



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:08 AM UTC

PDB ID : 3OOJ / pdb_00003ooj
Title : C1A mutant of E. coli GlmS in complex with glucose-6P and glutamate
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on : 2010-08-31
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

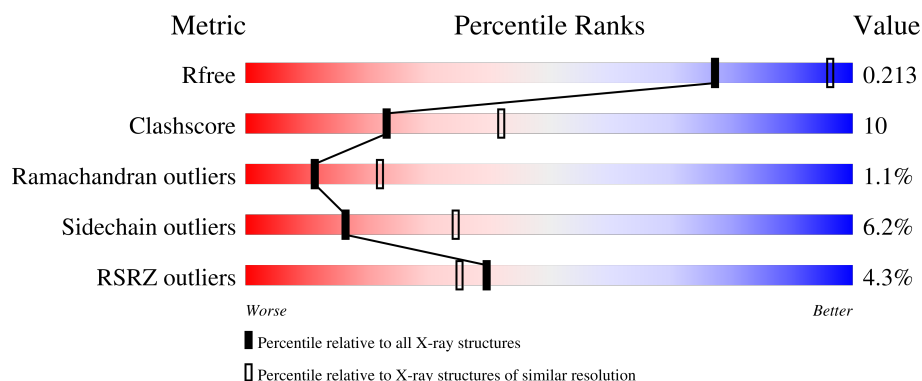
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	608	2% 82% 17% .
1	B	608	4% 76% 21% .
1	C	608	2% 77% 19% ..
1	D	608	5% 75% 21% ..
1	E	608	2% 75% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	608	
1	G	608	
1	H	608	

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
2	GLU	F	701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39092 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 Glucosamine/fructose-6-phosphate aminotransferase, isomerizing.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	5	0
			4718	2966	838	898	16			
1	B	608	Total	C	N	O	S	0	2	0
			4697	2953	834	894	16			
1	C	601	Total	C	N	O	S	0	2	0
			4631	2915	819	881	16			
1	D	602	Total	C	N	O	S	0	3	0
			4634	2915	821	882	16			
1	E	602	Total	C	N	O	S	0	2	0
			4647	2925	826	880	16			
1	F	594	Total	C	N	O	S	0	0	0
			4583	2887	811	869	16			
1	G	605	Total	C	N	O	S	0	1	0
			4653	2929	823	885	16			
1	H	608	Total	C	N	O	S	0	2	0
			4692	2954	828	894	16			

There are 8 discrepancies between the modelled and reference sequences:

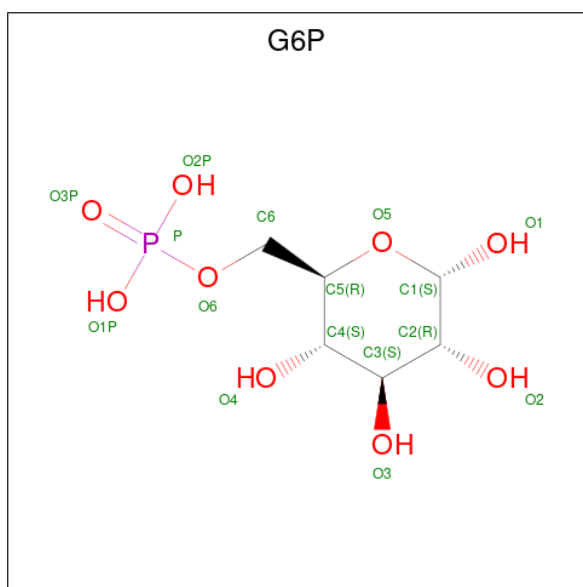
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP C9QXA7
B	1	ALA	CYS	engineered mutation	UNP C9QXA7
C	1	ALA	CYS	engineered mutation	UNP C9QXA7
D	1	ALA	CYS	engineered mutation	UNP C9QXA7
E	1	ALA	CYS	engineered mutation	UNP C9QXA7
F	1	ALA	CYS	engineered mutation	UNP C9QXA7
G	1	ALA	CYS	engineered mutation	UNP C9QXA7
H	1	ALA	CYS	engineered mutation	UNP C9QXA7

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

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



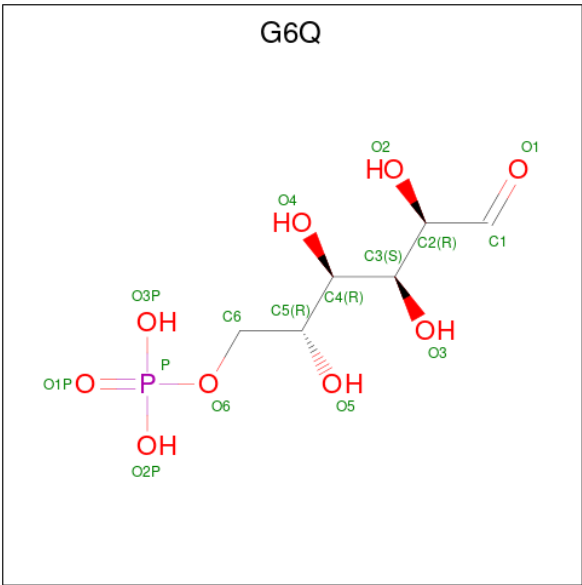
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is GLUCOSE-6-PHOSPHATE (CCD ID: G6Q) (formula: C₆H₁₃O₉P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O	0	0
			231	231		
6	B	192	Total	O	0	0
			192	192		
6	C	196	Total	O	0	0
			196	196		
6	D	244	Total	O	0	0
			244	244		

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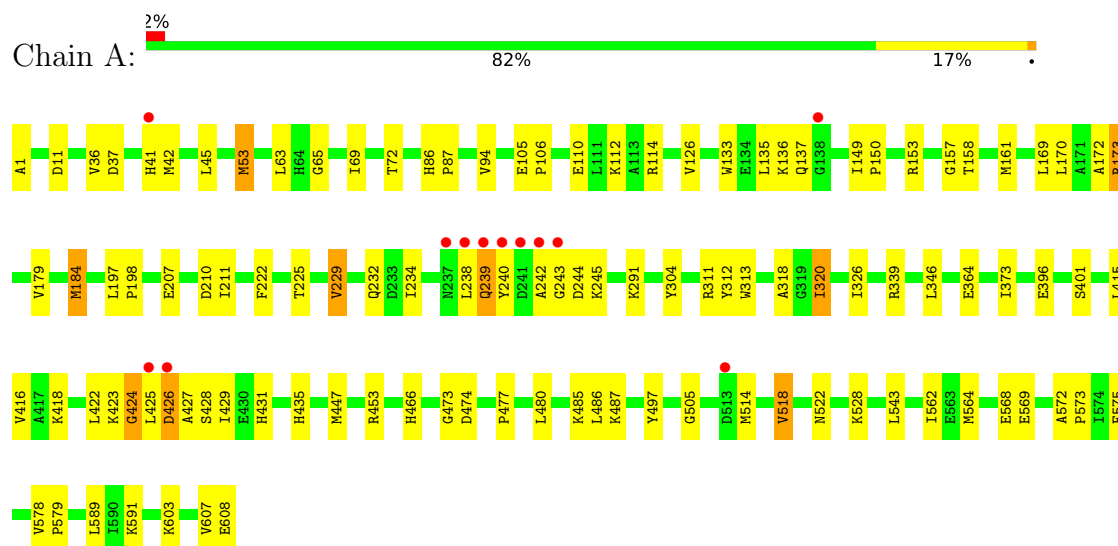
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	123	Total 123	O 123	0	0
6	F	123	Total 123	O 123	0	0
6	G	175	Total 175	O 175	0	0
6	H	169	Total 169	O 169	0	0

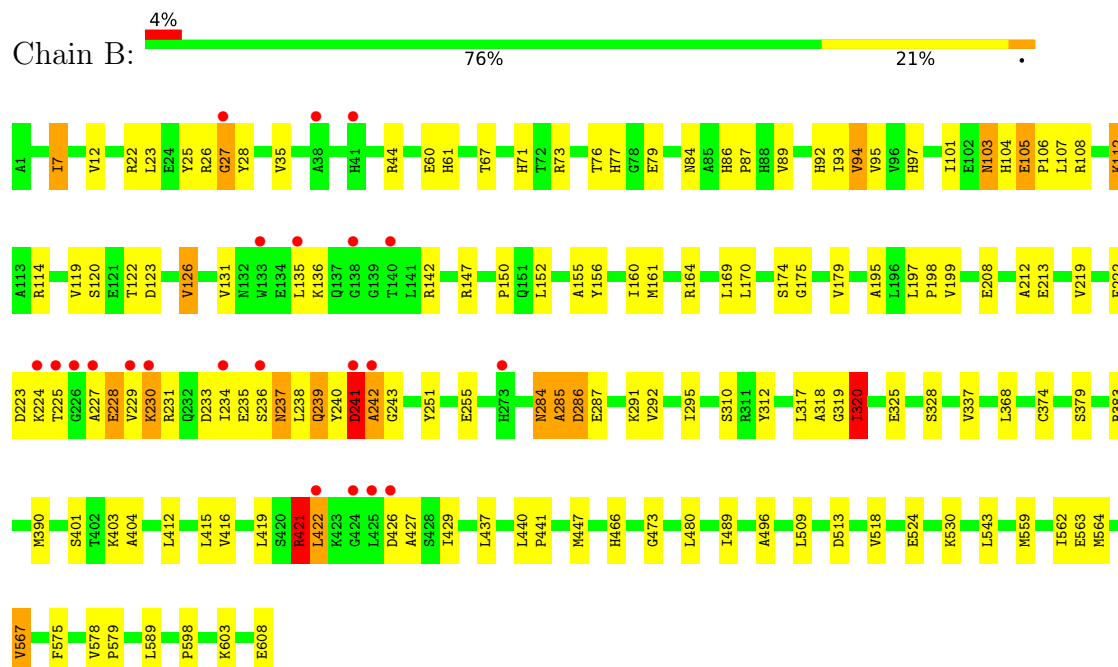
3 Residue-property plots

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: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



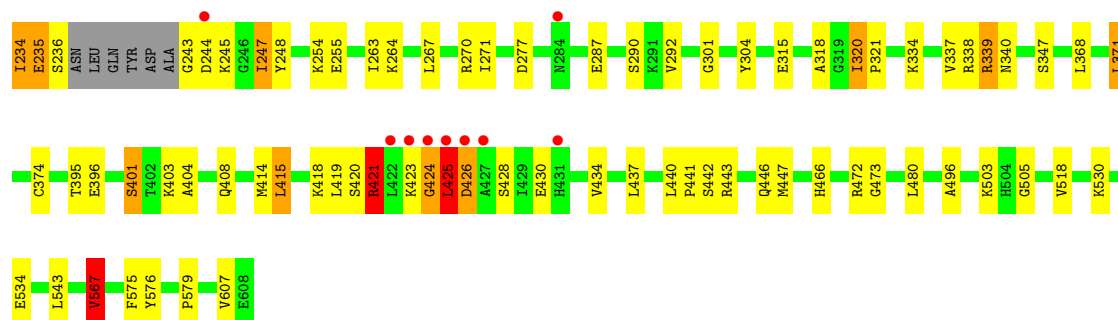
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



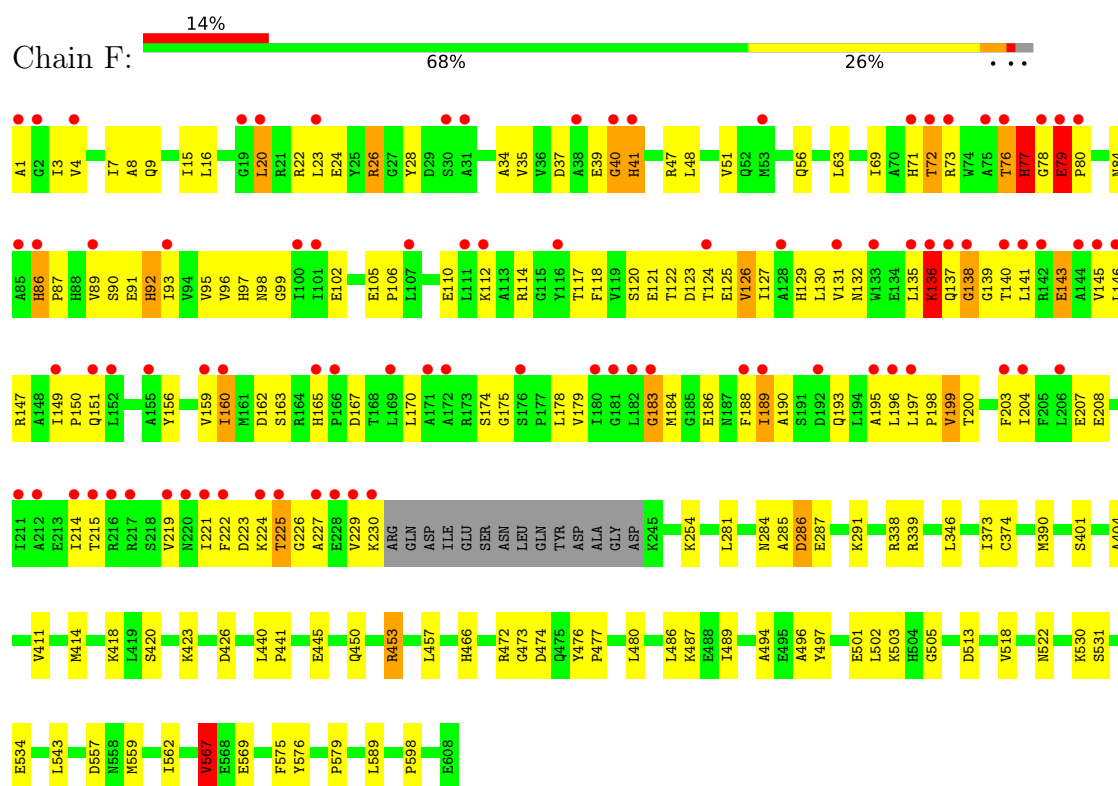
- Chain C:
- | Label | Value | Category |
|-------|-------|----------|
| A1 | 1 | Red |
| G2 | 2 | Green |
| I3 | 3 | Green |
| D11 | 4 | Green |
| E14 | 5 | Green |
| R21 | 6 | Red |
| R22 | 7 | Green |
| L23 | 8 | Green |
| E24 | 9 | Green |
| Y28 | 10 | Green |
| H41 | 11 | Red |
| K50 | 12 | Orange |
| V51 | 13 | Green |
| Q52 | 14 | Green |
| M53 | 15 | Green |
| L54 | 16 | Green |
| L63 | 17 | Green |
| H64 | 18 | Green |
| G65 | 19 | Green |
| H71 | 20 | Green |
| H77 | 21 | Green |
| H86 | 22 | Green |
| S90 | 23 | Green |
| E91 | 24 | Orange |
| H97 | 25 | Green |
| I101 | 26 | Green |
| E102 | 27 | Green |
| E105 | 28 | Green |
| P106 | 29 | Red |
| E110 | 30 | Green |
| L111 | 31 | Red |
| K112 | 32 | Green |
| A113 | 33 | Green |
| F118 | 34 | Red |
| V119 | 35 | Green |
| T122 | 36 | Orange |
| D123 | 37 | Orange |
| T124 | 38 | Orange |
| E125 | 39 | Green |
| V126 | 40 | Orange |
| T127 | 41 | Orange |
| A128 | 42 | Orange |
| W133 | 43 | Red |
| E134 | 44 | Green |
| L135 | 45 | Green |
| K136 | 46 | Red |
| Q137 | 47 | Green |
| G138 | 48 | Green |
| G139 | 49 | Green |
| T140 | 50 | Green |
| E143 | 51 | Green |
| A144 | 52 | Green |
| V145 | 53 | Green |
| L146 | 54 | Green |
| R147 | 55 | Green |
| ASP | 56 | Grey |
| A148 | 57 | Green |
| I149 | 58 | Green |
| P150 | 59 | Orange |
| Q151 | 60 | Green |
| R152 | 61 | Green |
| G157 | 62 | Green |
| M161 | 63 | Green |
| R164 | 64 | Orange |
| L169 | 65 | Green |
| L170 | 66 | Green |
| A171 | 67 | Green |
| A172 | 68 | Green |
| R173 | 69 | Green |
| S176 | 70 | Green |
| P177 | 71 | Green |
| T180 | 72 | Green |
| G181 | 73 | Green |
| L182 | 74 | Green |
| G183 | 75 | Green |
| M184 | 76 | Green |
| A190 | 77 | Green |
| Q193 | 78 | Green |
| L194 | 79 | Orange |
| A195 | 80 | Green |
| L196 | 81 | Green |
| L197 | 82 | Green |
| P198 | 83 | Green |
| V199 | 84 | Green |
| T200 | 85 | Orange |
| F203 | 86 | Orange |
| I204 | 87 | Orange |
| F205 | 88 | Orange |
| L206 | 89 | Orange |
| T221 | 90 | Green |
| F222 | 91 | Green |
| E228 | 92 | Green |
| V229 | 93 | Green |
| K230 | 94 | Orange |
| R231 | 95 | Orange |
| Q232 | 96 | Green |
| D233 | 97 | Green |
| I234 | 98 | Green |
| E235 | 99 | Green |
| S236 | 100 | Green |
| ASN | 101 | Grey |
| LEU | 102 | Grey |
| GLN | 103 | Grey |
| TYR | 104 | Grey |
| ALA | 105 | Grey |
| GLY | 106 | Grey |
| D244 | 107 | Green |
| K254 | 108 | Green |
| E258 | 109 | Green |
| N261 | 110 | Green |
| A285 | 111 | Orange |
| D286 | 112 | Orange |
| L295 | 113 | Green |
| L298 | 114 | Green |
| G301 | 115 | Green |
| Y304 | 116 | Green |
| V309 | 117 | Green |
| F330 | 118 | Green |
| R339 | 119 | Green |
| L346 | 120 | Green |
| I373 | 121 | Green |
| A400 | 122 | Green |
| L415 | 123 | Green |
| K418 | 124 | Green |
| L419 | 125 | Green |
| S420 | 126 | Orange |
| R421 | 127 | Orange |
| L430 | 128 | Orange |
| H431 | 129 | Red |
| R443 | 130 | Orange |
| M477 | 131 | Orange |
| K464 | 132 | Green |
| H465 | 133 | Green |
| H466 | 134 | Green |
| D474 | 135 | Green |
| P477 | 136 | Green |
| L480 | 137 | Green |
| K485 | 138 | Green |
| L486 | 139 | Green |
| K487 | 140 | Green |
| E488 | 141 | Green |
| A496 | 142 | Green |
| Y497 | 143 | Green |
| K503 | 144 | Green |
| H504 | 145 | Green |
| G505 | 146 | Green |
| A512 | 147 | Green |
| D513 | 148 | Green |
| A520 | 149 | Green |
| E524 | 150 | Green |
| K530 | 151 | Green |
| L543 | 152 | Green |
| D557 | 153 | Green |
| M558 | 154 | Green |
| M559 | 155 | Green |
| I562 | 156 | Green |
| E563 | 157 | Green |
| M564 | 158 | Green |
| V567 | 159 | Green |
| E568 | | |

