



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:33 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 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:

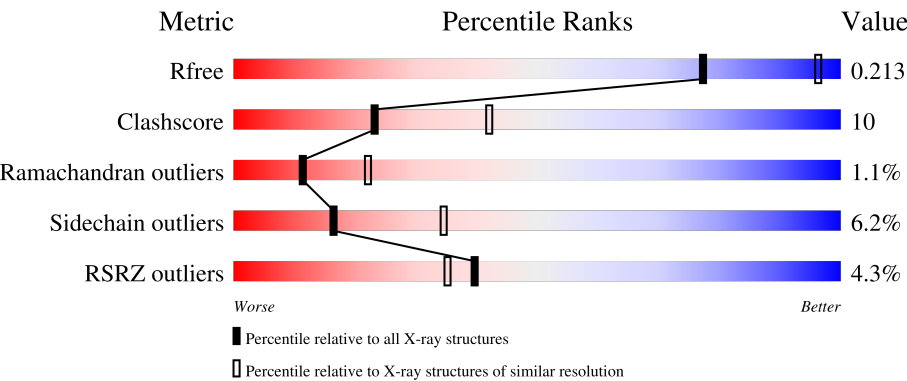
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.50 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:

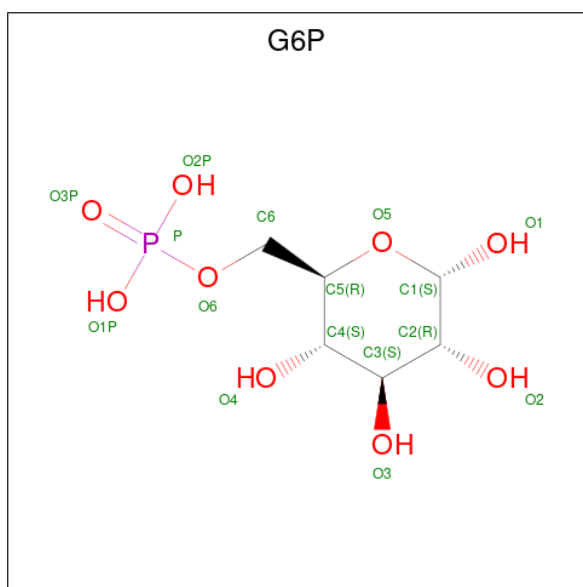
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP C9QXA7
B	1	ALA	CYS	engineered mutation	UNP C9QXA7
C	1	ALA	CYS	engineered mutation	UNP C9QXA7
D	1	ALA	CYS	engineered mutation	UNP C9QXA7
E	1	ALA	CYS	engineered mutation	UNP C9QXA7
F	1	ALA	CYS	engineered mutation	UNP C9QXA7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



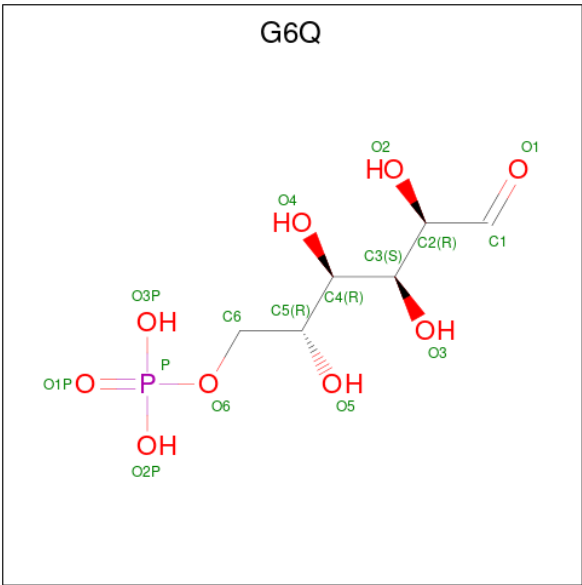
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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: $C_6H_{13}O_9P$).



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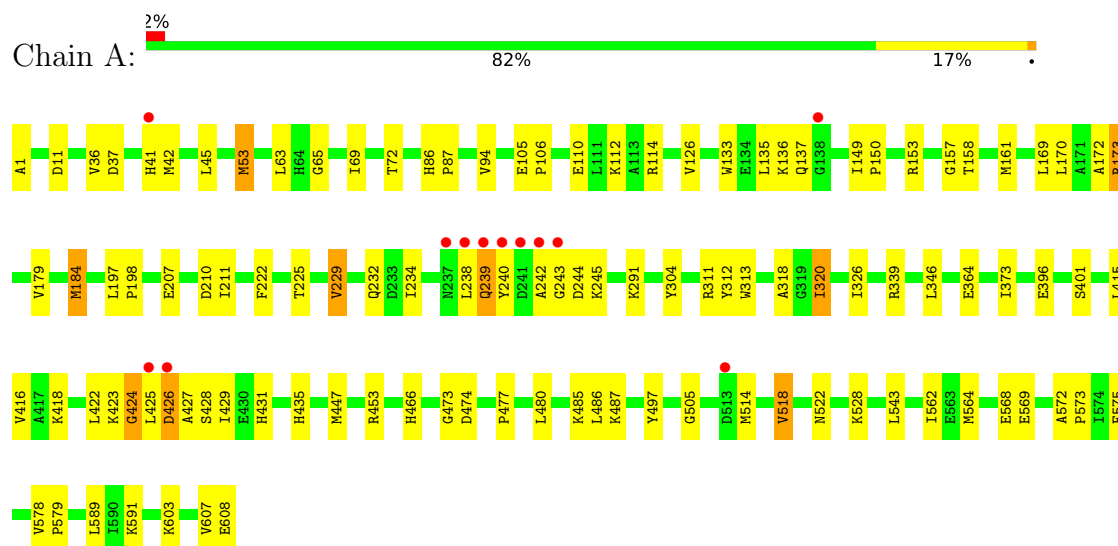
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	123	Total 123	O 123	0	0
6	F	123	Total 123	O 123	0	0
6	G	175	Total 175	O 175	0	0
6	H	169	Total 169	O 169	0	0

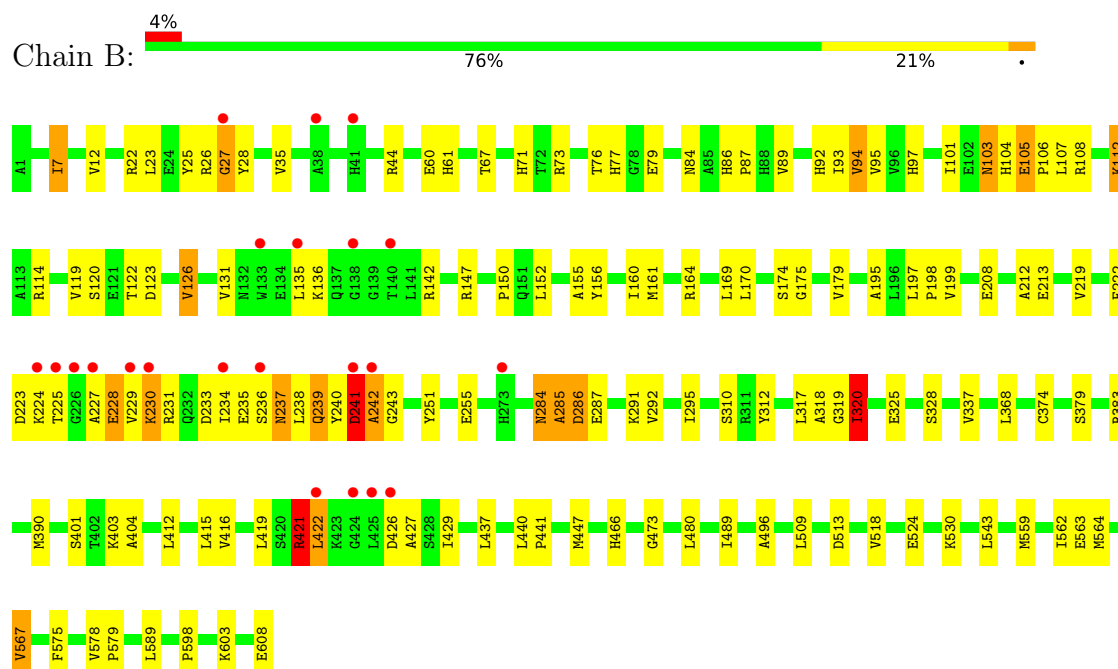
3 Residue-property plots

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



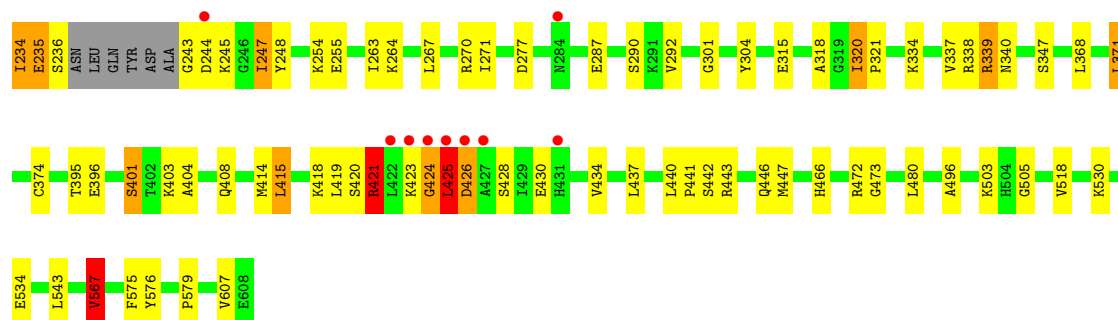
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



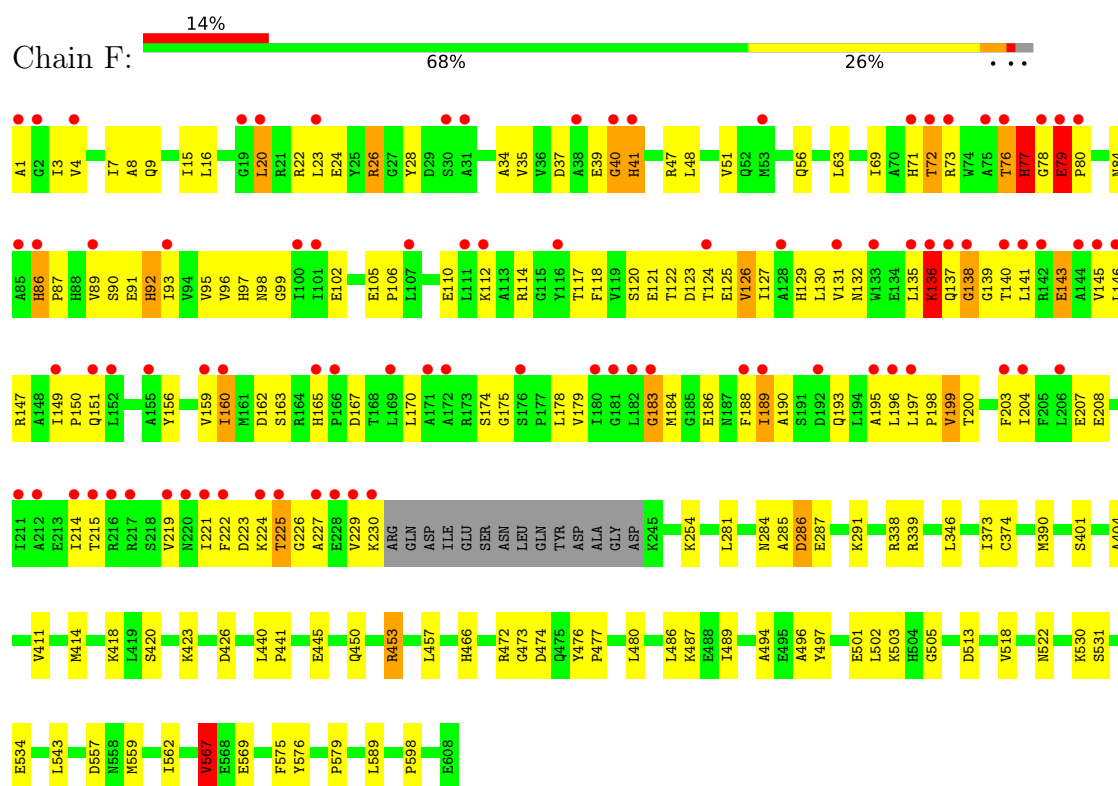
- Chain C:
- | Label | Value | Category |
|-------|-------|----------|
| A1 | 1 | Red |
| G2 | 2 | Green |
| I3 | 3 | Green |
| D11 | 4 | Green |
| E14 | 5 | Green |
| R21 | 6 | Red |
| R22 | 7 | Green |
| L23 | 8 | Green |
| E24 | 9 | Green |
| Y28 | 10 | Green |
| H41 | 11 | Red |
| K50 | 12 | Orange |
| 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:

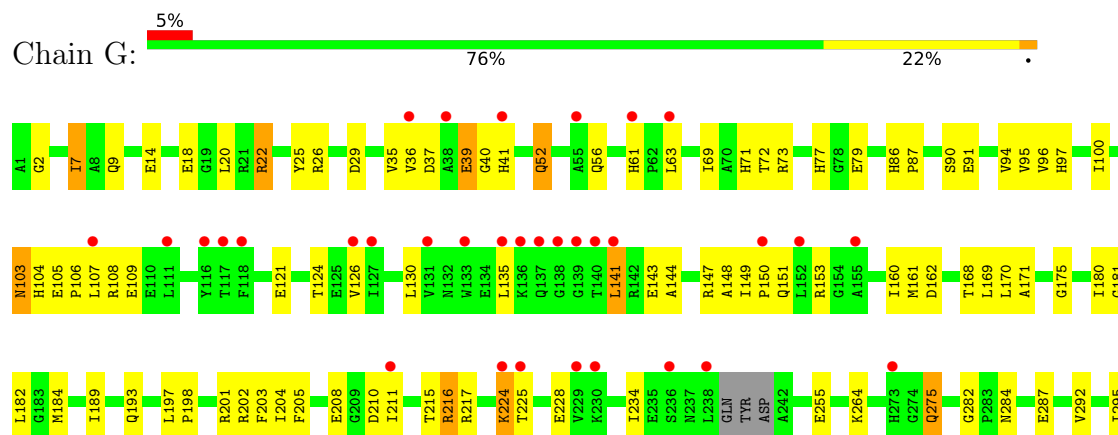
- Chain E:
-
- 2% 75% 20%
- A1 G2 I7 A8 Q9 E14 L20 L23 E24 Y25 D37 A38 E39 G40 H41 M63 E60 T67 H71 T72 R73 W74 A75 T76 H86 P87 S90 V95 V96 H97 N103 H104 E105 P106 L107 R114 T124 E125 V126 H129 N132 W133 F124 L135 G136 Q137 G138 R142 V145 L146 R147 A148 L149 P150 A155 Y156 G157 T158 V159 I160 R164 L170 A171 R172 R173 S174 G175 S176 V179 M184 D192 L197 P198 R202 F205 L206 E207 E208 I211 R216 D222 F223 K224 E228 R231 Q232 Q233

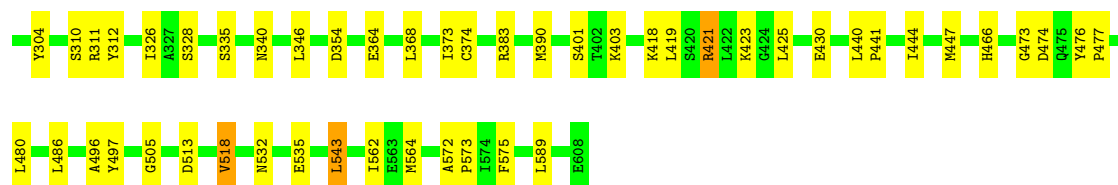


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

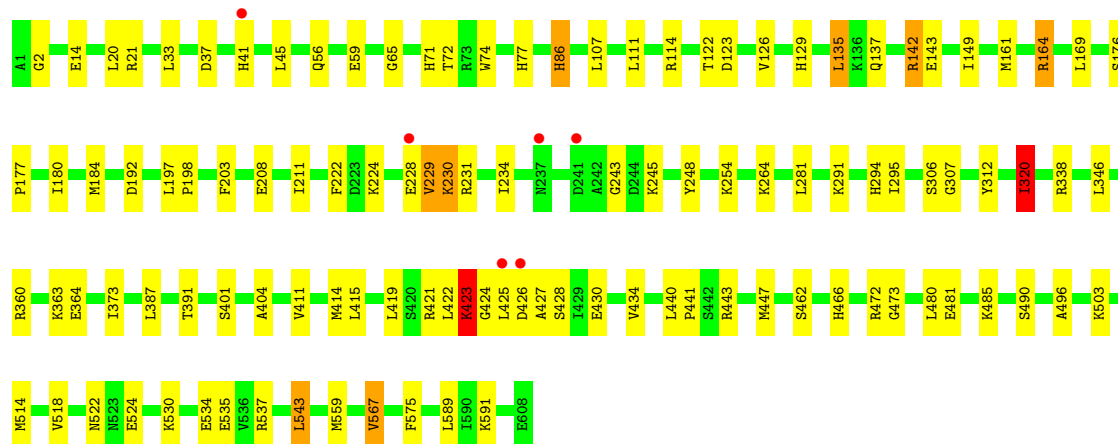
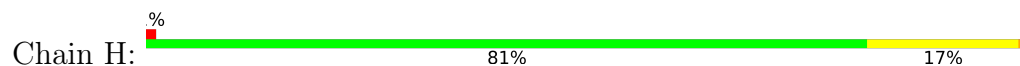


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing





- 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 ⓘ

5.1 Standard geometry ⓘ

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

All (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
1	A	245	LYS	N-CA-C	-6.74	105.06	113.28
1	B	320	ILE	CB-CA-C	-6.69	103.44	110.53
1	D	518	VAL	CB-CA-C	-6.54	100.87	110.81
1	G	423	LYS	CB-CA-C	-6.35	109.26	116.63
1	H	514	MET	CA-C-N	6.33	126.30	119.78
1	H	514	MET	C-N-CA	6.33	126.30	119.78
1	E	157	GLY	N-CA-C	-6.17	98.57	113.18
1	B	421	ARG	CA-C-N	6.06	132.61	121.70
1	B	421	ARG	C-N-CA	6.06	132.61	121.70
1	A	243	GLY	N-CA-C	-6.01	103.58	114.46
1	A	313	TRP	N-CA-C	5.97	117.45	111.07
1	G	282	GLY	CA-C-N	5.78	125.64	119.28
1	G	282	GLY	C-N-CA	5.78	125.64	119.28
1	A	320	ILE	CB-CA-C	-5.64	101.09	111.36
1	B	61	HIS	CA-C-N	5.53	125.45	119.76
1	B	61	HIS	C-N-CA	5.53	125.45	119.76
1	D	61	HIS	CA-C-N	5.26	126.41	119.84
1	D	61	HIS	C-N-CA	5.26	126.41	119.84
1	A	518	VAL	CB-CA-C	-5.20	102.90	110.81
1	B	567	VAL	CB-CA-C	-5.14	102.47	110.69
1	A	239	GLN	N-CA-C	-5.11	99.93	110.80
1	C	151	GLN	N-CA-C	-5.10	107.73	114.31
1	B	12	VAL	N-CA-C	5.05	117.83	112.83
1	E	567	VAL	CB-CA-C	-5.04	101.78	110.30
1	F	225	THR	N-CA-C	5.04	117.54	111.40
1	E	424	GLY	N-CA-C	-5.03	101.27	113.18

