Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 06:45 PM EDT

PDB ID	:	5SUK
Title	:	G6P bound activated state of yeast glycogen synthase 2
Authors	:	Baskaran, S.; Mahalingan, K.K.; Hurley, T.D.
Deposited on	:	2016-08-03
Resolution	:	2.88 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 (i) 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 (i)) were used in the production of this report:

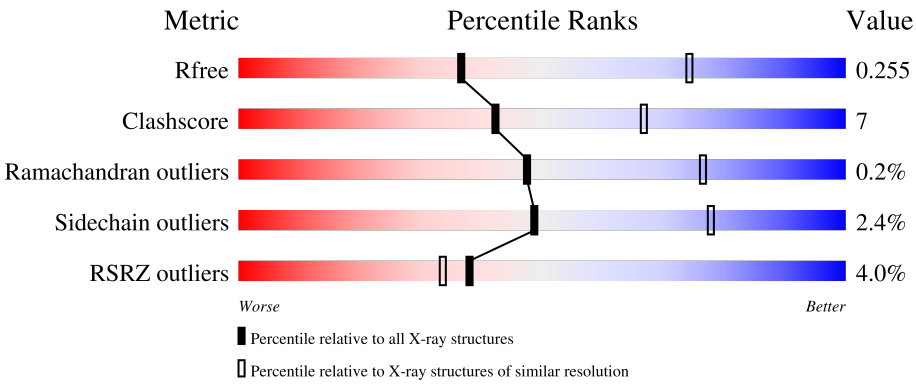
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	725	2% 76% 12% 12%
1	B	725	3% 76% 12% 12%
1	C	725	4% 75% 12% • 12%
1	D	725	5% 69% 14% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19585 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	638	5020	3207	869	925	19	0	0	0
			Total	C	N	O	S			
1	B	637	5018	3198	877	925	18	0	0	0
			Total	C	N	O	S			
1	C	639	4869	3095	847	909	18	0	0	0
			Total	C	N	O	S			
1	D	604	4582	2921	797	847	17	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	conflict	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
C	-19	MET	-	initiating methionine	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	conflict	UNP P27472

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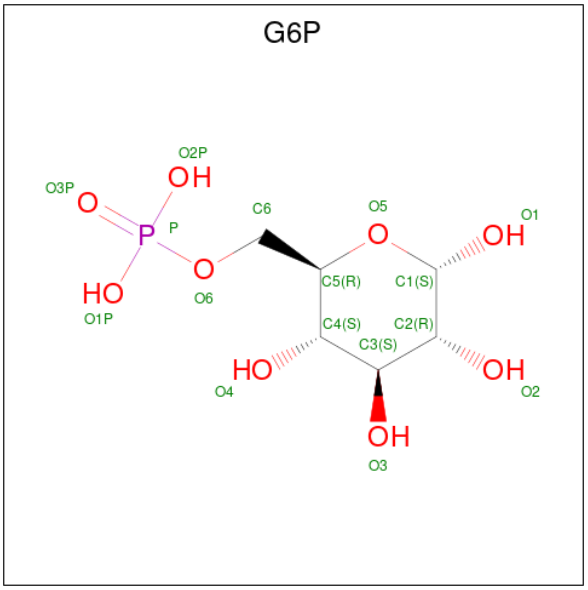
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	conflict	UNP P27472

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



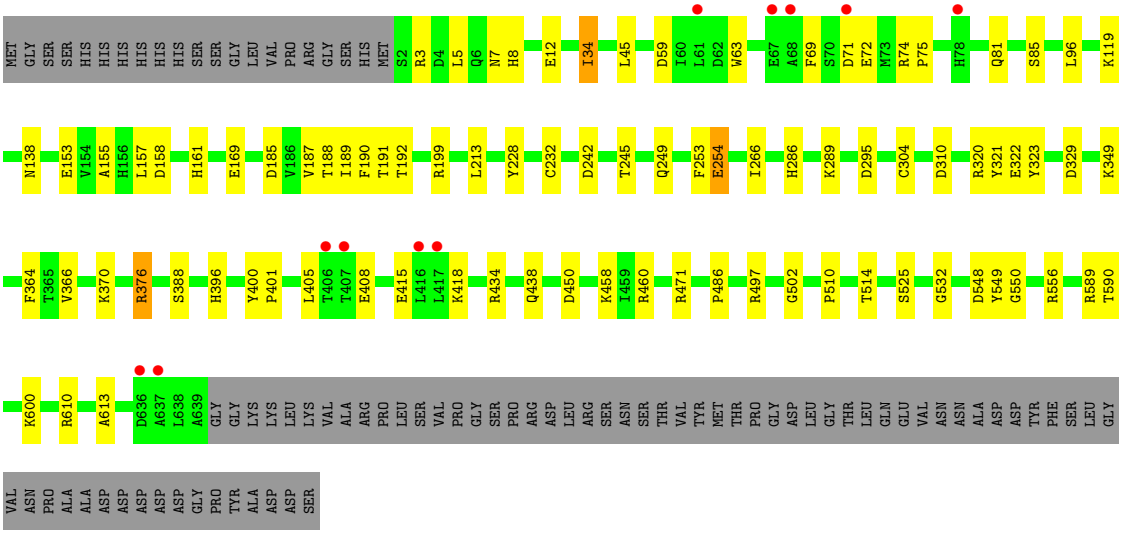
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0
			Total	C	O	P		
2	A	1	16	6	9	1	0	0
			Total	C	O	P		
2	B	1	16	6	9	1	0	0
			Total	C	O	P		
2	B	1	16	6	9	1	0	0
			Total	C	O	P		
2	C	1	16	6	9	1	0	0
			Total	C	O	P		
2	D	1	16	6	9	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

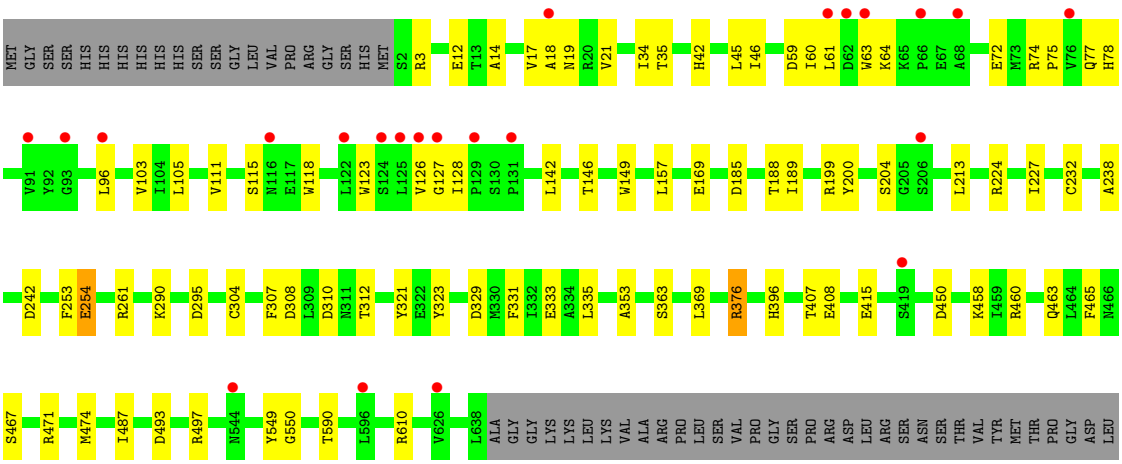
• Molecule 1: Glycogen [starch] synthase isoform 2