- Chain D:

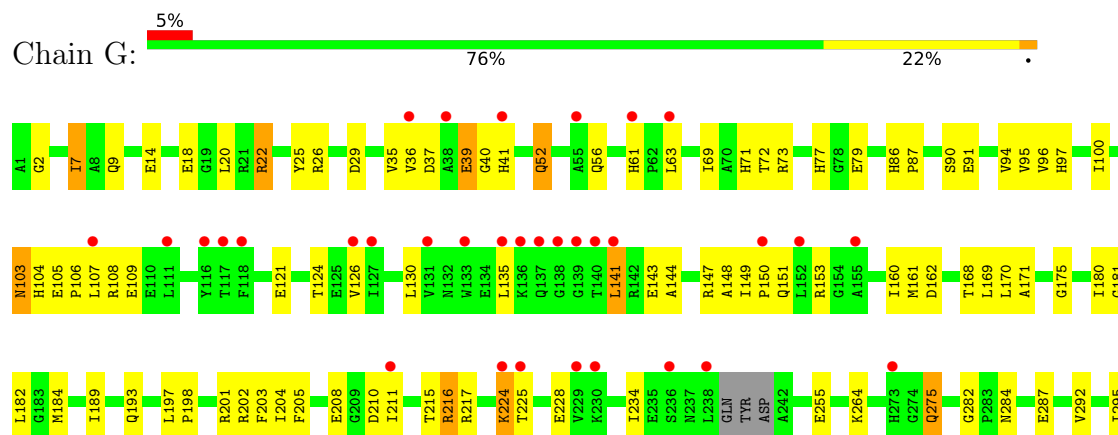
- Chain E:

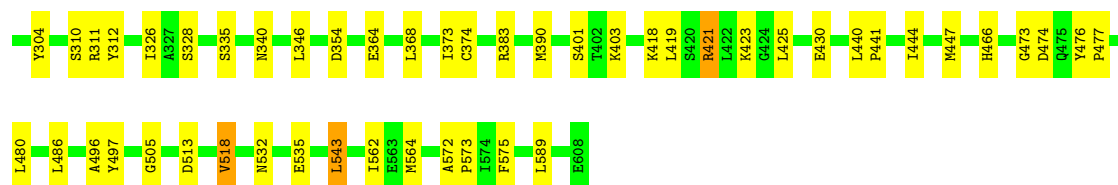


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

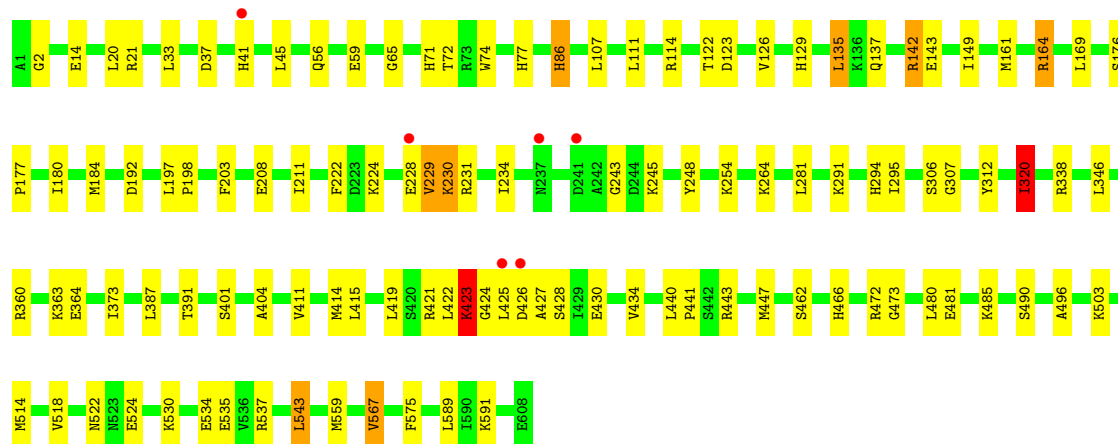
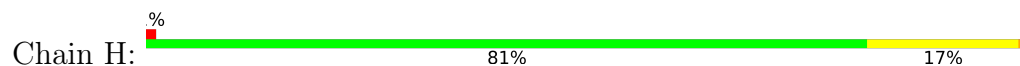


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing





- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	247.60Å 247.60Å 630.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.99-2.50) 98.3 (19.99-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.178 , 0.220 0.170 , 0.213	Depositor DCC
R_{free} test set	12633 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.000 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.000 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39092	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: GOL, G6Q, 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	0.57	0/4805	0.87	6/6510 (0.1%)
1	B	0.54	0/4783	0.89	8/6478 (0.1%)
1	C	0.56	1/4714 (0.0%)	0.87	1/6384 (0.0%)
1	D	0.55	0/4712	0.85	3/6380 (0.0%)
1	E	0.52	0/4734	0.84	3/6409 (0.0%)
1	F	0.53	0/4662	0.86	4/6312 (0.1%)
1	G	0.51	0/4736	0.84	3/6414 (0.0%)
1	H	0.53	0/4780	0.85	3/6475 (0.0%)
All	All	0.54	1/37926 (0.0%)	0.86	31/51362 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	ALA	CA-CB	5.22	1.57	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	ARG	N-CA-C	10.32	126.44	113.43
1	H	320	ILE	CB-CA-C	-7.39	102.70	110.53
1	F	567	VAL	CB-CA-C	-7.05	99.84	110.55
1	F	423	LYS	CB-CA-C	-6.97	108.55	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	136	LYS	N-CA-C	-6.75	103.61	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	LEU	Peptide

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	4718	0	4704	76	0
1	B	4697	0	4698	108	0
1	C	4631	0	4638	107	0
1	D	4634	0	4640	93	0
1	E	4647	0	4666	89	0
1	F	4583	0	4617	152	0
1	G	4653	0	4669	81	0
1	H	4692	0	4703	74	0
2	A	10	0	5	0	0
2	B	10	0	5	2	0
2	C	10	0	5	2	0
2	D	10	0	5	1	0
2	E	10	0	5	2	0
2	F	10	0	5	4	0
2	G	10	0	5	0	0
2	H	10	0	5	1	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	0	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	0	0
4	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	16	0	11	3	0
5	B	16	0	11	0	0
5	C	16	0	11	3	0
5	D	16	0	11	1	0
5	E	16	0	11	1	0
5	F	16	0	11	3	0
5	G	16	0	11	2	0
5	H	16	0	11	0	0
6	A	231	0	0	2	0
6	B	192	0	0	3	0
6	C	196	0	0	3	0
6	D	244	0	0	5	0
6	E	123	0	0	1	0
6	F	123	0	0	2	0
6	G	175	0	0	2	0
6	H	169	0	0	2	0
All	All	39092	0	37615	772	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 10.

The worst 5 of 772 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HB3	1:B:243:GLY:HA3	1.32	1.10
1:H:230:LYS:HE3	1:H:231:ARG:H	1.11	1.10
1:B:236:SER:HA	1:B:237:ASN:HB2	1.14	1.07
1:B:236:SER:HA	1:B:237:ASN:CB	1.92	0.97
1:F:569:GLU:HG3	5:F:610:G6Q:O2	1.66	0.94

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	611/608 (100%)	586 (96%)	21 (3%)	4 (1%)	18	34
1	B	608/608 (100%)	577 (95%)	21 (4%)	10 (2%)	7	14
1	C	599/608 (98%)	572 (96%)	20 (3%)	7 (1%)	10	20
1	D	601/608 (99%)	576 (96%)	18 (3%)	7 (1%)	10	20
1	E	600/608 (99%)	566 (94%)	28 (5%)	6 (1%)	12	24
1	F	590/608 (97%)	531 (90%)	47 (8%)	12 (2%)	6	10
1	G	602/608 (99%)	576 (96%)	22 (4%)	4 (1%)	18	34
1	H	608/608 (100%)	587 (96%)	19 (3%)	2 (0%)	36	55
All	All	4819/4864 (99%)	4571 (95%)	196 (4%)	52 (1%)	11	22

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	B	241	ASP
1	B	242	ALA
1	B	284	ASN
1	B	285	ALA

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	498/499 (100%)	469 (94%)	29 (6%)	18	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	497/499 (100%)	464 (93%)	33 (7%)	15	32
1	C	490/499 (98%)	466 (95%)	24 (5%)	22	45
1	D	488/499 (98%)	458 (94%)	30 (6%)	17	35
1	E	492/499 (99%)	458 (93%)	34 (7%)	14	30
1	F	487/499 (98%)	452 (93%)	35 (7%)	13	28
1	G	493/499 (99%)	465 (94%)	28 (6%)	18	39
1	H	497/499 (100%)	466 (94%)	31 (6%)	16	34
All	All	3942/3992 (99%)	3698 (94%)	244 (6%)	16	34

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	589	LEU
1	H	135	LEU
1	E	423	LYS
1	H	114	ARG
1	H	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	446	GLN
1	F	98	ASN
1	G	165	HIS
1	F	86	HIS
1	F	104	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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
5	G6Q	D	611	-	14,15,15	1.67	4 (28%)	19,21,21	1.20	2 (10%)
5	G6Q	F	610	-	14,15,15	1.32	3 (21%)	19,21,21	1.32	3 (15%)
5	G6Q	E	610	-	14,15,15	1.46	2 (14%)	19,21,21	1.18	2 (10%)
3	G6P	H	614	-	16,16,16	1.49	2 (12%)	23,24,24	1.04	2 (8%)
2	GLU	D	701	-	8,9,9	1.07	1 (12%)	8,11,11	1.16	1 (12%)
4	GOL	E	609	-	5,5,5	0.35	0	5,5,5	0.86	0
2	GLU	B	701	-	8,9,9	1.12	1 (12%)	8,11,11	1.23	1 (12%)
3	G6P	C	610	-	16,16,16	1.47	2 (12%)	23,24,24	1.03	2 (8%)
4	GOL	A	609	-	5,5,5	0.36	0	5,5,5	0.54	0
2	GLU	A	701	-	8,9,9	1.11	1 (12%)	8,11,11	1.12	1 (12%)
3	G6P	D	609	-	16,16,16	1.48	3 (18%)	23,24,24	1.11	1 (4%)
5	G6Q	G	610	-	14,15,15	1.48	3 (21%)	19,21,21	1.03	2 (10%)
5	G6Q	A	610	-	14,15,15	1.52	3 (21%)	19,21,21	1.03	1 (5%)
3	G6P	B	612	-	16,16,16	1.46	2 (12%)	23,24,24	0.87	0
2	GLU	F	701	-	8,9,9	1.15	1 (12%)	8,11,11	1.07	1 (12%)
5	G6Q	C	611	-	14,15,15	1.44	2 (14%)	19,21,21	1.23	2 (10%)
3	G6P	E	616	-	16,16,16	1.53	2 (12%)	23,24,24	1.65	5 (21%)
2	GLU	C	701	-	8,9,9	1.08	1 (12%)	8,11,11	1.22	1 (12%)
4	GOL	H	609	-	5,5,5	0.48	0	5,5,5	0.47	0
2	GLU	E	701	-	8,9,9	1.28	1 (12%)	8,11,11	1.04	0
4	GOL	B	609	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GLU	H	701	-	8,9,9	1.10	1 (12%)	8,11,11	1.22	1 (12%)
4	GOL	C	609	-	5,5,5	0.33	0	5,5,5	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G6P	A	611	-	16,16,16	1.45	2 (12%)	23,24,24	0.96	1 (4%)
3	G6P	F	615	-	16,16,16	1.49	2 (12%)	23,24,24	0.89	0
2	GLU	G	701	-	8,9,9	1.11	1 (12%)	8,11,11	1.24	1 (12%)
3	G6P	G	613	-	16,16,16	1.52	2 (12%)	23,24,24	1.22	3 (13%)
5	G6Q	H	610	-	14,15,15	1.44	2 (14%)	19,21,21	1.20	2 (10%)
5	G6Q	B	610	-	14,15,15	1.49	3 (21%)	19,21,21	1.10	1 (5%)
4	GOL	D	610	-	5,5,5	0.33	0	5,5,5	0.48	0
4	GOL	G	609	-	5,5,5	0.32	0	5,5,5	0.60	0
4	GOL	F	609	-	5,5,5	0.30	0	5,5,5	0.57	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
5	G6Q	D	611	-	-	8/19/20/20	-
5	G6Q	F	610	-	-	9/19/20/20	-
5	G6Q	E	610	-	-	11/19/20/20	-
3	G6P	H	614	-	-	0/6/26/26	0/1/1/1
2	GLU	D	701	-	-	2/9/9/9	-
4	GOL	E	609	-	-	2/4/4/4	-
2	GLU	B	701	-	-	2/9/9/9	-
3	G6P	C	610	-	-	0/6/26/26	0/1/1/1
4	GOL	A	609	-	-	4/4/4/4	-
2	GLU	A	701	-	-	2/9/9/9	-
3	G6P	D	609	-	-	0/6/26/26	0/1/1/1
5	G6Q	G	610	-	-	4/19/20/20	-
5	G6Q	A	610	-	-	11/19/20/20	-
3	G6P	B	612	-	-	2/6/26/26	0/1/1/1
2	GLU	F	701	-	-	3/9/9/9	-
5	G6Q	C	611	-	-	10/19/20/20	-
3	G6P	E	616	-	-	0/6/26/26	0/1/1/1
2	GLU	C	701	-	-	0/9/9/9	-
4	GOL	H	609	-	-	4/4/4/4	-
2	GLU	E	701	-	-	2/9/9/9	-
4	GOL	B	609	-	-	0/4/4/4	-
2	GLU	H	701	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	609	-	-	2/4/4/4	-
3	G6P	A	611	-	-	1/6/26/26	0/1/1/1
3	G6P	F	615	-	-	1/6/26/26	0/1/1/1
2	GLU	G	701	-	-	2/9/9/9	-
3	G6P	G	613	-	-	0/6/26/26	0/1/1/1
5	G6Q	H	610	-	-	9/19/20/20	-
5	G6Q	B	610	-	-	5/19/20/20	-
4	GOL	D	610	-	-	0/4/4/4	-
4	GOL	G	609	-	-	4/4/4/4	-
4	GOL	F	609	-	-	3/4/4/4	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	G6Q	O2-C2	-3.23	1.37	1.43
5	D	611	G6Q	O2-C2	-3.11	1.37	1.43
5	G	610	G6Q	O2-C2	-3.02	1.38	1.43
5	B	610	G6Q	O2-C2	-2.98	1.38	1.43
3	G	613	G6P	P-O2P	2.95	1.65	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	616	G6P	C1-O5-C5	4.21	121.79	113.65
5	H	610	G6Q	O6-C6-C5	3.74	119.33	109.36
5	C	611	G6Q	O6-C6-C5	3.54	118.82	109.36
5	B	610	G6Q	O6-C6-C5	3.46	118.59	109.36
5	E	610	G6Q	O6-C6-C5	3.43	118.52	109.36