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 ⓘ

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:F:99:GLY:O	2:F:701:GLU:HB2	1.67	0.93
1:B:242:ALA:CB	1:B:243:GLY:HA3	1.99	0.92
1:H:424:GLY:HA3	1:H:425:LEU:HB3	1.51	0.91
1:F:86:HIS:HD2	1:F:97:HIS:H	1.14	0.89
1:G:9:GLN:HB2	1:G:216:ARG:HH21	1.38	0.89
1:D:411:VAL:HA	1:D:414:MET:HE3	1.56	0.88
1:C:485:LYS:HE3	1:C:488:GLU:OE1	1.74	0.87
1:B:236:SER:CA	1:B:237:ASN:HB2	2.04	0.86
1:D:328[A]:SER:OG	6:D:1385:HOH:O	1.94	0.85
1:H:423:LYS:CB	1:H:424:GLY:HA2	2.06	0.84
1:D:9:GLN:HB2	1:D:216:ARG:NH1	1.93	0.84
1:A:239:GLN:O	1:A:240:TYR:HD1	1.61	0.83
1:B:319:GLY:HA3	1:B:422:LEU:HD13	1.59	0.83
1:F:71:HIS:HB2	1:F:96:VAL:HG23	1.60	0.82
1:C:105:GLU:HB2	1:C:106:PRO:HD3	1.60	0.82
1:H:222:PHE:HA	1:H:229:VAL:HG13	1.62	0.81
1:H:230:LYS:HE3	1:H:231:ARG:N	1.95	0.81
1:D:153:ARG:HG2	1:D:154:GLY:H	1.45	0.81
1:C:24:GLU:OE1	1:C:28:TYR:OH	1.98	0.80
1:B:292:VAL:O	1:B:421:ARG:NH2	2.15	0.80
1:D:136:LYS:HA	1:D:136:LYS:HE2	1.64	0.79
1:H:423:LYS:HB2	1:H:424:GLY:HA2	1.66	0.78
1:A:239:GLN:C	1:A:240:TYR:HD1	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HB2	1:A:427:ALA:H	1.50	0.77
1:F:73:ARG:NH2	1:F:78:GLY:O	2.17	0.77
1:F:480:LEU:HD23	1:F:496:ALA:HB3	1.66	0.76
1:B:27:GLY:HA3	1:B:28:TYR:HB3	1.66	0.76
1:D:69:ILE:HD12	1:D:96:VAL:HG13	1.68	0.76
1:C:149:ILE:HB	1:C:150:PRO:HD3	1.68	0.75
1:D:135:LEU:HD21	1:D:164:ARG:HH22	1.51	0.75
1:B:150:PRO:HG3	1:B:224:LYS:HD2	1.69	0.75
1:A:447:MET:HE2	1:A:575:PHE:CE2	2.20	0.75
1:E:426:ASP:HB3	1:E:428:SER:HB3	1.68	0.74
1:A:425:LEU:HA	1:A:426:ASP:CB	2.16	0.74
1:F:530:LYS:NZ	1:F:534:GLU:OE2	2.19	0.74
1:D:143:GLU:HA	1:D:146:LEU:HD12	1.69	0.74
1:B:230:LYS:HE2	1:B:230:LYS:HA	1.68	0.74
1:C:204:ILE:HD11	1:C:221:ILE:HD11	1.70	0.74
1:G:7:ILE:HG12	1:G:216:ARG:HB3	1.69	0.73
1:E:224:LYS:H	1:E:224:LYS:HD2	1.53	0.73
1:F:86:HIS:CD2	1:F:97:HIS:H	2.03	0.73
1:D:130:LEU:O	1:D:130:LEU:HD12	1.88	0.72
1:E:443:ARG:HH11	1:E:446:GLN:HE22	1.36	0.72
1:F:71:HIS:HB2	1:F:96:VAL:CG2	2.20	0.72
1:A:425:LEU:CB	1:A:427:ALA:H	2.03	0.72
1:G:105:GLU:O	1:G:109:GLU:HG2	1.90	0.72
1:D:93:ILE:HG21	1:D:131:VAL:HG23	1.71	0.71
1:G:20:LEU:HD22	1:G:72:THR:HG23	1.71	0.70
1:H:208:GLU:OE2	6:H:1507:HOH:O	2.08	0.70
1:B:240:TYR:HB2	1:B:241:ASP:HB2	1.73	0.70
1:F:285:ALA:O	1:F:286:ASP:CB	2.40	0.70
1:E:426:ASP:C	1:E:428:SER:H	2.00	0.70
1:H:424:GLY:CA	1:H:425:LEU:HB3	2.21	0.70
1:G:71:HIS:HE1	1:G:73:ARG:HB2	1.57	0.69
1:C:231:ARG:HG2	1:C:231:ARG:HH11	1.56	0.69
1:F:40:GLY:HA3	1:F:41:HIS:HB2	1.75	0.69
1:B:318:ALA:HB1	1:B:320:ILE:HD11	1.74	0.69
1:C:261:ASN:OD1	6:C:809:HOH:O	2.11	0.69
1:H:142:ARG:HG3	1:H:143:GLU:N	2.08	0.68
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.76	0.68
1:H:567:VAL:HG11	1:H:575:PHE:CD1	2.29	0.68
1:D:234:ILE:HG22	1:D:235:GLU:H	1.59	0.68
1:C:138:GLY:HA3	1:C:147:ARG:NH2	2.09	0.68
1:F:291:LYS:HD2	1:F:291:LYS:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:PHE:HB3	1:E:228:GLU:HA	1.76	0.67
1:G:284:ASN:O	1:G:287:GLU:HB2	1.93	0.67
1:F:4:VAL:HG12	1:F:16:LEU:HD23	1.77	0.67
1:F:97:HIS:HB3	1:F:124:THR:HG23	1.77	0.67
1:F:149:ILE:HG21	1:F:224:LYS:HZ2	1.60	0.67
1:B:230:LYS:HE2	1:B:231:ARG:H	1.60	0.67
1:F:3:ILE:HG12	1:F:96:VAL:HG22	1.76	0.67
1:B:223:ASP:OD1	1:B:225:THR:HG22	1.95	0.66
1:D:7:ILE:HD13	1:D:215:THR:HA	1.77	0.66
1:H:423:LYS:CG	1:H:424:GLY:HA2	2.25	0.66
1:G:210:ASP:O	1:G:211:ILE:HD13	1.95	0.66
1:F:93:ILE:HD13	1:F:131:VAL:HG22	1.76	0.66
1:B:285:ALA:C	1:B:287:GLU:H	2.04	0.66
5:A:610:G6Q:O5	5:A:610:G6Q:O3	2.10	0.66
1:E:425:LEU:O	1:E:426:ASP:HB2	1.96	0.66
1:B:236:SER:CA	1:B:237:ASN:CB	2.69	0.65
1:D:339:ARG:NH1	6:D:743:HOH:O	2.28	0.65
1:F:40:GLY:CA	1:F:41:HIS:HB2	2.27	0.65
1:F:140:THR:HG22	1:F:141:LEU:H	1.60	0.65
1:C:21:ARG:O	1:C:24:GLU:HG3	1.96	0.65
1:G:9:GLN:HB2	1:G:216:ARG:NH2	2.10	0.65
1:B:255:GLU:HG2	1:B:403:LYS:HE2	1.77	0.65
1:F:188:PHE:CE2	1:F:199:VAL:HG11	2.31	0.65
1:E:576:TYR:O	1:E:579:PRO:HD2	1.97	0.64
1:B:161:MET:HB3	1:B:169:LEU:HD23	1.79	0.64
1:E:426:ASP:HB3	1:E:428:SER:CB	2.28	0.64
1:D:95:VAL:HG22	1:D:160:ILE:HG12	1.80	0.64
1:F:136:LYS:O	1:F:137:GLN:HG3	1.96	0.64
1:A:173:ARG:HG2	1:A:207:GLU:O	1.97	0.64
1:B:240:TYR:CA	1:B:241:ASP:HB2	2.28	0.64
1:B:240:TYR:CZ	1:H:243:GLY:HA3	2.33	0.63
1:H:426:ASP:OD2	1:H:427:ALA:N	2.31	0.63
1:D:173:ARG:HG3	1:D:176:SER:O	1.98	0.63
1:H:447:MET:HE2	1:H:575:PHE:CE2	2.33	0.63
1:C:400:ALA:HB1	1:C:485:LYS:HE2	1.80	0.63
1:A:431[B]:HIS:NE2	1:A:435[B]:HIS:CD2	2.67	0.63
1:E:95:VAL:HG22	1:E:160:ILE:HG12	1.80	0.63
1:E:207:GLU:HG3	1:E:231:ARG:NH1	2.14	0.63
1:F:138:GLY:O	1:F:143:GLU:HB3	1.99	0.63
1:H:422:LEU:O	1:H:423:LYS:HG2	1.97	0.63
1:C:204:ILE:HD11	1:C:221:ILE:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:TYR:CB	1:F:72:THR:HG23	2.28	0.62
1:A:63:LEU:N	1:A:63:LEU:HD12	2.13	0.62
1:A:239:GLN:C	1:A:240:TYR:CD1	2.76	0.62
1:F:162:ASP:OD1	1:F:163:SER:N	2.32	0.62
1:C:608:GLU:O	1:D:528:LYS:HE3	1.99	0.62
1:B:222:PHE:CE1	1:B:228:GLU:HG2	2.34	0.62
1:C:138:GLY:HA3	1:C:147:ARG:HH22	1.63	0.62
1:H:480:LEU:HD23	1:H:496:ALA:HB3	1.80	0.62
1:A:425:LEU:HB2	1:A:427:ALA:N	2.14	0.62
1:C:77:HIS:O	1:C:122:THR:HA	1.99	0.62
1:C:149:ILE:C	1:C:151:GLN:H	2.07	0.62
1:F:149:ILE:HG23	1:F:156:TYR:OH	1.99	0.62
1:B:95:VAL:HG22	1:B:160:ILE:HG12	1.82	0.61
1:F:71:HIS:CG	1:F:96:VAL:HG23	2.35	0.61
1:G:71:HIS:CE1	1:G:73:ARG:HB2	2.35	0.61
1:E:263:ILE:HG21	1:E:440:LEU:HD23	1.82	0.61
1:D:118:PHE:HA	1:D:125:GLU:OE2	2.00	0.61
1:E:243:GLY:O	1:E:245:LYS:N	2.33	0.61
1:B:230:LYS:HA	1:B:230:LYS:CE	2.31	0.61
1:F:71:HIS:CB	1:F:96:VAL:HG23	2.29	0.61
1:F:411:VAL:HA	1:F:414:MET:HE3	1.82	0.61
1:B:447:MET:HE2	1:B:575:PHE:CZ	2.35	0.61
1:H:530:LYS:HD3	1:H:559:MET:SD	2.41	0.61
1:F:7:ILE:HD13	1:F:215:THR:HA	1.83	0.61
1:B:242:ALA:CB	1:B:243:GLY:CA	2.77	0.61
1:E:103:ASN:ND2	1:E:107:LEU:HD11	2.16	0.61
1:B:285:ALA:O	1:B:287:GLU:N	2.33	0.61
1:C:477:PRO:HA	1:C:480:LEU:HD12	1.81	0.61
1:E:447:MET:HE2	1:E:575:PHE:CE2	2.36	0.60
1:F:76:THR:O	1:F:76:THR:OG1	2.19	0.60
1:G:180:ILE:O	1:G:203:PHE:HA	2.01	0.60
1:D:107:LEU:HD13	1:D:152:LEU:HD23	1.82	0.60
1:F:346:LEU:HD23	1:F:373:ILE:HB	1.84	0.60
1:G:480:LEU:HD23	1:G:496:ALA:HB3	1.83	0.60
1:E:235:GLU:OE2	1:E:236:SER:N	2.34	0.60
1:B:447:MET:HE2	1:B:575:PHE:CE2	2.37	0.60
1:D:86:HIS:HB3	1:D:87:PRO:HA	1.84	0.60
1:G:105:GLU:HB2	1:G:106:PRO:HD3	1.83	0.60
1:D:90:SER:HB2	1:D:128:ALA:HB1	1.82	0.60
1:G:447:MET:HE2	1:G:575:PHE:CZ	2.36	0.60
1:F:112:LYS:HE2	1:F:117:THR:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:611:G6Q:O5	5:C:611:G6Q:O3	2.11	0.60
1:B:76:THR:HG1	2:B:701:GLU:N	2.00	0.59
1:F:15:ILE:HD13	1:F:188:PHE:CE1	2.37	0.59
1:A:346:LEU:HD23	1:A:373:ILE:HB	1.84	0.59
1:C:101:ILE:HD12	1:C:152:LEU:HD22	1.84	0.59
1:C:513:ASP:HB3	6:C:1513:HOH:O	2.02	0.59
1:A:562:ILE:HG22	1:A:564:MET:HE2	1.84	0.59
1:B:320:ILE:CD1	1:B:421:ARG:HG2	2.32	0.59
1:H:222:PHE:HB3	1:H:228:GLU:HA	1.84	0.59
1:D:22:ARG:HD3	6:D:1429:HOH:O	2.01	0.59
1:B:105:GLU:HG3	1:B:106:PRO:HD3	1.84	0.59
1:B:427:ALA:N	6:B:631:HOH:O	2.34	0.58
1:B:480:LEU:HD23	1:B:496:ALA:HB3	1.84	0.58
1:G:255:GLU:HG2	1:G:403:LYS:HE2	1.83	0.58
1:F:76:THR:O	1:F:77:HIS:HB2	2.02	0.58
1:B:240:TYR:CB	1:B:241:ASP:HB2	2.32	0.58
1:E:292:VAL:O	1:E:421:ARG:NH1	2.33	0.58
1:F:4:VAL:HG11	1:F:16:LEU:HA	1.85	0.58
1:F:92:HIS:CD2	1:F:93:ILE:HG13	2.38	0.58
1:H:37:ASP:OD2	1:H:41[A]:HIS:HB2	2.03	0.58
1:B:240:TYR:HA	1:B:241:ASP:CB	2.33	0.58
1:F:71:HIS:CB	1:F:86:HIS:HB2	2.34	0.58
1:F:1:ALA:HB3	1:F:72:THR:HG22	1.85	0.58
1:F:28:TYR:HB3	1:F:72:THR:HG23	1.85	0.57
1:F:95:VAL:HG22	1:F:160:ILE:HG23	1.86	0.57
1:B:318:ALA:HB2	1:B:416:VAL:HG13	1.85	0.57
1:F:149:ILE:HG21	1:F:224:LYS:NZ	2.19	0.57
1:C:229:VAL:CG2	1:C:231:ARG:HH12	2.17	0.57
1:E:426:ASP:C	1:E:428:SER:N	2.61	0.57
1:E:567:VAL:HG11	1:E:575:PHE:CD1	2.39	0.57
1:A:514:MET:HE3	4:A:609:GOL:H2	1.87	0.57
1:B:285:ALA:C	1:B:287:GLU:N	2.62	0.57
1:C:474:ASP:OD2	5:C:611:G6Q:H3	2.05	0.57
1:C:591:LYS:NZ	6:C:1346:HOH:O	2.38	0.57
5:G:610:G6Q:O5	5:G:610:G6Q:O3	2.13	0.57
1:H:534:GLU:OE1	1:H:537:ARG:NH1	2.38	0.57
1:C:161:MET:HB3	1:C:169:LEU:CD2	2.34	0.57
1:G:513:ASP:HB3	6:G:1354:HOH:O	2.04	0.56
1:A:425:LEU:HA	1:A:426:ASP:HB3	1.88	0.56
1:C:285:ALA:O	1:C:286:ASP:CB	2.53	0.56
1:F:22:ARG:NE	1:F:198:PRO:HG3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:HIS:CD2	1:F:96:VAL:HG23	2.40	0.56
1:F:139:GLY:HA3	1:F:143:GLU:OE1	2.04	0.56
1:G:69:ILE:HD12	1:G:96:VAL:HG22	1.86	0.56
1:G:466:HIS:CE1	1:H:466:HIS:CE1	2.93	0.56
1:E:146:LEU:HD23	1:E:211:ILE:HD12	1.86	0.56
1:A:86:HIS:HB3	1:A:87:PRO:HA	1.87	0.56
1:E:142:ARG:HA	1:E:170:LEU:HD11	1.88	0.56
1:C:466:HIS:CE1	1:D:466:HIS:CE1	2.94	0.56
1:F:106:PRO:O	1:F:110:GLU:HB2	2.06	0.56
1:A:431[B]:HIS:CD2	1:A:435[B]:HIS:HD2	2.23	0.56
1:A:466:HIS:CE1	1:B:466:HIS:CE1	2.94	0.56
1:C:197:LEU:N	1:C:198:PRO:HD2	2.21	0.56
1:D:225:THR:HA	6:D:694:HOH:O	2.06	0.56
1:E:466:HIS:CE1	1:F:466:HIS:CE1	2.94	0.56
1:F:474:ASP:OD1	5:F:610:G6Q:H3	2.05	0.56
1:B:103:ASN:C	1:B:103:ASN:HD22	2.14	0.56
1:H:423:LYS:HG2	1:H:424:GLY:HA2	1.87	0.56
1:C:196:LEU:HB2	1:C:203:PHE:HE1	1.70	0.56
1:E:90:SER:OG	1:E:129:HIS:ND1	2.30	0.56
1:G:86:HIS:HB3	1:G:87:PRO:HA	1.87	0.56
1:A:466:HIS:CG	1:A:514:MET:HE2	2.41	0.55
1:D:93:ILE:HG21	1:D:131:VAL:CG2	2.35	0.55
1:F:71:HIS:HB3	1:F:86:HIS:HB2	1.87	0.55
1:A:426:ASP:H	1:A:429:ILE:HD12	1.70	0.55
1:C:149:ILE:O	1:C:151:GLN:N	2.38	0.55
1:B:240:TYR:HA	1:B:241:ASP:HB2	1.89	0.55
1:F:93:ILE:HD12	1:F:132:ASN:HA	1.88	0.55
1:C:50:LYS:HB3	1:C:50:LYS:NZ	2.22	0.55
1:H:184:MET:HE2	1:H:184:MET:HA	1.88	0.55
1:A:53:MET:HE2	1:A:53:MET:HA	1.89	0.55
1:C:14:GLU:HG2	1:G:184:MET:HE2	1.89	0.55
1:E:136:LYS:C	1:E:138:GLY:H	2.15	0.55
1:F:167:ASP:O	1:F:215:THR:HG22	2.07	0.55
1:F:440:LEU:HB3	1:F:441:PRO:HD3	1.88	0.55
1:A:291:LYS:HD2	1:A:291:LYS:N	2.21	0.55
1:F:69:ILE:HD12	1:F:96:VAL:HG12	1.89	0.55
1:B:84:ASN:OD1	1:B:120:SER:HB2	2.07	0.55
1:C:339:ARG:NH1	6:D:743:HOH:O	2.40	0.55
1:E:301:GLY:O	1:E:304:TYR:HB3	2.07	0.55
1:D:222:PHE:HA	1:D:228:GLU:CA	2.37	0.54
1:F:450:GLN:OE1	1:F:453:ARG:NH2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ASN:OD1	1:G:153:ARG:HB2	2.06	0.54
1:F:63:LEU:HD12	1:F:63:LEU:H	1.72	0.54
1:G:149:ILE:HB	1:G:150:PRO:HD3	1.89	0.54
1:G:295:ILE:HD11	1:G:419:LEU:HD13	1.90	0.54
1:E:103:ASN:O	1:E:107:LEU:HD12	2.08	0.54
1:F:141:LEU:HD23	1:F:170:LEU:HD23	1.88	0.54
1:D:63:LEU:N	1:D:63:LEU:HD12	2.23	0.54
1:D:127:ILE:O	1:D:131:VAL:HG22	2.07	0.54
1:A:425:LEU:CA	1:A:427:ALA:H	2.21	0.54
1:B:174:SER:HA	1:B:208:GLU:OE2	2.08	0.54
1:C:285:ALA:O	1:C:286:ASP:HB2	2.08	0.54
1:C:447:MET:HE2	1:C:575:PHE:CZ	2.42	0.54
1:F:77:HIS:HB2	2:F:701:GLU:N	2.23	0.54
1:G:95:VAL:HG22	1:G:160:ILE:HG23	1.89	0.54
1:B:319:GLY:CA	1:B:422:LEU:HD13	2.35	0.54
1:F:105:GLU:HB3	1:F:106:PRO:HD3	1.88	0.54
1:F:199:VAL:HG12	1:F:200:THR:HG22	1.88	0.54
1:F:188:PHE:CZ	1:F:199:VAL:HG11	2.43	0.54
1:B:241:ASP:O	1:B:242:ALA:CB	2.56	0.53
1:D:447:MET:HE2	1:D:575:PHE:CE2	2.43	0.53
1:G:141:LEU:HD11	1:G:162:ASP:HB2	1.90	0.53
1:G:2:GLY:O	1:G:71:HIS:HA	2.08	0.53
1:D:48:LEU:HD13	1:D:81:SER:HA	1.90	0.53
1:C:222:PHE:HB3	1:C:228:GLU:HA	1.88	0.53
1:B:71:HIS:HE1	1:B:73:ARG:HB2	1.74	0.53
1:D:20:LEU:HD22	1:D:72:THR:HG23	1.91	0.53
1:F:79:GLU:HG2	1:F:84:ASN:ND2	2.23	0.53
1:B:320:ILE:HD12	1:B:421:ARG:HG2	1.91	0.53
1:D:170:LEU:HD13	1:D:212:ALA:O	2.08	0.53
1:F:183:GLY:HA2	1:F:186:GLU:O	2.09	0.53
1:G:22:ARG:HG2	1:G:22:ARG:HH11	1.74	0.53
1:C:197:LEU:HD23	1:C:203:PHE:HZ	1.73	0.53
1:E:39:GLU:HB3	1:E:41[A]:HIS:CE1	2.44	0.53
1:E:149:ILE:HB	1:E:150:PRO:HD3	1.90	0.53
1:H:422:LEU:O	1:H:424:GLY:HA3	2.08	0.53
1:D:90:SER:OG	1:D:129:HIS:HA	2.09	0.53
1:A:234:ILE:HD12	1:A:234:ILE:C	2.33	0.53
1:A:466:HIS:HB3	1:A:514:MET:HE2	1.91	0.53
1:C:105:GLU:OE2	1:C:105:GLU:HA	2.09	0.53
1:B:92:HIS:CD2	1:B:93:ILE:HD12	2.44	0.52
1:F:285:ALA:O	1:F:286:ASP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HG12	1:B:235:GLU:N	2.24	0.52
1:C:234:ILE:HD12	1:C:234:ILE:C	2.34	0.52
1:E:270:ARG:HD3	1:E:414:MET:HE1	1.91	0.52
1:H:360:ARG:O	1:H:363:LYS:HB2	2.08	0.52
1:A:222:PHE:HA	1:A:229:VAL:HG13	1.92	0.52
1:E:86:HIS:HB3	1:E:87:PRO:HA	1.92	0.52
1:F:4:VAL:O	1:F:16:LEU:HD22	2.10	0.52
1:G:401:SER:HB2	6:G:1455:HOH:O	2.09	0.52
1:H:2:GLY:O	1:H:71:HIS:HA	2.10	0.52
1:B:241:ASP:O	1:B:242:ALA:HB3	2.09	0.52
1:F:127:ILE:O	1:F:131:VAL:HG12	2.09	0.52
1:F:576:TYR:O	1:F:579:PRO:HD2	2.09	0.52
1:F:472:ARG:HG2	1:F:473:GLY:N	2.24	0.52
1:G:61:HIS:CG	1:G:61:HIS:O	2.63	0.52
1:G:201:ARG:HA	1:G:203:PHE:HE1	1.75	0.52
1:B:104:HIS:HD2	1:B:108:ARG:HH12	1.58	0.52
1:B:108:ARG:O	1:B:112:LYS:HB2	2.10	0.52
1:E:480:LEU:HD23	1:E:496:ALA:HB3	1.92	0.52
1:F:90:SER:O	1:F:91:GLU:HB3	2.09	0.51
1:G:39:GLU:CD	1:G:39:GLU:H	2.18	0.51
1:H:530:LYS:NZ	1:H:534:GLU:OE2	2.31	0.51
1:E:339:ARG:NE	1:F:339:ARG:NH2	2.58	0.51
1:D:145:VAL:HG13	1:D:149:ILE:HD13	1.92	0.51
1:H:426:ASP:CG	1:H:427:ALA:H	2.17	0.51
1:A:466:HIS:CB	1:A:514:MET:HE2	2.41	0.51
1:C:123:ASP:O	1:C:126:VAL:HG13	2.10	0.51
1:C:231:ARG:HG2	1:C:231:ARG:NH1	2.23	0.51
1:D:489:ILE:HG22	1:D:598:PRO:HG3	1.92	0.51
1:H:37:ASP:OD2	1:H:41[B]:HIS:HB3	2.10	0.51
1:C:464:LYS:HE3	1:C:512:ALA:O	2.11	0.51
1:E:7:ILE:HD12	1:E:67:THR:OG1	2.11	0.51
1:E:371:LEU:HD21	1:E:415:LEU:HD21	1.92	0.51
1:F:22:ARG:CZ	1:F:198:PRO:HG3	2.40	0.51
1:H:77:HIS:O	1:H:122:THR:HA	2.10	0.51
1:D:155:ALA:HA	1:D:175:GLY:HA3	1.93	0.51
1:F:1:ALA:O	1:F:26:ARG:HD3	2.11	0.51
1:F:8:ALA:HB2	1:F:186:GLU:HB2	1.92	0.51
1:H:86:HIS:N	1:H:86:HIS:CD2	2.79	0.51
1:H:518:VAL:HG23	1:H:543:LEU:HD21	1.92	0.51
1:G:346:LEU:HD23	1:G:373:ILE:HB	1.93	0.51
1:A:304:TYR:CD1	1:A:326:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LEU:HD11	1:F:71:HIS:C	2.36	0.51
1:E:255:GLU:HG2	1:E:403:LYS:HE2	1.93	0.50
1:H:422:LEU:O	1:H:425:LEU:HB3	2.11	0.50
1:B:170:LEU:HD13	1:B:212:ALA:O	2.11	0.50
1:B:197:LEU:N	1:B:198:PRO:CD	2.74	0.50
1:D:410:THR:HG22	1:D:414:MET:HE2	1.94	0.50
1:G:143:GLU:HB3	1:G:147:ARG:NH1	2.26	0.50
1:B:23:LEU:HD21	1:B:195:ALA:HB2	1.93	0.50
1:C:2:GLY:O	1:C:71:HIS:HA	2.11	0.50
1:E:105:GLU:HB2	1:E:106:PRO:HD3	1.92	0.50
1:F:156:TYR:N	1:F:175:GLY:HA3	2.25	0.50
1:H:490:SER:O	1:H:591:LYS:NZ	2.40	0.50
1:C:135:LEU:O	1:C:136:LYS:C	2.55	0.50
1:G:161:MET:HB3	1:G:169:LEU:CD2	2.41	0.50
1:D:86:HIS:HE1	1:D:97:HIS:HB3	1.77	0.50
2:F:701:GLU:O	2:F:701:GLU:HG2	2.11	0.50
1:B:147:ARG:O	1:B:150:PRO:HD2	2.11	0.50
1:G:77:HIS:HE1	1:G:100:ILE:HD13	1.76	0.50
1:A:425:LEU:HD12	1:A:425:LEU:O	2.11	0.50
1:B:97:HIS:NE2	1:B:156:TYR:HB2	2.26	0.50
1:D:105:GLU:OE2	1:D:105:GLU:HA	2.12	0.50
1:E:248:TYR:CD2	1:E:254:LYS:HB2	2.47	0.50
1:B:284:ASN:O	1:B:286:ASP:N	2.44	0.50
1:C:254:LYS:HE2	1:C:258:GLU:OE2	2.12	0.50
1:E:224:LYS:H	1:E:224:LYS:CD	2.21	0.50
1:F:140:THR:HG22	1:F:141:LEU:N	2.27	0.50
1:G:107:LEU:HD11	1:G:151:GLN:O	2.12	0.50
1:H:248:TYR:CD2	1:H:254:LYS:HB2	2.47	0.50
1:E:20:LEU:HD22	1:E:72:THR:HG23	1.94	0.50
1:B:320:ILE:CD1	1:B:419:LEU:O	2.60	0.49
1:C:145:VAL:O	1:C:149:ILE:HG12	2.12	0.49
1:D:346:LEU:HD23	1:D:373:ILE:HB	1.94	0.49
1:E:76:THR:HG1	2:E:701:GLU:N	2.10	0.49
1:H:161:MET:HB3	1:H:169:LEU:CD2	2.42	0.49
1:C:137:GLN:O	1:C:137:GLN:HG2	2.12	0.49
1:H:20:LEU:HD22	1:H:72:THR:HG23	1.94	0.49
1:B:103:ASN:O	1:B:107:LEU:HG	2.13	0.49
1:F:71:HIS:CD2	1:F:96:VAL:CG2	2.96	0.49
1:C:102:GLU:N	1:C:153:ARG:O	2.41	0.49
1:D:103:ASN:O	1:D:107:LEU:HD12	2.13	0.49
1:D:426:ASP:O	1:D:427:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:VAL:HG21	1:G:63:LEU:HB3	1.95	0.49
1:E:2:GLY:O	1:E:71:HIS:HA	2.12	0.49
1:G:36:VAL:HG12	1:G:37:ASP:O	2.13	0.49
1:B:77:HIS:O	1:B:122:THR:HA	2.11	0.49
1:C:569:GLU:HB3	5:C:611:G6Q:O2	2.12	0.49
1:D:12:VAL:O	1:D:16:LEU:HG	2.13	0.49
1:G:171:ALA:O	1:G:211:ILE:HA	2.12	0.49
1:H:401:SER:OG	1:H:404:ALA:HB3	2.13	0.49
1:B:421:ARG:H	1:B:422:LEU:HB3	1.77	0.49
1:C:235:GLU:HG3	1:C:236:SER:N	2.25	0.49
1:H:423:LYS:CB	1:H:424:GLY:CA	2.87	0.49
1:C:567:VAL:HG11	1:C:575:PHE:CG	2.47	0.49
1:E:129:HIS:O	1:E:132:ASN:HB3	2.13	0.49
1:F:204:ILE:HG21	1:F:221:ILE:HD11	1.94	0.49
1:G:205:PHE:HE1	1:G:234:ILE:HD11	1.77	0.49
1:G:328:SER:HB3	1:G:354:ASP:OD2	2.12	0.49
1:G:86:HIS:CE1	1:G:124:THR:HG21	2.48	0.48
1:H:312:TYR:CE2	1:H:473:GLY:HA2	2.48	0.48
1:A:431[B]:HIS:CD2	1:A:435[B]:HIS:CD2	3.01	0.48
5:D:611:G6Q:O5	5:D:611:G6Q:O3	2.25	0.48
1:F:214:ILE:HG23	1:F:219:VAL:HG22	1.95	0.48
1:F:225:THR:OG1	1:F:226:GLY:HA2	2.13	0.48
1:H:567:VAL:HG11	1:H:575:PHE:CG	2.47	0.48
1:C:295:ILE:HD11	1:C:419:LEU:HD13	1.94	0.48
1:F:76:THR:O	1:F:77:HIS:CB	2.61	0.48
1:F:285:ALA:O	1:F:286:ASP:HB3	2.11	0.48
1:H:281:LEU:HD22	1:H:387:LEU:HB3	1.95	0.48
1:H:430:GLU:O	1:H:434:VAL:HG23	2.13	0.48
1:H:472:ARG:HG2	1:H:473:GLY:N	2.28	0.48
1:B:93:ILE:HG12	1:B:131:VAL:HG12	1.95	0.48
1:C:480:LEU:HD23	1:C:496:ALA:HB3	1.96	0.48
1:E:135:LEU:HD23	1:E:135:LEU:HA	1.56	0.48
1:E:567:VAL:HG11	1:E:575:PHE:CG	2.49	0.48