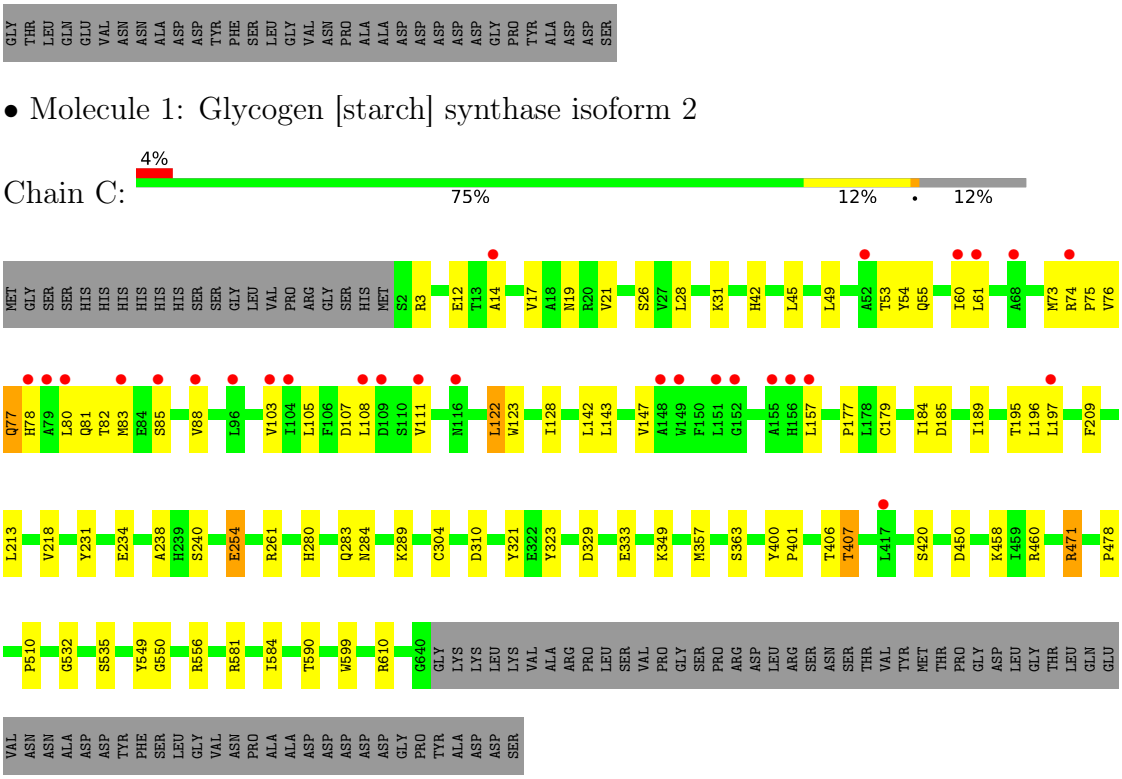
Chain A:



• Molecule 1: Glycogen [starch] synthase isoform 2

Chain B:




GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP ASP ASP ASP GLY PRO TYR ALA ASP ASP SER
• Molecule 1: Glycogen [starch] synthase isoform 2
Chain C:
4%
75%
12%
12%
MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET S2 R3 E12 T13 A14 V17 A18 N19 R20 V21 S26 V27 L28 K31 H42 L45 L49 A52 T53 Y54 Q55 I60 L61 A63 M73 R74 P75 V76
Q77 H78 A79 L80 Q81 T82 M83 E84 S85 V88 L96 V103 I104 L105 F106 D107 L108 D109 S110 V111 N116 L122 W123 I128 L142 L143 V147 A148 W149 F150 L151 G152 A155 H156 L157 P177 L178 C179 I184 D185 I189 T195 L196 L197 F209
L213 V218 Y231 E234 A238 H239 S240 E254 R261 H280 Q283 N284 K289 C304 D310 Y321 E322 Y323 D329 E333 K349 M357 S363 Y400 P401 T406 T407 L417 S420 D450 K458 I459 R460 R471 P478
P510 G532 S535 Y549 G550 R556 R581 I584 T590 W599 R610 G640 GLY LYS LYS LEU LYS VAL ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR VAL TYR MET THR PRO GLY ASP LEU GLY THR LEU GLN GLU
VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP ASP ASP GLY PRO TYR ALA ASP ASP SER
• Molecule 1: Glycogen [starch] synthase isoform 2
Chain D:
5%
69%
14%
17%
MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER R3 L10 F11 E12 E16 V17 A18 N19 R20 V21 I24 A32 P33 I34 Y43 H44 L45 L49 N50 T53 Y54 Q55 N56 E57 V58 ASP ILE LEU ASP TRP LYS
LYS PRO GLU ALA F69 E72 M73 R74 P75 Q81 S85 R86 G87 VAL HIS F90 V91 Y92 GLY ARG TRP L96 I97 A100 P101 K102 V103 I104 L108 D109 S110 V111 L122 W123 S124 L125 V126 G127 I128 P129 S130 N133 D134 F135 I141 G144 A148 L151 G152
E153 L157 D158 H161 A162 I163 F167 V174 A175 L176 P177 L178 C179 R180 V186 V187 T188 I189 L197 Y200 A203 S204 G205 SER PHE D208 L213 V218 A222 G223 R224 F225 G226 I227 Y228 H229 R230 Y231 S240 A241 D242 F253 L259 G265
F282 Q283 N284 K289 H302 G303 C304 Y321 E322 Y323 K326 D329 K349 T350 S363 E367 H383 T387 Y400 P401 T406 T407 L432 R433 R471 G502 P510 E517 S525 N529 G532 Y549 G550 D555 T590 E591
W599 L604 V607 R610 A613 L614 R615 R616 D620 R623 GLU LEU VAL GLY GLU GLU LEU ASN ASP SER ASN MET ASP ALA LEU ALA GLY GLY LYS LYS LEU LYS VAL ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR VAL TYR MET
THR PRO GLY ASP LEU GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP ASP ASP ASP GLY PRO TYR ALA ASP ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	191.98Å 204.56Å 205.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.09 – 2.88 45.80 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.0 (145.09-2.88) 98.0 (45.80-2.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.219 , 0.260 0.217 , 0.255	Depositor DCC
R_{free} test set	4461 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19585	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/5140	0.60	0/6983
1	B	0.39	0/5136	0.60	0/6977
1	C	0.39	0/4975	0.59	0/6776
1	D	0.41	0/4677	0.61	0/6363
All	All	0.40	0/19928	0.60	0/27099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5020	0	4846	54	0
1	B	5018	0	4844	50	0
1	C	4869	0	4619	73	0
1	D	4582	0	4371	87	0
2	A	32	0	22	2	0
2	B	32	0	22	3	0
2	C	16	0	11	0	0
2	D	16	0	11	1	0
All	All	19585	0	18746	263	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (263) 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:D:167:PHE:CD2	1:D:176:LEU:HD21	1.87	1.09
1:C:83:MET:C	1:C:88:VAL:HG22	1.73	1.09
1:C:83:MET:CA	1:C:88:VAL:HG22	1.92	0.98
1:D:176:LEU:HD11	1:D:188:THR:OG1	1.67	0.95
1:D:134:ASP:OD2	1:D:229:HIS:NE2	2.04	0.90
1:D:227:ILE:O	1:D:229:HIS:N	2.08	0.87
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.13	0.84
1:C:82:THR:HG22	1:C:83:MET:H	1.41	0.83
1:C:122:LEU:HD12	1:C:128:ILE:HB	1.64	0.79
1:C:83:MET:CB	1:C:88:VAL:CG2	2.62	0.77
1:A:7:ASN:ND2	1:A:72:GLU:OE2	2.17	0.77
1:D:148:ALA:HB1	1:D:178:LEU:HD11	1.67	0.77
1:C:83:MET:CA	1:C:88:VAL:CG2	2.63	0.76
2:B:902:G6P:O1P	2:B:902:G6P:O4	2.00	0.75
1:C:83:MET:O	1:C:88:VAL:HG22	1.86	0.75
1:D:163:ILE:HB	1:D:186:VAL:HG22	1.68	0.75
1:D:167:PHE:CG	1:D:176:LEU:HD21	2.23	0.73
1:C:196:LEU:HD12	1:C:234:GLU:OE2	1.89	0.72
1:D:549:TYR:O	1:D:590:THR:HG22	1.89	0.72
1:D:176:LEU:CD1	1:D:188:THR:OG1	2.38	0.72
1:A:153:GLU:O	1:A:157:LEU:HD13	1.91	0.70
1:C:143:LEU:O	1:C:147:VAL:HG23	1.91	0.70
1:D:187:VAL:HG11	1:D:613:ALA:HB1	1.73	0.69
1:D:167:PHE:CD2	1:D:176:LEU:CD2	2.71	0.69
1:A:3:ARG:NH2	1:A:158:ASP:O	2.24	0.69
1:B:123:TRP:O	1:B:127:GLY:HA2	1.91	0.69
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.25	0.69
1:C:53:THR:O	1:C:55:GLN:N	2.24	0.69
1:A:549:TYR:O	1:A:590:THR:HG22	1.95	0.67
1:D:178:LEU:HD12	1:D:179:CYS:N	2.09	0.67
1:C:49:LEU:HD23	1:C:107:ASP:CB	2.25	0.66
1:A:5:LEU:O	1:A:8:HIS:HB3	1.95	0.66
1:B:74:ARG:NH1	1:B:77:GLN:OE1	2.29	0.66
1:D:302:HIS:HD2	1:D:432:LEU:O	1.79	0.65
1:C:179:CYS:HA	1:C:184:ILE:HD12	1.78	0.65
1:D:187:VAL:CG1	1:D:613:ALA:HB1	2.27	0.65
1:A:415:GLU:O	1:A:418:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:HIS:NE2	1:B:72:GLU:OE2	2.30	0.65
1:C:83:MET:O	1:C:88:VAL:N	2.27	0.65
1:A:71:ASP:HA	1:A:74:ARG:HG2	1.79	0.65
1:C:218:VAL:HG11	1:C:231:TYR:CZ	2.32	0.65
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.98	0.64
1:C:42:HIS:HA	1:C:73:MET:CE	2.28	0.64
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.45	0.64
1:C:42:HIS:HA	1:C:73:MET:HE1	1.79	0.63
1:C:122:LEU:CD1	1:C:128:ILE:HB	2.27	0.63
1:C:49:LEU:HB3	1:C:107:ASP:HA	1.81	0.63
1:C:77:GLN:HA	1:C:80:LEU:HB2	1.79	0.63
1:A:71:ASP:HA	1:A:74:ARG:CG	2.29	0.63
1:C:197:LEU:HD11	1:C:218:VAL:HG13	1.81	0.63
1:D:167:PHE:CG	1:D:176:LEU:CD2	2.82	0.63
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.79	0.62
1:C:83:MET:HA	1:C:88:VAL:HG22	1.81	0.62
1:C:510:PRO:O	1:C:532:GLY:HA3	2.00	0.62
1:C:77:GLN:O	1:C:81:GLN:N	2.32	0.62
1:C:45:LEU:HB2	1:C:103:VAL:HG22	1.82	0.61
1:D:227:ILE:HG23	1:D:230:ARG:CB	2.32	0.60
1:B:549:TYR:O	1:B:590:THR:HG22	2.01	0.59
1:D:188:THR:CG2	1:D:242:ASP:H	2.14	0.59
1:C:78:HIS:CB	1:C:157:LEU:HD13	2.33	0.59
1:D:97:ILE:HD13	1:D:97:ILE:H	1.67	0.59
1:D:148:ALA:CB	1:D:178:LEU:HD11	2.33	0.59
1:C:218:VAL:HG11	1:C:231:TYR:OH	2.03	0.58
1:A:187:VAL:HG12	1:A:613:ALA:HB1	1.83	0.58
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.36	0.58
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.85	0.58
1:C:78:HIS:CB	1:C:157:LEU:CD1	2.82	0.58
1:C:195:THR:OG1	1:C:254:GLU:OE1	2.19	0.58
1:B:18:ALA:HB2	1:B:105:LEU:CD2	2.34	0.57
1:D:176:LEU:N	1:D:177:PRO:HD2	2.19	0.57
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.34	0.57
1:C:108:LEU:O	1:C:111:VAL:N	2.32	0.57
1:D:188:THR:HG23	1:D:242:ASP:H	1.70	0.57
1:A:158:ASP:OD2	1:A:161:HIS:ND1	2.30	0.56
1:C:73:MET:C	1:C:75:PRO:HD2	2.26	0.56
1:D:177:PRO:HA	1:D:240:SER:OG	2.05	0.55
1:A:187:VAL:CG1	1:A:613:ALA:HB1	2.36	0.55
1:B:353:ALA:HB3	1:B:474:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HD12	1:C:234:GLU:CD	2.26	0.55
1:C:82:THR:HA	1:C:85:SER:HB3	1.87	0.55
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.40	0.55
1:A:5:LEU:N	1:A:5:LEU:HD23	2.22	0.55
1:D:510:PRO:O	1:D:532:GLY:HA3	2.07	0.55
1:D:74:ARG:N	1:D:75:PRO:HD2	2.21	0.54
1:D:3:ARG:NH2	1:D:158:ASP:O	2.40	0.54
1:A:213:LEU:HD21	1:A:254:GLU:HA	1.89	0.54
1:D:227:ILE:HG22	1:D:231:TYR:H	1.73	0.54
1:B:213:LEU:HD21	1:B:254:GLU:HA	1.90	0.54
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.90	0.54
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.89	0.54
1:C:82:THR:HG22	1:C:83:MET:N	2.15	0.53
1:C:122:LEU:HD11	1:C:128:ILE:HD12	1.91	0.53
1:A:434:ARG:NH1	1:A:438:GLN:OE1	2.42	0.52
1:D:96:LEU:N	1:D:100:ALA:HA	2.24	0.52
1:C:83:MET:CB	1:C:88:VAL:HG21	2.39	0.52
1:C:80:LEU:O	1:C:82:THR:O	2.27	0.52
1:A:199:ARG:NH2	2:A:902:G6P:O3P	2.33	0.52
1:C:14:ALA:O	1:C:17:VAL:HG23	2.09	0.52
1:B:323:TYR:OH	1:B:458:LYS:HG2	2.10	0.52
1:B:115:SER:HB3	1:B:142:LEU:HD21	1.92	0.52
1:D:73:MET:HA	1:D:73:MET:CE	2.39	0.51
1:D:123:TRP:O	1:D:127:GLY:HA2	2.10	0.51
1:B:308:ASP:O	1:B:312:THR:HG23	2.10	0.51
1:D:133:ASN:O	1:D:135:PHE:N	2.44	0.51
1:D:383:HIS:O	1:D:387:THR:HG23	2.11	0.51
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.93	0.51