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	GOL	O2-C2-C3-O3
4	C	609	GOL	O1-C1-C2-O2
4	C	609	GOL	O1-C1-C2-C3
4	E	609	GOL	O1-C1-C2-C3
4	F	609	GOL	O1-C1-C2-C3

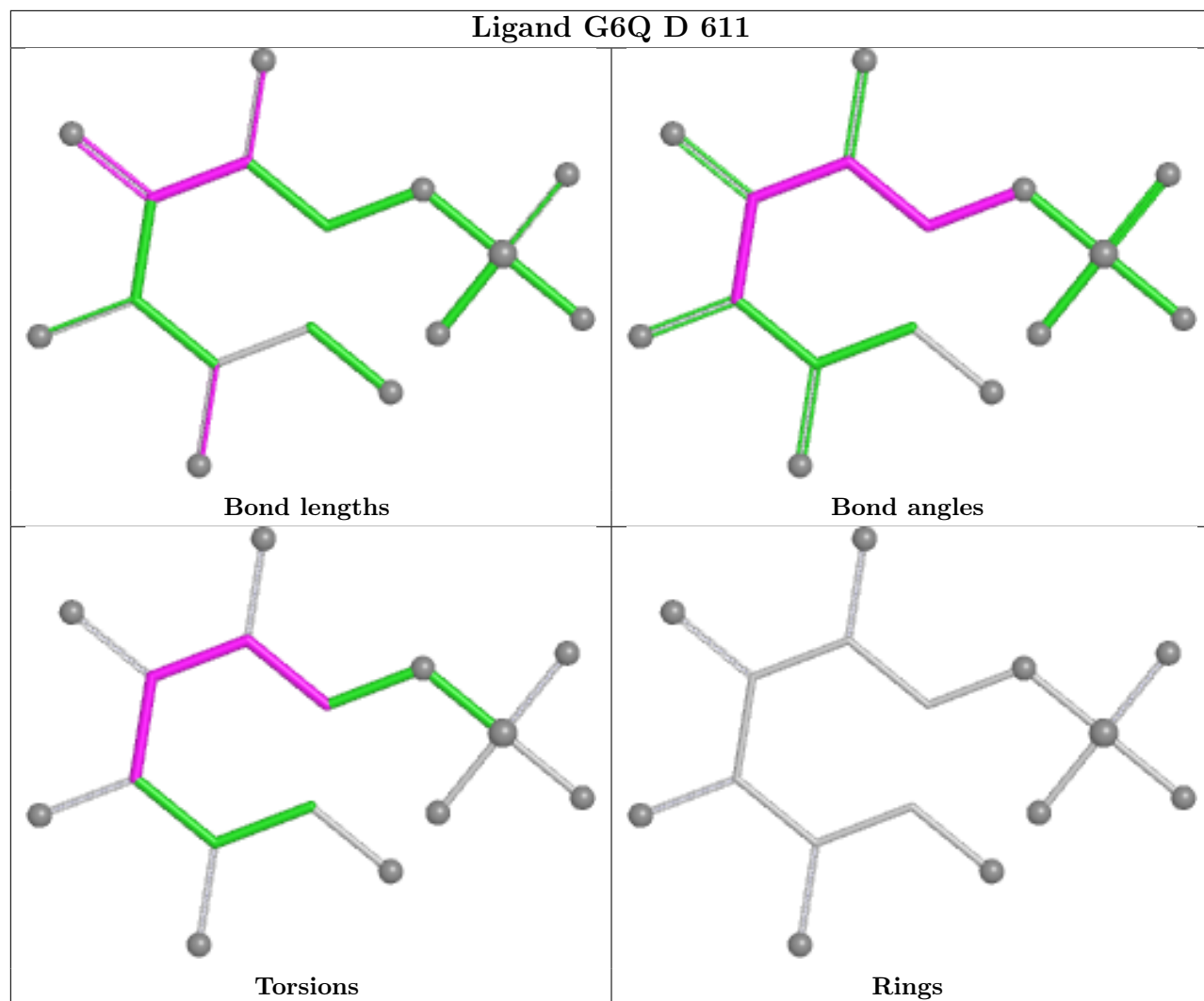
There are no ring outliers.

14 monomers are involved in 27 short contacts:

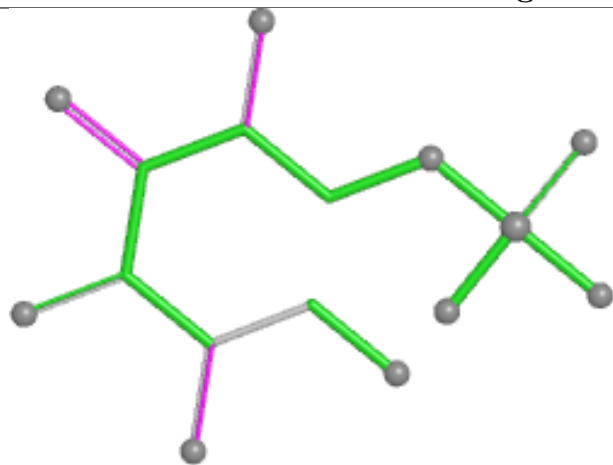
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	611	G6Q	1	0
5	F	610	G6Q	3	0
5	E	610	G6Q	1	0
2	D	701	GLU	1	0
4	E	609	GOL	1	0
2	B	701	GLU	2	0
4	A	609	GOL	1	0
5	G	610	G6Q	2	0
5	A	610	G6Q	3	0
2	F	701	GLU	4	0
5	C	611	G6Q	3	0
2	C	701	GLU	2	0
2	E	701	GLU	2	0
2	H	701	GLU	1	0

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.