1:G:275:GLN:HG3	1:G:430:GLU:OE2	2.14	0.48
1:B:44:ARG:NH1	1:B:89:VAL:HG13	2.29	0.48
1:E:7:ILE:HG23	1:E:7:ILE:O	2.14	0.48
1:C:63:LEU:HD12	1:C:63:LEU:N	2.29	0.48
1:C:137:GLN:N	1:C:137:GLN:OE1	2.47	0.48
1:D:52:GLN:NE2	1:D:56:GLN:OE1	2.46	0.48
4:E:609:GOL:H12	6:E:1521:HOH:O	2.13	0.48
1:F:89:VAL:HG22	1:F:90:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:LEU:HD13	1:H:129:HIS:HB2	1.93	0.48
1:A:1:ALA:N	1:A:72:THR:O	2.47	0.48
1:D:148:ALA:O	1:D:151:GLN:HG3	2.14	0.48
1:D:304:TYR:CD1	1:D:326:ILE:HD13	2.49	0.48
1:A:110:GLU:O	1:A:114:ARG:HG3	2.14	0.48
1:E:184:MET:HE2	1:E:184:MET:HA	1.95	0.48
1:F:284:ASN:O	1:F:285:ALA:C	2.55	0.48
1:C:447:MET:HE2	1:C:575:PHE:CE2	2.49	0.47
1:D:453:ARG:NH2	1:D:563:GLU:O	2.36	0.47
1:F:15:ILE:HG21	1:F:188:PHE:CE1	2.48	0.47
1:H:245:LYS:NZ	6:H:891:HOH:O	2.47	0.47
1:E:145:VAL:O	1:E:149:ILE:HG12	2.14	0.47
1:F:513:ASP:HB3	6:F:1392:HOH:O	2.14	0.47
1:H:56:GLN:HA	1:H:59:GLU:HG2	1.95	0.47
1:B:89:VAL:HG12	1:B:94:VAL:HG13	1.95	0.47
1:C:90:SER:O	1:C:91:GLU:HB3	2.14	0.47
1:D:73:ARG:NH1	1:D:75:ALA:HB2	2.29	0.47
1:E:205:PHE:HD1	1:E:234:ILE:HD11	1.79	0.47
1:E:396:GLU:OE1	1:E:401:SER:HB2	2.14	0.47
1:F:457:LEU:HD22	1:F:562:ILE:HD13	1.95	0.47
1:F:522:ASN:ND2	6:F:694:HOH:O	2.47	0.47
1:G:104:HIS:CD2	1:G:108:ARG:HH22	2.33	0.47
1:A:240:TYR:CD1	1:A:240:TYR:N	2.83	0.47
1:B:155:ALA:HA	1:B:175:GLY:HA3	1.96	0.47
1:C:447:MET:HG2	1:C:578:VAL:HB	1.97	0.47
1:D:173:ARG:NH2	1:D:177:PRO:HB3	2.29	0.47
1:B:320:ILE:HD13	1:B:421:ARG:HG2	1.97	0.47
1:C:400:ALA:HB1	1:C:485:LYS:CE	2.44	0.47
1:E:9:GLN:HB2	1:E:216:ARG:HH21	1.79	0.47
1:E:37:ASP:OD2	1:E:41[A]:HIS:HB2	2.15	0.47
1:F:149:ILE:N	1:F:150:PRO:CD	2.77	0.47
1:H:295:ILE:HD11	1:H:320:ILE:HD12	1.97	0.47
1:A:591:LYS:HE3	6:A:1520:HOH:O	2.14	0.47
1:D:142:ARG:HG2	1:D:146:LEU:HD11	1.96	0.47
1:D:134:GLU:OE2	1:D:147:ARG:NH2	2.43	0.47
1:F:136:LYS:C	1:F:137:GLN:HG3	2.40	0.47
1:F:188:PHE:CE2	1:F:199:VAL:CG1	2.97	0.47
1:H:518:VAL:CG2	1:H:543:LEU:HD21	2.45	0.47
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.95	0.47
1:D:130:LEU:HD12	1:D:130:LEU:C	2.40	0.47
1:E:197:LEU:N	1:E:198:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:SER:OG	1:F:224:LYS:NZ	2.48	0.47
1:B:71:HIS:CE1	1:B:73:ARG:HB2	2.50	0.47
1:F:503:LYS:O	1:F:503:LYS:HG3	2.14	0.47
1:C:567:VAL:HG11	1:C:575:PHE:CD1	2.50	0.46
1:F:23:LEU:HG	1:F:195:ALA:HB2	1.96	0.46
1:F:489:ILE:HG22	1:F:598:PRO:HG3	1.97	0.46
1:A:161:MET:HB3	1:A:169:LEU:CD2	2.44	0.46
1:C:90:SER:HB2	1:C:128:ALA:HB1	1.95	0.46
1:C:562:ILE:HG22	1:C:564:MET:HE2	1.96	0.46
1:F:420:SER:HB2	1:F:426:ASP:CG	2.40	0.46
1:A:474:ASP:OD2	5:A:610:G6Q:H3	2.15	0.46
1:E:267:LEU:HD21	1:E:437:LEU:HD22	1.97	0.46
1:D:119:VAL:N	1:D:125:GLU:OE2	2.48	0.46
1:F:223:ASP:O	1:F:226:GLY:HA3	2.14	0.46
1:G:215:THR:C	1:G:217:ARG:H	2.24	0.46
1:B:240:TYR:CE2	1:H:243:GLY:HA3	2.51	0.46
1:C:97:HIS:HB3	1:C:124:THR:HG23	1.97	0.46
1:E:74:TRP:CG	1:E:264:LYS:HE2	2.50	0.46
1:F:40:GLY:HA3	1:F:41:HIS:CB	2.38	0.46
1:F:401:SER:OG	1:F:404:ALA:HB3	2.16	0.46
1:A:447:MET:HE1	1:A:564:MET:HG3	1.98	0.46
1:B:401:SER:OG	1:B:404:ALA:HB3	2.15	0.46
1:C:1:ALA:N	2:C:701:GLU:OE1	2.44	0.46
1:C:346:LEU:HD23	1:C:373:ILE:HB	1.97	0.46
1:C:578:VAL:N	1:C:579:PRO:HD2	2.31	0.46
1:E:9:GLN:HB2	1:E:216:ARG:NH2	2.30	0.46
1:F:3:ILE:HG12	1:F:96:VAL:CG2	2.44	0.46
1:A:447:MET:HG2	1:A:575:PHE:CE1	2.51	0.46
1:F:227:ALA:O	1:F:229:VAL:HG23	2.15	0.46
1:B:86:HIS:HB3	1:B:87:PRO:HA	1.98	0.46
1:C:229:VAL:O	1:C:230:LYS:HD2	2.16	0.46
1:B:7:ILE:HD13	1:B:67:THR:OG1	2.15	0.46
1:D:142:ARG:HD3	1:D:222:PHE:CE2	2.51	0.46
1:F:145:VAL:C	1:F:147:ARG:H	2.24	0.46
1:G:474:ASP:OD1	5:G:610:G6Q:H3	2.16	0.46
1:C:105:GLU:HB2	1:C:106:PRO:CD	2.40	0.46
1:C:105:GLU:CB	1:C:106:PRO:HD3	2.38	0.46
1:D:197:LEU:N	1:D:198:PRO:CD	2.79	0.46
1:D:255:GLU:HA	1:D:258:GLU:HG2	1.97	0.46
1:F:130:LEU:C	1:F:130:LEU:HD23	2.41	0.46
1:C:199:VAL:HG23	1:C:200:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:ILE:N	1:F:150:PRO:HD2	2.31	0.45
1:H:423:LYS:HB2	1:H:424:GLY:CA	2.42	0.45
1:D:295:ILE:HD11	1:D:419:LEU:HD13	1.98	0.45
1:E:371:LEU:CD2	1:E:415:LEU:HD21	2.46	0.45
1:F:15:ILE:HD13	1:F:188:PHE:HE1	1.79	0.45
1:B:241:ASP:HB3	1:B:251:TYR:HE1	1.80	0.45
1:H:164:ARG:HE	1:H:164:ARG:HB2	1.57	0.45
1:B:295:ILE:HD11	1:B:419:LEU:HD13	1.97	0.45
1:B:562:ILE:HG22	1:B:564:MET:CE	2.47	0.45
1:C:298:LEU:HD11	1:C:330:PHE:CD2	2.51	0.45
1:H:346:LEU:HD23	1:H:373:ILE:HB	1.99	0.45
1:D:567:VAL:HG11	1:D:575:PHE:CD1	2.52	0.45
1:E:76:THR:OG1	2:E:701:GLU:N	2.50	0.45
1:C:222:PHE:CB	1:C:228:GLU:HA	2.46	0.45
1:D:90:SER:HB2	1:D:128:ALA:C	2.41	0.45
1:D:194:LEU:HD11	1:D:383:ARG:HD3	1.99	0.45
1:E:149:ILE:HG23	1:E:156:TYR:OH	2.16	0.45
1:F:28:TYR:CG	1:F:72:THR:HG23	2.52	0.45
1:F:190:ALA:HB2	1:F:196:LEU:HD21	1.99	0.45
1:D:193:GLN:OE1	1:D:205:PHE:HZ	2.00	0.45
1:E:97:HIS:HB3	1:E:124:THR:HG23	1.99	0.45
1:F:136:LYS:HB2	1:F:136:LYS:HE2	1.70	0.45
1:F:196:LEU:HB2	1:F:203:PHE:HE1	1.81	0.45
1:F:457:LEU:CD2	1:F:562:ILE:HD13	2.47	0.45
1:G:476:TYR:HB3	1:G:477:PRO:HD3	1.99	0.45
1:H:135:LEU:HD23	1:H:135:LEU:HA	1.61	0.45
1:H:180:ILE:O	1:H:203:PHE:HA	2.17	0.45
1:C:557:ASP:N	1:C:557:ASP:OD1	2.49	0.45
1:E:472:ARG:HG2	1:E:473:GLY:N	2.31	0.45
1:G:440:LEU:HB3	1:G:441:PRO:HD3	1.98	0.45
1:G:486:LEU:HD12	1:G:486:LEU:HA	1.70	0.45
1:A:425:LEU:HA	1:A:427:ALA:H	1.81	0.45
1:B:291:LYS:HA	1:B:291:LYS:HD3	1.82	0.45
1:G:175:GLY:N	1:G:208:GLU:OE2	2.50	0.45
1:C:3:ILE:O	1:C:190:ALA:HA	2.17	0.45
1:F:123:ASP:OD1	1:F:124:THR:N	2.50	0.45
1:H:74:TRP:CG	1:H:264:LYS:HE2	2.52	0.45
1:B:225:THR:HG23	1:B:227:ALA:H	1.81	0.44
1:B:240:TYR:CA	1:B:241:ASP:CB	2.92	0.44
1:B:578:VAL:HB	1:B:579:PRO:HD3	1.99	0.44
1:D:203:PHE:O	1:D:233:ASP:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLY:HA2	1:D:381:LEU:HD12	1.99	0.44
1:E:247:ILE:HG13	1:E:247:ILE:O	2.16	0.44
1:E:334:LYS:HB3	1:E:334:LYS:HE2	1.76	0.44
1:F:118:PHE:CE2	1:F:126:VAL:HG12	2.52	0.44
1:H:503:LYS:O	1:H:503:LYS:HG3	2.17	0.44
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.18	0.44
1:E:576:TYR:C	1:E:579:PRO:HD2	2.42	0.44
1:G:205:PHE:CE1	1:G:234:ILE:HD11	2.51	0.44
1:H:440:LEU:HB3	1:H:441:PRO:HD3	1.98	0.44
1:A:63:LEU:HD12	1:A:63:LEU:H	1.82	0.44
1:C:503:LYS:O	1:C:503:LYS:HG3	2.18	0.44
1:E:340:ASN:HA	1:E:368:LEU:HG	1.99	0.44
1:B:320:ILE:HD11	1:B:419:LEU:O	2.17	0.44
1:D:135:LEU:C	1:D:135:LEU:HD23	2.42	0.44
1:E:430:GLU:O	1:E:434:VAL:HG23	2.18	0.44
1:F:531:SER:O	1:F:534:GLU:HB2	2.16	0.44
1:G:18:GLU:O	1:G:22:ARG:HD2	2.18	0.44
1:G:224:LYS:HD2	1:G:225:THR:N	2.32	0.44
1:A:197:LEU:N	1:A:198:PRO:CD	2.81	0.44
1:A:239:GLN:O	1:A:240:TYR:CD1	2.53	0.44
1:D:3:ILE:O	1:D:190:ALA:HA	2.17	0.44
1:F:441:PRO:O	1:F:445:GLU:HG3	2.18	0.44
1:G:141:LEU:CD1	1:G:162:ASP:HB2	2.47	0.44
1:H:294:HIS:CD2	1:H:338:ARG:HG2	2.52	0.44
1:A:311:ARG:HH22	1:B:325:GLU:CD	2.26	0.44
1:A:572:ALA:N	1:A:573:PRO:CD	2.81	0.44
1:B:237:ASN:N	1:B:239:GLN:OE1	2.45	0.44
1:C:51:VAL:O	1:C:54:LEU:N	2.51	0.44
1:D:105:GLU:H	1:D:106:PRO:HD2	1.83	0.44
1:D:440:LEU:HB3	1:D:441:PRO:HD3	1.98	0.44
1:A:318:ALA:HB2	1:A:416:VAL:HG13	1.99	0.44
1:G:97:HIS:HB3	1:G:124:THR:HG23	2.00	0.44
1:H:320:ILE:HG23	1:H:421:ARG:HG3	1.99	0.44
1:B:312:TYR:CE2	1:B:473:GLY:HA2	2.52	0.44
1:B:489:ILE:HG22	1:B:598:PRO:HG3	2.00	0.44
1:C:180:ILE:HD12	1:C:206:LEU:HD21	2.00	0.44
1:C:232:GLN:HE21	1:C:234:ILE:HG22	1.83	0.44
1:D:99:GLY:O	2:D:701:GLU:N	2.51	0.44
1:G:25:TYR:CD2	1:G:383:ARG:HB3	2.52	0.44
1:B:22:ARG:CZ	1:B:198:PRO:HG3	2.48	0.44
1:D:167:ASP:O	1:D:215:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:LYS:HE3	1:G:264:LYS:HB2	1.75	0.44
1:A:423:LYS:O	1:A:424:GLY:C	2.60	0.43
1:B:92:HIS:CD2	1:B:164:ARG:NE	2.85	0.43
1:D:318:ALA:HB2	1:D:416:VAL:HG13	1.98	0.43
1:D:379:SER:O	1:D:383:ARG:HG3	2.17	0.43
1:H:176:SER:HA	1:H:177:PRO:HD3	1.85	0.43
1:A:234:ILE:HD12	1:A:234:ILE:O	2.18	0.43
1:B:230:LYS:HE2	1:B:231:ARG:N	2.31	0.43
1:C:86:HIS:CE1	1:C:124:THR:HG21	2.52	0.43
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.78	0.43
1:H:295:ILE:CD1	1:H:320:ILE:HD12	2.48	0.43
1:H:426:ASP:O	1:H:427:ALA:HB3	2.18	0.43
1:A:242:ALA:HA	1:D:242:ALA:N	2.33	0.43
1:C:140:THR:OG1	1:C:143:GLU:OE1	2.37	0.43
1:C:530:LYS:HG2	1:C:559:MET:SD	2.58	0.43
1:G:104:HIS:HD2	1:G:108:ARG:HH12	1.67	0.43
1:B:123:ASP:O	1:B:126:VAL:HG22	2.18	0.43
1:C:149:ILE:C	1:C:151:GLN:N	2.73	0.43
1:C:229:VAL:HG23	1:C:231:ARG:HH12	1.83	0.43
1:D:141:LEU:HD21	1:D:162:ASP:CB	2.48	0.43
1:F:37:ASP:OD1	1:F:41:HIS:HB3	2.19	0.43
1:A:69:ILE:HD11	1:A:94:VAL:HG12	2.00	0.43
1:A:149:ILE:HB	1:A:150:PRO:HD3	2.00	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.80	0.43
1:C:157:GLY:HA2	1:C:172:ALA:O	2.18	0.43
1:C:196:LEU:HB2	1:C:203:PHE:CE1	2.53	0.43
1:E:530:LYS:NZ	1:E:534:GLU:OE2	2.35	0.43
1:F:77:HIS:O	1:F:122:THR:HA	2.18	0.43
1:G:518:VAL:CG2	1:G:543:LEU:HD21	2.49	0.43
1:C:11:ASP:HA	1:C:65:GLY:O	2.19	0.43
5:E:610:G6Q:O5	5:E:610:G6Q:O3	2.24	0.43
1:H:443:ARG:HD2	1:H:567:VAL:HG12	2.00	0.43
1:F:3:ILE:HD12	1:F:98:ASN:ND2	2.34	0.43
1:A:157:GLY:HA2	1:A:172:ALA:O	2.19	0.43
1:C:204:ILE:CD1	1:C:221:ILE:HD11	2.43	0.43
1:E:155:ALA:HB2	1:E:446:GLN:CD	2.44	0.43
1:E:425:LEU:HD13	1:E:426:ASP:OD2	2.18	0.43
1:F:178:LEU:HB3	1:F:189:ILE:HD11	2.01	0.43
1:F:487:LYS:NZ	1:F:494:ALA:O	2.49	0.43
1:G:130:LEU:HD23	1:G:148:ALA:HB1	2.01	0.43
1:G:292:VAL:O	1:G:421:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:ASP:HA	1:H:65:GLY:HA2	2.01	0.43
1:B:76:THR:OG1	2:B:701:GLU:N	2.52	0.43
1:C:197:LEU:HD23	1:C:203:PHE:CZ	2.53	0.43
1:D:8:ALA:HA	1:D:216:ARG:HG2	2.00	0.43
1:E:86:HIS:N	1:E:86:HIS:CD2	2.85	0.43
1:E:440:LEU:HB3	1:E:441:PRO:HD3	2.00	0.43
1:B:320:ILE:H	1:B:320:ILE:HG12	1.67	0.42
1:C:193:GLN:O	1:C:195:ALA:N	2.52	0.42
1:D:86:HIS:CE1	1:D:97:HIS:HB3	2.53	0.42
1:D:110:GLU:HG3	1:D:114:ARG:NH2	2.34	0.42
1:D:567:VAL:HG11	1:D:575:PHE:CG	2.53	0.42
1:E:315:GLU:HG2	1:E:320:ILE:O	2.19	0.42
1:E:424:GLY:O	1:E:425:LEU:HB2	2.19	0.42
1:F:35:VAL:CG2	1:F:63:LEU:HB3	2.49	0.42
1:F:196:LEU:HB2	1:F:203:PHE:CE1	2.53	0.42
1:F:221:ILE:O	1:F:229:VAL:HB	2.18	0.42
1:G:572:ALA:N	1:G:573:PRO:CD	2.82	0.42
1:A:133:TRP:O	1:A:136:LYS:HB2	2.19	0.42
1:B:174:SER:O	1:B:174:SER:OG	2.28	0.42
1:E:425:LEU:HA	1:E:425:LEU:HD23	1.74	0.42
1:F:530:LYS:HD3	1:F:559:MET:SD	2.59	0.42
1:G:52:GLN:NE2	1:G:52:GLN:C	2.77	0.42
1:G:310:SER:O	1:G:311:ARG:C	2.62	0.42
1:B:437:LEU:HD23	1:B:437:LEU:HA	1.90	0.42
1:G:197:LEU:N	1:G:198:PRO:CD	2.82	0.42
1:A:11:ASP:HA	1:A:65:GLY:O	2.19	0.42
1:A:396:GLU:OE1	1:A:401:SER:HB2	2.20	0.42
1:B:513:ASP:HB3	6:B:618:HOH:O	2.20	0.42
1:E:233:ASP:OD2	1:E:233:ASP:C	2.62	0.42
1:E:321:PRO:HB3	1:F:338:ARG:CZ	2.49	0.42
1:G:304:TYR:CD1	1:G:326:ILE:HD13	2.54	0.42
1:A:173:ARG:O	1:A:173:ARG:HG3	2.12	0.42
1:A:425:LEU:HD13	1:A:428:SER:CB	2.50	0.42
1:A:487:LYS:HG2	1:B:509:LEU:HD11	2.02	0.42
1:C:193:GLN:O	1:C:194:LEU:C	2.63	0.42
1:E:134:GLU:O	1:E:147:ARG:NH2	2.52	0.42
1:E:174:SER:HA	1:E:208:GLU:OE2	2.19	0.42
1:E:337:VAL:HG12	1:E:338:ARG:O	2.18	0.42
1:F:125:GLU:HG2	1:F:129:HIS:CD2	2.54	0.42
1:F:175:GLY:N	1:F:208:GLU:OE2	2.53	0.42
1:B:379:SER:O	1:B:383:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:SER:HB2	1:D:128:ALA:CB	2.48	0.42
1:E:25:TYR:OH	1:E:192:ASP:OD2	2.29	0.42
1:F:4:VAL:CG1	1:F:16:LEU:HA	2.50	0.42
1:F:35:VAL:HG21	1:F:63:LEU:HB3	2.00	0.42
1:F:374:CYS:O	1:F:390:MET:HA	2.20	0.42
1:A:431[B]:HIS:NE2	1:A:435[B]:HIS:HD2	2.16	0.42
1:B:603:LYS:HD2	1:B:603:LYS:HA	1.80	0.42
1:C:309:VAL:HG23	1:C:477:PRO:HB2	2.02	0.42
1:D:411:VAL:HA	1:D:414:MET:CE	2.37	0.42
1:F:71:HIS:CG	1:F:86:HIS:HB2	2.54	0.42
1:A:528:LYS:HE3	1:B:608:GLU:O	2.20	0.42
1:B:142:ARG:NE	1:B:213:GLU:OE1	2.52	0.42
1:D:165:HIS:C	1:D:167:ASP:H	2.27	0.42
1:F:223:ASP:OD2	1:F:224:LYS:N	2.49	0.42
1:G:182:LEU:HD11	1:G:204:ILE:HD11	2.02	0.42
1:H:197:LEU:N	1:H:198:PRO:CD	2.82	0.42
1:A:184:MET:HE3	1:A:184:MET:HB3	1.75	0.42
1:A:311:ARG:HD3	6:A:707:HOH:O	2.19	0.42
1:A:568:GLU:H	1:A:568:GLU:CD	2.28	0.42
1:C:134:GLU:HB3	1:C:144:ALA:HA	2.02	0.42
1:C:488:GLU:O	1:C:598:PRO:HB3	2.19	0.42
1:D:18:GLU:O	1:D:22:ARG:HG3	2.20	0.42
1:D:86:HIS:CE1	1:D:124:THR:HG21	2.55	0.42
1:D:111:LEU:HD22	1:D:116:TYR:CE2	2.55	0.42
1:E:404:ALA:O	1:E:408:GLN:HG3	2.19	0.42
1:H:530:LYS:O	1:H:534:GLU:HG2	2.20	0.42
1:C:486:LEU:HD12	1:C:486:LEU:HA	1.89	0.42
1:D:56:GLN:O	1:D:57:ALA:C	2.63	0.42
1:G:340:ASN:OD1	1:G:368:LEU:HD21	2.20	0.42
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.82	0.41
1:G:217:ARG:HA	1:G:217:ARG:HD3	1.60	0.41
1:A:569:GLU:HB2	5:A:610:G6Q:O2	2.20	0.41
1:C:193:GLN:OE1	1:C:205:PHE:HZ	2.03	0.41
1:D:447:MET:HE2	1:D:575:PHE:CZ	2.54	0.41
1:E:158:THR:HG22	1:E:172:ALA:HB3	2.02	0.41
1:F:3:ILE:HG21	1:F:159:VAL:HG21	2.02	0.41
1:F:24:GLU:HG2	1:F:28:TYR:CE1	2.55	0.41
1:F:569:GLU:HG2	5:F:610:G6Q:O4	2.19	0.41
1:G:143:GLU:O	1:G:144:ALA:C	2.63	0.41
1:B:25:TYR:CE2	1:B:26:ARG:HG3	2.55	0.41
1:C:301:GLY:O	1:C:304:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ARG:HE	1:E:164:ARG:HB2	1.54	0.41
1:F:34:ALA:HB2	1:F:87:PRO:HG2	2.02	0.41
1:F:287:GLU:O	1:F:291:LYS:HD3	2.21	0.41
1:F:557:ASP:OD1	1:F:557:ASP:N	2.53	0.41
1:F:567:VAL:CG2	1:F:575:PHE:CD2	3.03	0.41
1:G:90:SER:O	1:G:91:GLU:HB2	2.20	0.41
1:G:181:GLY:HA2	1:G:202:ARG:O	2.20	0.41
1:G:447:MET:HE2	1:G:575:PHE:CE2	2.55	0.41
1:H:411:VAL:HA	1:H:414:MET:HE2	2.01	0.41
1:A:37:ASP:OD2	1:A:41[A]:HIS:HB2	2.20	0.41
1:B:101:ILE:HG21	1:B:152:LEU:HD22	2.02	0.41
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.83	0.41
1:F:476:TYR:HB3	1:F:477:PRO:HD3	2.02	0.41
1:H:423:LYS:HD2	1:H:423:LYS:N	2.35	0.41
1:C:164:ARG:HE	1:C:164:ARG:HB2	1.42	0.41
1:D:90:SER:O	1:D:132:ASN:ND2	2.54	0.41
1:F:47:ARG:HD3	1:F:47:ARG:HA	1.83	0.41
1:G:374:CYS:O	1:G:390:MET:HA	2.20	0.41
1:C:443:ARG:HD2	1:C:567:VAL:HG12	2.03	0.41
1:D:179:VAL:HG22	1:D:180:ILE:N	2.36	0.41
1:E:287:GLU:O	1:E:290:SER:OG	2.34	0.41
1:E:318:ALA:HB1	1:E:420:SER:HA	2.02	0.41
1:D:107:LEU:CD1	1:D:152:LEU:HD23	2.50	0.41
1:F:3:ILE:HG13	1:F:98:ASN:ND2	2.35	0.41
1:H:481:GLU:OE2	1:H:485:LYS:NZ	2.43	0.41
1:B:101:ILE:HD12	1:B:152:LEU:HB3	2.01	0.41
1:B:230:LYS:HE2	1:B:230:LYS:CA	2.45	0.41
1:C:138:GLY:O	1:C:139:GLY:C	2.64	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.74	0.41
1:C:184:MET:HE2	1:G:14:GLU:HG2	2.02	0.41
1:E:347:SER:O	1:E:374:CYS:HA	2.21	0.41
1:A:105:GLU:HB2	1:A:106:PRO:HD3	2.03	0.41
1:A:312:TYR:CE2	1:A:473:GLY:HA2	2.55	0.41
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.92	0.41
1:A:522:ASN:OD1	1:A:522:ASN:C	2.63	0.41
1:A:578:VAL:N	1:A:579:PRO:HD2	2.36	0.41
1:C:71:HIS:ND1	1:C:86:HIS:HB2	2.36	0.41
1:C:176:SER:HA	1:C:177:PRO:HD3	1.83	0.41
1:C:309:VAL:CG2	1:C:477:PRO:HB2	2.50	0.41
1:D:80:PRO:O	1:D:81:SER:HB3	2.20	0.41
1:D:95:VAL:HG22	1:D:160:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:LEU:N	1:F:198:PRO:CD	2.83	0.41
1:F:224:LYS:HE2	1:F:224:LYS:HB2	1.89	0.41
1:F:281:LEU:HD23	1:F:281:LEU:HA	1.93	0.41
1:F:486:LEU:HD12	1:F:486:LEU:HA	1.91	0.41
1:B:401:SER:HB2	6:B:659:HOH:O	2.20	0.41
1:C:196:LEU:C	1:C:198:PRO:HD2	2.45	0.41
1:F:34:ALA:CB	1:F:87:PRO:HG2	2.51	0.41
1:F:196:LEU:HD12	1:F:203:PHE:CE1	2.56	0.41
1:G:193:GLN:HB2	1:G:203:PHE:CE2	2.56	0.41
1:B:310:SER:HB3	1:B:412:LEU:HD13	2.02	0.40
1:E:277:ASP:C	1:E:277:ASP:OD1	2.64	0.40
1:E:426:ASP:HB3	1:E:428:SER:H	1.86	0.40
1:F:9:GLN:O	1:F:9:GLN:HG2	2.22	0.40
1:F:84:ASN:OD1	1:F:120:SER:HB2	2.22	0.40
1:F:501:GLU:O	1:F:502:LEU:C	2.64	0.40
1:G:532:ASN:O	1:G:535:GLU:HB2	2.21	0.40
1:H:123:ASP:OD1	2:H:701:GLU:N	2.54	0.40
1:A:210:ASP:C	1:A:211:ILE:HG13	2.46	0.40
1:A:431[B]:HIS:CE1	1:A:435[B]:HIS:NE2	2.90	0.40
1:B:317:LEU:O	1:B:429:ILE:HD13	2.22	0.40
1:B:374:CYS:O	1:B:390:MET:HA	2.20	0.40
1:B:530:LYS:HD3	1:B:559:MET:SD	2.61	0.40
1:C:123:ASP:OD1	2:C:701:GLU:N	2.54	0.40
1:C:222:PHE:HA	1:C:228:GLU:HA	2.03	0.40
1:E:23:LEU:HD21	1:E:192:ASP:HB3	2.02	0.40
1:E:136:LYS:C	1:E:138:GLY:N	2.79	0.40
1:F:37:ASP:OD1	1:F:37:ASP:C	2.64	0.40
1:G:562:ILE:HG22	1:G:564:MET:HE2	2.02	0.40
1:H:306:SER:O	1:H:307:GLY:C	2.64	0.40
1:B:320:ILE:HD12	1:B:419:LEU:O	2.20	0.40
1:F:76:THR:HG23	2:F:701:GLU:HB3	2.02	0.40
1:F:141:LEU:CG	1:F:170:LEU:HD23	2.50	0.40
1:G:35:VAL:CG2	1:G:63:LEU:HB3	2.52	0.40
1:G:312:TYR:CE2	1:G:473:GLY:HA2	2.56	0.40
1:H:192:ASP:C	1:H:192:ASP:OD1	2.65	0.40
1:A:603:LYS:HA	1:A:603:LYS:HD2	1.97	0.40
1:C:232:GLN:NE2	1:C:234:ILE:HG22	2.37	0.40
1:D:52:GLN:O	1:D:56:GLN:HG3	2.21	0.40
1:E:503:LYS:HG3	1:E:503:LYS:O	2.21	0.40
1:A:36:VAL:HG22	1:A:42:MET:HG2	2.02	0.40
1:A:158:THR:HG22	1:A:172:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HG13	1:D:190:ALA:N	2.37	0.40
1:D:589:LEU:HD23	1:D:589:LEU:HA	1.95	0.40
1:F:79:GLU:HA	1:F:80:PRO:HD3	1.89	0.40
1:G:168:THR:HG22	1:G:169:LEU:N	2.37	0.40
1:G:440:LEU:O	1:G:444:ILE:HG12	2.21	0.40
1:H:522:ASN:OD1	1:H:522:ASN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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