1:C:60:ILE:HG22	1:C:61:LEU:N	2.26	0.51
1:C:76:VAL:O	1:C:77:GLN:CB	2.58	0.51
1:A:74:ARG:N	1:A:75:PRO:CD	2.74	0.50
1:D:227:ILE:HG22	1:D:231:TYR:N	2.27	0.50
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.46	0.50
1:D:34:ILE:HD13	1:D:599:TRP:HB3	1.94	0.50
1:B:126:VAL:HG12	1:B:128:ILE:HG13	1.93	0.50
1:A:188:THR:O	1:A:242:ASP:HB2	2.12	0.50
1:C:82:THR:O	1:C:83:MET:CB	2.60	0.50
1:B:45:LEU:HB2	1:B:103:VAL:HG12	1.94	0.50
1:B:333:GLU:OE1	1:B:458:LYS:NZ	2.45	0.49
1:B:369:LEU:HA	1:B:487:ILE:HD11	1.94	0.49
1:D:49:LEU:HD11	1:D:91:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:HIS:HE1	1:B:407:THR:O	1.94	0.49
1:C:83:MET:HA	1:C:88:VAL:CG2	2.40	0.49
1:C:218:VAL:CG1	1:C:231:TYR:CZ	2.95	0.49
1:C:406:THR:O	1:C:407:THR:OG1	2.15	0.49
1:B:63:TRP:O	1:B:77:GLN:NE2	2.44	0.49
1:C:213:LEU:HD21	1:C:254:GLU:HA	1.94	0.49
1:D:10:LEU:HD13	1:D:610:ARG:HD3	1.94	0.49
1:D:72:GLU:O	1:D:161:HIS:HE1	1.95	0.49
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.43	0.49
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.44	0.48
1:C:549:TYR:O	1:C:590:THR:HG22	2.12	0.48
1:D:97:ILE:HD13	1:D:97:ILE:N	2.28	0.48
1:B:60:ILE:C	1:B:61:LEU:HD12	2.33	0.48
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.95	0.48
1:C:83:MET:C	1:C:88:VAL:CG2	2.64	0.48
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.78	0.48
1:A:510:PRO:O	1:A:532:GLY:HA3	2.14	0.48
1:B:18:ALA:HB2	1:B:105:LEU:HD22	1.96	0.48
1:A:34:ILE:CD1	1:A:600:LYS:HA	2.44	0.47
1:B:493:ASP:O	1:B:497:ARG:HG3	2.14	0.47
1:D:187:VAL:HG11	1:D:613:ALA:O	2.15	0.47
1:B:200:TYR:CD1	1:B:227:ILE:HD11	2.49	0.47
1:D:322:GLU:HB2	1:D:326:LYS:HG2	1.96	0.47
1:D:49:LEU:CD1	1:D:91:VAL:HG21	2.45	0.47
1:B:146:THR:O	1:B:149:TRP:HB3	2.15	0.47
1:B:396:HIS:HD2	1:B:415:GLU:OE2	1.97	0.47
1:D:49:LEU:CD1	1:D:91:VAL:CG2	2.92	0.47
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.14	0.47
1:C:123:TRP:CD1	1:C:123:TRP:C	2.88	0.47
1:D:97:ILE:HD13	1:D:101:PRO:HD2	1.95	0.47
1:D:126:VAL:HG12	1:D:126:VAL:O	2.15	0.47
1:C:49:LEU:HB3	1:C:107:ASP:CA	2.45	0.47
1:A:295:ASP:CG	1:A:376:ARG:HH22	2.19	0.47
1:D:43:TYR:OH	1:D:45:LEU:HD21	2.15	0.47
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.96	0.47
1:B:74:ARG:N	1:B:75:PRO:CD	2.78	0.47
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.50	0.47
1:C:14:ALA:CB	1:C:28:LEU:HD11	2.45	0.47
1:C:19:ASN:OD1	1:C:21:VAL:HG23	2.15	0.47
1:D:187:VAL:HG12	1:D:188:THR:N	2.31	0.46
1:A:349:LYS:O	1:A:471:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ALA:O	1:B:17:VAL:HG23	2.16	0.46
1:A:3:ARG:NH2	1:A:155:ALA:O	2.42	0.46
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.49	0.46
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.45	0.46
1:D:49:LEU:HD12	1:D:91:VAL:CG2	2.45	0.46
1:A:169:GLU:HA	1:A:169:GLU:OE2	2.16	0.46
1:A:249:GLN:HG2	1:A:266:ILE:HD11	1.98	0.46
1:C:238:ALA:O	1:C:261:ARG:NH1	2.47	0.46
1:D:81:GLN:O	1:D:85:SER:N	2.44	0.46
1:B:335:LEU:HD13	1:B:474:MET:CE	2.46	0.46
1:D:187:VAL:HG11	1:D:613:ALA:C	2.36	0.46
1:A:502:GLY:O	1:A:525:SER:HA	2.15	0.46
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.97	0.46
1:B:295:ASP:CG	1:B:376:ARG:HH22	2.19	0.46
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.50	0.46
1:C:60:ILE:CG2	1:C:61:LEU:N	2.79	0.46
1:C:357:MET:O	1:C:478:PRO:HA	2.16	0.46
1:C:283:GLN:NE2	1:C:584:ILE:HG23	2.31	0.45
1:A:400:TYR:CD1	1:A:401:PRO:HA	2.51	0.45
1:D:73:MET:HA	1:D:73:MET:HE2	1.98	0.45
1:D:200:TYR:O	1:D:203:ALA:HB2	2.16	0.45
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.97	0.45
1:C:31:LYS:HD3	1:C:599:TRP:CH2	2.51	0.45
1:B:126:VAL:HG12	1:B:126:VAL:O	2.16	0.45
1:D:19:ASN:OD1	1:D:21:VAL:HG23	2.16	0.45
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.97	0.45
1:D:187:VAL:HG11	1:D:613:ALA:CB	2.44	0.45
1:C:108:LEU:HD13	1:C:142:LEU:HB2	1.98	0.45
1:D:134:ASP:OD2	1:D:229:HIS:CD2	2.69	0.45
1:B:200:TYR:CE1	1:B:227:ILE:HD11	2.52	0.45
1:A:396:HIS:CE1	1:A:405:LEU:HD22	2.52	0.44
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.48	0.44
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.52	0.44
1:D:283:GLN:HG3	2:D:901:G6P:O1	2.18	0.44
1:A:157:LEU:N	1:A:157:LEU:HD12	2.32	0.44
1:A:190:PHE:CE2	1:A:192:THR:HG23	2.52	0.44
1:A:514:THR:OG1	2:A:902:G6P:H1	2.17	0.44
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.99	0.44
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.50	0.44
1:C:196:LEU:CD1	1:C:234:GLU:CD	2.86	0.44
1:D:69:PHE:CD2	1:D:69:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:HD23	1:D:253:PHE:CE2	2.52	0.44
1:C:177:PRO:HA	1:C:240:SER:OG	2.18	0.44
1:A:72:GLU:OE2	1:A:161:HIS:NE2	2.51	0.44
1:A:400:TYR:HA	1:A:405:LEU:HD12	1.99	0.44
1:C:209:PHE:O	1:C:213:LEU:HB2	2.18	0.43
1:D:227:ILE:CG2	1:D:230:ARG:CB	2.96	0.43
1:B:111:VAL:HG11	1:B:118:TRP:CH2	2.53	0.43
1:C:74:ARG:N	1:C:75:PRO:HD2	2.33	0.43
1:D:111:VAL:HG22	1:D:111:VAL:O	2.18	0.43
1:D:163:ILE:HG22	1:D:186:VAL:HG13	2.00	0.43
1:A:249:GLN:OE1	1:A:266:ILE:HD11	2.19	0.43
1:A:320:ARG:NH1	1:A:322:GLU:OE1	2.52	0.43
1:A:63:TRP:O	1:A:69:PHE:HE2	2.01	0.43
1:D:529:ASN:ND2	1:D:555:ASP:OD2	2.52	0.43
1:A:364:PHE:CE2	1:A:486:PRO:HD2	2.53	0.42
1:D:122:LEU:HA	1:D:125:LEU:HB2	2.01	0.42
1:A:34:ILE:HD11	1:A:600:LYS:HA	2.02	0.42
1:B:126:VAL:HG11	1:B:128:ILE:HD12	2.02	0.42
1:A:548:ASP:O	1:A:589:ARG:NH1	2.52	0.42
1:B:290:LYS:NZ	2:B:901:G6P:O1P	2.43	0.42
1:A:228:TYR:CE2	1:A:232:CYS:SG	3.12	0.42
1:B:78:HIS:HB2	1:B:157:LEU:HD13	2.01	0.42
1:C:333:GLU:OE1	1:C:458:LYS:NZ	2.52	0.42
1:D:122:LEU:CD1	1:D:141:ILE:HG12	2.50	0.42
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.54	0.42
1:A:323:TYR:OH	1:A:458:LYS:HG2	2.20	0.42
1:B:238:ALA:O	1:B:261:ARG:NH1	2.53	0.42
1:D:50:ASN:ND2	1:D:53:THR:OG1	2.53	0.42
1:D:180:ARG:HA	1:D:180:ARG:HD3	1.83	0.42
1:D:200:TYR:CE2	1:D:227:ILE:HD11	2.55	0.42
1:B:213:LEU:HD23	1:B:253:PHE:CE2	2.55	0.41
1:D:163:ILE:HG22	1:D:186:VAL:CG1	2.49	0.41
1:A:191:THR:HA	1:A:245:THR:O	2.19	0.41
1:D:32:ALA:HB3	1:D:33:PRO:HD3	2.02	0.41
1:D:302:HIS:HE1	1:D:367:GLU:OE2	2.02	0.41
1:A:295:ASP:OD1	1:A:376:ARG:NH2	2.53	0.41
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.55	0.41
1:B:128:ILE:HG12	1:B:232:CYS:HB3	2.03	0.41
1:D:174:VAL:O	1:D:177:PRO:HG2	2.21	0.41
1:C:323:TYR:OH	1:C:458:LYS:HG2	2.21	0.41
1:C:400:TYR:CD1	1:C:401:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:NZ	1:A:138:ASN:OD1	2.53	0.41
1:D:16:GLU:HG3	1:D:24:ILE:HB	2.03	0.41
1:D:58:VAL:O	1:D:58:VAL:HG12	2.20	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:D:400:TYR:CD1	1:D:401:PRO:HA	2.56	0.41
1:B:188:THR:O	1:B:242:ASP:HB2	2.21	0.41
1:B:369:LEU:HD23	1:B:487:ILE:HD11	2.03	0.41
1:D:349:LYS:O	1:D:471:ARG:HD3	2.21	0.41
1:A:213:LEU:HD23	1:A:253:PHE:CE1	2.56	0.41
1:D:282:PHE:CD1	1:D:591:GLU:OE1	2.73	0.41
1:A:366:VAL:O	1:A:370:LYS:HB2	2.21	0.41
1:B:199:ARG:HH22	2:B:902:G6P:P	2.44	0.41
1:B:17:VAL:HG21	1:B:46:ILE:O	2.21	0.40
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.03	0.40
1:D:97:ILE:CD1	1:D:101:PRO:HD2	2.51	0.40
1:D:502:GLY:O	1:D:525:SER:HA	2.21	0.40
1:D:607:VAL:HA	1:D:610:ARG:NH1	2.36	0.40
1:C:349:LYS:O	1:C:471:ARG:HG3	2.21	0.40
1:A:286:HIS:ND1	1:A:497:ARG:O	2.54	0.40
1:D:153:GLU:O	1:D:157:LEU:HG	2.21	0.40
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.53	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	636/725 (88%)	607 (95%)	29 (5%)	0	100	100
1	B	635/725 (88%)	612 (96%)	22 (4%)	1 (0%)	47	76
1	C	637/725 (88%)	605 (95%)	29 (5%)	3 (0%)	29	59
1	D	594/725 (82%)	570 (96%)	22 (4%)	2 (0%)	41	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2502/2900 (86%)	2394 (96%)	102 (4%)	6 (0%)	47 76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	TYR
1	D	228	TYR
1	D	363	SER
1	B	169	GLU
1	C	407	THR
1	C	77	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	524/625 (84%)	512 (98%)	12 (2%)	50 79
1	B	524/625 (84%)	510 (97%)	14 (3%)	44 75
1	C	494/625 (79%)	480 (97%)	14 (3%)	43 75
1	D	463/625 (74%)	454 (98%)	9 (2%)	57 82
All	All	2005/2500 (80%)	1956 (98%)	49 (2%)	49 78