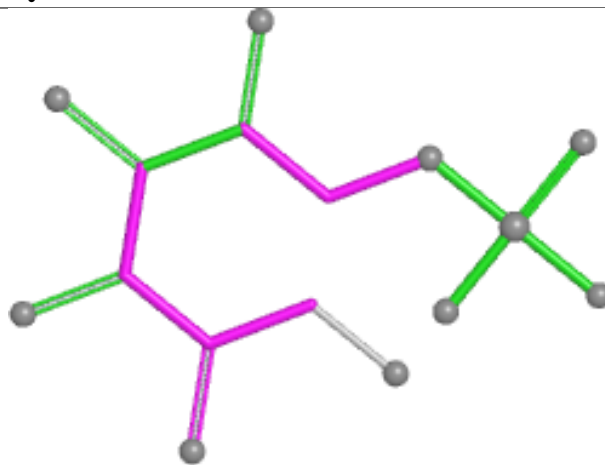
Ligand G6Q D 611



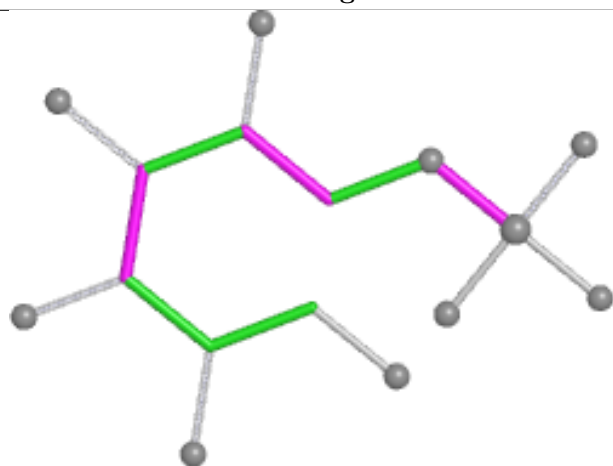
Ligand G6Q F 610



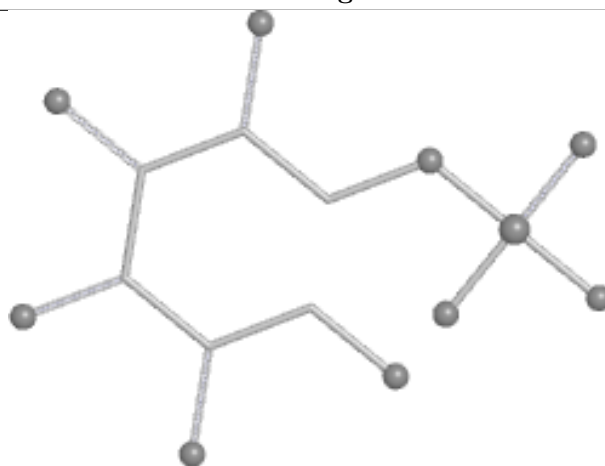
Bond lengths



Bond angles

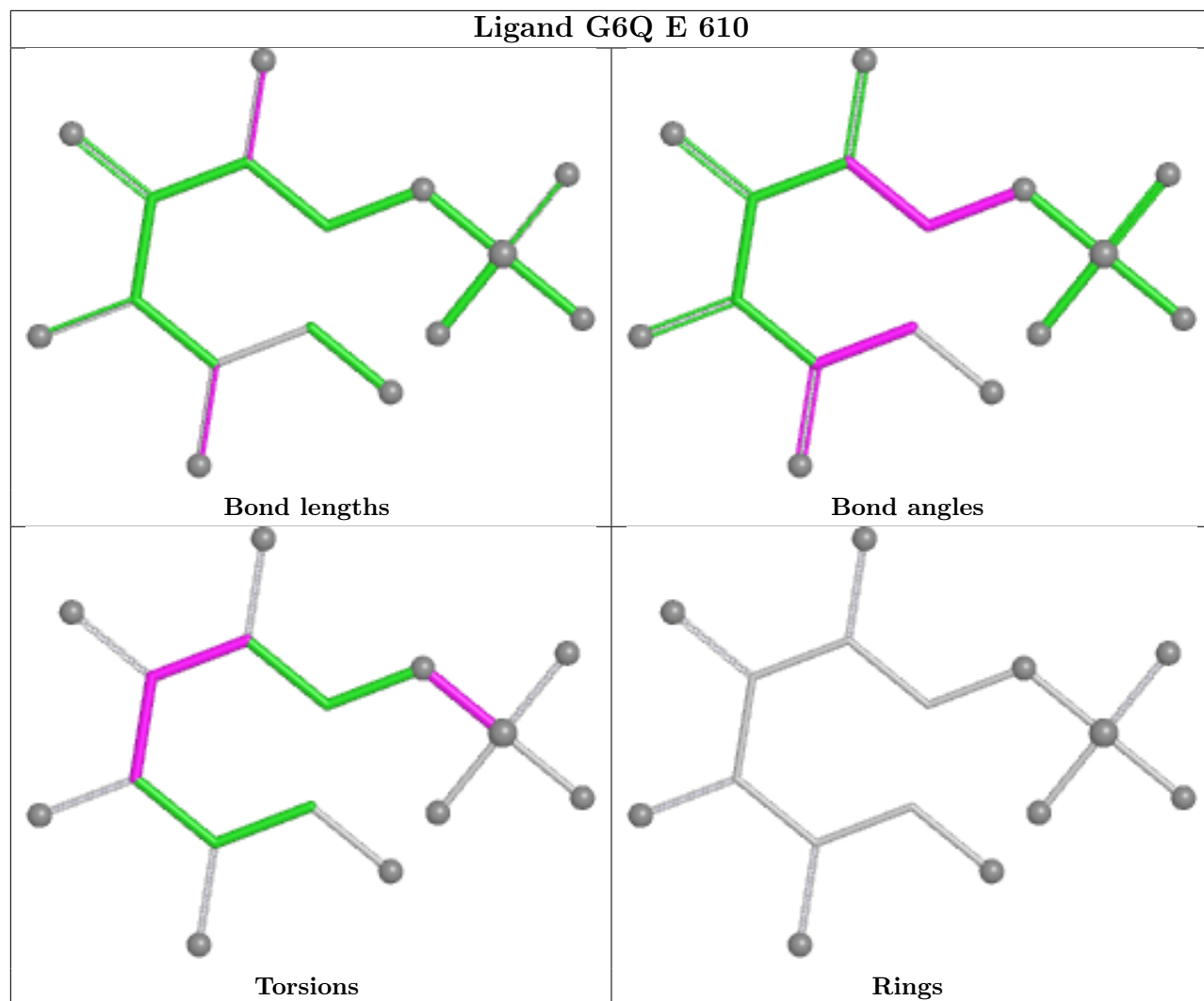


Torsions

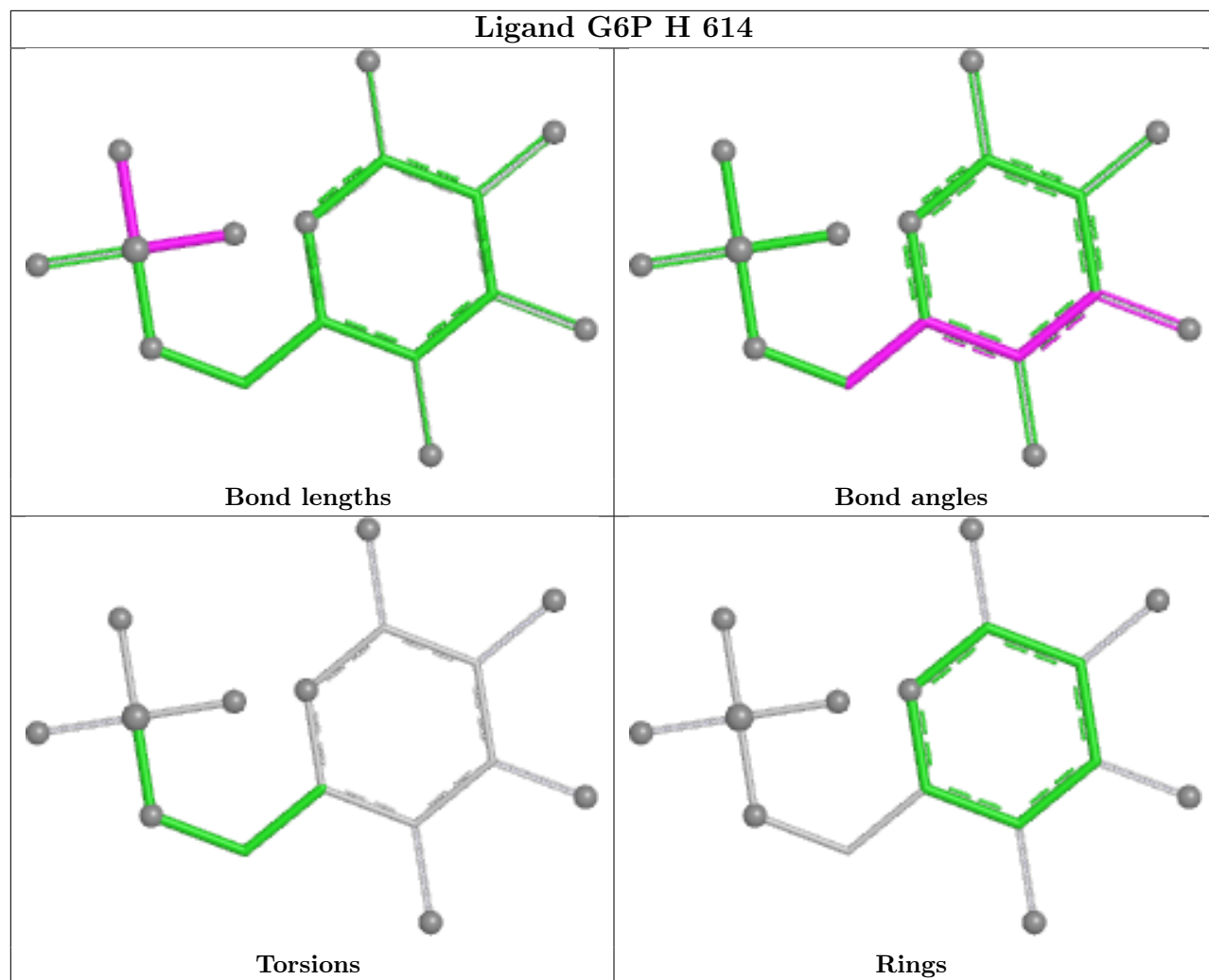


Rings

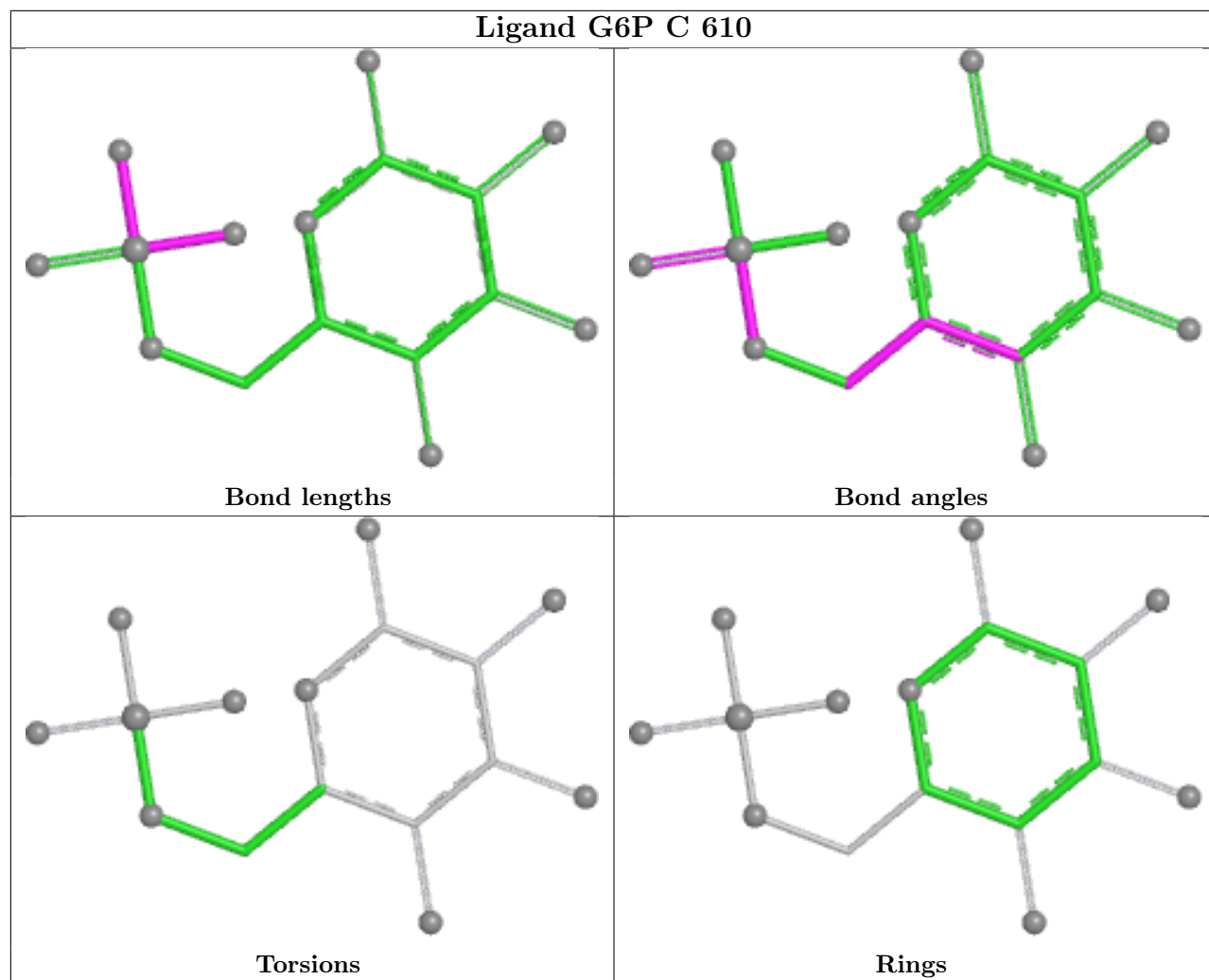
Ligand G6Q E 610



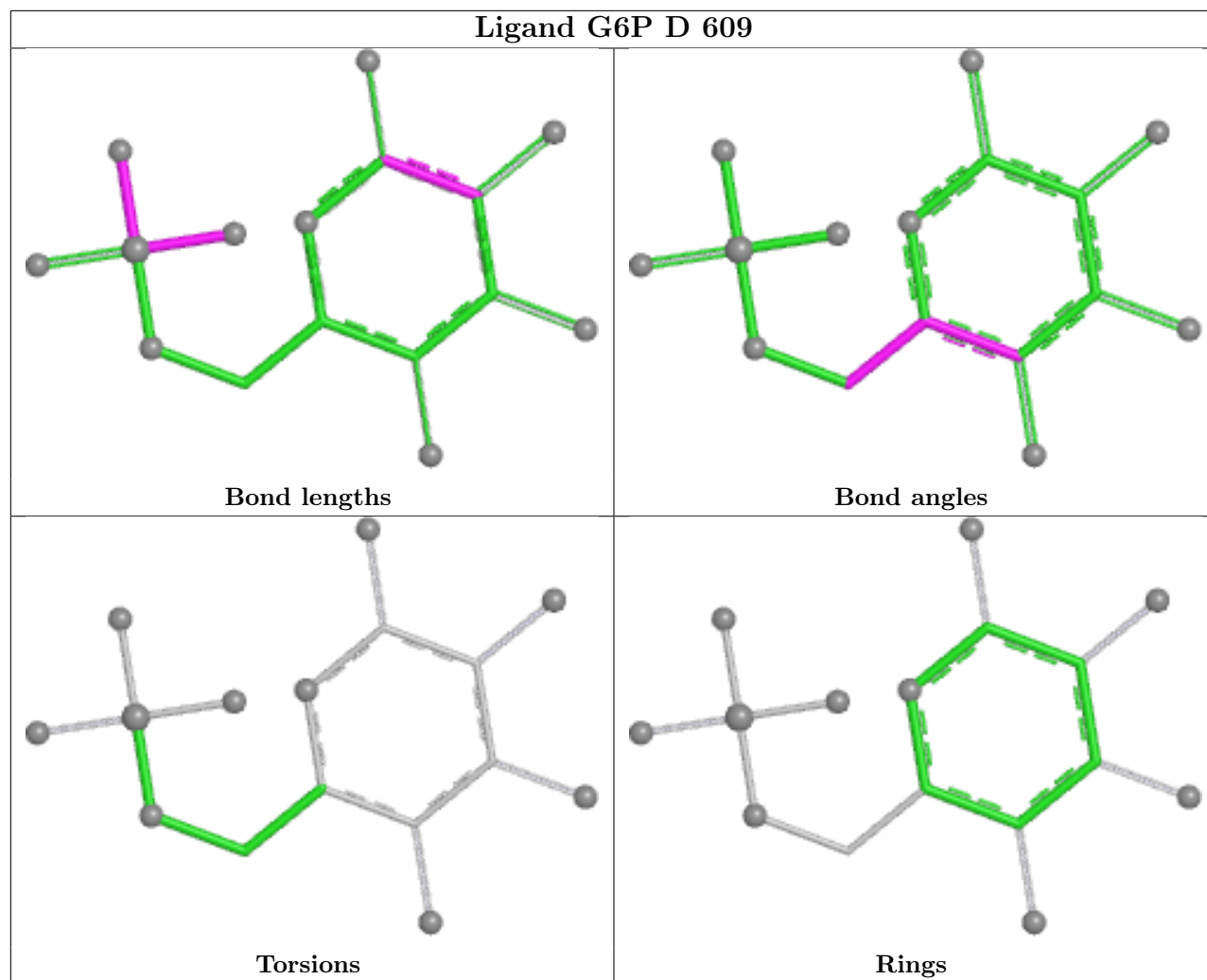
Ligand G6P H 614



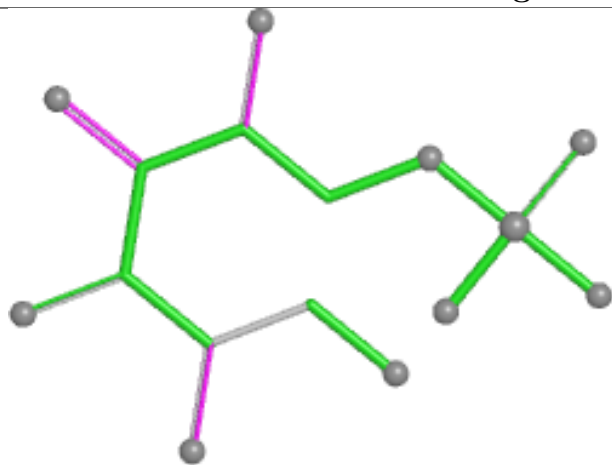
Ligand G6P C 610



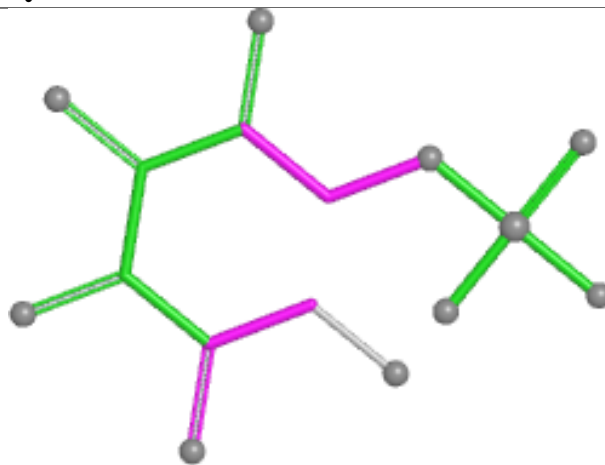
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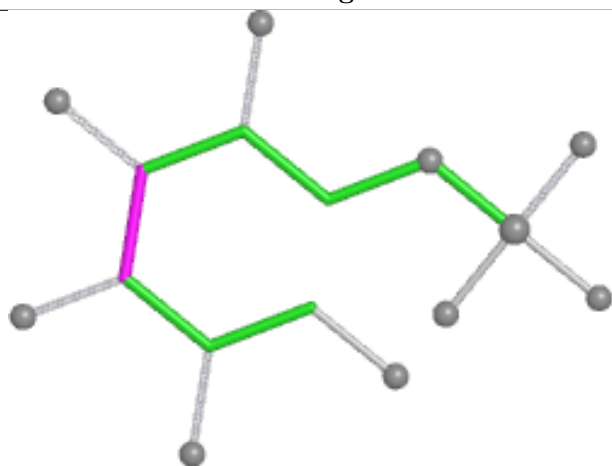
Ligand G6Q G 610