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Mol	Chain	Res	Type
1	B	285	ALA
1	C	139	GLY
1	E	114	ARG
1	E	426	ASP
1	F	77	HIS
1	F	114	ARG
1	F	286	ASP
1	A	424	GLY
1	B	228	GLU
1	B	286	ASP
1	B	426	ASP
1	C	286	ASP
1	D	114	ARG
1	D	227	ALA
1	D	426	ASP
1	E	244	ASP
1	E	419	LEU
1	F	40	GLY
1	A	238	LEU
1	A	244	ASP
1	C	194	LEU
1	D	224	LYS
1	F	41	HIS
1	G	41	HIS
1	G	228	GLU
1	B	114	ARG
1	C	91	GLU
1	C	136	LYS
1	E	421	ARG
1	F	138	GLY
1	F	222	PHE
1	G	40	GLY
1	H	423	LYS
1	H	535	GLU
1	D	91	GLU
1	F	79	GLU
1	F	92	HIS
1	F	146	LEU
1	F	183	GLY
1	F	505	GLY
1	G	505	GLY
1	C	505	GLY

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Mol	Chain	Res	Type
1	D	40	GLY
1	D	105	GLU
1	E	505	GLY
1	A	505	GLY
1	B	27	GLY
1	C	150	PRO

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
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

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	53	MET
1	A	112	LYS
1	A	126	VAL
1	A	135	LEU
1	A	137	GLN
1	A	153	ARG
1	A	170	LEU
1	A	173	ARG

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	184	MET
1	A	225	THR
1	A	229	VAL
1	A	232	GLN
1	A	320	ILE
1	A	339	ARG
1	A	364	GLU
1	A	415	LEU
1	A	418	LYS
1	A	422	LEU
1	A	426	ASP
1	A	453	ARG
1	A	485	LYS
1	A	497	TYR
1	A	518	VAL
1	A	543	LEU
1	A	589	LEU
1	A	607	VAL
1	A	608	GLU
1	B	7	ILE
1	B	35	VAL
1	B	60	GLU
1	B	79	GLU
1	B	94	VAL
1	B	103	ASN
1	B	105	GLU
1	B	112	LYS
1	B	119	VAL
1	B	126	VAL
1	B	135	LEU
1	B	136	LYS
1	B	179	VAL
1	B	199	VAL
1	B	219	VAL
1	B	229	VAL
1	B	230	LYS
1	B	233	ASP
1	B	238	LEU
1	B	239	GLN
1	B	241	ASP
1	B	320	ILE

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Mol	Chain	Res	Type
1	B	328	SER
1	B	337	VAL
1	B	415	LEU
1	B	421	ARG
1	B	422	LEU
1	B	518	VAL
1	B	524	GLU
1	B	543	LEU
1	B	563	GLU
1	B	567	VAL
1	B	589	LEU
1	C	50	LYS
1	C	52	GLN
1	C	119	VAL
1	C	122	THR
1	C	126	VAL
1	C	135	LEU
1	C	143	GLU
1	C	164	ARG
1	C	170	LEU
1	C	173	ARG
1	C	200	THR
1	C	204	ILE
1	C	230	LYS
1	C	235	GLU
1	C	415	LEU
1	C	418	LYS
1	C	421	ARG
1	C	485	LYS
1	C	497	TYR
1	C	524	GLU
1	C	543	LEU
1	C	567	VAL
1	C	589	LEU
1	C	608	GLU
1	D	50	LYS
1	D	63	LEU
1	D	95	VAL
1	D	109	GLU
1	D	121	GLU
1	D	126	VAL
1	D	130	LEU

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Mol	Chain	Res	Type
1	D	136	LYS
1	D	141	LEU
1	D	149	ILE
1	D	151	GLN
1	D	169	LEU
1	D	170	LEU
1	D	189	ILE
1	D	207	GLU
1	D	218	SER
1	D	230	LYS
1	D	261	ASN
1	D	328[A]	SER
1	D	328[B]	SER
1	D	339	ARG
1	D	415	LEU
1	D	423	LYS
1	D	428	SER
1	D	445	GLU
1	D	497	TYR
1	D	518	VAL
1	D	543	LEU
1	D	567	VAL
1	D	589	LEU
1	E	7	ILE
1	E	14	GLU
1	E	53	MET
1	E	60	GLU
1	E	90	SER
1	E	126	VAL
1	E	170	LEU
1	E	176	SER
1	E	179	VAL
1	E	184	MET
1	E	202	ARG
1	E	208	GLU
1	E	216	ARG
1	E	224	LYS
1	E	232	GLN
1	E	234	ILE
1	E	235	GLU
1	E	247	ILE
1	E	271	ILE

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Mol	Chain	Res	Type
1	E	320	ILE
1	E	339	ARG
1	E	371	LEU
1	E	395	THR
1	E	401	SER
1	E	415	LEU
1	E	418	LYS
1	E	421	ARG
1	E	423	LYS
1	E	425	LEU
1	E	442	SER
1	E	518	VAL
1	E	543	LEU
1	E	567	VAL
1	E	607	VAL
1	F	20	LEU
1	F	26	ARG
1	F	39	GLU
1	F	48	LEU
1	F	51	VAL
1	F	56	GLN
1	F	72	THR
1	F	76	THR
1	F	77	HIS
1	F	79	GLU
1	F	86	HIS
1	F	102	GLU
1	F	121	GLU
1	F	126	VAL
1	F	135	LEU
1	F	136	LYS
1	F	143	GLU
1	F	151	GLN
1	F	160	ILE
1	F	165	HIS
1	F	179	VAL
1	F	184	MET
1	F	189	ILE
1	F	193	GLN
1	F	199	VAL
1	F	207	GLU
1	F	230	LYS

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Mol	Chain	Res	Type
1	F	254	LYS
1	F	418	LYS
1	F	453	ARG
1	F	497	TYR
1	F	518	VAL
1	F	543	LEU
1	F	567	VAL
1	F	589	LEU
1	G	7	ILE
1	G	22	ARG
1	G	26	ARG
1	G	29	ASP
1	G	39	GLU
1	G	52	GLN
1	G	56	GLN
1	G	79	GLU
1	G	94	VAL
1	G	103	ASN
1	G	121	GLU
1	G	126	VAL
1	G	135	LEU
1	G	141	LEU
1	G	170	LEU
1	G	189	ILE
1	G	216	ARG
1	G	224	LYS
1	G	275	GLN
1	G	335	SER
1	G	364	GLU
1	G	418	LYS
1	G	421	ARG
1	G	425	LEU
1	G	497	TYR
1	G	518	VAL
1	G	543	LEU
1	G	589	LEU
1	H	14	GLU
1	H	21	ARG
1	H	33	LEU
1	H	45	LEU
1	H	86	HIS
1	H	107	LEU

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Mol	Chain	Res	Type
1	H	114	ARG
1	H	126	VAL
1	H	135	LEU
1	H	137	GLN
1	H	142	ARG
1	H	149	ILE
1	H	164	ARG
1	H	211	ILE
1	H	224	LYS
1	H	229	VAL
1	H	230	LYS
1	H	234	ILE
1	H	291	LYS
1	H	320	ILE
1	H	364	GLU
1	H	391	THR
1	H	415	LEU
1	H	419	LEU
1	H	423	LYS
1	H	428	SER
1	H	462	SER
1	H	524	GLU
1	H	543	LEU
1	H	567	VAL
1	H	589	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	261	ASN
1	A	275	GLN
1	A	597	GLN
1	B	64	HIS
1	B	103	ASN
1	B	104	HIS
1	B	435	HIS
1	B	532	ASN
1	C	232	GLN
1	C	532	ASN
1	D	52	GLN
1	D	549	GLN

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Mol	Chain	Res	Type
1	E	232	GLN
1	E	446	GLN
1	E	532	ASN
1	F	86	HIS
1	F	98	ASN
1	F	104	HIS
1	F	259	GLN
1	F	581	GLN
1	G	52	GLN
1	G	71	HIS
1	G	104	HIS
1	G	165	HIS
1	H	56	GLN

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](#)

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
5	E	610	G6Q	O2-C2	-2.94	1.38	1.43
3	E	616	G6P	P-O2P	2.93	1.65	1.54
3	D	609	G6P	P-O2P	2.93	1.65	1.54
3	F	615	G6P	P-O2P	2.93	1.65	1.54
5	H	610	G6Q	O2-C2	-2.93	1.38	1.43
3	B	612	G6P	P-O2P	2.84	1.65	1.54
3	H	614	G6P	P-O2P	2.82	1.65	1.54
3	C	610	G6P	P-O2P	2.81	1.65	1.54
3	H	614	G6P	P-O1P	2.79	1.65	1.54
3	B	612	G6P	P-O1P	2.79	1.65	1.54
3	E	616	G6P	P-O1P	2.76	1.65	1.54
5	F	610	G6Q	O2-C2	-2.75	1.38	1.43
3	G	613	G6P	P-O1P	2.70	1.64	1.54
5	C	611	G6Q	O2-C2	-2.67	1.38	1.43
3	A	611	G6P	P-O2P	2.63	1.64	1.54
3	F	615	G6P	P-O1P	2.58	1.64	1.54
3	D	609	G6P	P-O1P	2.57	1.64	1.54
3	C	610	G6P	P-O1P	2.49	1.64	1.54
3	A	611	G6P	P-O1P	2.48	1.64	1.54
5	D	611	G6Q	O4-C4	-2.33	1.37	1.43
5	C	611	G6Q	O5-C5	-2.33	1.38	1.43
5	D	611	G6Q	O5-C5	-2.32	1.38	1.43
5	B	610	G6Q	O5-C5	-2.32	1.38	1.43
2	B	701	GLU	OXT-C	-2.31	1.23	1.30
2	F	701	GLU	OXT-C	-2.28	1.23	1.30
5	G	610	G6Q	O5-C5	-2.21	1.38	1.43
2	E	701	GLU	OXT-C	-2.17	1.23	1.30
5	A	610	G6Q	O5-C5	-2.16	1.38	1.43
2	D	701	GLU	OXT-C	-2.15	1.23	1.30
5	H	610	G6Q	O4-C4	-2.14	1.37	1.43
5	F	610	G6Q	O4-C4	-2.14	1.37	1.43
2	C	701	GLU	OXT-C	-2.11	1.23	1.30
2	G	701	GLU	OXT-C	-2.11	1.23	1.30
3	D	609	G6P	C1-C2	2.10	1.57	1.52
5	B	610	G6Q	O4-C4	-2.10	1.37	1.43
2	A	701	GLU	OXT-C	-2.10	1.23	1.30
5	E	610	G6Q	O5-C5	-2.10	1.38	1.43
5	F	610	G6Q	O5-C5	-2.09	1.39	1.43
5	A	610	G6Q	O4-C4	-2.07	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	701	GLU	OXT-C	-2.04	1.24	1.30
5	G	610	G6Q	O4-C4	-2.04	1.37	1.43
5	D	611	G6Q	C5-C4	-2.01	1.49	1.53

All (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
5	F	610	G6Q	O6-C6-C5	3.17	117.81	109.36
5	G	610	G6Q	O6-C6-C5	3.15	117.76	109.36
2	B	701	GLU	OXT-C-O	-2.85	117.61	124.08
3	E	616	G6P	O5-C1-C2	2.81	115.23	110.30
3	D	609	G6P	C6-C5-C4	-2.77	106.25	112.07
2	G	701	GLU	OXT-C-O	-2.76	117.81	124.08
5	D	611	G6Q	C5-C4-C3	-2.75	108.25	112.48
3	G	613	G6P	C1-O5-C5	2.75	118.97	113.65
5	F	610	G6Q	O2-C2-C1	-2.70	104.34	110.48
3	E	616	G6P	O3-C3-C4	2.68	116.70	110.38
5	A	610	G6Q	O6-C6-C5	2.62	116.35	109.36
5	C	611	G6Q	C5-C4-C3	-2.59	108.51	112.48
2	H	701	GLU	OXT-C-O	-2.58	118.22	124.08
3	A	611	G6P	C6-C5-C4	-2.55	106.72	112.07
2	D	701	GLU	OXT-C-O	-2.51	118.39	124.08
2	A	701	GLU	OXT-C-O	-2.45	118.51	124.08
2	F	701	GLU	OXT-C-O	-2.45	118.52	124.08
3	H	614	G6P	O3-C3-C4	2.45	116.15	110.38
5	D	611	G6Q	O6-C6-C5	2.41	115.80	109.36
3	G	613	G6P	O6-P-O3P	2.38	112.88	106.44
3	E	616	G6P	O3-C3-C2	2.38	115.98	110.38
2	C	701	GLU	OXT-C-O	-2.31	118.84	124.08
3	C	610	G6P	O6-P-O3P	2.29	112.62	106.44
3	C	610	G6P	C6-C5-C4	-2.26	107.32	112.07
5	F	610	G6Q	C4-C3-C2	2.24	117.42	113.49
3	E	616	G6P	O6-P-O3P	2.24	112.50	106.44
3	G	613	G6P	O3-C3-C2	2.23	115.62	110.38
5	G	610	G6Q	O2-C2-C1	-2.19	105.49	110.48
3	H	614	G6P	C6-C5-C4	-2.17	107.51	112.07
5	H	610	G6Q	O2-C2-C1	-2.09	105.72	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	610	G6Q	O2-C2-C1	-2.06	105.80	110.48

There are no chirality outliers.