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	81	GLN
1	A	85	SER
1	A	254	GLU
1	A	289	LYS
1	A	304	CYS
1	A	310	ASP
1	A	321	TYR
1	A	376	ARG

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Mol	Chain	Res	Type
1	A	388	SER
1	A	408	GLU
1	A	556	ARG
1	B	34	ILE
1	B	35	THR
1	B	64	LYS
1	B	204	SER
1	B	224	ARG
1	B	254	GLU
1	B	304	CYS
1	B	310	ASP
1	B	321	TYR
1	B	363	SER
1	B	376	ARG
1	B	408	GLU
1	B	467	SER
1	B	471	ARG
1	C	26	SER
1	C	105	LEU
1	C	122	LEU
1	C	254	GLU
1	C	289	LYS
1	C	304	CYS
1	C	310	ASP
1	C	321	TYR
1	C	363	SER
1	C	420	SER
1	C	471	ARG
1	C	535	SER
1	C	556	ARG
1	C	581	ARG
1	D	69	PHE
1	D	73	MET
1	D	97	ILE
1	D	180	ARG
1	D	289	LYS
1	D	304	CYS
1	D	321	TYR
1	D	433	ARG
1	D	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	283	GLN
1	A	484	ASN
1	B	6	GLN
1	B	161	HIS
1	B	396	HIS
1	B	452	ASN
1	B	582	GLN
1	B	585	ASN
1	C	283	GLN
1	C	284	ASN
1	C	403	ASN
1	D	50	ASN
1	D	161	HIS
1	D	168	HIS
1	D	211	ASN
1	D	302	HIS
1	D	403	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
2	G6P	A	901	-	16,16,16	0.50	0	24,24,24	0.94	2 (8%)
2	G6P	B	902	-	16,16,16	0.65	0	24,24,24	1.72	8 (33%)
2	G6P	B	901	-	16,16,16	0.53	0	24,24,24	0.84	0
2	G6P	D	901	-	16,16,16	0.69	0	24,24,24	1.31	2 (8%)
2	G6P	C	901	-	16,16,16	0.55	0	24,24,24	0.93	1 (4%)
2	G6P	A	902	-	16,16,16	0.57	0	24,24,24	1.18	3 (12%)

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
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
2	G6P	B	902	-	-	3/6/26/26	0/1/1/1
2	G6P	B	901	-	-	2/6/26/26	0/1/1/1
2	G6P	D	901	-	-	5/6/26/26	0/1/1/1
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
2	G6P	A	902	-	-	5/6/26/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	G6P	O2P-P-O6	-4.03	96.00	106.73
2	B	902	G6P	O5-C5-C6	3.44	113.60	106.67
2	B	902	G6P	C3-C4-C5	-3.20	104.52	110.24
2	B	902	G6P	C4-C3-C2	-3.16	105.30	110.82
2	D	901	G6P	O2P-P-O1P	2.78	118.25	107.64
2	A	901	G6P	C1-O5-C5	2.57	118.52	113.66
2	A	902	G6P	O5-C5-C6	2.47	111.66	106.67
2	B	902	G6P	O5-C5-C4	-2.43	105.28	109.69
2	B	902	G6P	O4-C4-C3	2.42	115.94	110.35
2	B	902	G6P	O3-C3-C4	2.36	115.81	110.35
2	A	902	G6P	C6-C5-C4	-2.23	107.43	112.09
2	B	902	G6P	O1P-P-O6	-2.20	100.88	106.73
2	C	901	G6P	O2P-P-O1P	2.19	116.02	107.64
2	B	902	G6P	O5-C1-C2	2.17	114.16	110.28
2	A	901	G6P	O2P-P-O1P	2.09	115.64	107.64
2	A	902	G6P	C4-C3-C2	-2.01	107.31	110.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	G6P	C4-C5-C6-O6
2	A	902	G6P	O5-C5-C6-O6
2	A	902	G6P	C6-O6-P-O1P
2	A	902	G6P	C6-O6-P-O2P
2	A	902	G6P	C6-O6-P-O3P
2	B	901	G6P	C4-C5-C6-O6
2	B	901	G6P	O5-C5-C6-O6
2	B	902	G6P	C4-C5-C6-O6
2	B	902	G6P	O5-C5-C6-O6
2	D	901	G6P	C6-O6-P-O1P
2	D	901	G6P	C6-O6-P-O2P
2	D	901	G6P	C6-O6-P-O3P
2	B	902	G6P	C5-C6-O6-P
2	D	901	G6P	C4-C5-C6-O6
2	D	901	G6P	O5-C5-C6-O6