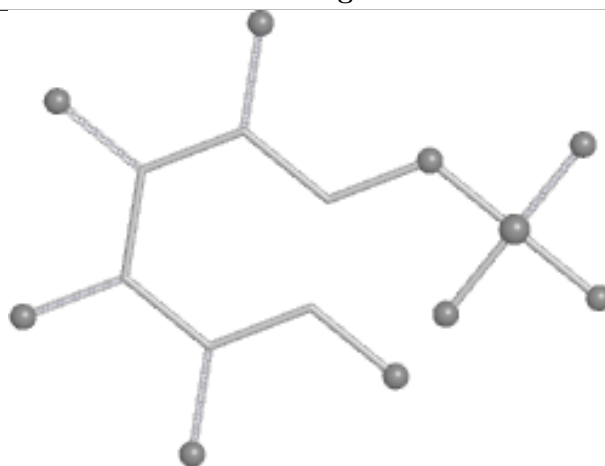
Bond lengths



Bond angles

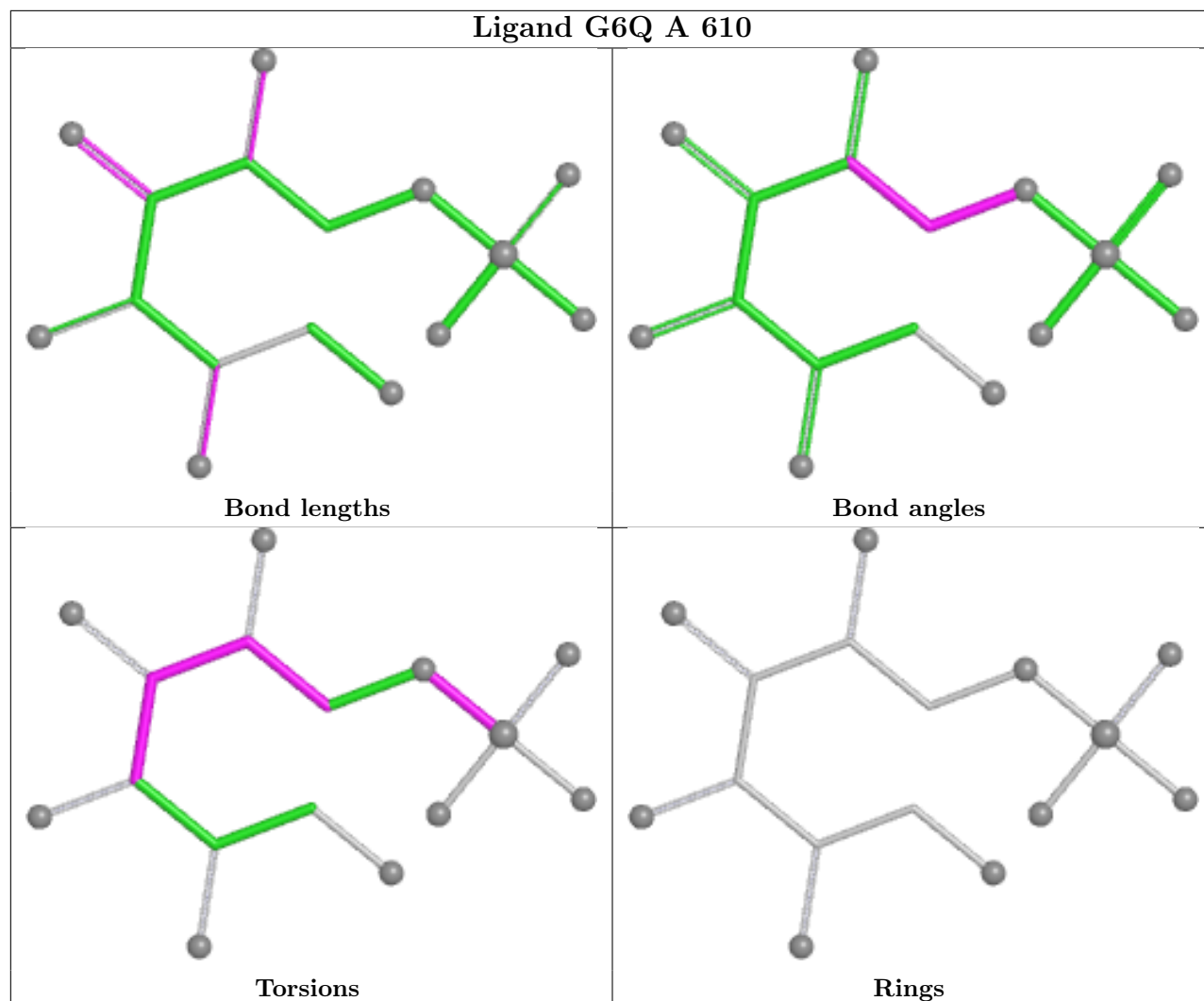


Torsions

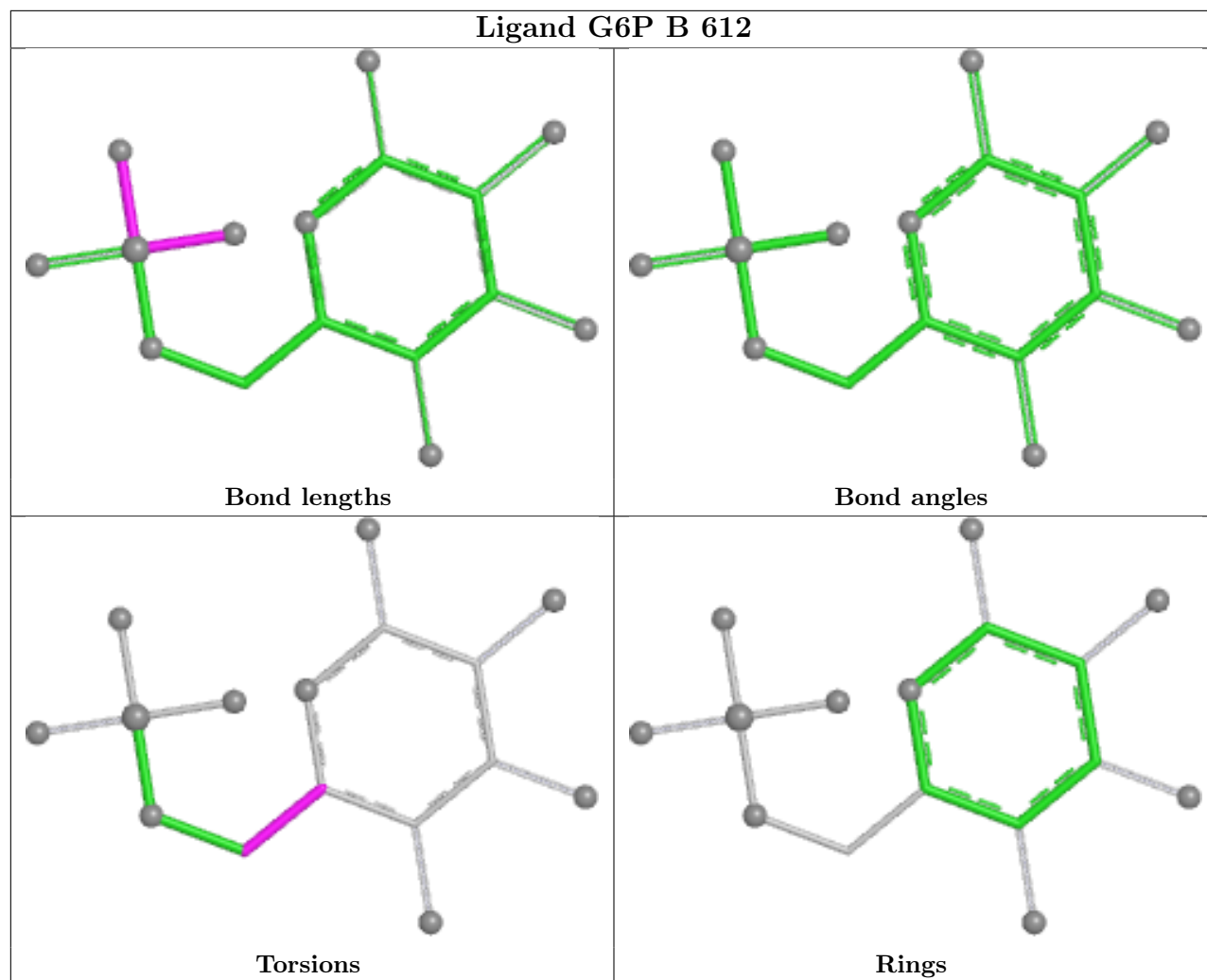


Rings

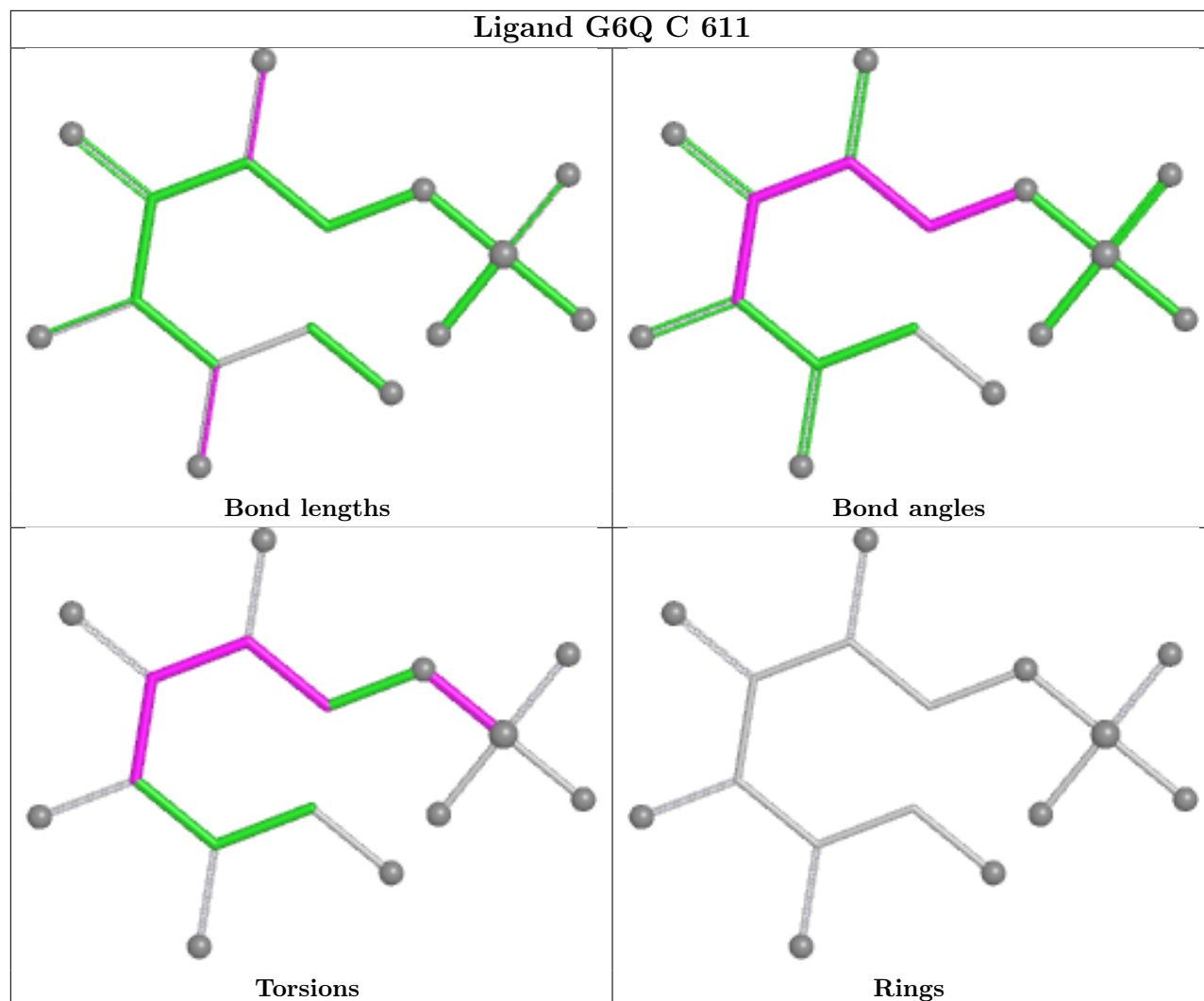
Ligand G6Q A 610



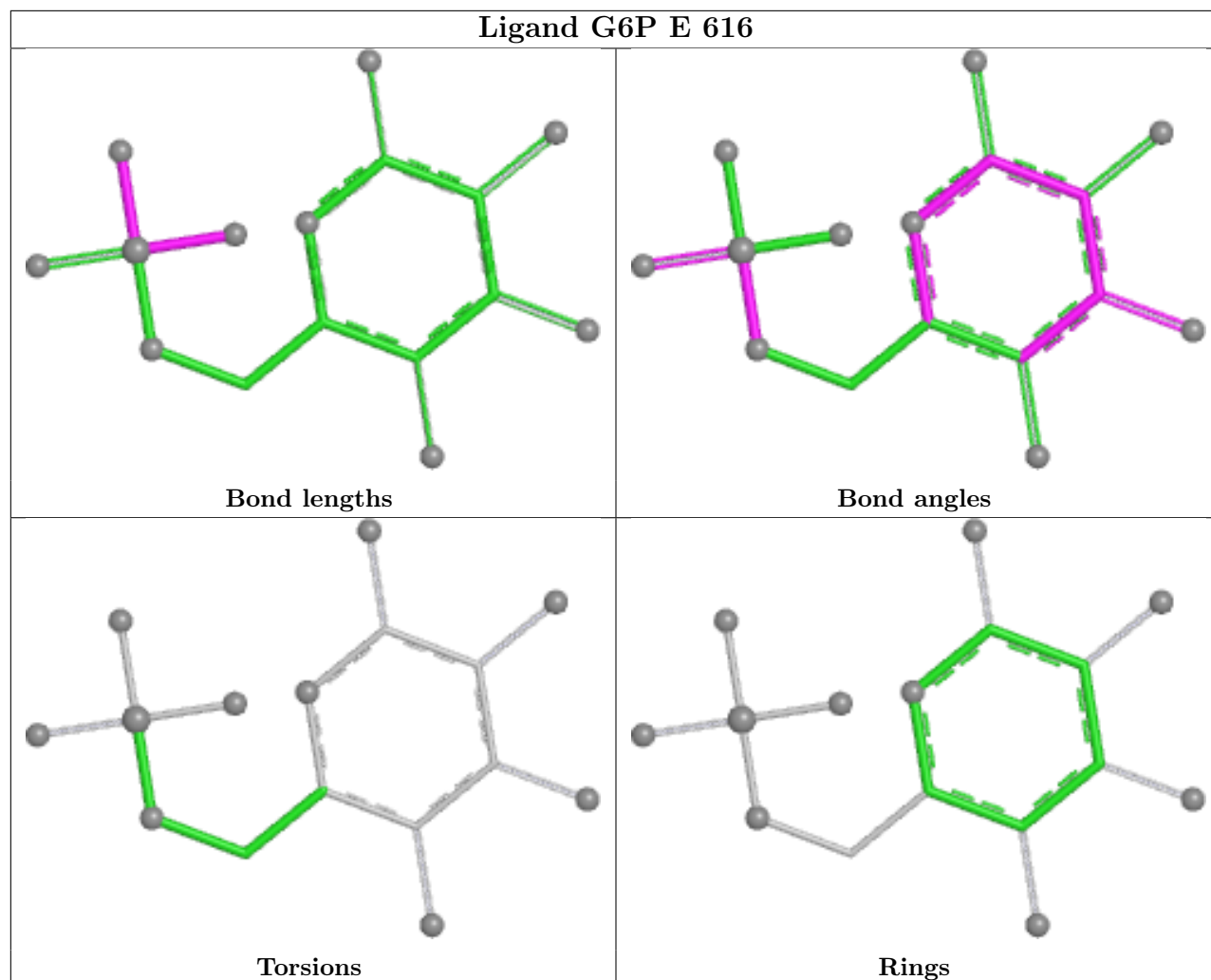
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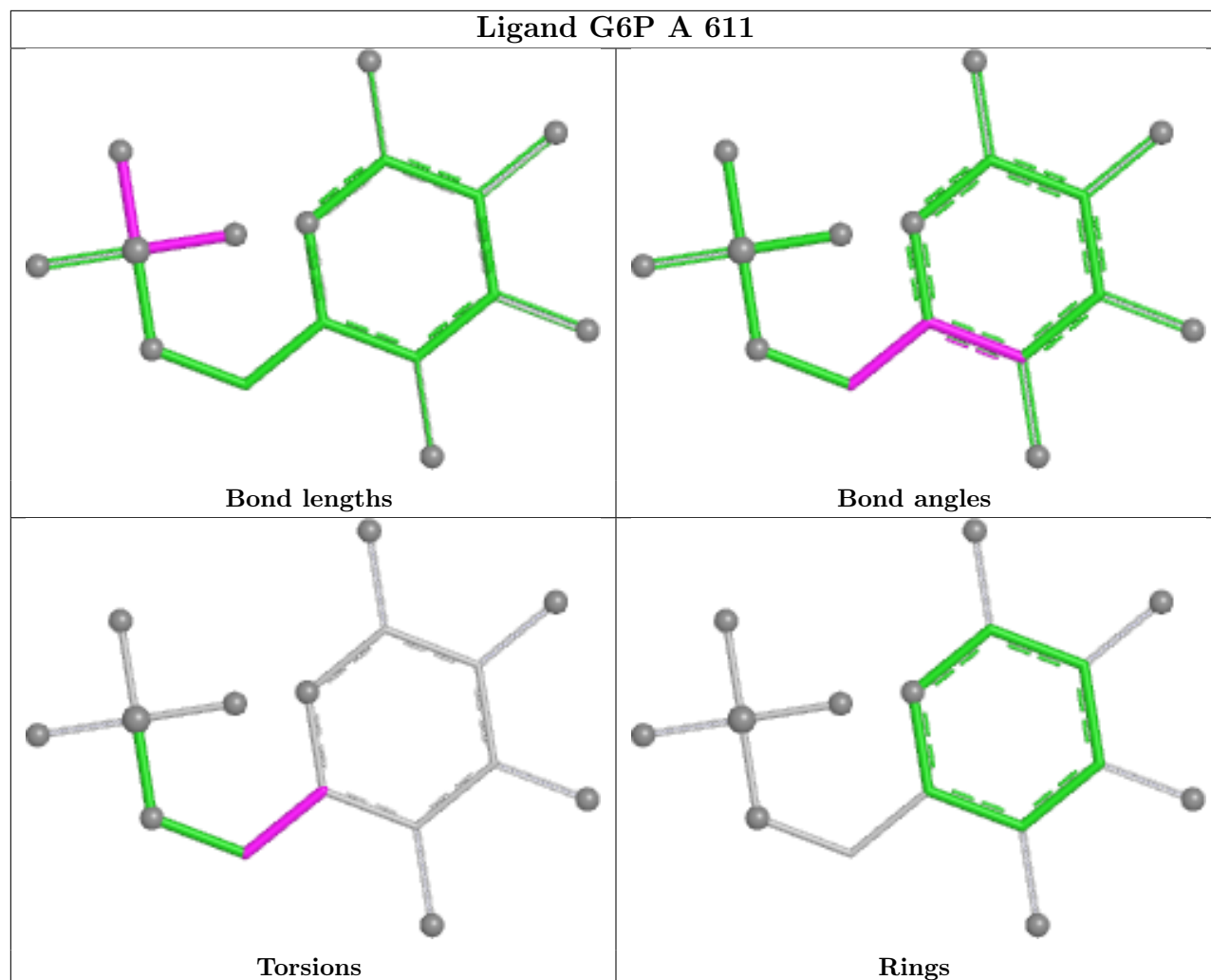
Ligand G6Q C 611