All (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
4	G	609	GOL	O1-C1-C2-O2
4	G	609	GOL	O1-C1-C2-C3
4	G	609	GOL	C1-C2-C3-O3
4	G	609	GOL	O2-C2-C3-O3
4	H	609	GOL	O1-C1-C2-C3
5	A	610	G6Q	C2-C3-C4-C5
5	A	610	G6Q	C2-C3-C4-O4
5	A	610	G6Q	O3-C3-C4-C5
5	A	610	G6Q	O3-C3-C4-O4
5	A	610	G6Q	C4-C5-C6-O6
5	A	610	G6Q	O5-C5-C6-O6
5	A	610	G6Q	C6-O6-P-O2P
5	A	610	G6Q	C6-O6-P-O3P
5	B	610	G6Q	C2-C3-C4-C5
5	B	610	G6Q	C2-C3-C4-O4
5	B	610	G6Q	O3-C3-C4-C5
5	B	610	G6Q	O3-C3-C4-O4
5	C	611	G6Q	C2-C3-C4-C5
5	C	611	G6Q	C2-C3-C4-O4
5	C	611	G6Q	O3-C3-C4-C5
5	C	611	G6Q	O3-C3-C4-O4
5	C	611	G6Q	C4-C5-C6-O6
5	C	611	G6Q	O5-C5-C6-O6
5	C	611	G6Q	C6-O6-P-O1P
5	C	611	G6Q	C6-O6-P-O2P
5	D	611	G6Q	O3-C3-C4-C5
5	D	611	G6Q	O5-C5-C6-O6
5	E	610	G6Q	C2-C3-C4-C5
5	E	610	G6Q	C2-C3-C4-O4
5	E	610	G6Q	O3-C3-C4-C5
5	E	610	G6Q	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	E	610	G6Q	C6-O6-P-O2P
5	F	610	G6Q	C2-C3-C4-C5
5	F	610	G6Q	C2-C3-C4-O4
5	F	610	G6Q	O3-C3-C4-C5
5	F	610	G6Q	O3-C3-C4-O4
5	F	610	G6Q	C4-C5-C6-O6
5	F	610	G6Q	O5-C5-C6-O6
5	F	610	G6Q	C6-O6-P-O1P
5	F	610	G6Q	C6-O6-P-O2P
5	F	610	G6Q	C6-O6-P-O3P
5	G	610	G6Q	C2-C3-C4-C5
5	G	610	G6Q	C2-C3-C4-O4
5	G	610	G6Q	O3-C3-C4-C5
5	G	610	G6Q	O3-C3-C4-O4
5	H	610	G6Q	C2-C3-C4-C5
5	H	610	G6Q	C2-C3-C4-O4
5	H	610	G6Q	O3-C3-C4-C5
5	H	610	G6Q	O3-C3-C4-O4
5	H	610	G6Q	C4-C5-C6-O6
5	H	610	G6Q	O5-C5-C6-O6
5	H	610	G6Q	C6-O6-P-O1P
5	H	610	G6Q	C6-O6-P-O2P
5	E	610	G6Q	O4-C4-C5-C6
5	E	610	G6Q	C3-C4-C5-C6
5	D	611	G6Q	O3-C3-C4-O4
5	D	611	G6Q	C2-C3-C4-O4
5	D	611	G6Q	C2-C3-C4-C5
4	H	609	GOL	O1-C1-C2-O2
5	E	610	G6Q	C3-C4-C5-O5
5	E	610	G6Q	O4-C4-C5-O5
4	A	609	GOL	O1-C1-C2-C3
4	A	609	GOL	C1-C2-C3-O3
4	H	609	GOL	C1-C2-C3-O3
4	E	609	GOL	O1-C1-C2-O2
5	B	610	G6Q	O5-C5-C6-O6
4	A	609	GOL	O1-C1-C2-O2
5	A	610	G6Q	C6-O6-P-O1P
4	F	609	GOL	O1-C1-C2-O2
3	B	612	G6P	O5-C5-C6-O6
5	C	611	G6Q	C6-O6-P-O3P
5	E	610	G6Q	C6-O6-P-O3P
5	E	610	G6Q	C6-O6-P-O1P

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Mol	Chain	Res	Type	Atoms
5	A	610	G6Q	C3-C4-C5-O5
5	D	611	G6Q	C4-C5-C6-O6
2	G	701	GLU	OE2-CD-CG-CB
4	F	609	GOL	C1-C2-C3-O3
3	A	611	G6P	O5-C5-C6-O6
3	F	615	G6P	O5-C5-C6-O6
2	H	701	GLU	OE2-CD-CG-CB
2	D	701	GLU	OE1-CD-CG-CB
2	E	701	GLU	OE1-CD-CG-CB
2	B	701	GLU	OE1-CD-CG-CB
2	E	701	GLU	OE2-CD-CG-CB
2	D	701	GLU	OE2-CD-CG-CB
2	G	701	GLU	OE1-CD-CG-CB
2	H	701	GLU	OE1-CD-CG-CB
2	A	701	GLU	OE2-CD-CG-CB
2	B	701	GLU	OE2-CD-CG-CB
4	H	609	GOL	O2-C2-C3-O3
5	H	610	G6Q	C6-O6-P-O3P
2	A	701	GLU	OE1-CD-CG-CB
5	C	611	G6Q	C3-C4-C5-O5
5	D	611	G6Q	C3-C4-C5-O5
2	F	701	GLU	OE1-CD-CG-CB
2	F	701	GLU	OE2-CD-CG-CB
5	A	610	G6Q	O4-C4-C5-C6
5	D	611	G6Q	O4-C4-C5-C6
2	F	701	GLU	OXT-C-CA-N
3	B	612	G6P	C4-C5-C6-O6

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

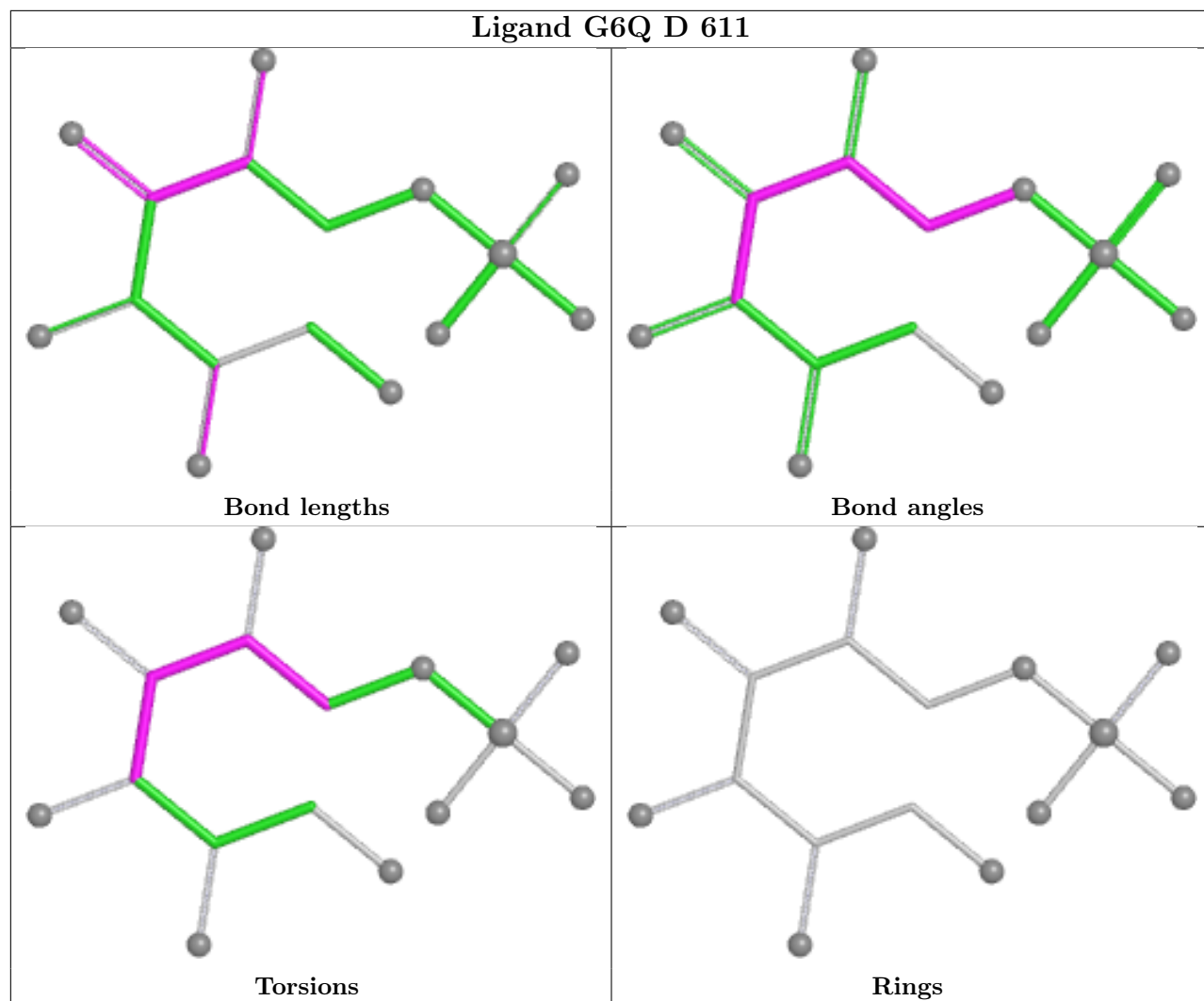
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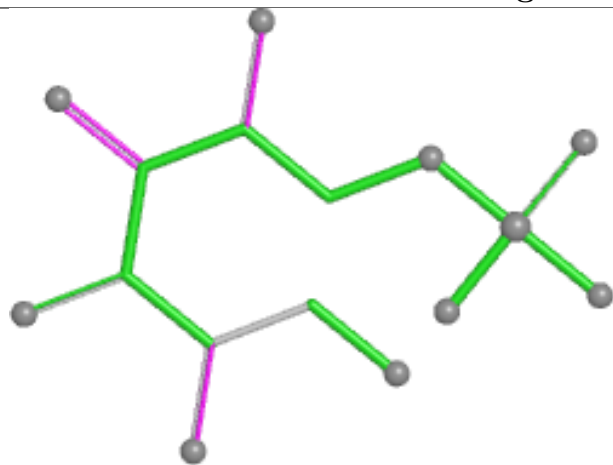
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	611	G6Q	3	0
2	C	701	GLU	2	0
2	E	701	GLU	2	0
2	H	701	GLU	1	0

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.