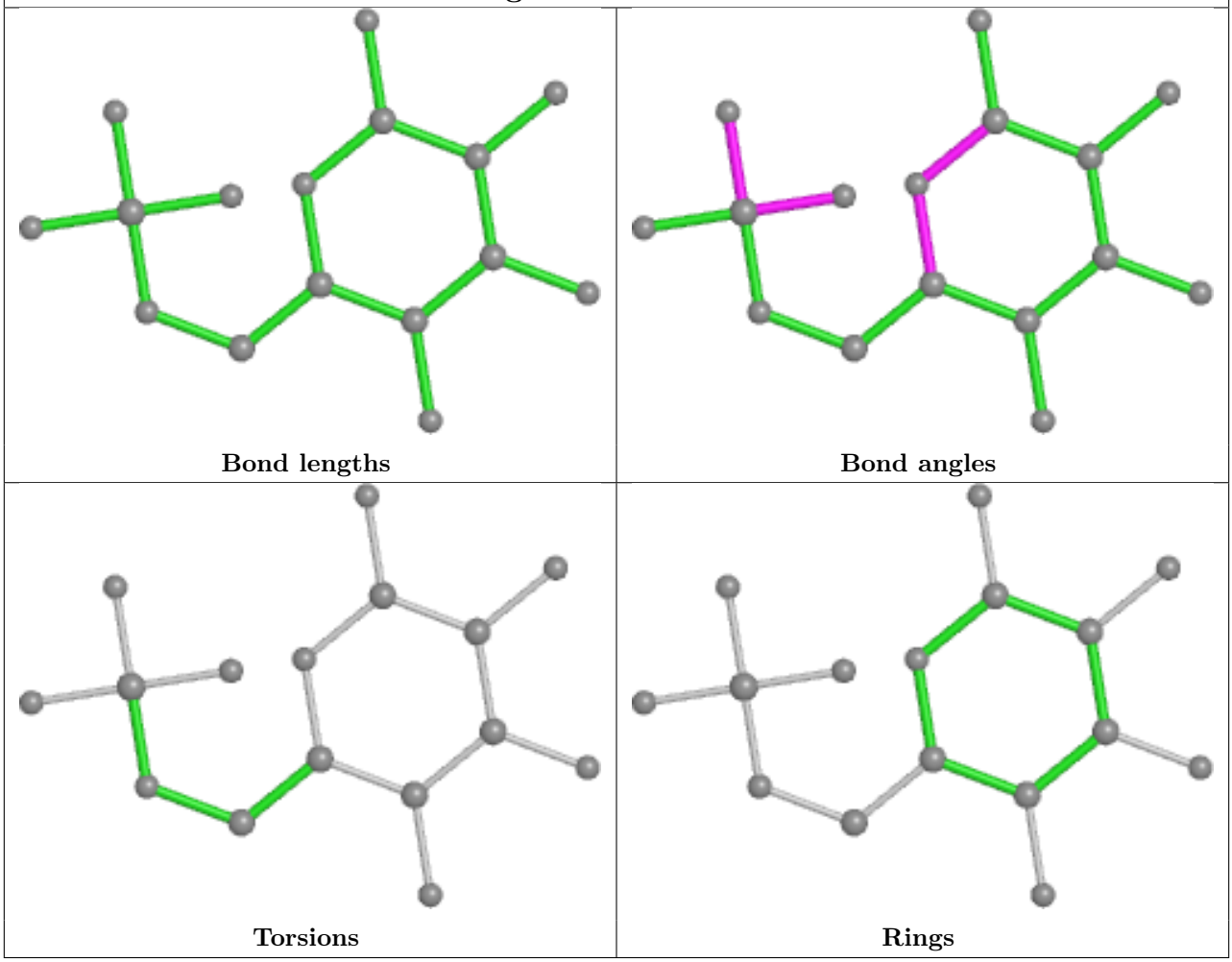
There are no ring outliers.

4 monomers are involved in 6 short contacts:

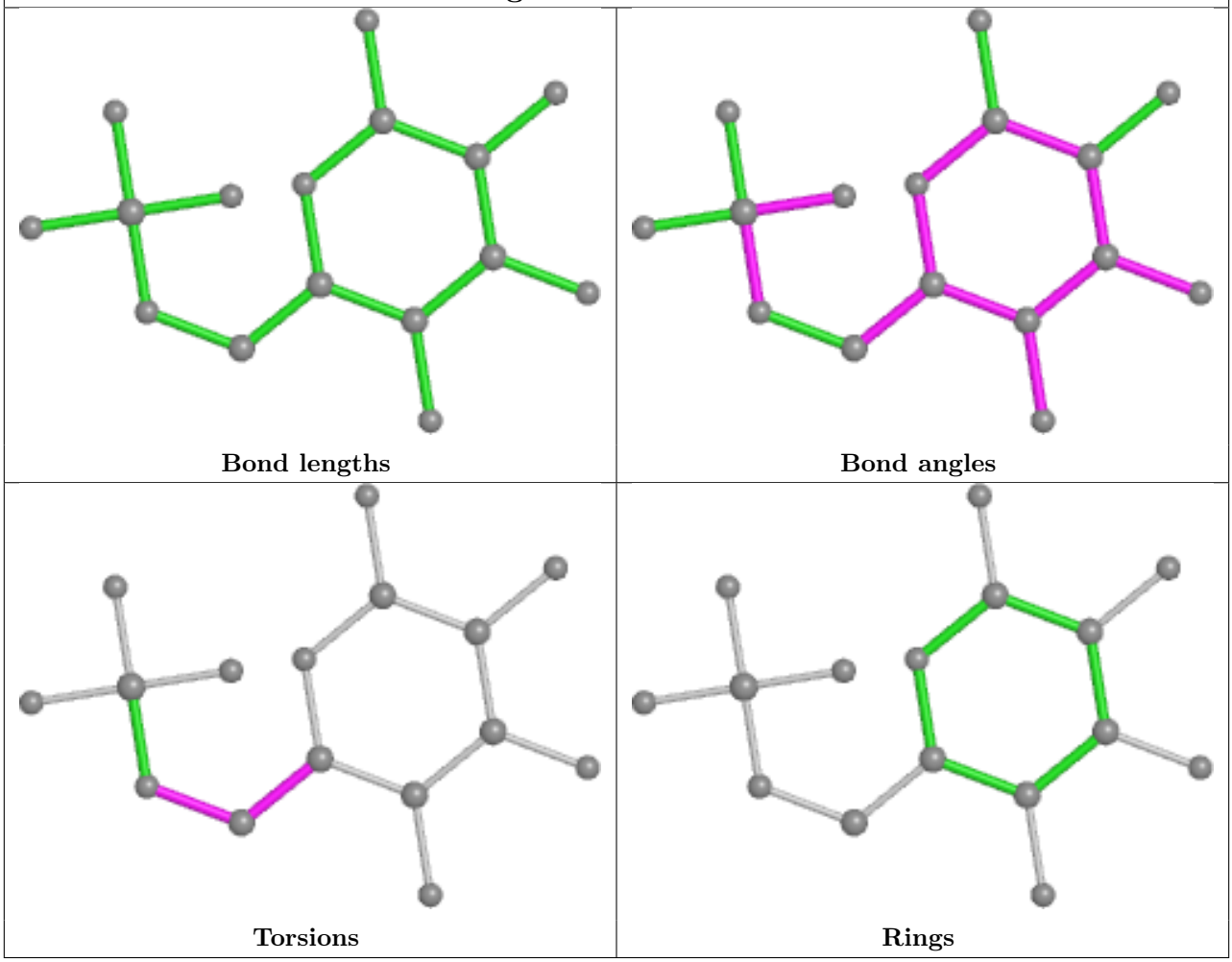
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	G6P	2	0
2	B	901	G6P	1	0
2	D	901	G6P	1	0
2	A	902	G6P	2	0