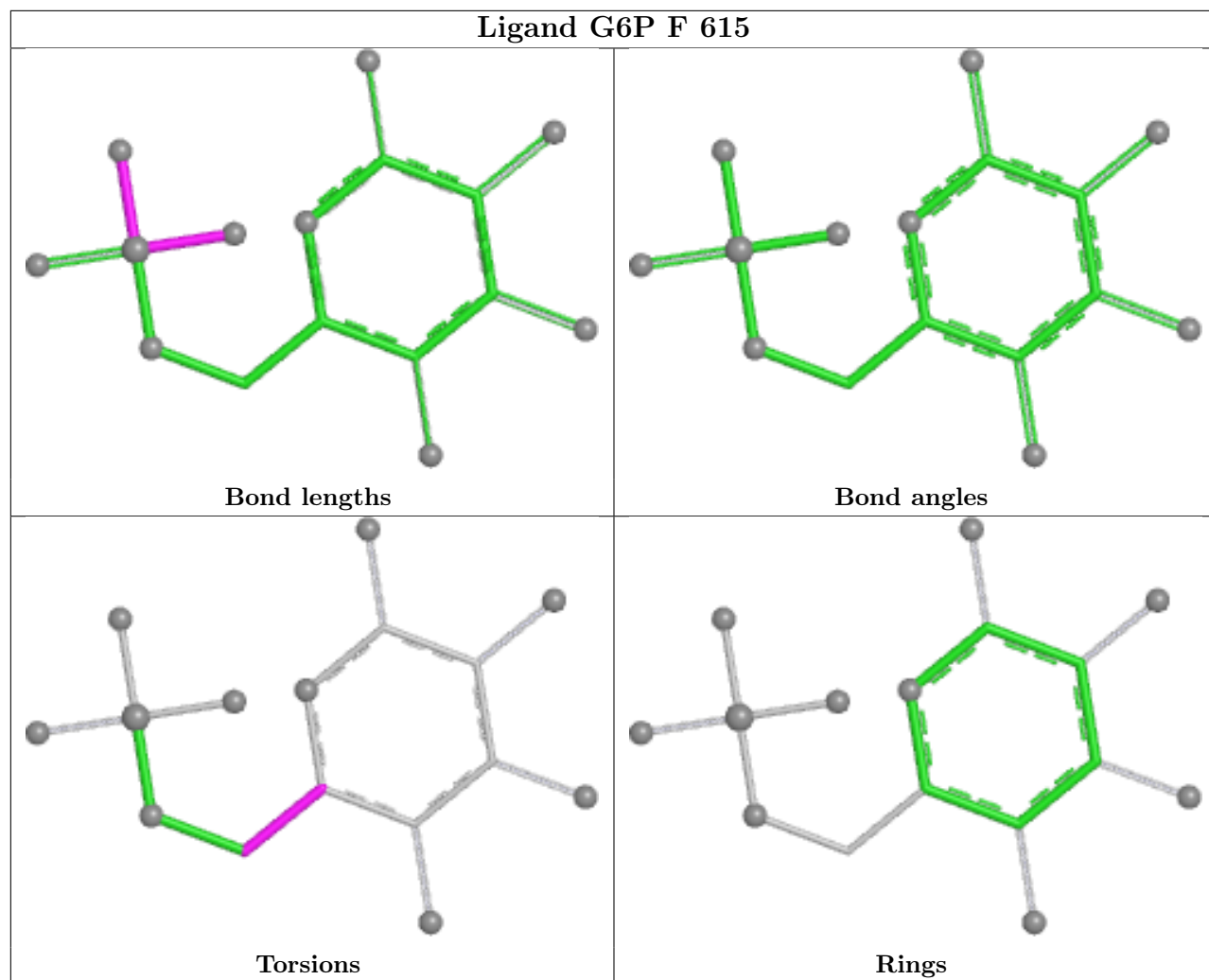
Ligand G6P E 616



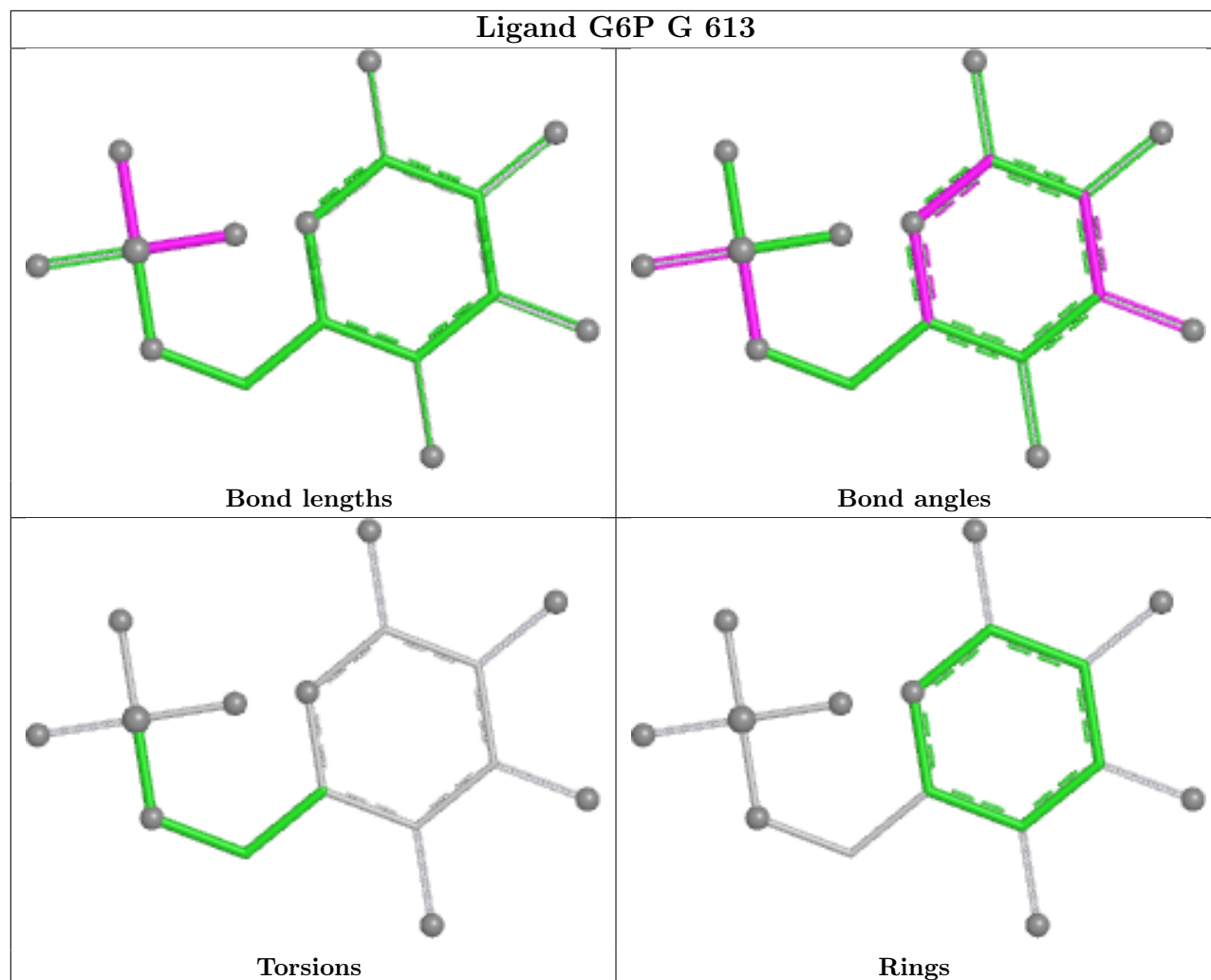
Ligand G6P A 611



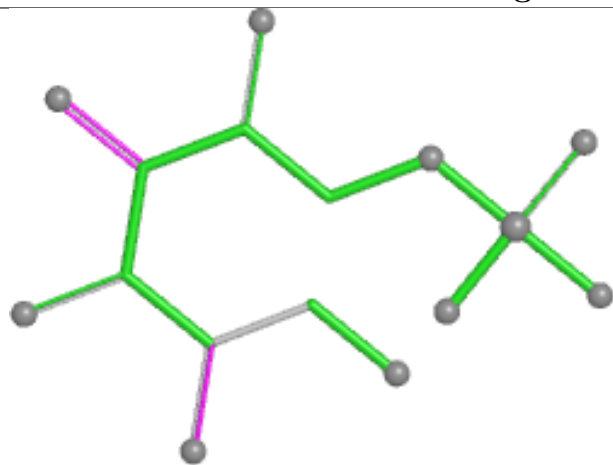
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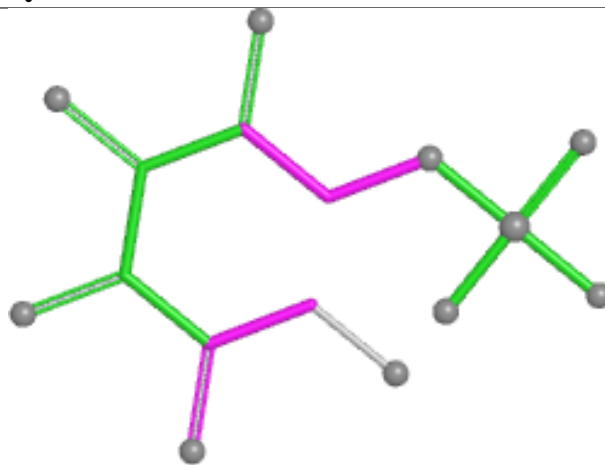
Ligand G6P G 613



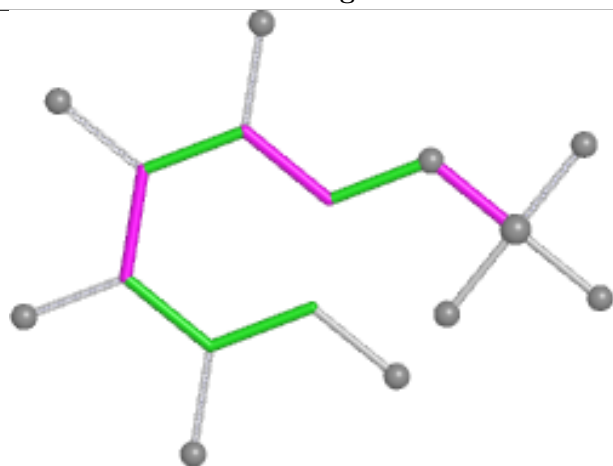
Ligand G6Q H 610



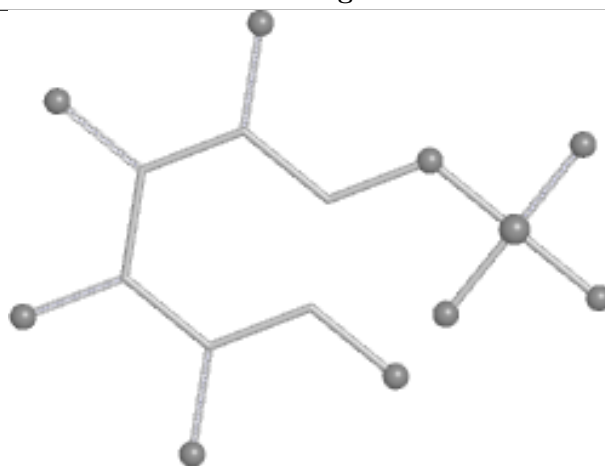
Bond lengths



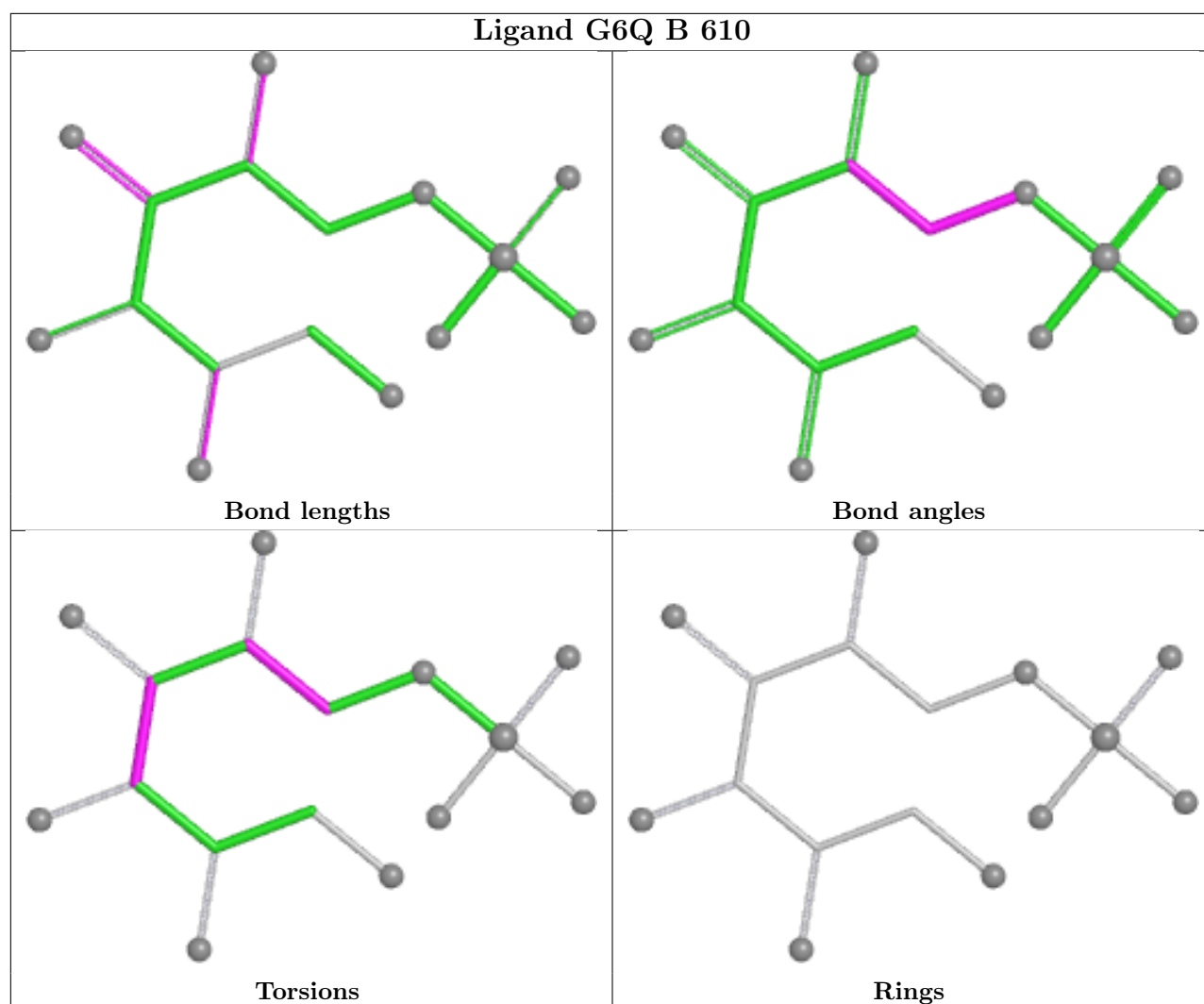
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	608/608 (100%)	-0.69	12 (1%) 65 61	15, 36, 72, 168	5 (0%)
1	B	608/608 (100%)	-0.40	22 (3%) 46 41	23, 43, 106, 131	2 (0%)
1	C	601/608 (98%)	-0.40	10 (1%) 69 65	15, 38, 96, 137	2 (0%)
1	D	602/608 (99%)	-0.40	29 (4%) 35 31	14, 37, 115, 142	3 (0%)
1	E	602/608 (99%)	-0.37	10 (1%) 69 65	23, 47, 90, 152	2 (0%)
1	F	594/608 (97%)	0.20	85 (14%) 6 5	24, 47, 129, 158	0
1	G	605/608 (99%)	-0.15	33 (5%) 30 27	20, 42, 131, 170	1 (0%)
1	H	608/608 (100%)	-0.51	6 (0%) 79 76	16, 44, 80, 135	2 (0%)
All	All	4828/4864 (99%)	-0.34	207 (4%) 40 35	14, 43, 109, 170	17 (0%)