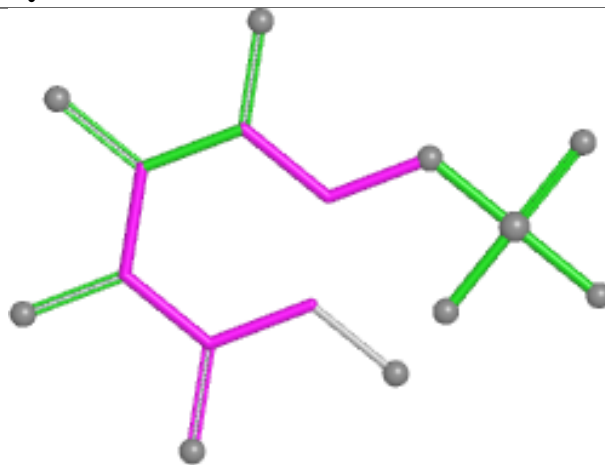
Ligand G6Q D 611



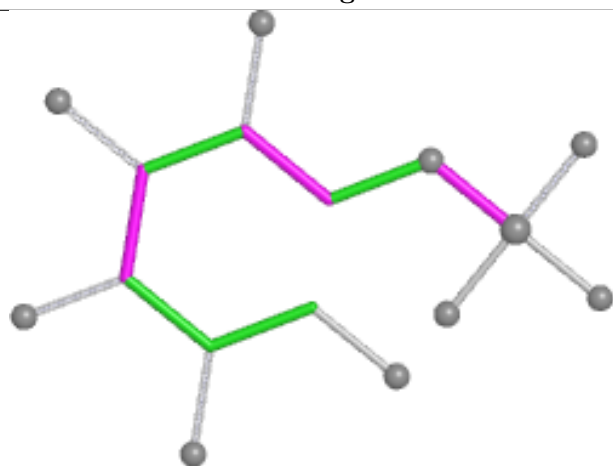
Ligand G6Q F 610



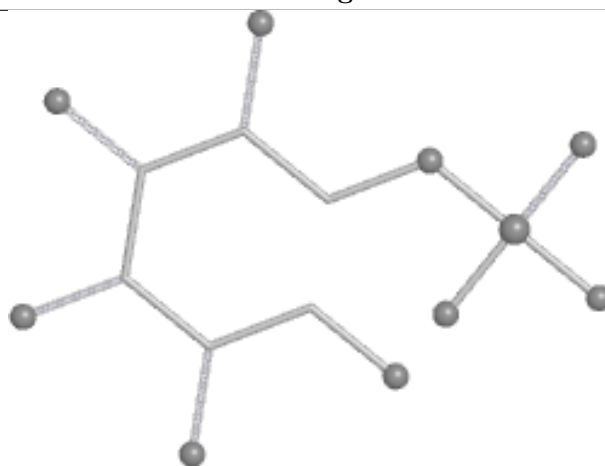
Bond lengths



Bond angles

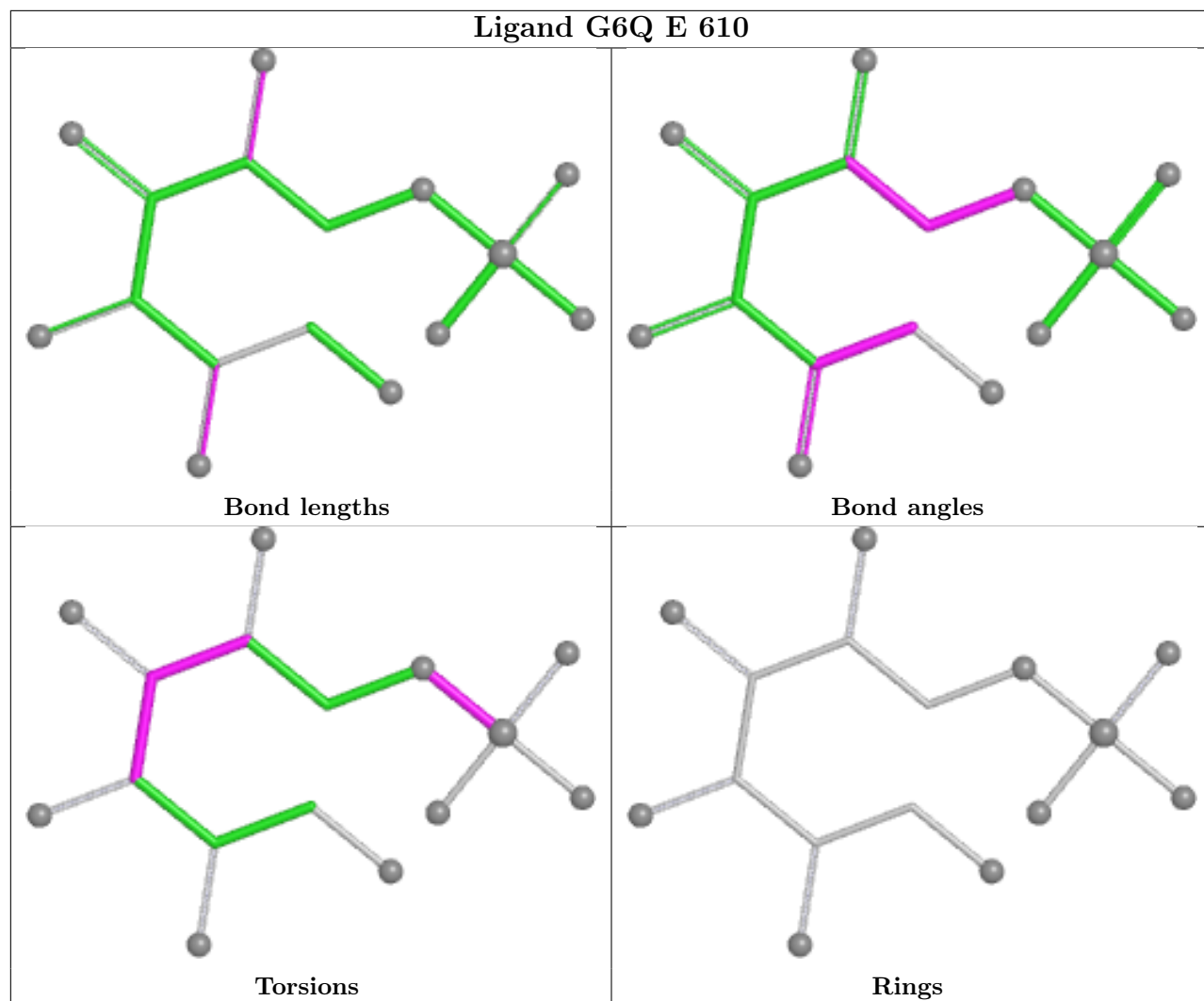


Torsions

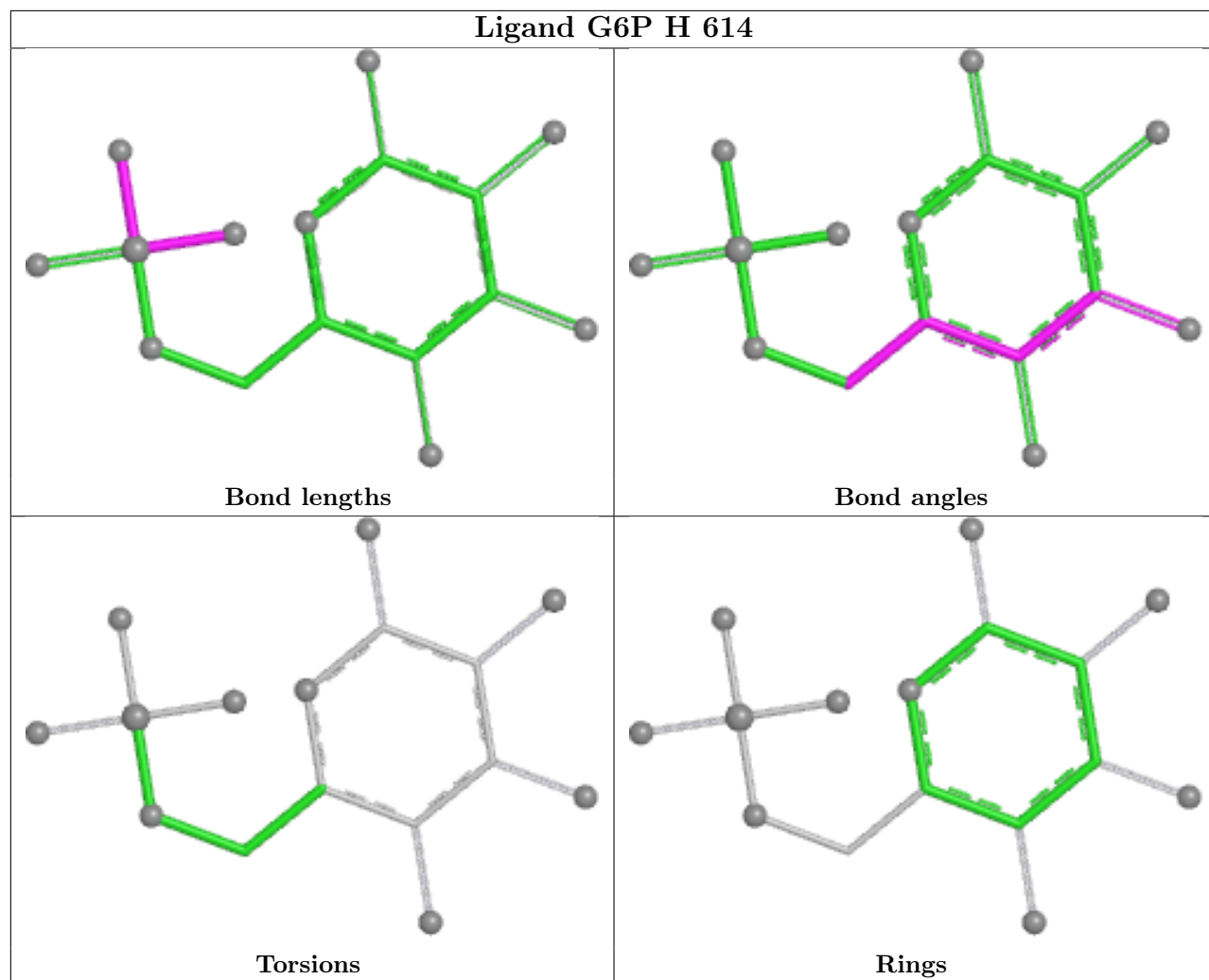


Rings

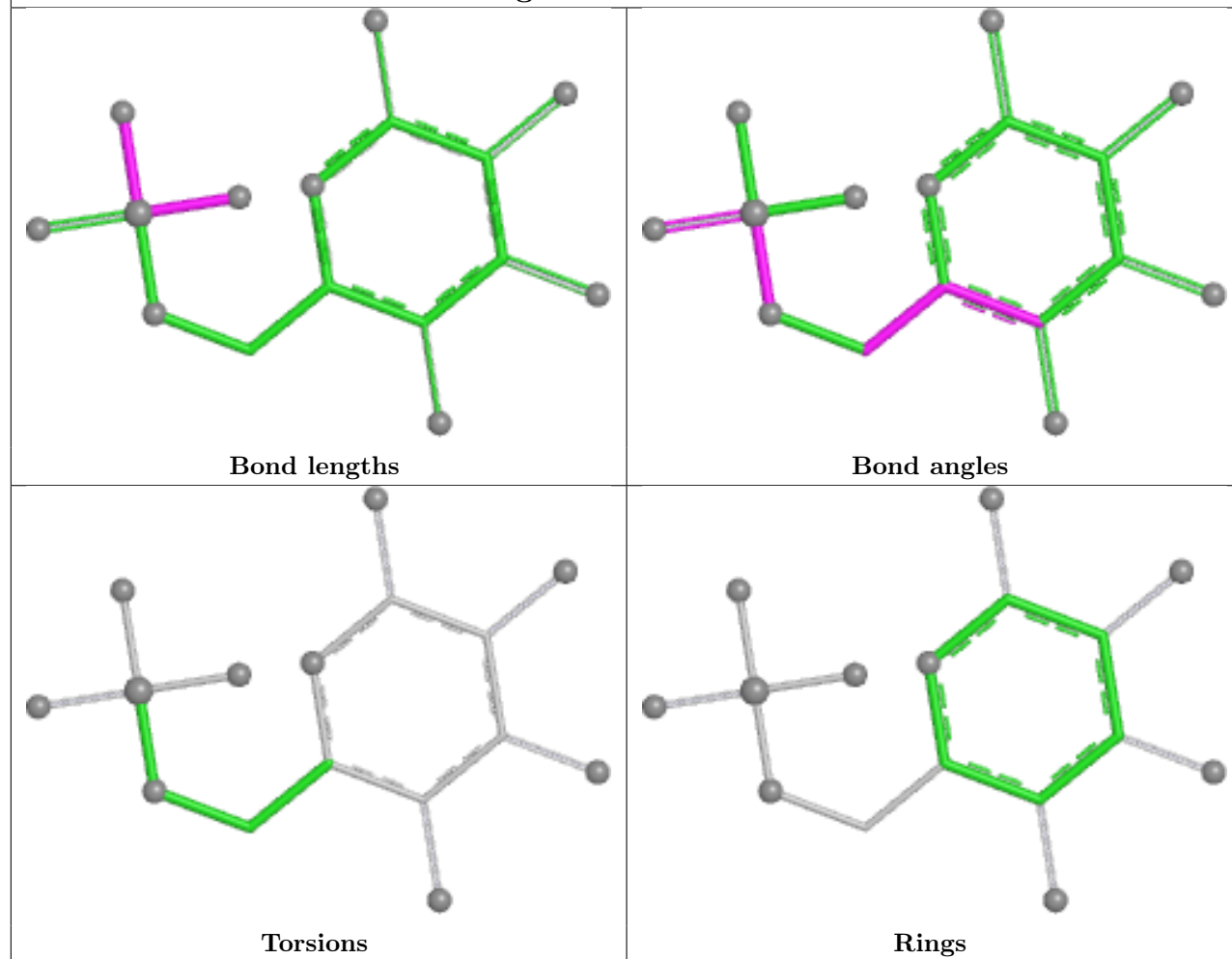
Ligand G6Q E 610



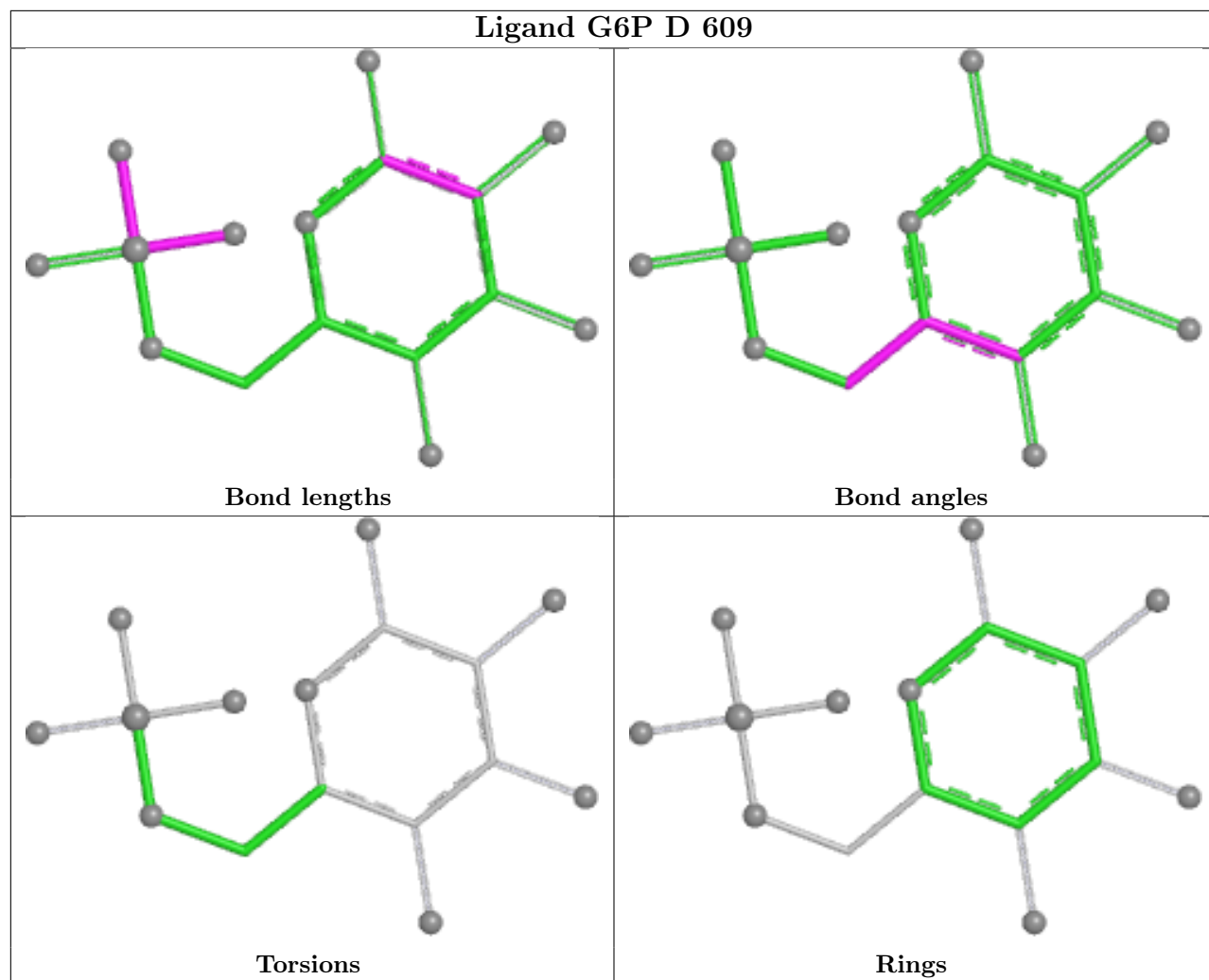
Ligand G6P H 614



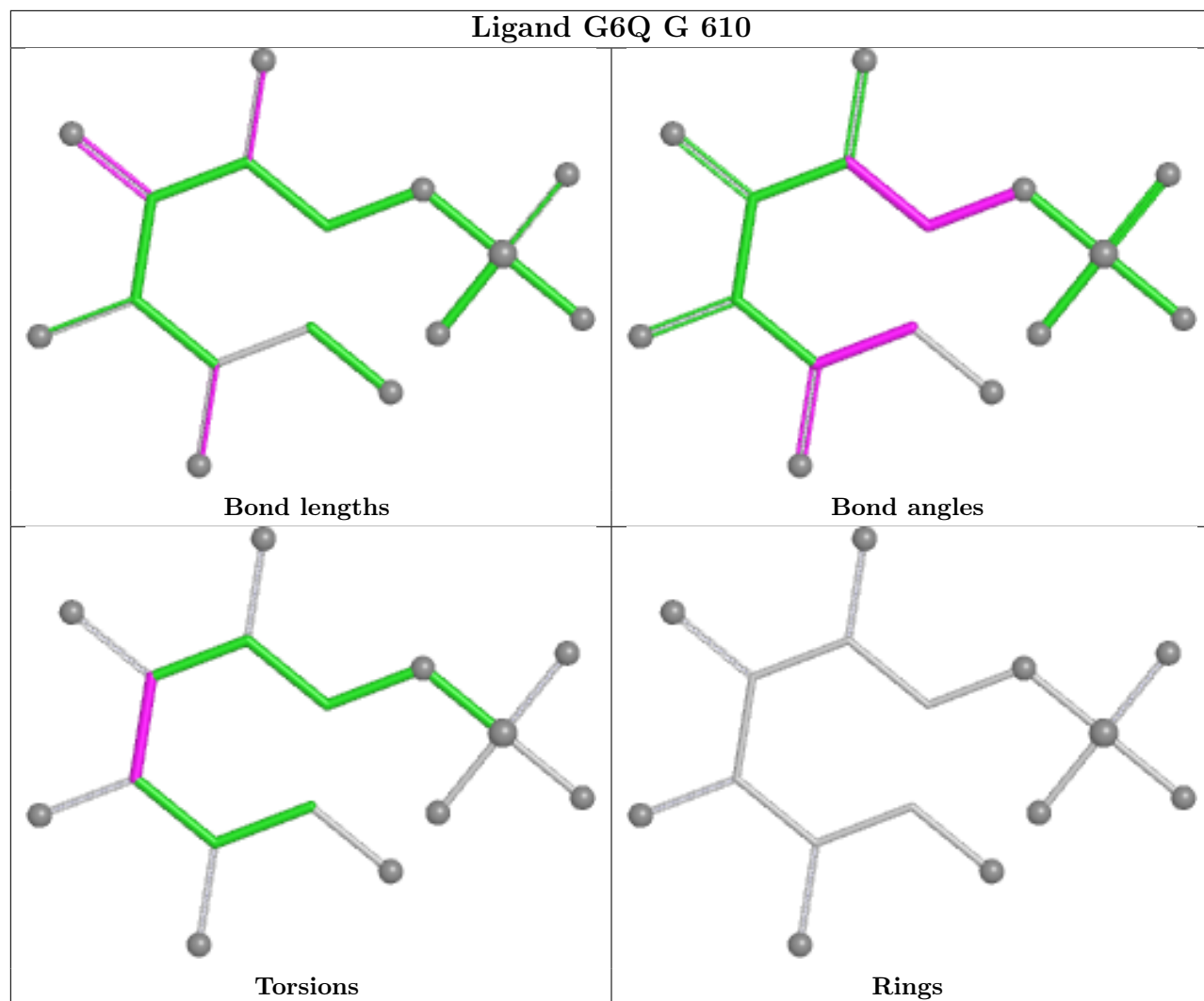
Ligand G6P C 610



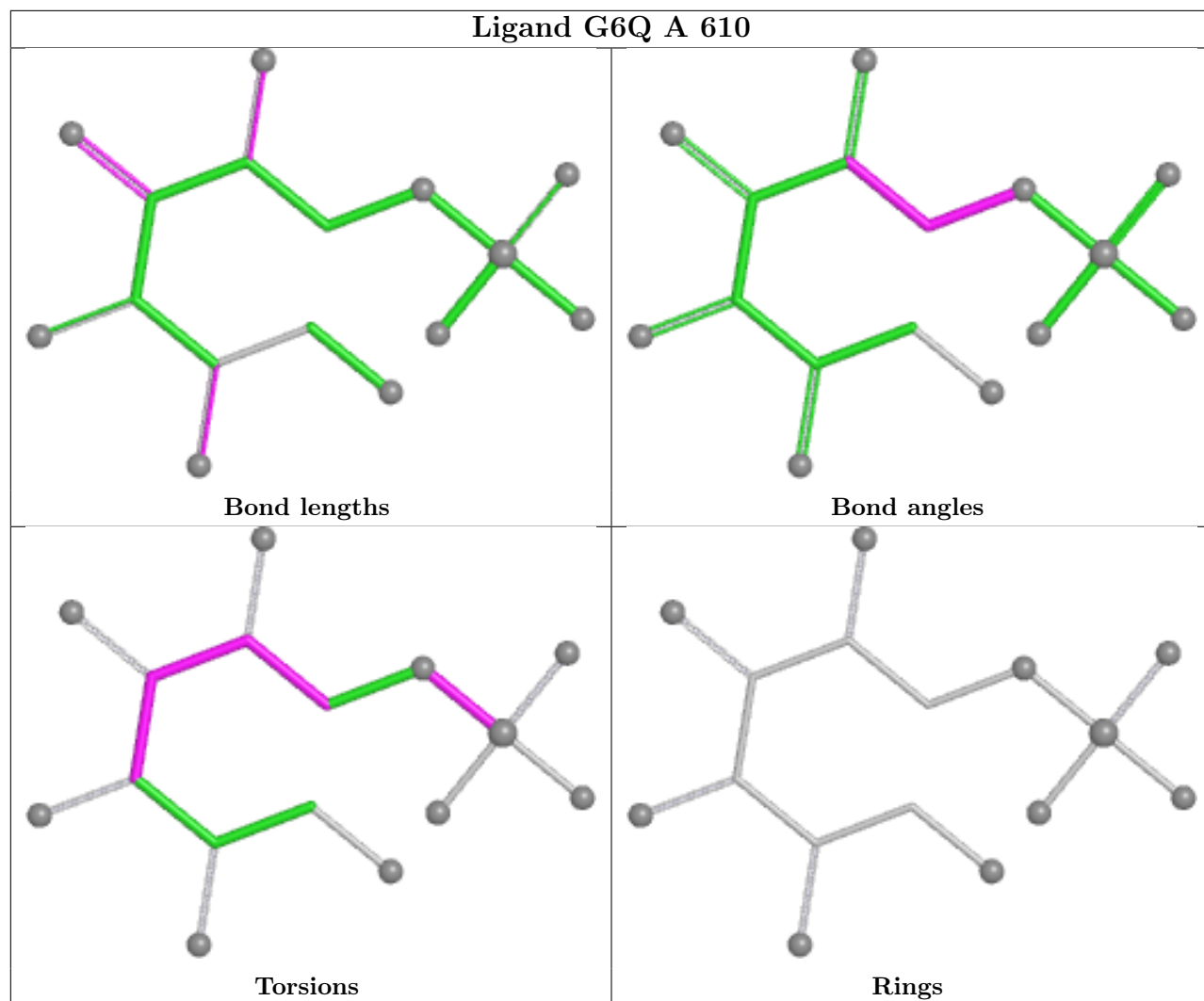
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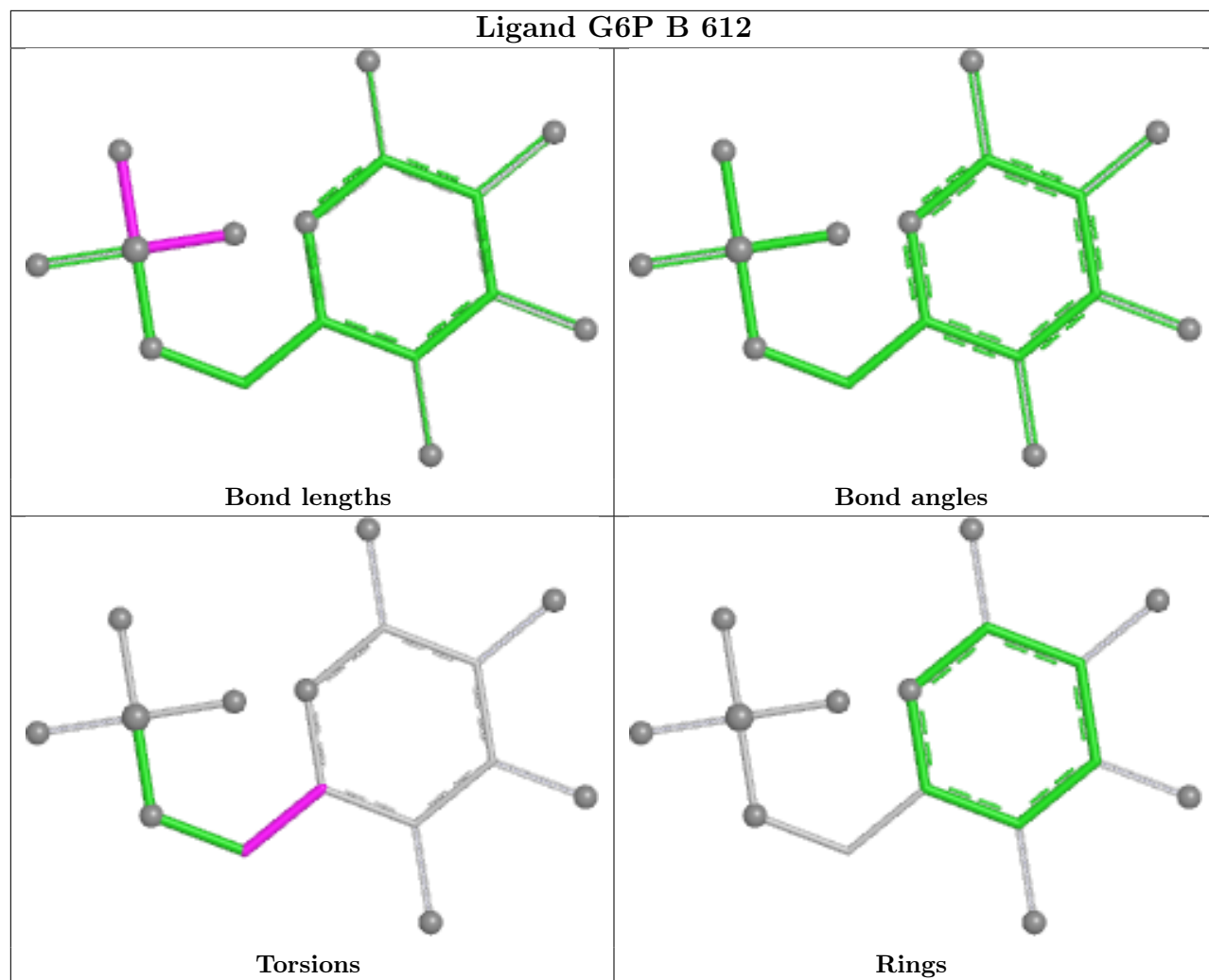
Ligand G6Q G 610



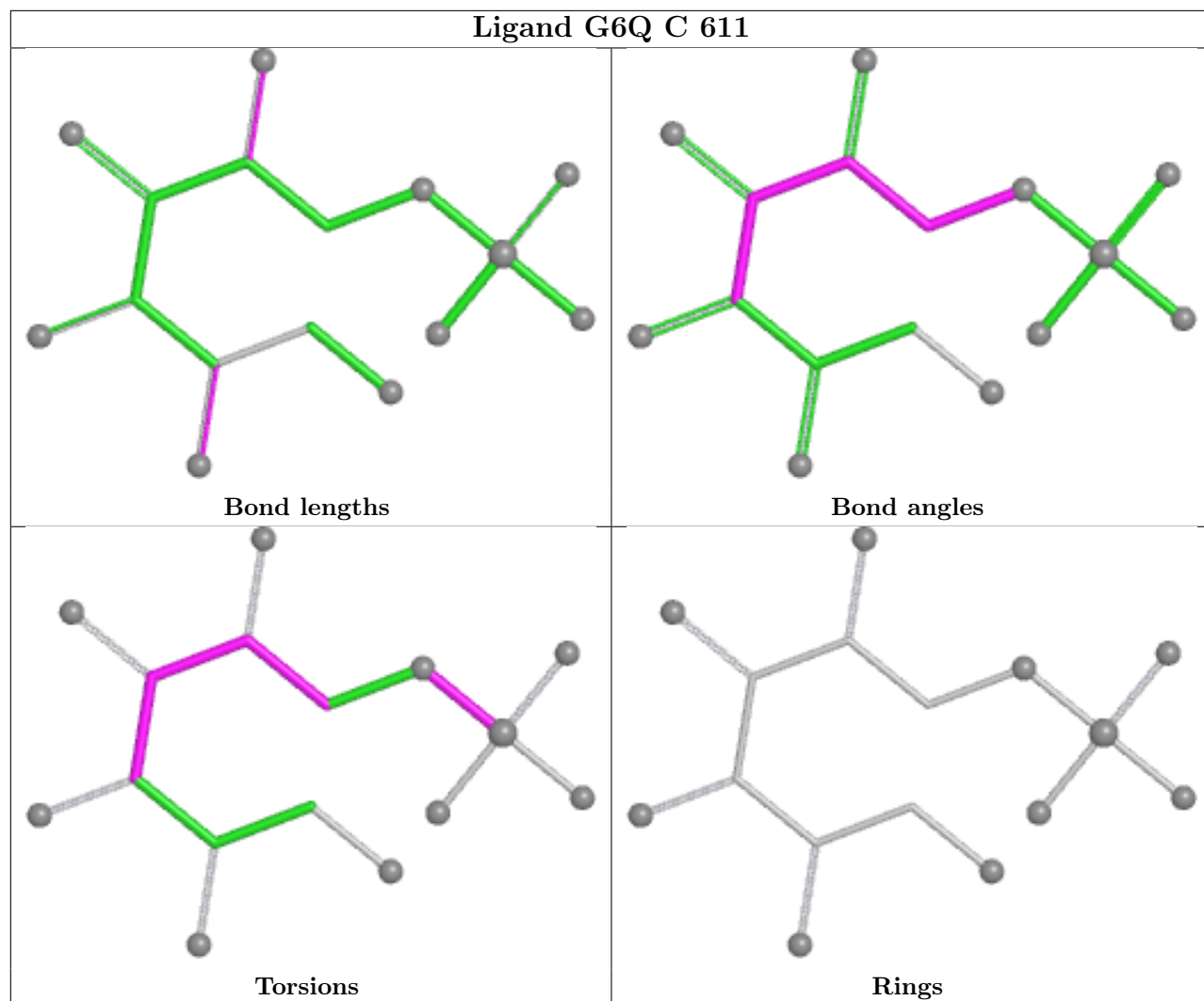
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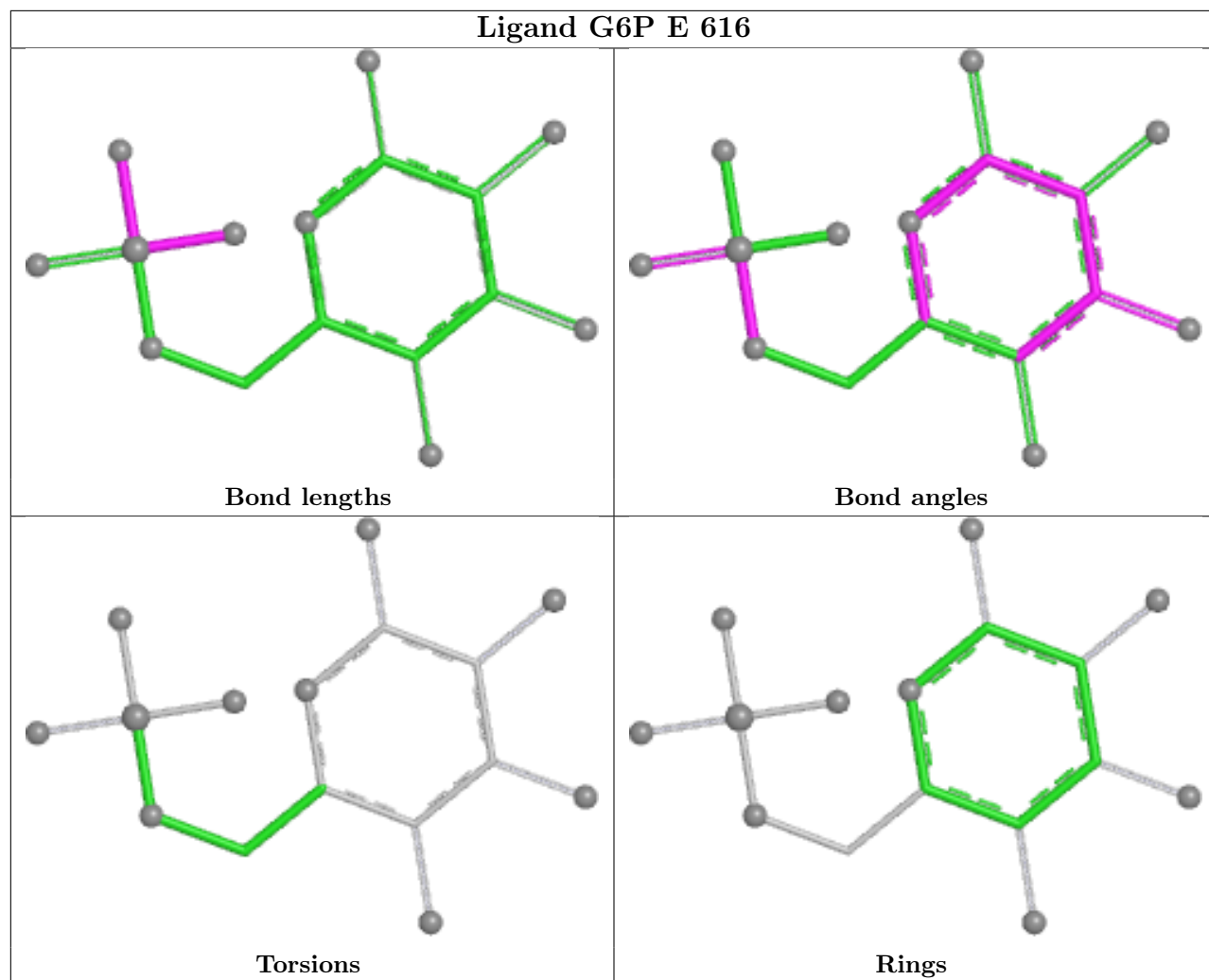
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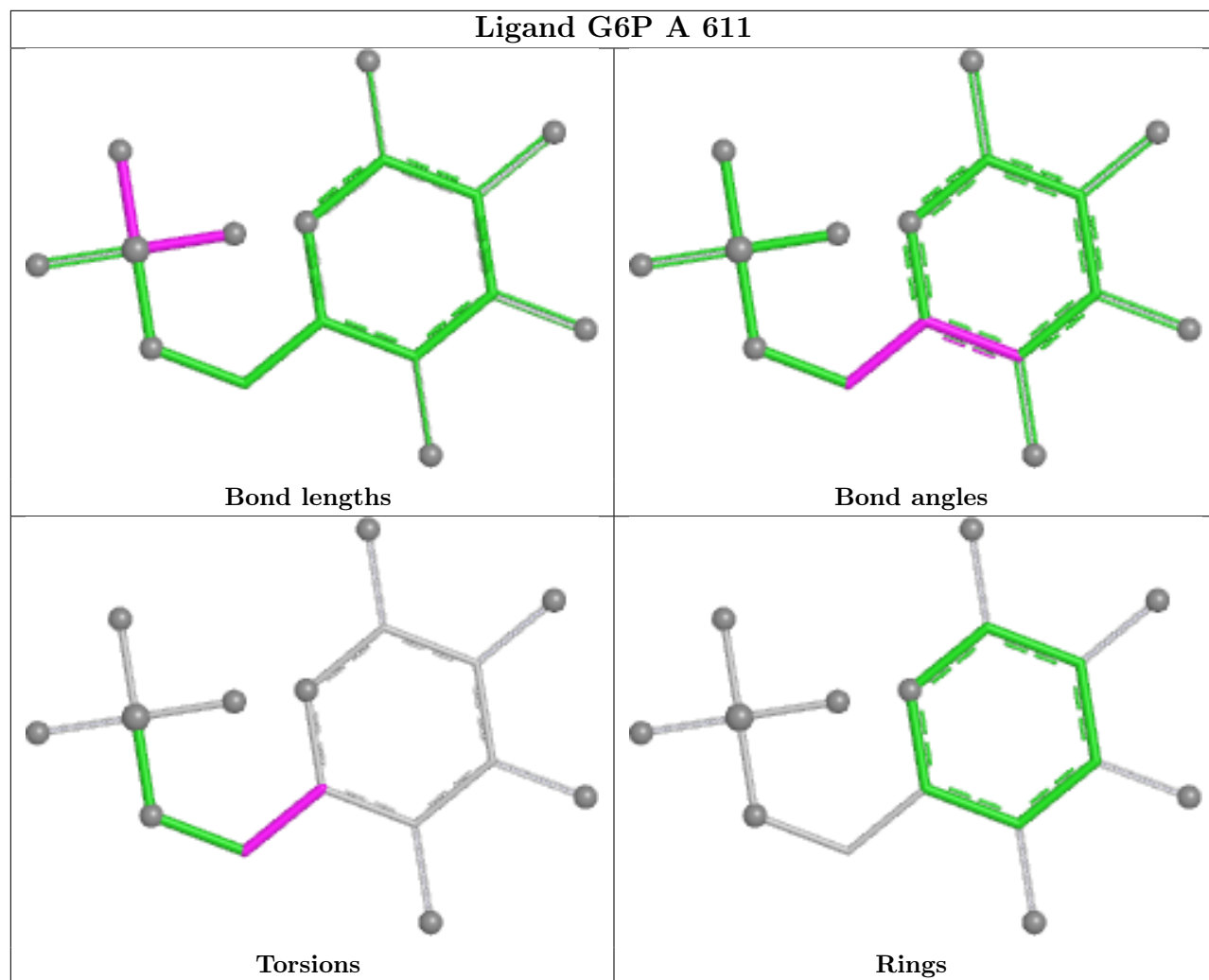
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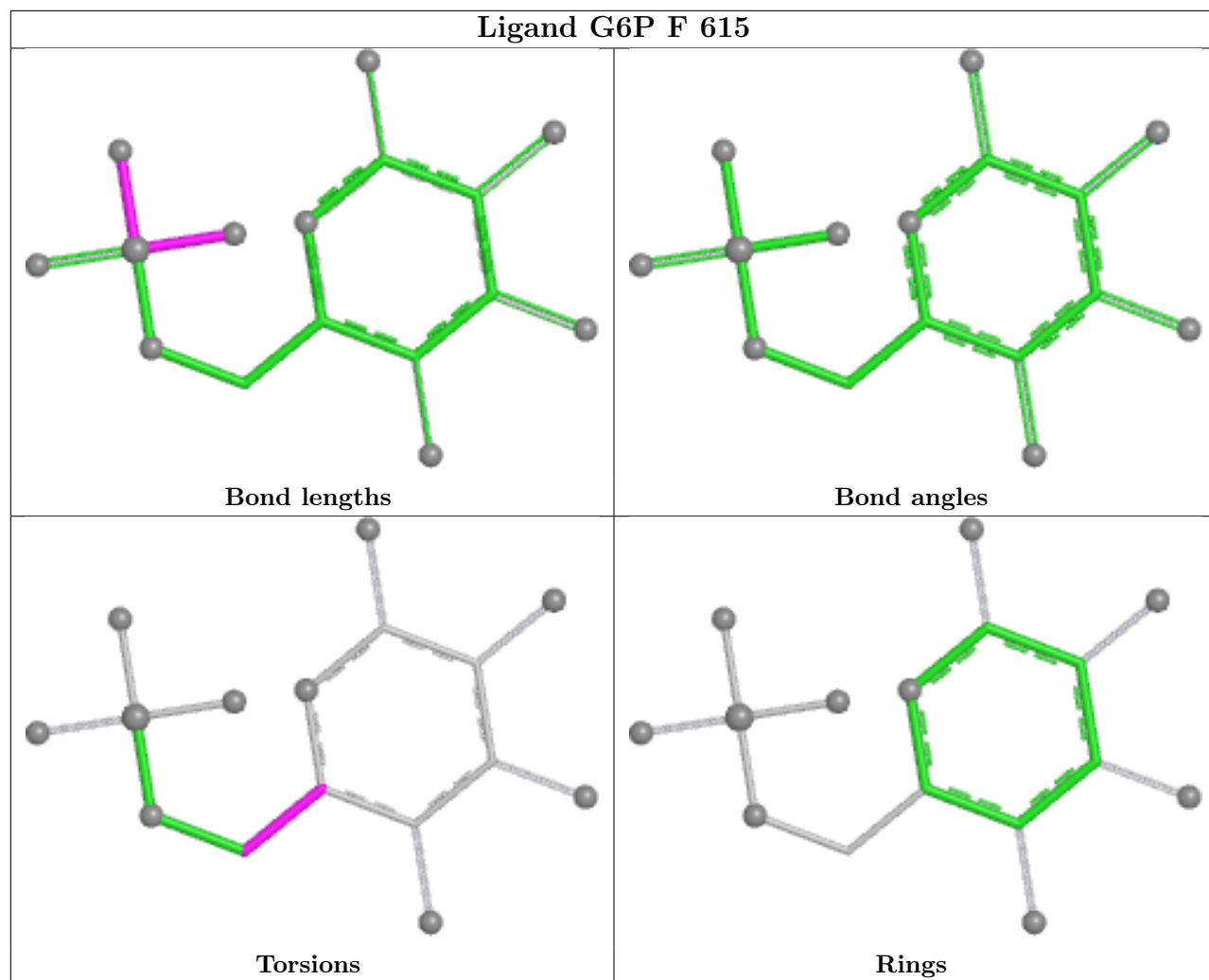
Ligand G6P E 616