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

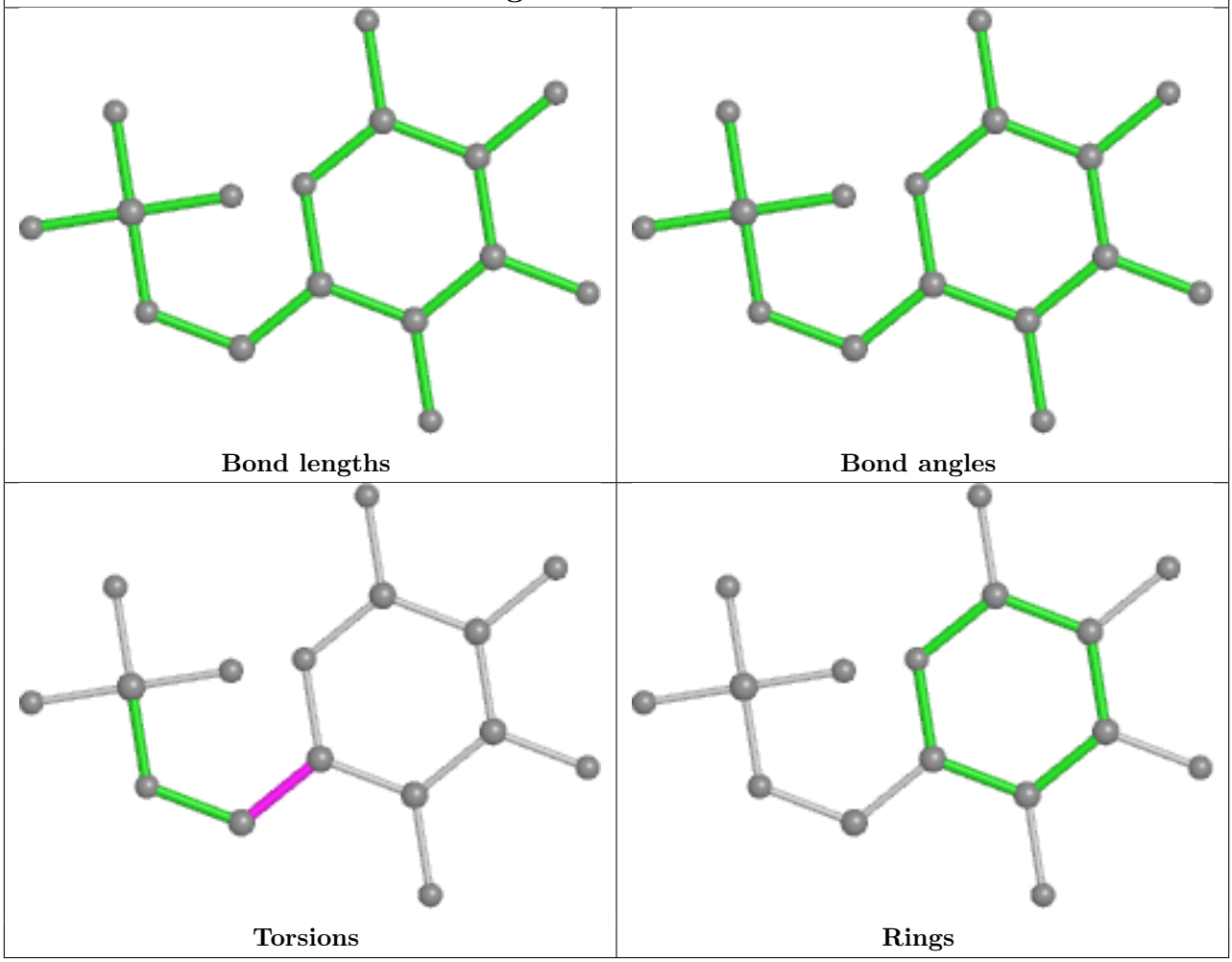
Ligand G6P A 901



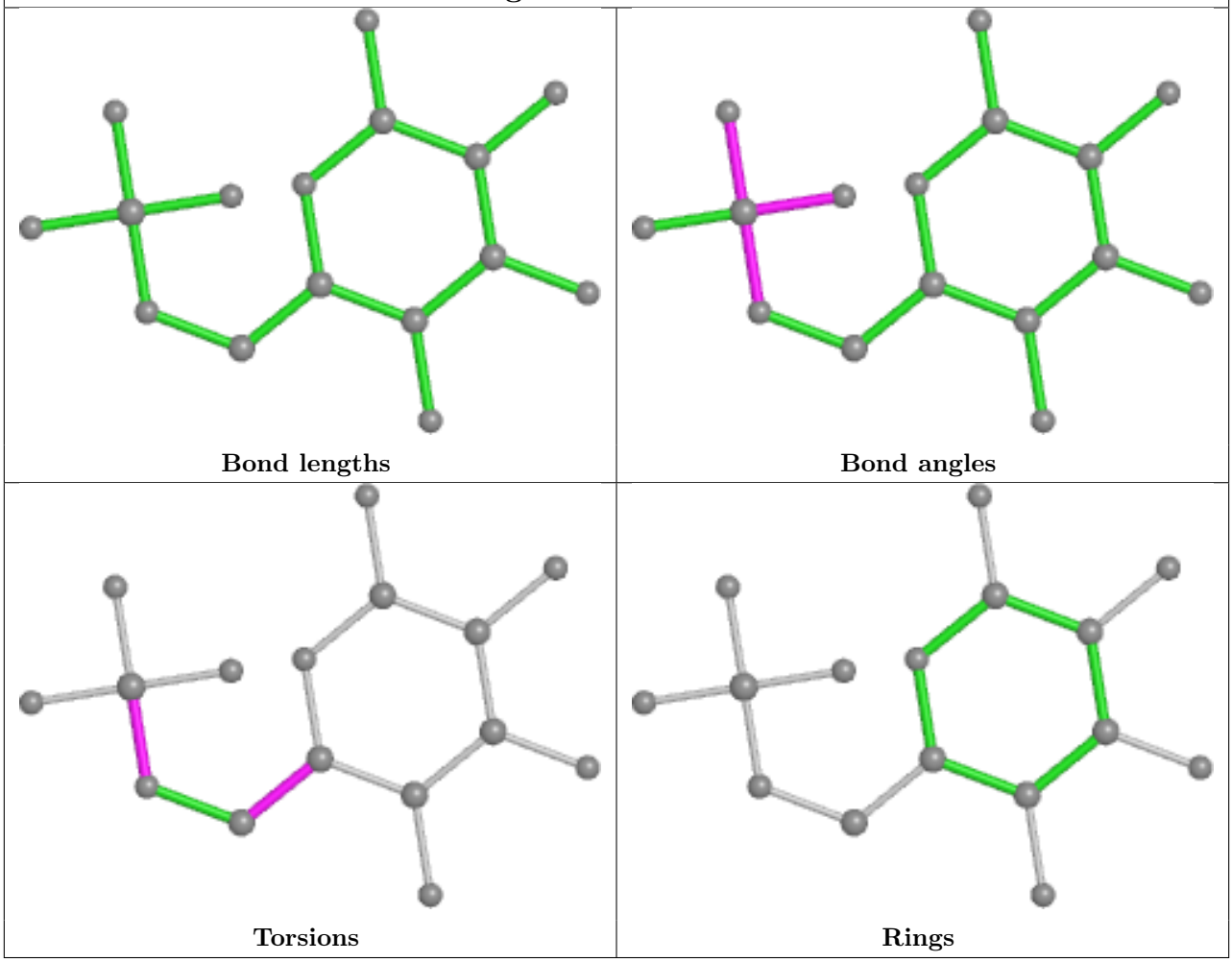
Ligand G6P B 902



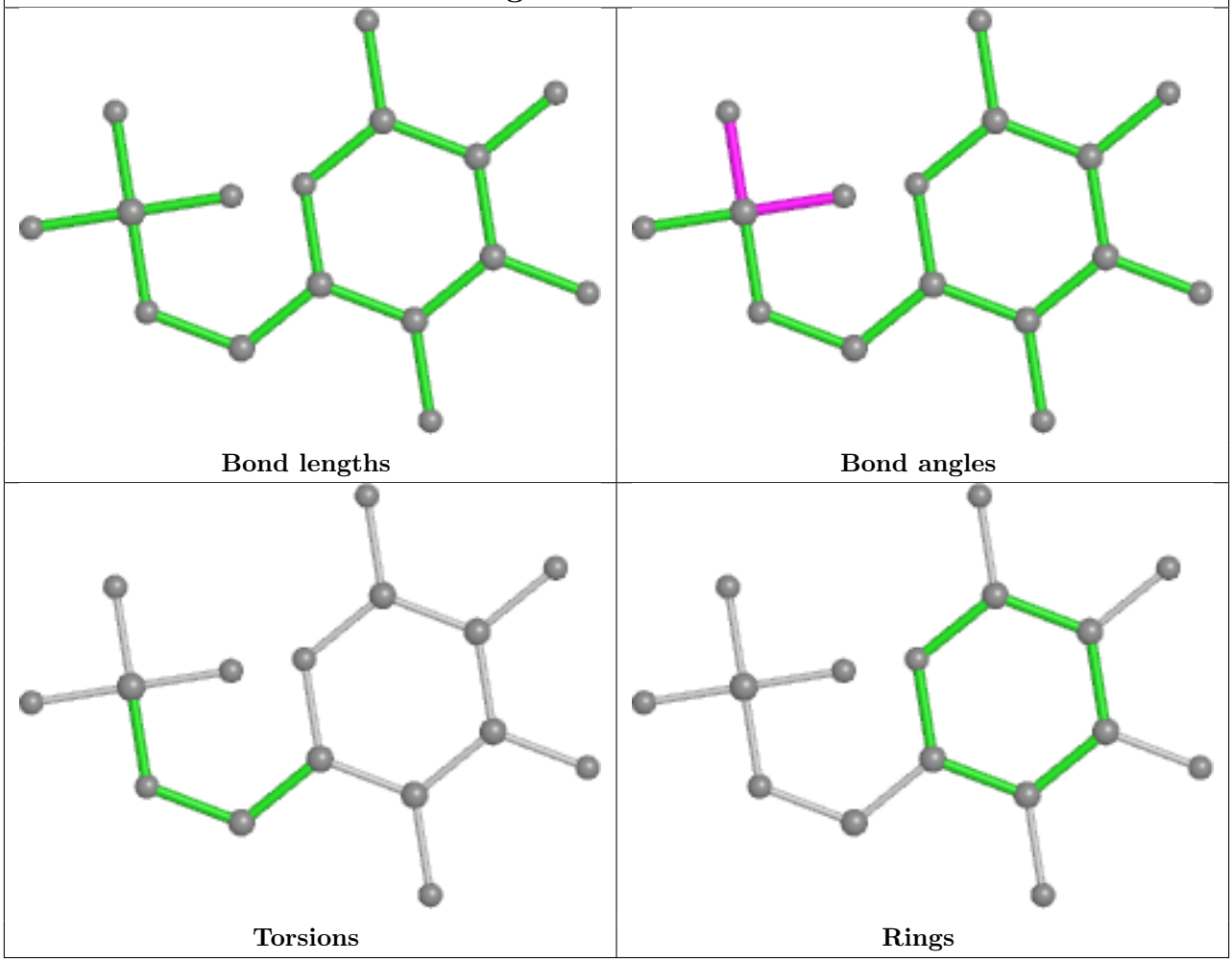
Ligand G6P B 901



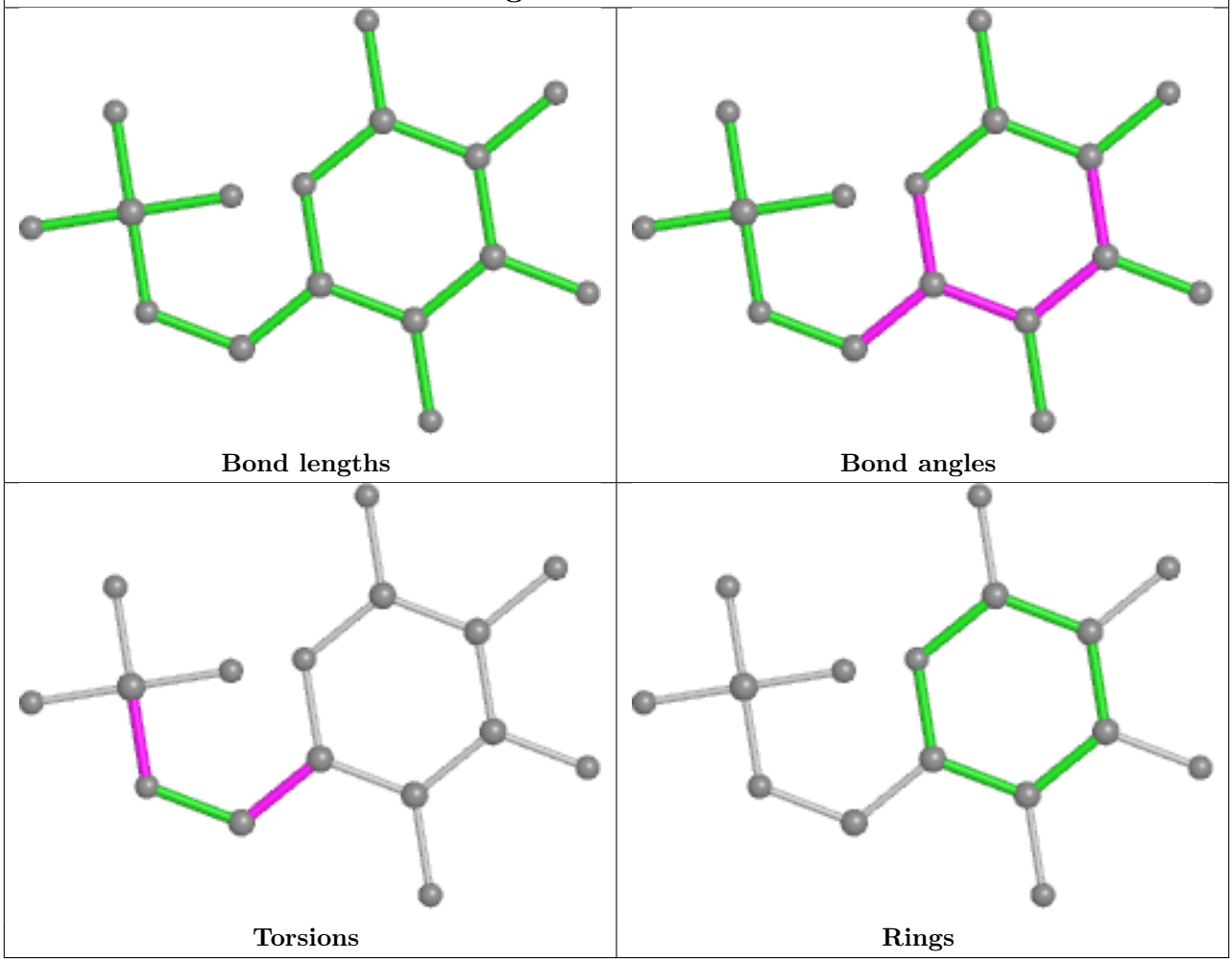
Ligand G6P D 901



Ligand G6P C 901



Ligand G6P A 902



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	638/725 (88%)	0.11	11 (1%)	70	70	32, 67, 119, 145	4 (0%)
1	B	637/725 (87%)	0.18	23 (3%)	42	38	44, 75, 119, 137	3 (0%)
1	C	639/725 (88%)	0.29	28 (4%)	34	30	47, 81, 135, 160	2 (0%)
1	D	604/725 (83%)	0.31	38 (6%)	20	16	37, 80, 146, 168	1 (0%)
All	All	2518/2900 (86%)	0.22	100 (3%)	38	33	32, 77, 133, 168	10 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	LEU	6.2
1	C	111	VAL	5.6
1	D	108	LEU	5.3
1	C	85	SER	5.0
1	C	79	ALA	4.9
1	C	96	LEU	4.4
1	B	124	SER	4.2
1	B	129	PRO	4.2
1	D	122	LEU	4.1
1	C	157	LEU	3.9
1	D	265	GLY	3.9
1	C	68	ALA	3.8
1	D	129	PRO	3.7
1	C	116	ASN	3.7