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	ALA	6.0
1	F	76	THR	5.8
1	F	100	ILE	5.6
1	G	238	LEU	5.2
1	F	230	LYS	5.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

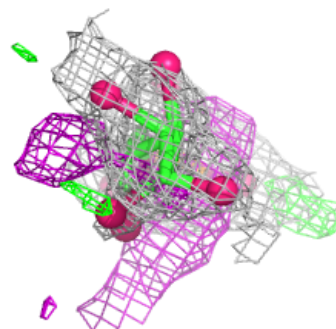
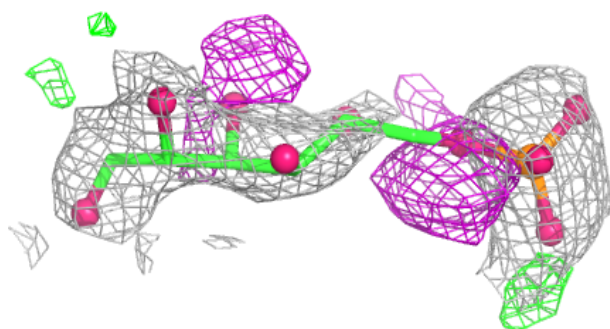
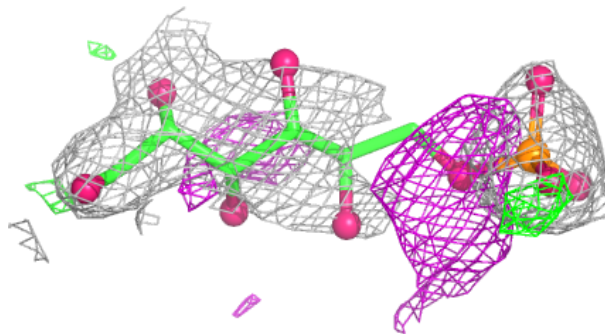
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G6Q	F	610	16/16	0.74	0.16	63,91,104,108	0
2	GLU	F	701	10/10	0.79	0.16	73,75,80,82	0
5	G6Q	E	610	16/16	0.83	0.18	95,104,115,118	0
5	G6Q	H	610	16/16	0.85	0.14	76,91,103,105	0
5	G6Q	G	610	16/16	0.87	0.15	59,90,102,107	0
2	GLU	G	701	10/10	0.88	0.13	68,78,81,82	0
5	G6Q	B	610	16/16	0.88	0.14	60,86,96,100	0
4	GOL	C	609	6/6	0.89	0.17	56,60,64,66	0
4	GOL	G	609	6/6	0.90	0.14	56,58,59,64	0
5	G6Q	C	611	16/16	0.90	0.13	57,77,89,94	0
5	G6Q	A	610	16/16	0.90	0.11	56,70,83,88	0
2	GLU	D	701	10/10	0.92	0.11	64,66,67,67	0
5	G6Q	D	611	16/16	0.92	0.11	63,71,78,82	0
4	GOL	A	609	6/6	0.93	0.13	59,62,65,68	0
4	GOL	E	609	6/6	0.93	0.11	47,51,53,57	0
4	GOL	F	609	6/6	0.93	0.12	55,56,57,59	0
4	GOL	B	609	6/6	0.93	0.10	51,54,54,56	0
4	GOL	H	609	6/6	0.94	0.11	47,53,55,58	0
2	GLU	B	701	10/10	0.94	0.12	74,83,85,88	0
2	GLU	E	701	10/10	0.94	0.10	34,42,44,44	0
2	GLU	C	701	10/10	0.95	0.09	36,46,61,62	0
2	GLU	H	701	10/10	0.96	0.07	39,43,48,49	0
4	GOL	D	610	6/6	0.96	0.09	56,56,57,57	0
2	GLU	A	701	10/10	0.98	0.05	30,35,36,38	0
3	G6P	E	616	16/16	0.98	0.05	31,37,43,44	0
3	G6P	F	615	16/16	0.98	0.05	29,32,38,39	0
3	G6P	H	614	16/16	0.98	0.05	22,29,34,36	0
3	G6P	A	611	16/16	0.99	0.04	22,26,31,32	0
3	G6P	B	612	16/16	0.99	0.04	24,28,34,39	0
3	G6P	G	613	16/16	0.99	0.04	24,28,34,34	0
3	G6P	C	610	16/16	0.99	0.04	20,25,27,31	0
3	G6P	D	609	16/16	0.99	0.04	23,27,29,29	0

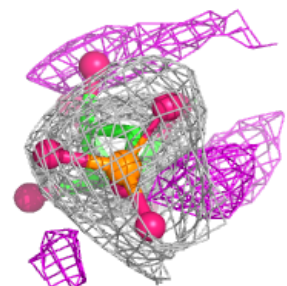
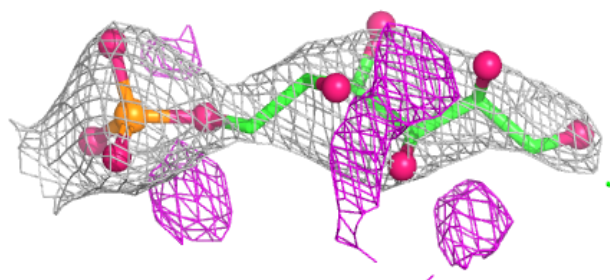
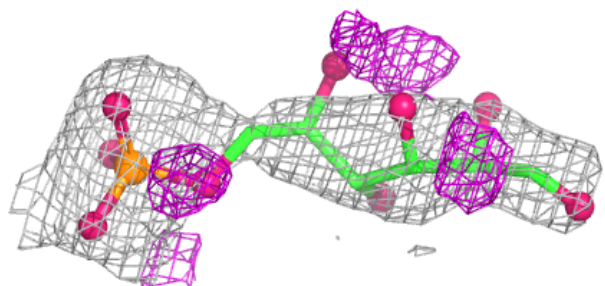
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6Q F 610:

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

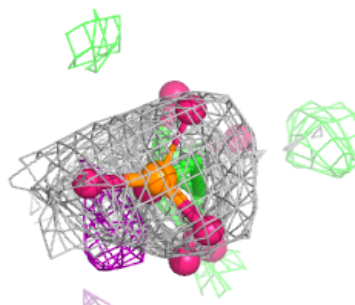
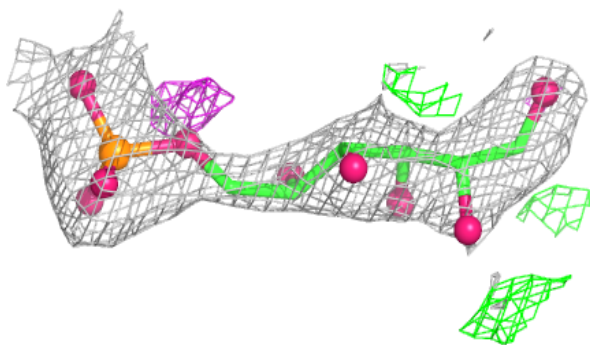
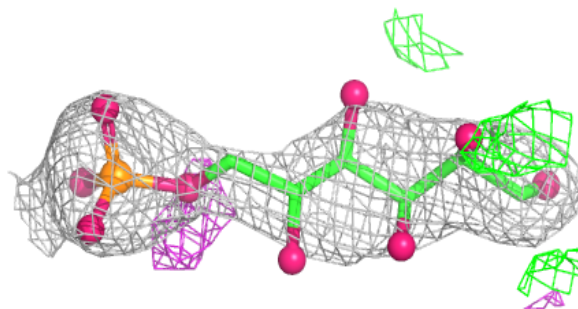
**Electron density around G6Q E 610:**

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

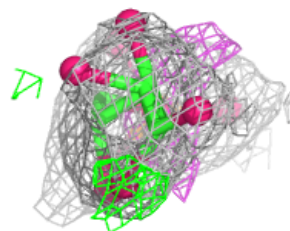
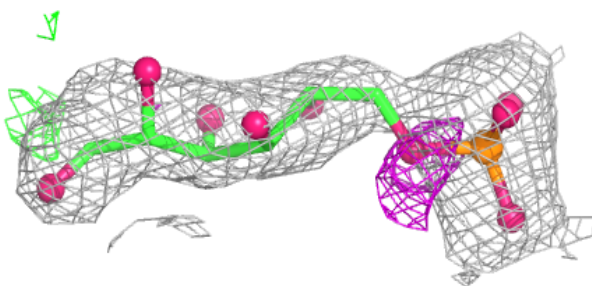
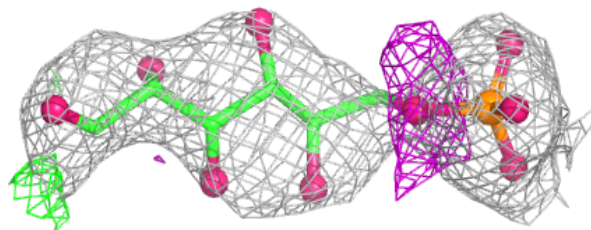


Electron density around G6Q H 610:

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

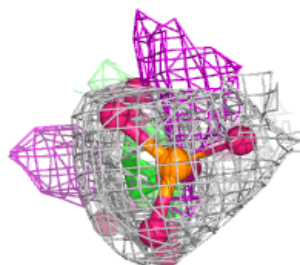
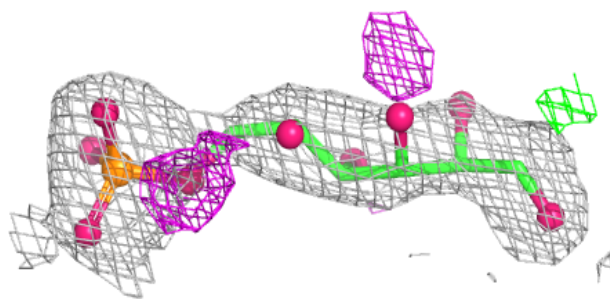
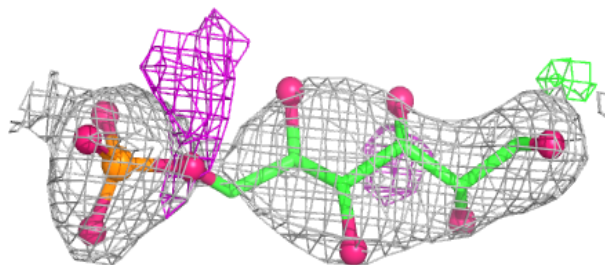
**Electron density around G6Q G 610:**

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

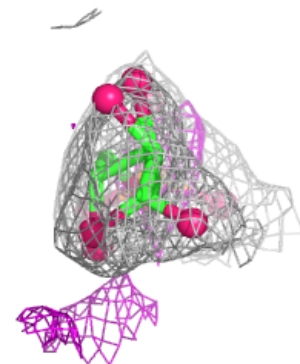
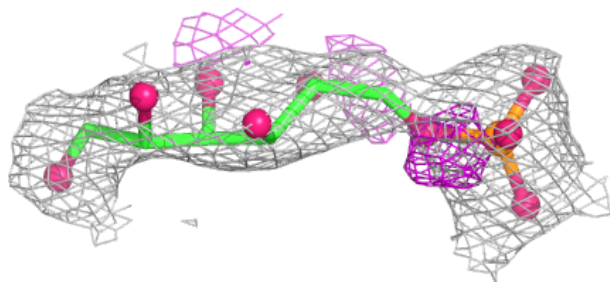
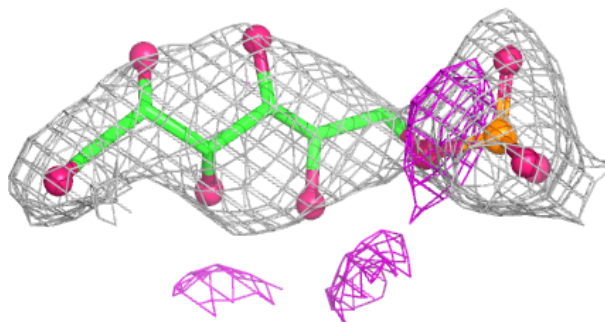


Electron density around G6Q B 610:

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

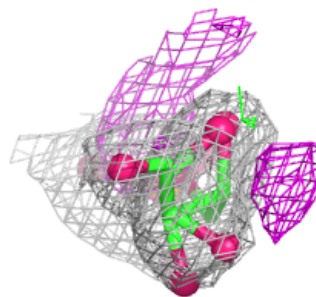
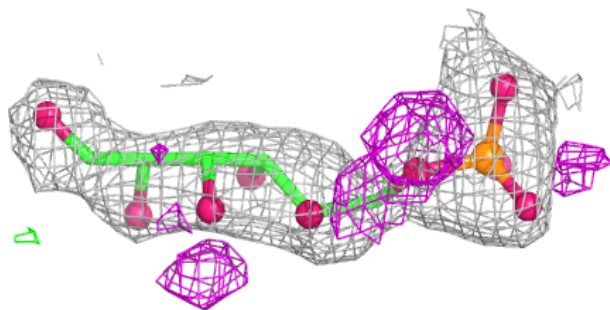
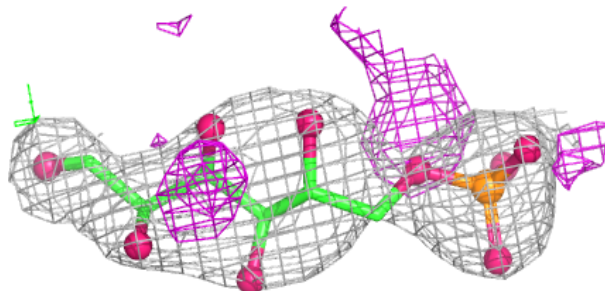
**Electron density around G6Q C 611:**

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

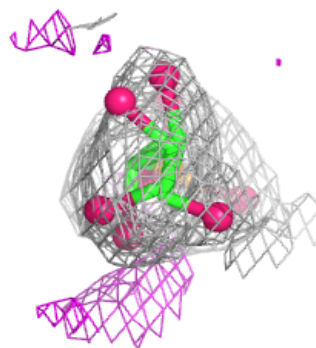
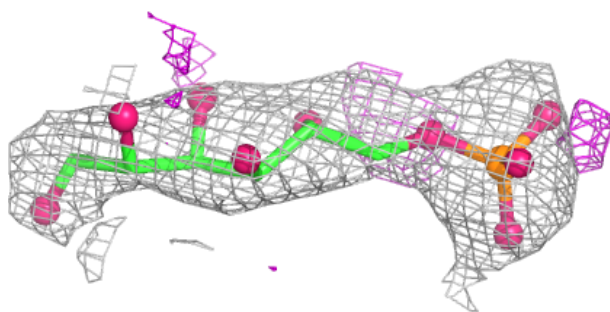
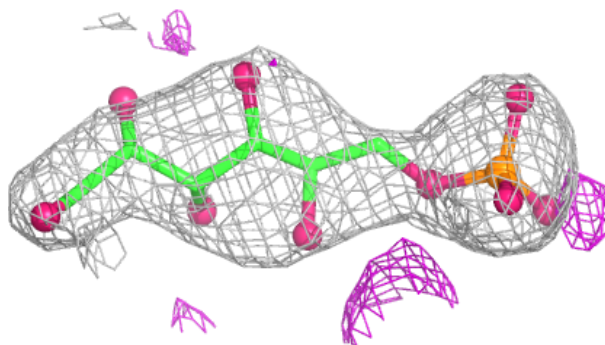