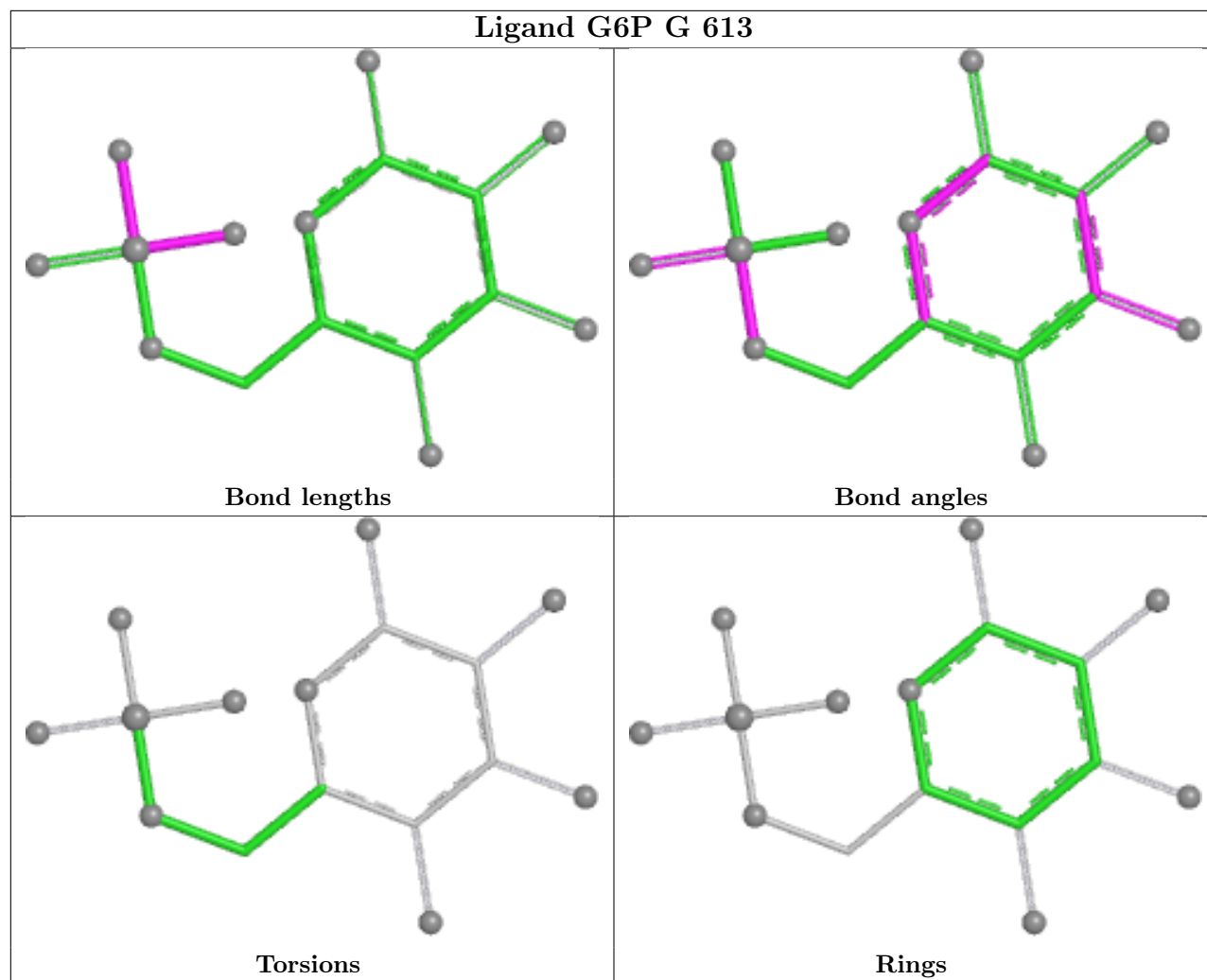
Ligand G6P A 611



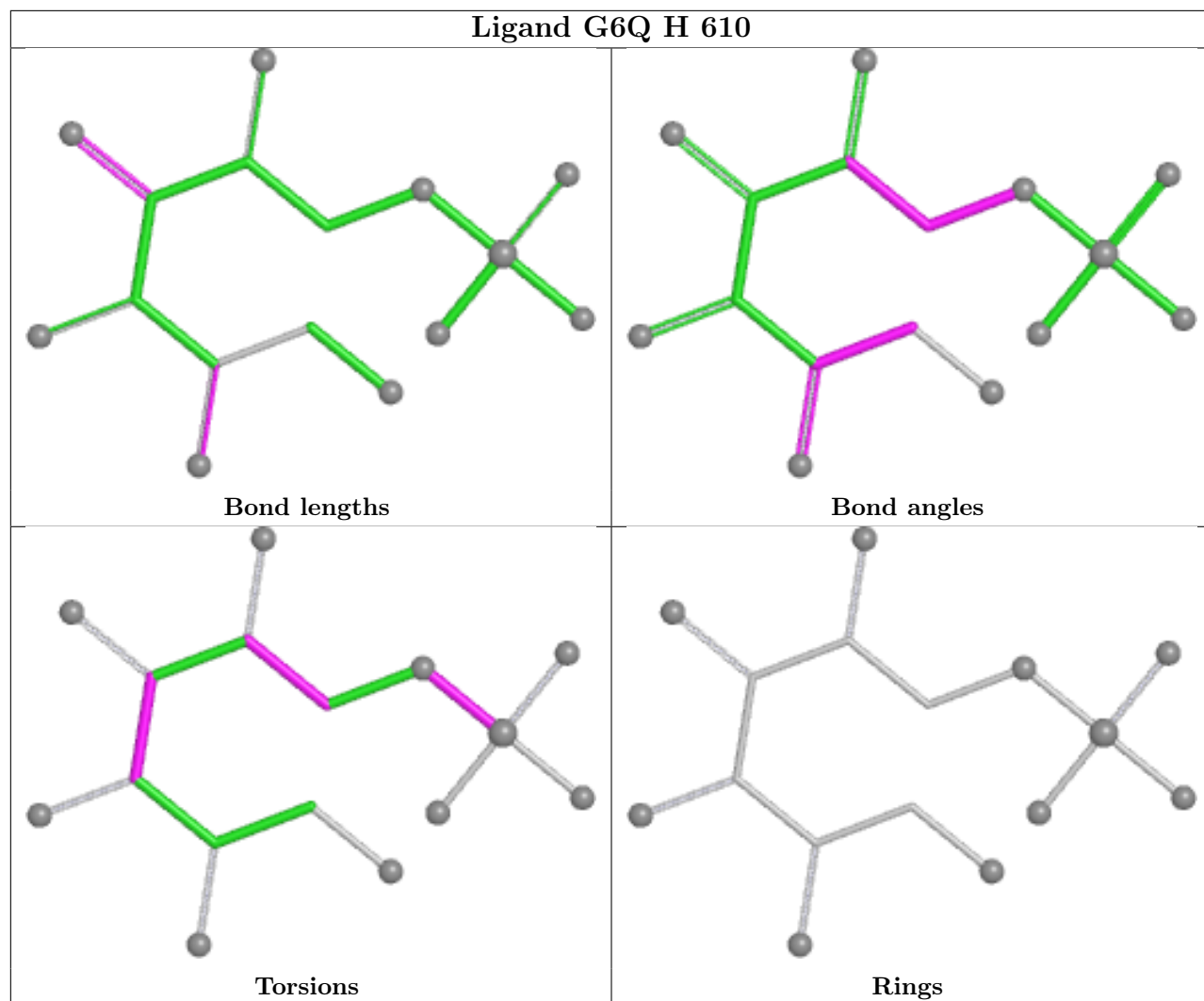
Ligand G6P F 615

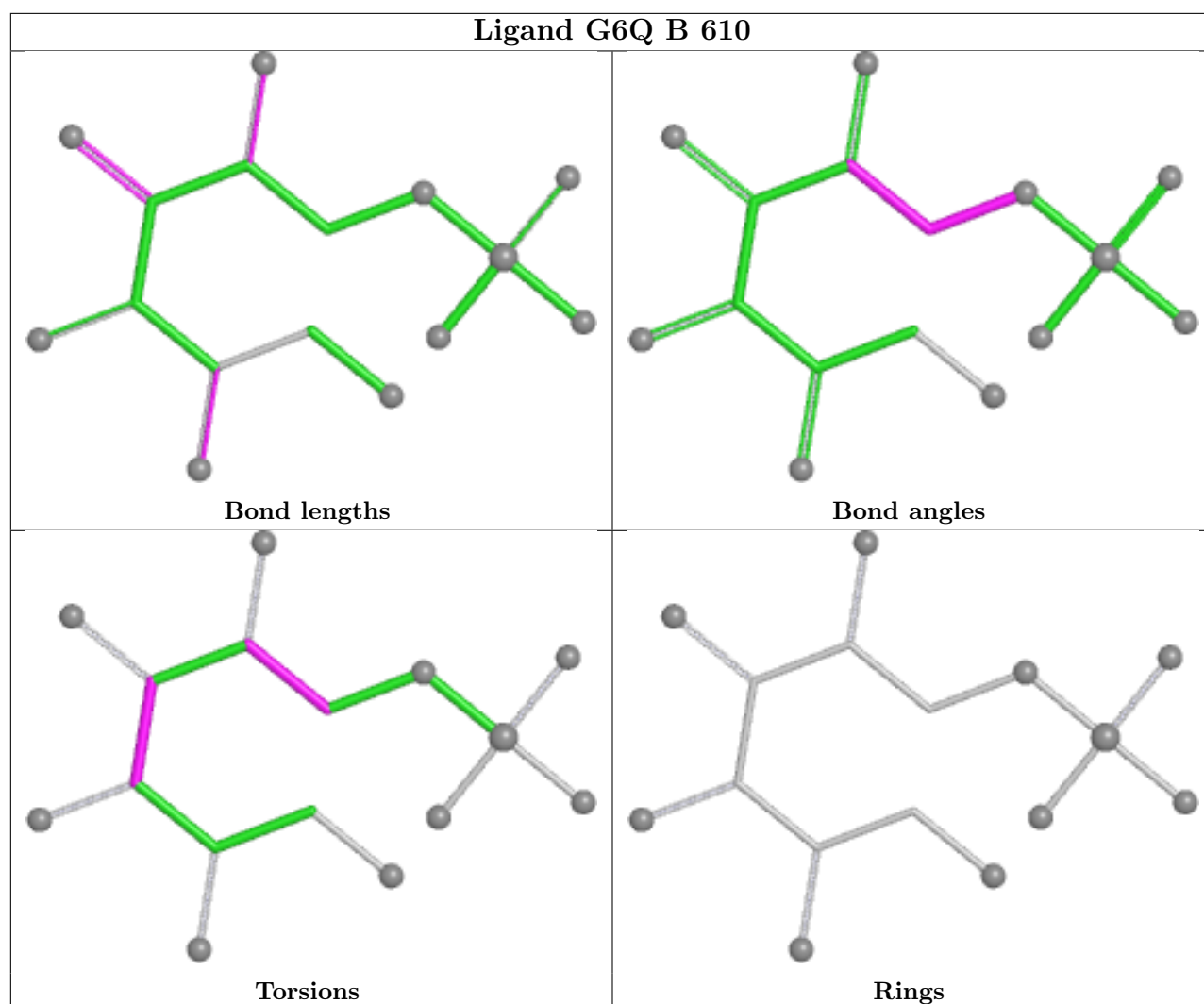


Ligand G6P G 613



Ligand G6Q H 610





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%)

All (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
1	F	181	GLY	5.1
1	B	422	LEU	4.9
1	G	133	TRP	4.9
1	G	116	TYR	4.9
1	A	240	TYR	4.8
1	F	145	VAL	4.7
1	A	238	LEU	4.7
1	F	141	LEU	4.6
1	F	227	ALA	4.5
1	F	72	THR	4.5
1	B	273[A]	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLN	4.4
1	F	229	VAL	4.3
1	H	425	LEU	4.3
1	E	422	LEU	4.3
1	E	425	LEU	4.2
1	F	75	ALA	4.2
1	A	425	LEU	4.1
1	A	242	ALA	4.1
1	G	273[A]	HIS	4.1
1	B	242	ALA	4.1
1	F	2	GLY	3.9
1	E	423	LYS	3.9
1	G	135	LEU	3.9
1	E	431[A]	HIS	3.8
1	H	41[A]	HIS	3.8
1	F	107	LEU	3.8
1	F	214	ILE	3.8
1	F	169	LEU	3.7
1	F	220	ASN	3.7
1	F	211	ILE	3.7
1	F	31	ALA	3.7
1	A	237	ASN	3.6
1	D	133	TRP	3.6
1	F	4	VAL	3.6
1	F	219	VAL	3.6
1	G	138	GLY	3.5
1	F	101	ILE	3.5
1	F	224	LYS	3.5
1	B	138	GLY	3.4
1	B	241	ASP	3.4
1	E	41[A]	HIS	3.4
1	G	41	HIS	3.4
1	F	152	LEU	3.4
1	G	126	VAL	3.4
1	F	135	LEU	3.3
1	F	144	ALA	3.3
1	D	111	LEU	3.3
1	G	141	LEU	3.3
1	F	73	ARG	3.2
1	E	424	GLY	3.2
1	C	110	GLU	3.2
1	A	513[A]	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	172	ALA	3.2
1	G	55	ALA	3.1
1	F	136	LYS	3.1
1	F	188	PHE	3.1
1	A	243	GLY	3.1
1	D	138	GLY	3.1
1	B	38	ALA	3.1
1	D	235	GLU	3.1
1	A	241	ASP	3.0
1	D	135	LEU	3.0
1	F	197	LEU	3.0
1	H	426	ASP	3.0
1	F	180	ILE	3.0
1	F	128	ALA	3.0
1	F	149	ILE	2.9
1	G	118	PHE	2.9
1	F	183	GLY	2.9
1	G	38	ALA	2.9
1	F	159	VAL	2.9
1	F	216	ARG	2.9
1	G	140	THR	2.9
1	F	85	ALA	2.9
1	F	221	ILE	2.8
1	G	225	THR	2.8
1	B	234	ILE	2.8
1	G	211	ILE	2.8
1	D	131	VAL	2.8
1	B	226	GLY	2.8
1	F	93	ILE	2.8
1	F	30	SER	2.8
1	F	89	VAL	2.8
1	F	206	LEU	2.8
1	C	41[A]	HIS	2.7
1	F	151	GLN	2.7
1	F	112	LYS	2.7
1	E	426	ASP	2.7
1	G	136	LYS	2.7
1	D	231	ARG	2.7
1	F	215	THR	2.7
1	B	27	GLY	2.6
1	B	424	GLY	2.6
1	F	189	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	237	ASN	2.6
1	D	144	ALA	2.6
1	E	427	ALA	2.6
1	B	41[A]	HIS	2.6
1	C	136	LYS	2.6
1	F	124	THR	2.6
1	F	222	PHE	2.6
1	D	425	LEU	2.6
1	F	23	LEU	2.6
1	C	113	ALA	2.6
1	D	112	LYS	2.6
1	F	196	LEU	2.6
1	G	224	LYS	2.6
1	C	133	TRP	2.5
1	A	138	GLY	2.5
1	D	106	PRO	2.5
1	G	139	GLY	2.5
1	G	150	PRO	2.5
1	B	229	VAL	2.5
1	B	225	THR	2.5
1	B	236	SER	2.5
1	E	244	ASP	2.5
1	D	141	LEU	2.5
1	F	111	LEU	2.5
1	F	203	PHE	2.5
1	F	195	ALA	2.5
1	F	53	MET	2.5
1	F	79	GLU	2.5
1	B	227	ALA	2.5
1	F	38	ALA	2.5
1	F	160	ILE	2.5
1	G	152	LEU	2.5
1	F	133	TRP	2.5
1	F	212	ALA	2.5
1	G	137	GLN	2.4
1	G	131	VAL	2.4
1	D	155	ALA	2.4
1	F	140	THR	2.4
1	G	230	LYS	2.4
1	D	426	ASP	2.4
1	F	192	ASP	2.4
1	D	137	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	20	LEU	2.4
1	F	217	ARG	2.4
1	F	131	VAL	2.4
1	F	80	PRO	2.4
1	G	229	VAL	2.4
1	E	284	ASN	2.4
1	F	171	ALA	2.4
1	F	204	ILE	2.3
1	F	165	HIS	2.3
1	F	155	ALA	2.3
1	F	225	THR	2.3
1	F	78	GLY	2.3
1	G	127	ILE	2.3
1	G	155	ALA	2.3
1	D	117	THR	2.3
1	B	133	TRP	2.3
1	F	138	GLY	2.3
1	G	107	LEU	2.3
1	B	224	LYS	2.3
1	D	227	ALA	2.3
1	D	225	THR	2.3
1	G	111	LEU	2.3
1	B	230	LYS	2.3
1	F	146	LEU	2.2
1	H	241	ASP	2.2
1	H	228	GLU	2.2
1	D	153	ARG	2.2
1	D	224	LYS	2.2
1	C	21	ARG	2.2
1	D	115	GLY	2.2
1	F	19	GLY	2.2
1	C	106	PRO	2.2
1	F	166	PRO	2.2
1	B	135	LEU	2.2
1	D	107	LEU	2.2
1	G	63	LEU	2.2
1	B	426	ASP	2.2
1	C	118	PHE	2.2
1	A	41[A]	HIS	2.1
1	D	140	THR	2.1
1	F	182	LEU	2.1
1	F	116	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	236	SER	2.1
1	B	140	THR	2.1
1	B	425	LEU	2.1
1	G	117	THR	2.1
1	F	176	SER	2.1
1	F	137	GLN	2.1
1	F	142	ARG	2.1
1	D	230	LYS	2.1
1	F	86	HIS	2.1
1	G	61	HIS	2.1
1	F	40	GLY	2.1
1	A	426	ASP	2.1
1	D	119	VAL	2.0
1	C	111	LEU	2.0
1	D	152	LEU	2.0
1	F	41	HIS	2.0
1	G	36	VAL	2.0
1	D	113	ALA	2.0
1	D	109	GLU	2.0
1	D	136	LYS	2.0
1	F	228	GLU	2.0
1	C	431[A]	HIS	2.0
1	F	71	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.

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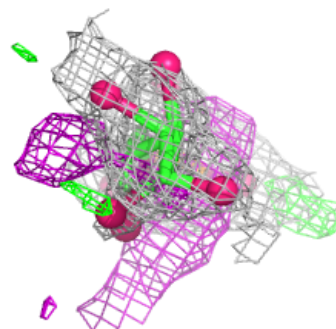
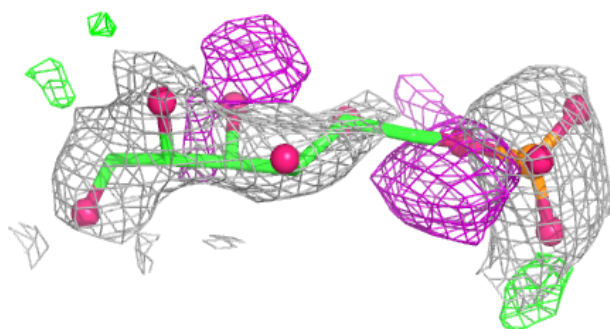
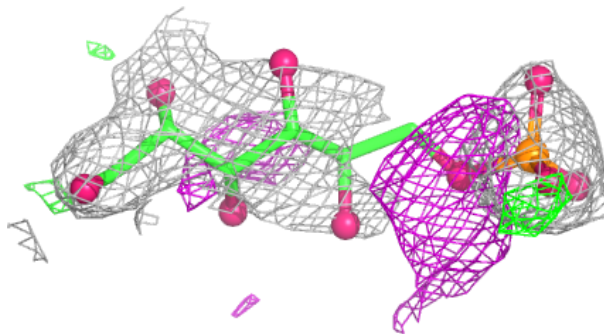
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	G6Q	F	610	16/16	0.74	0.16	63,91,104,108	0
2	GLU	F	701	10/10	0.79	0.16	73,75,80,82	0
5	G6Q	E	610	16/16	0.83	0.18	95,104,115,118	0
5	G6Q	H	610	16/16	0.85	0.14	76,91,103,105	0
5	G6Q	G	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

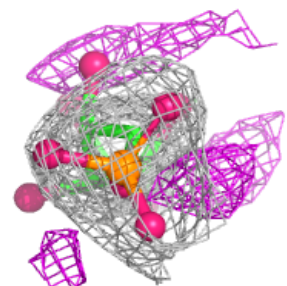
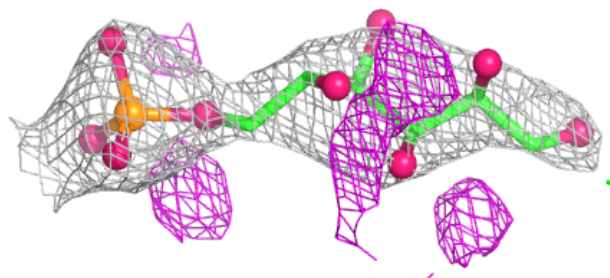
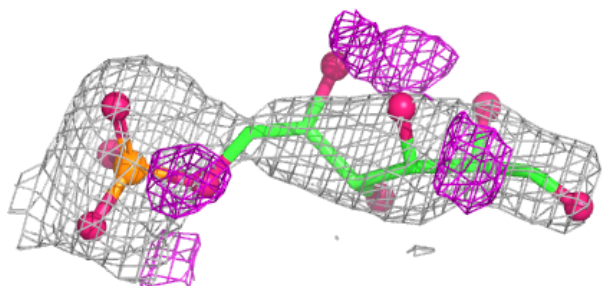
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

