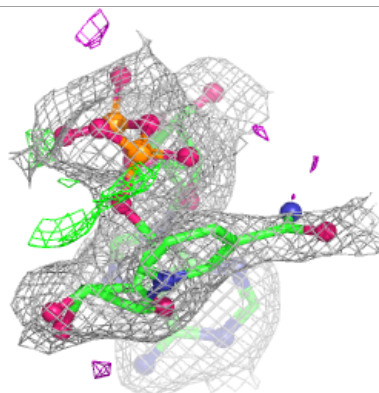
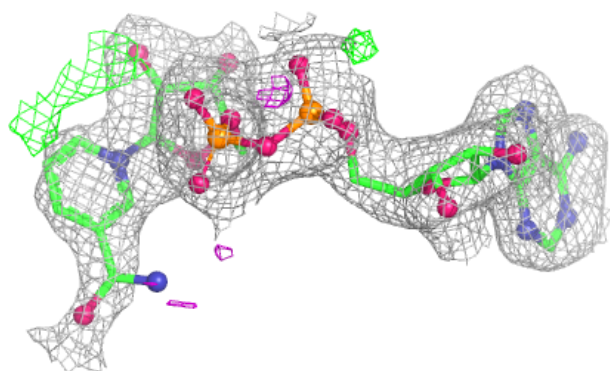
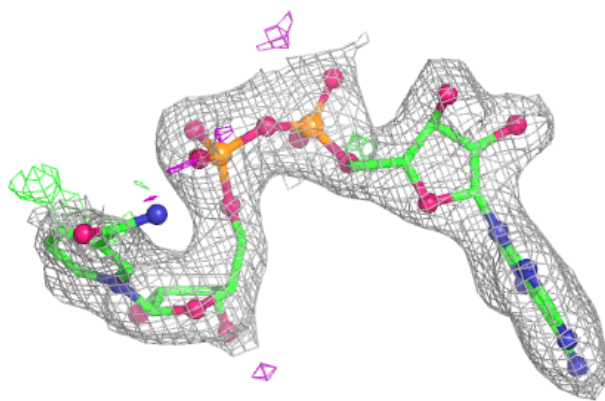
**Electron density around NAD B 1416:**

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

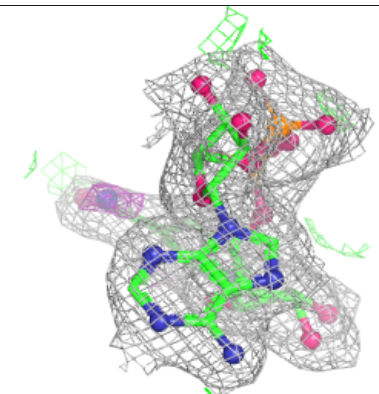
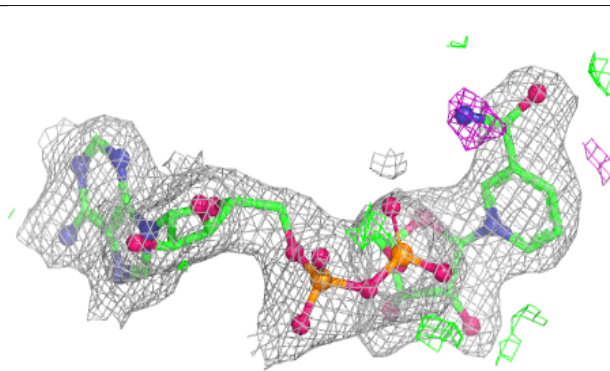
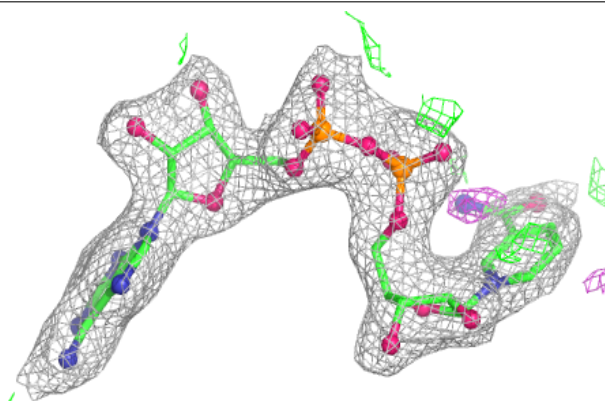


Electron density around NAD G 1416:

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

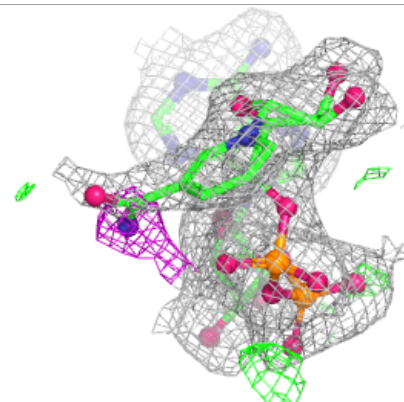
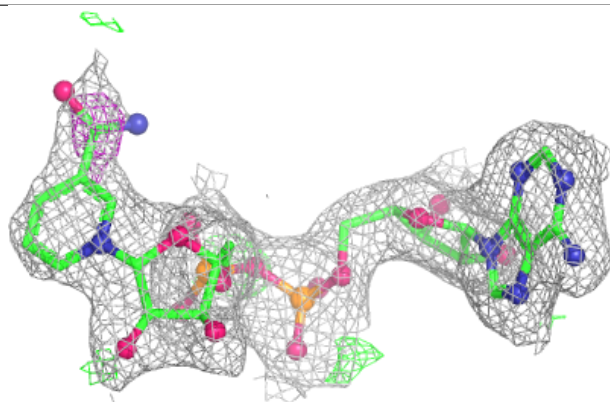
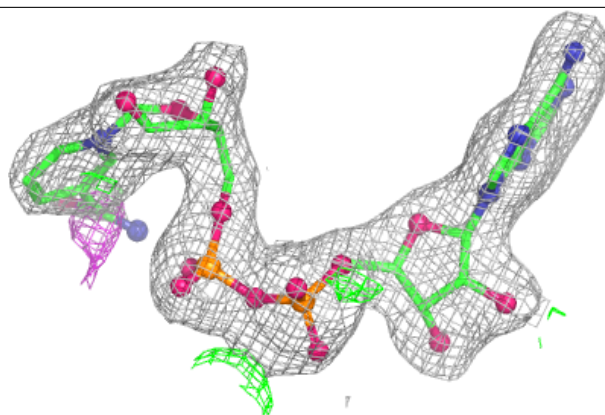
**Electron density around NAD D 1416:**

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

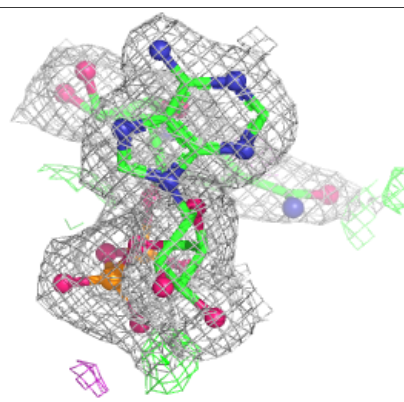
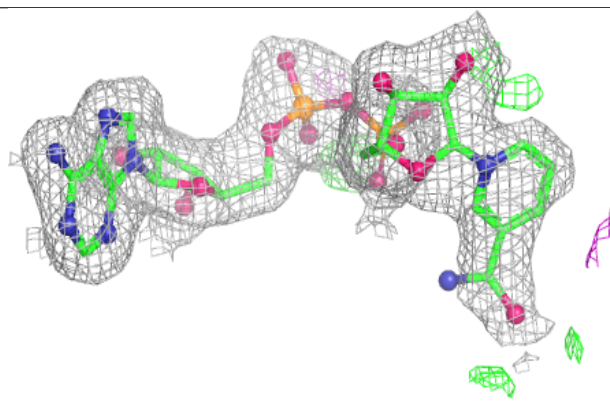
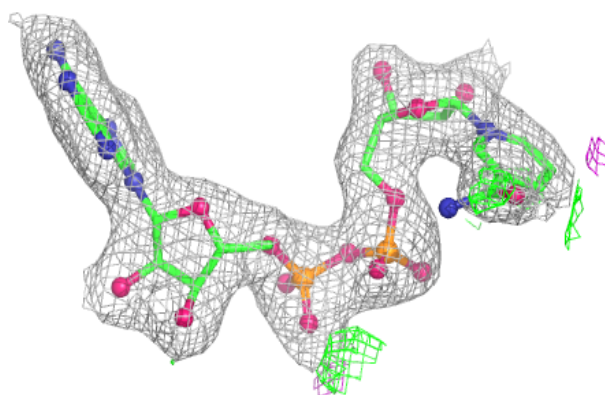


Electron density around NAD C 1416:

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

**Electron density around NAD A 1416:**

$2mF_o-DF_c$ (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.