Electron density around G6Q A 610:

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

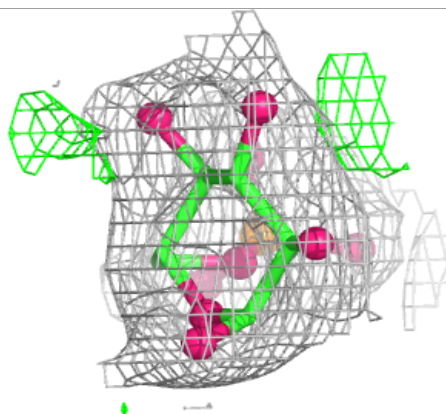
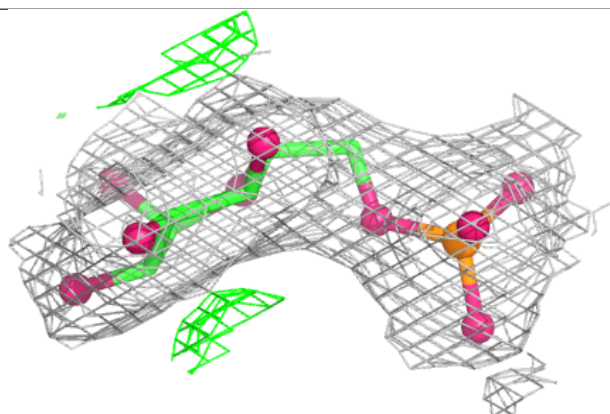
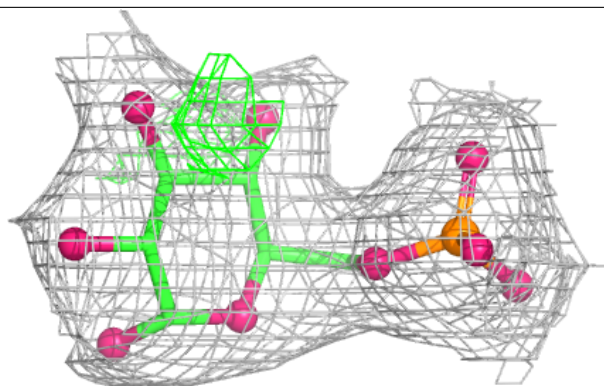
**Electron density around G6Q D 611:**

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

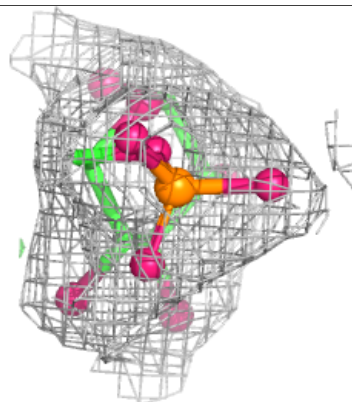
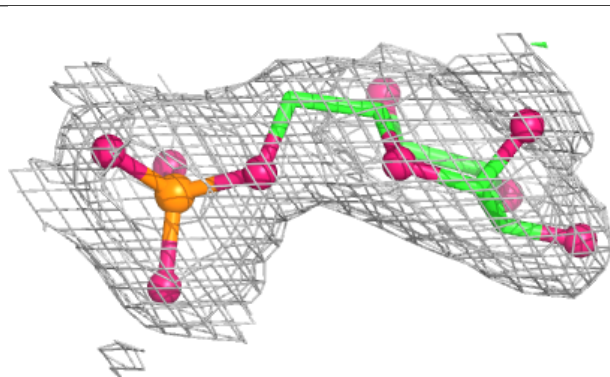
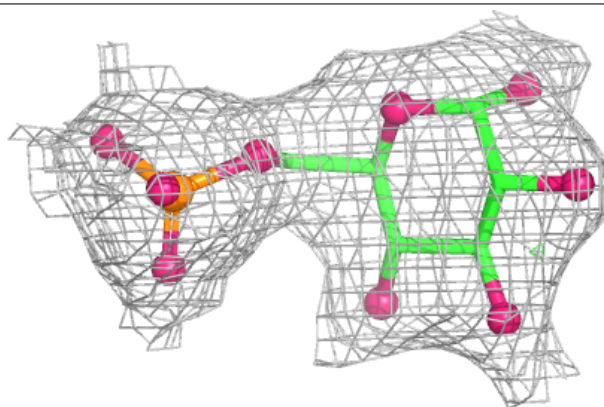


Electron density around G6P E 616:

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

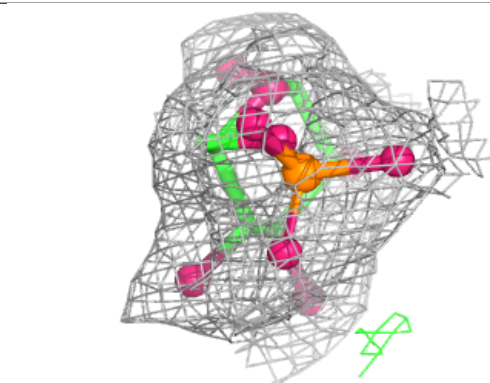
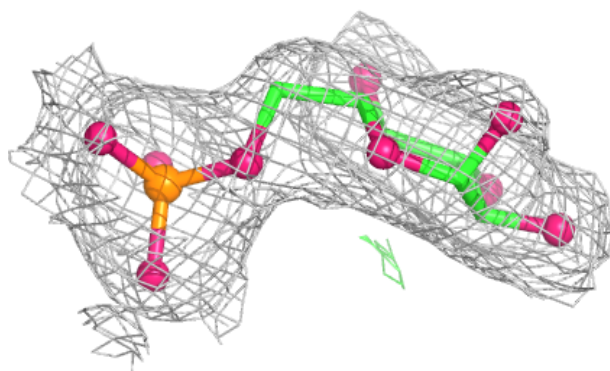
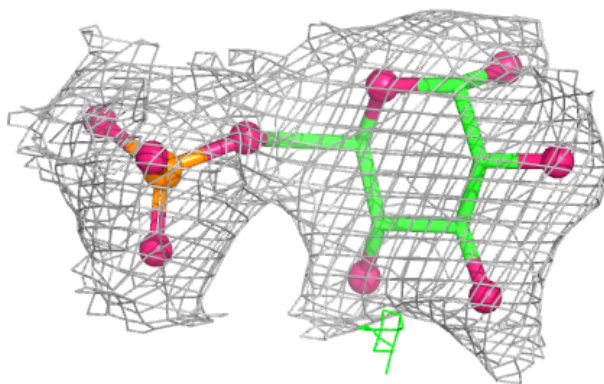
**Electron density around G6P F 615:**

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

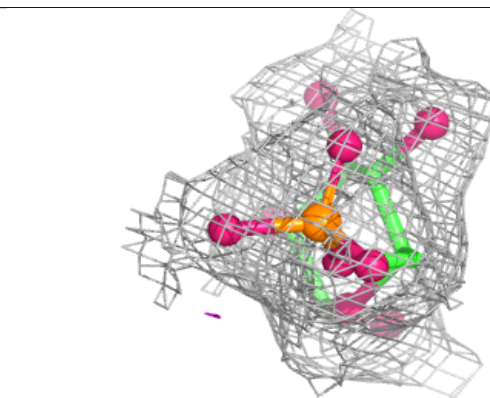
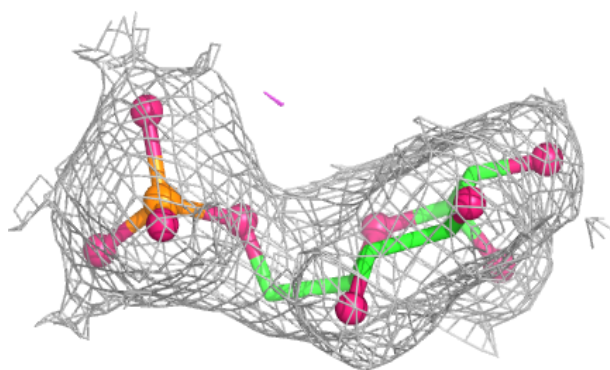
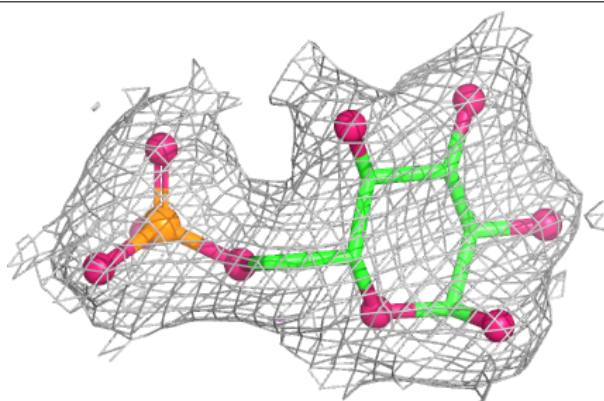


Electron density around G6P H 614:

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

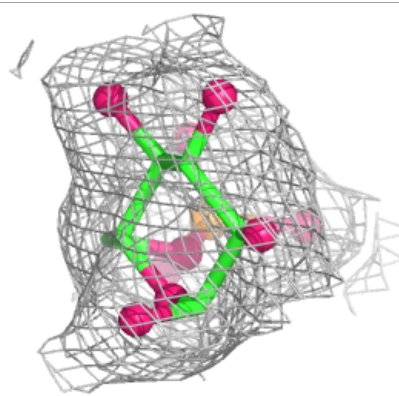
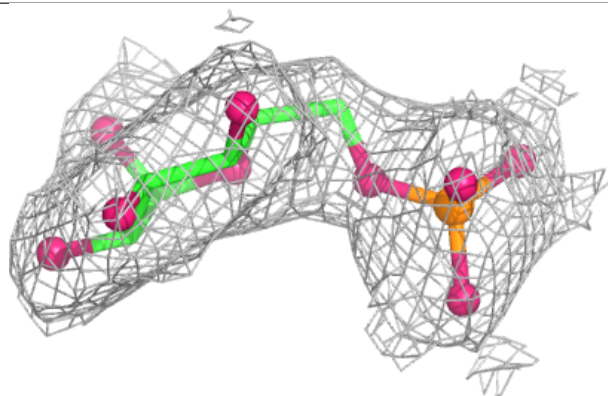
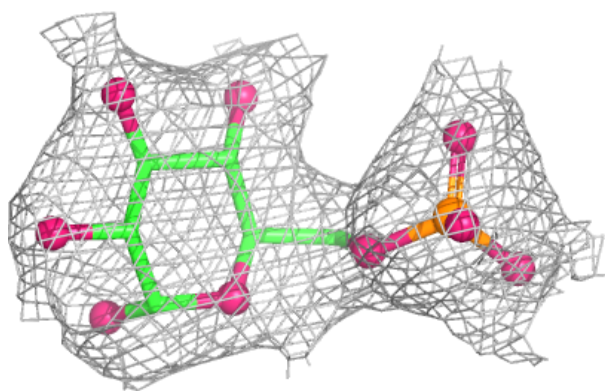
**Electron density around G6P A 611:**

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

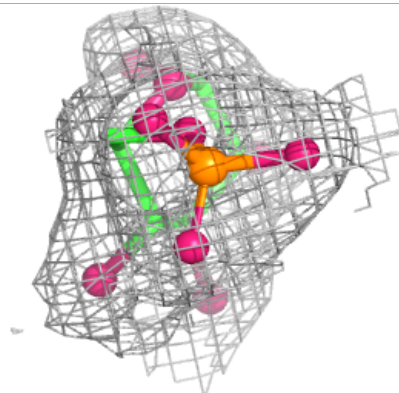
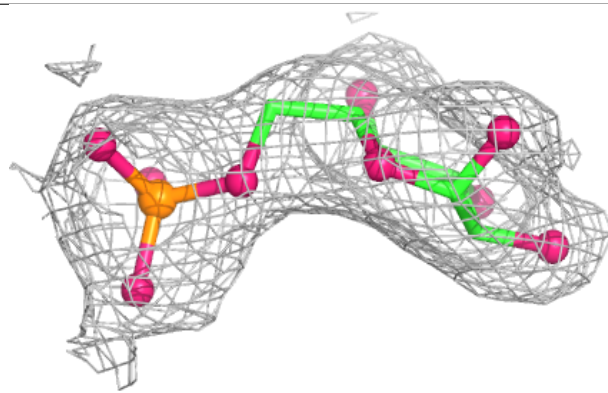
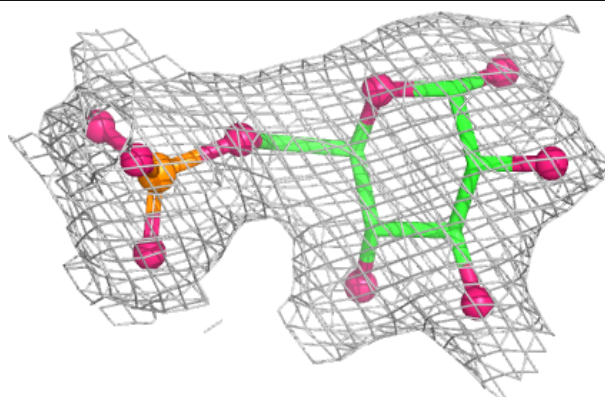


Electron density around G6P B 612:

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

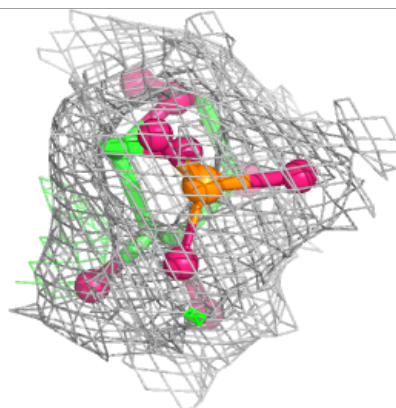
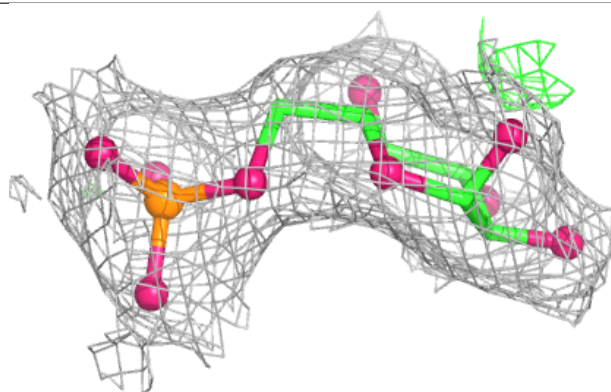
**Electron density around G6P G 613:**

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

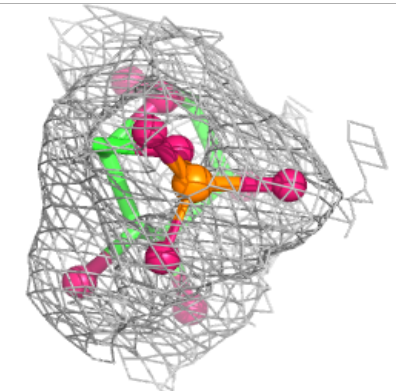
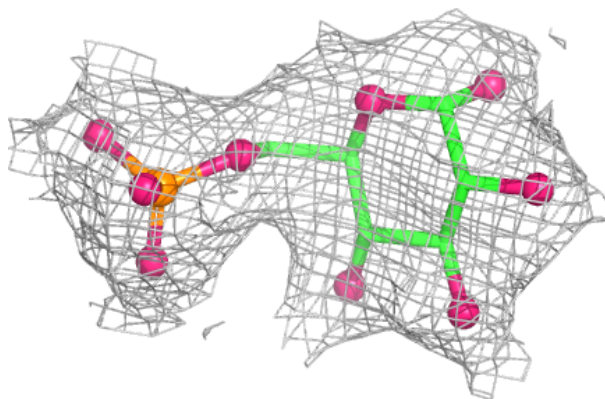


Electron density around G6P C 610:

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

**Electron density around G6P D 609:**

$2mF_o-DF_c$ (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.