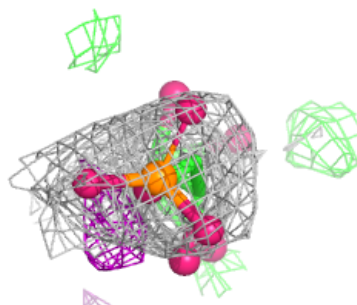
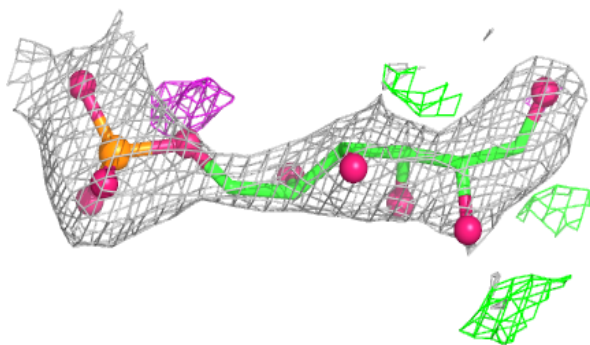
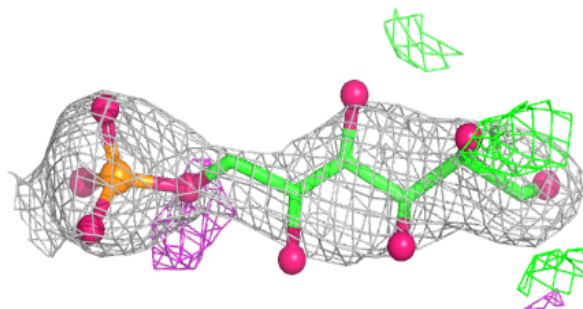
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and green (positive)

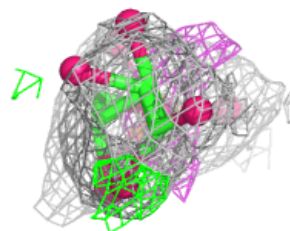
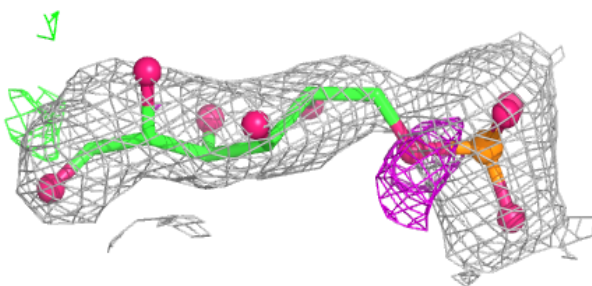
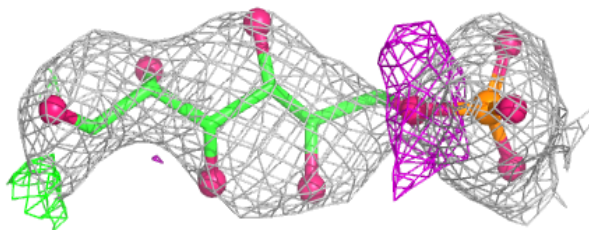


Electron density around G6Q H 610:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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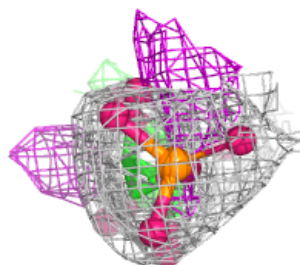
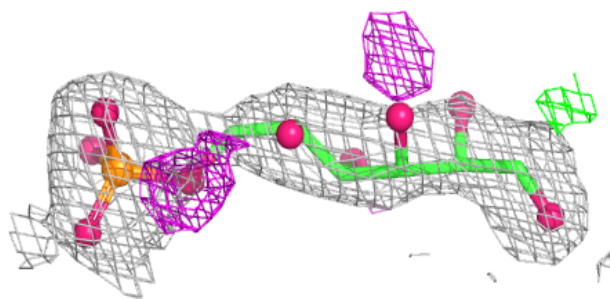
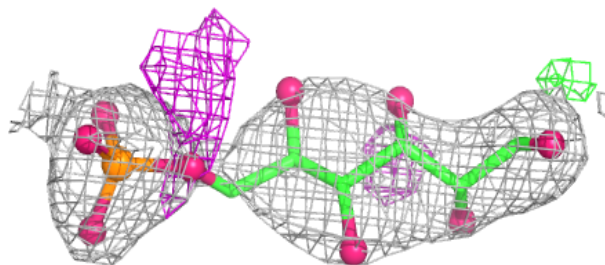
**Electron density around G6Q G 610:**

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and green (positive)

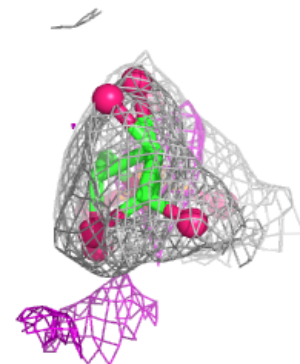
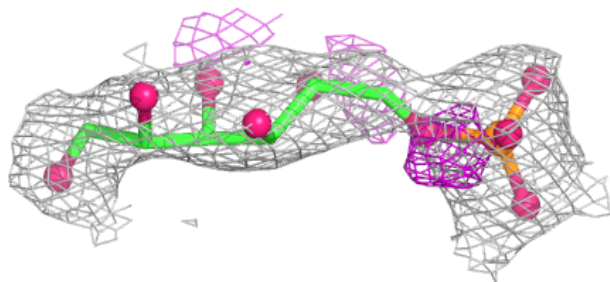
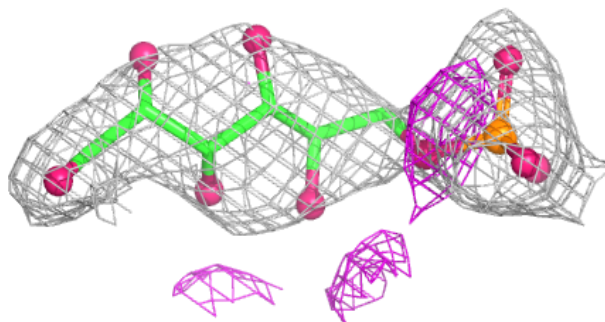


Electron density around G6Q B 610:

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and green (positive)

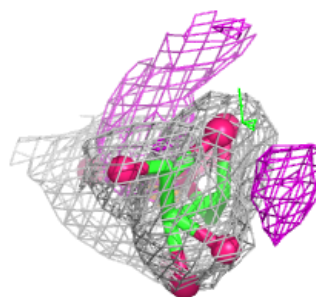
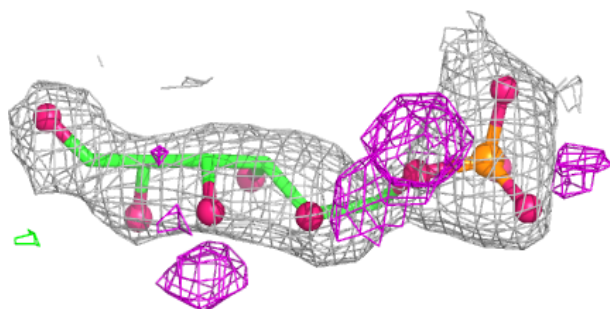
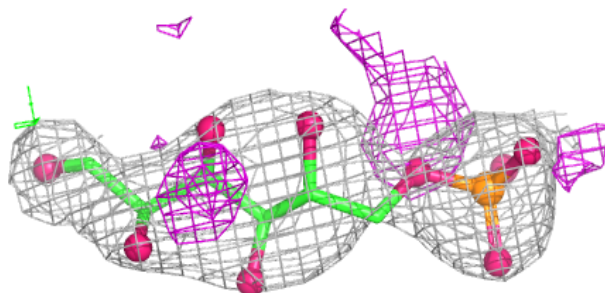
**Electron density around G6Q C 611:**

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and green (positive)

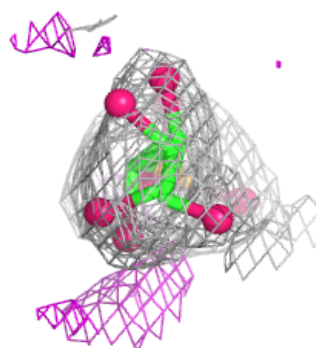
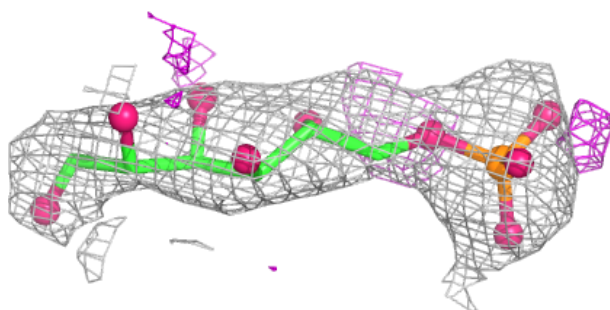
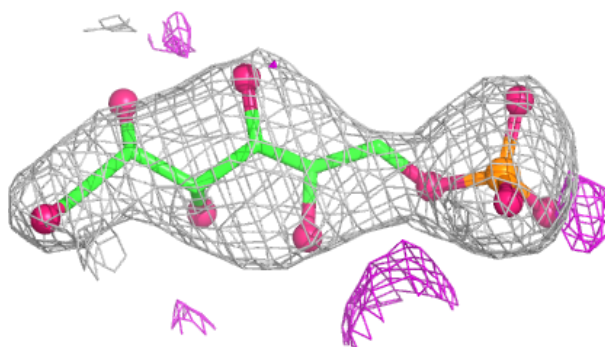


Electron density around G6Q A 610:

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and green (positive)

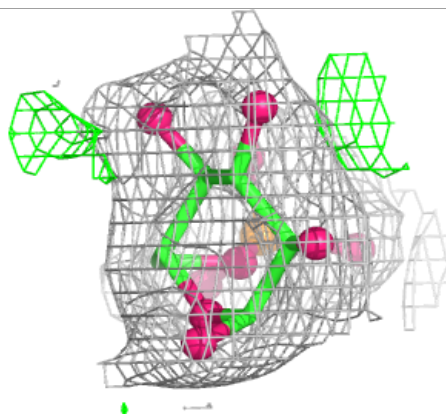
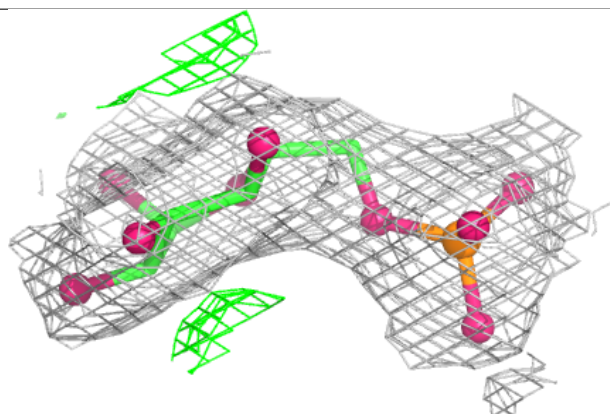
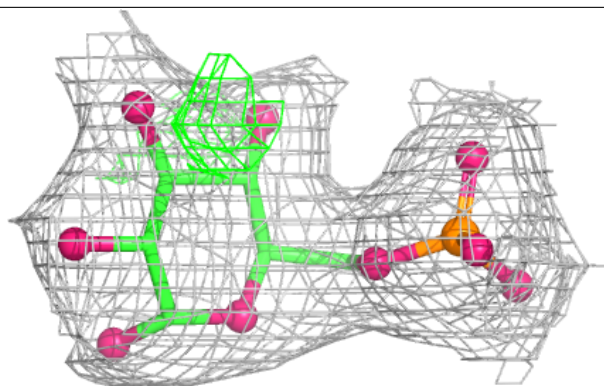
**Electron density around G6Q D 611:**

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

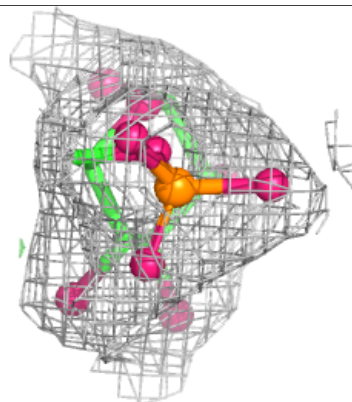
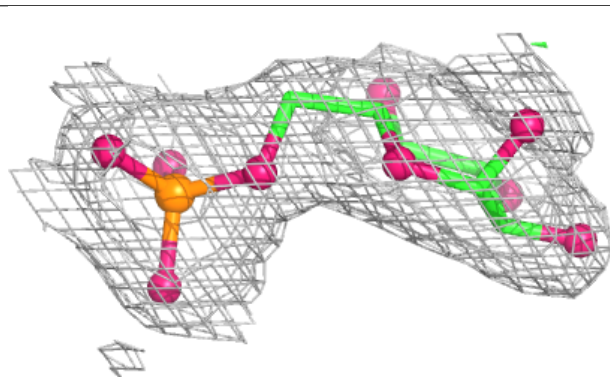
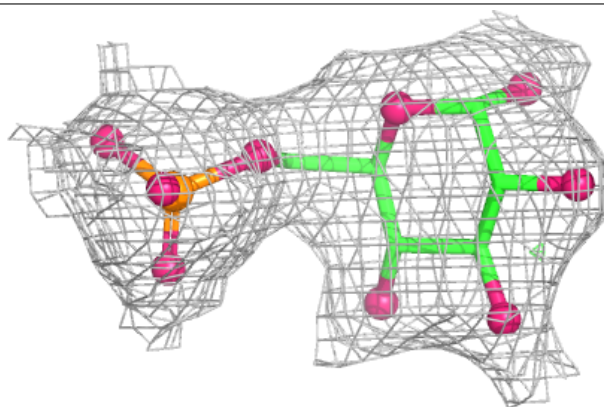


Electron density around G6P E 616:

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

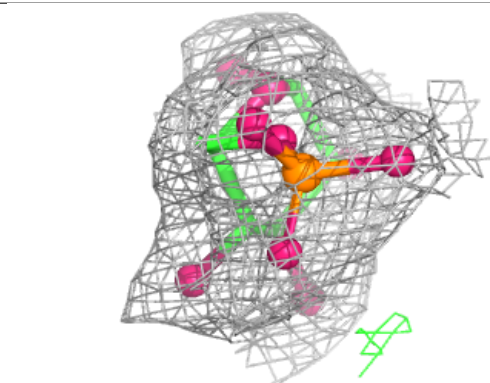
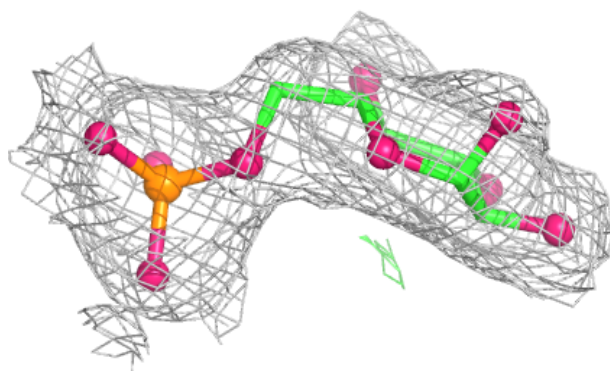
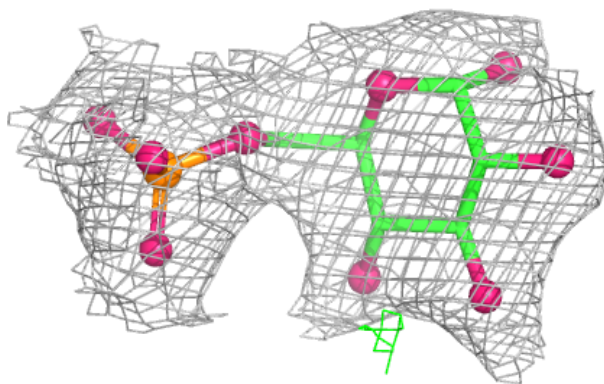
**Electron density around G6P F 615:**

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

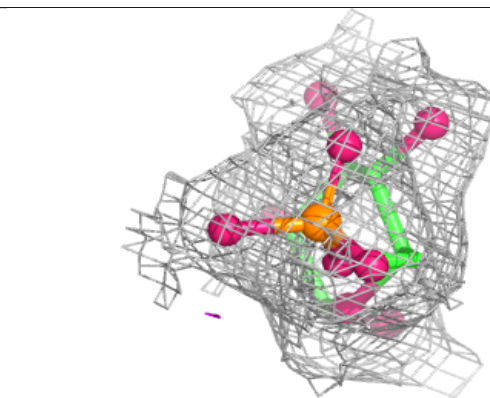
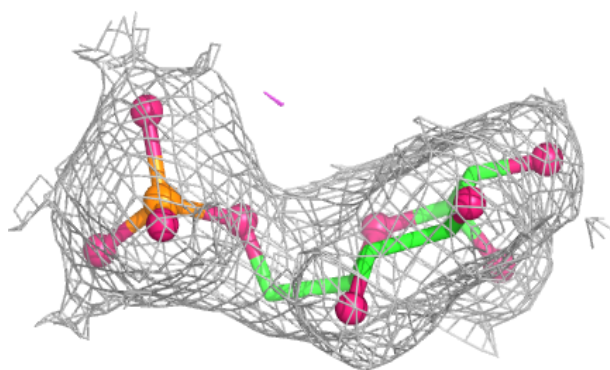
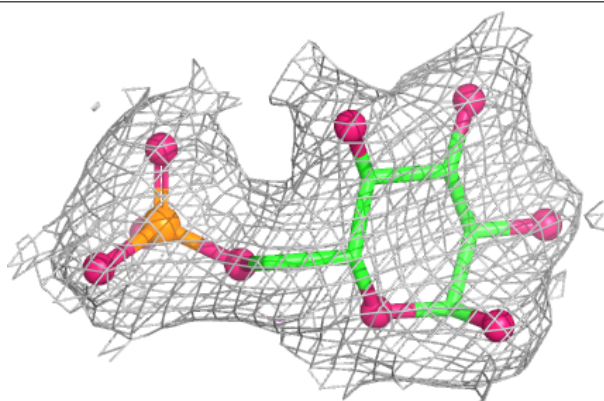


Electron density around G6P H 614:

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

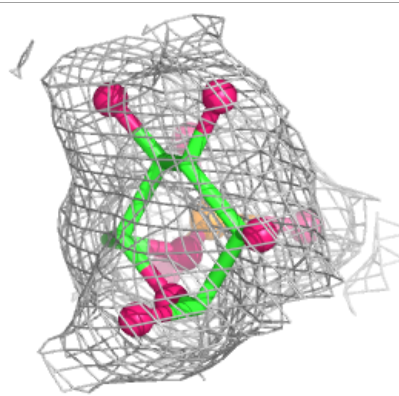
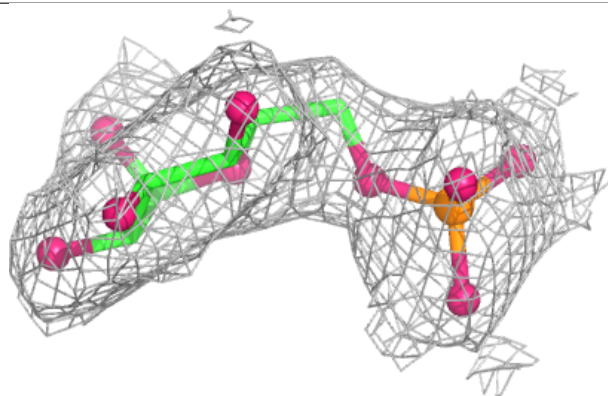
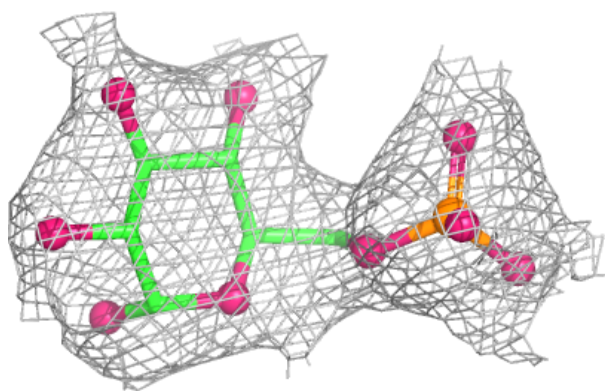
**Electron density around G6P A 611:**

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

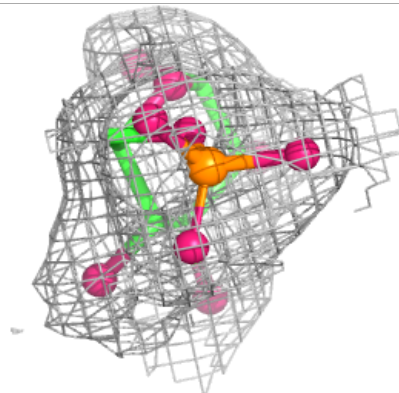
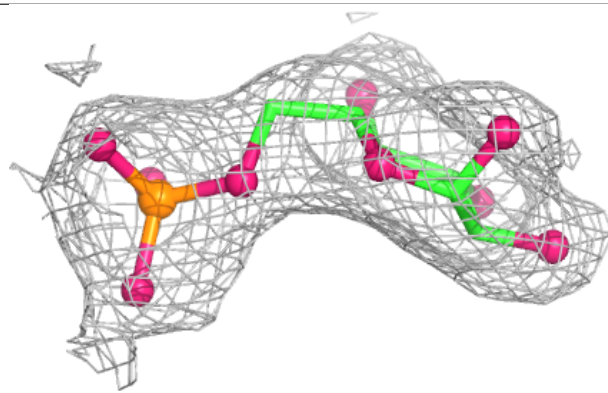
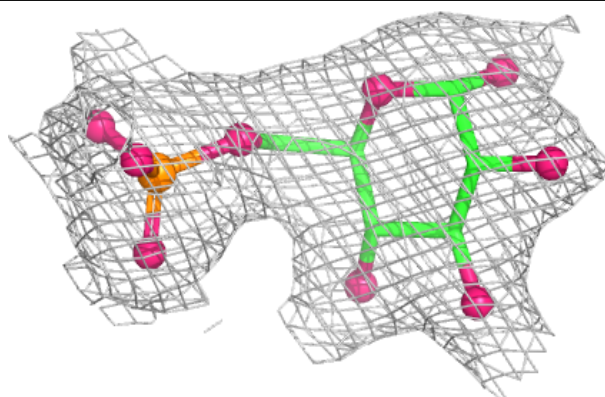


Electron density around G6P B 612:

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

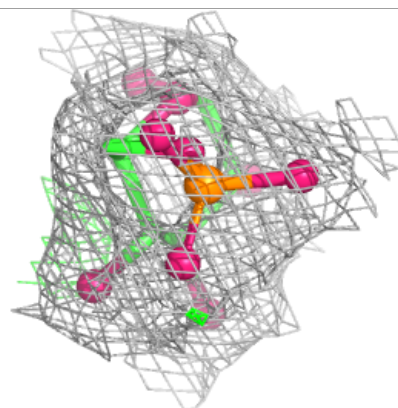
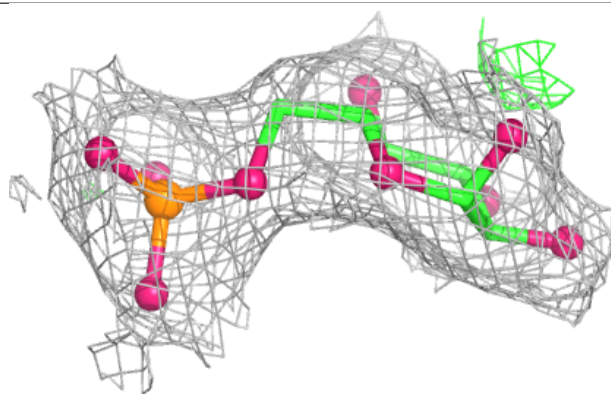
**Electron density around G6P G 613:**

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

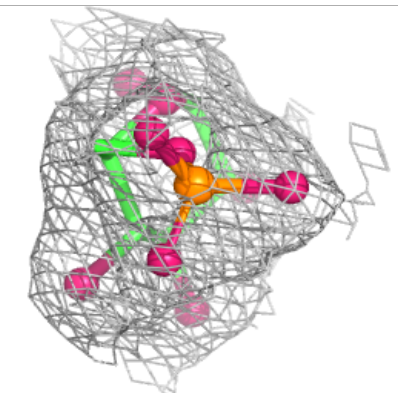
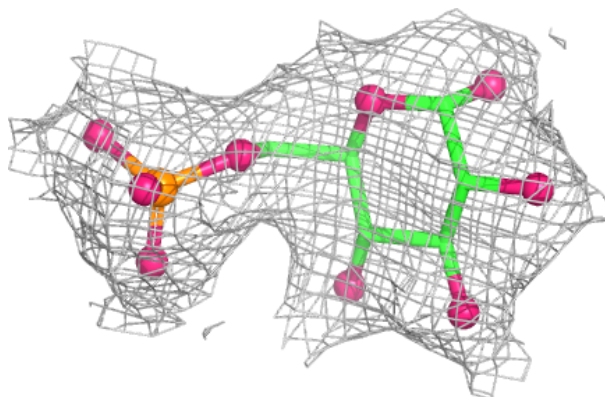


Electron density around G6P C 610:

$2mF_o-DF_c$ (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.