1	B	126	VAL	3.7
1	D	45	LEU	3.7
1	C	149	TRP	3.6
1	A	637	ALA	3.6
1	C	108	LEU	3.5
1	D	49	LEU	3.4
1	C	83	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	3.3
1	C	88	VAL	3.3
1	A	61	LEU	3.3
1	B	93	GLY	3.2
1	D	128	ILE	3.2
1	A	67	GLU	3.2
1	B	76	VAL	3.2
1	C	80	LEU	3.2
1	A	71	ASP	3.1
1	C	78	HIS	3.1
1	D	259	LEU	3.1
1	C	152	GLY	3.0
1	D	615	ARG	3.0
1	B	91	VAL	3.0
1	D	103	VAL	3.0
1	B	127	GLY	3.0
1	C	103	VAL	3.0
1	D	91	VAL	3.0
1	A	407	THR	3.0
1	D	616	ARG	2.9
1	B	206	SER	2.9
1	C	74	ARG	2.9
1	C	148	ALA	2.9
1	B	68	ALA	2.8
1	A	78	HIS	2.8
1	C	104	ILE	2.7
1	B	131	PRO	2.7
1	B	122	LEU	2.7
1	A	406	THR	2.7
1	D	407	THR	2.7
1	D	130	SER	2.7
1	C	60	ILE	2.7
1	D	218	VAL	2.7
1	B	596	LEU	2.7
1	D	104	ILE	2.6
1	B	66	PRO	2.6
1	B	63	TRP	2.6
1	D	614	LEU	2.5
1	D	225	PHE	2.5
1	A	417	LEU	2.4
1	D	227	ILE	2.4
1	C	52	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	10	LEU	2.4
1	D	109	ASP	2.3
1	B	62	ASP	2.3
1	A	68	ALA	2.3
1	D	604	LEU	2.3
1	A	636	ASP	2.3
1	B	96	LEU	2.3
1	C	197	LEU	2.3
1	D	229	HIS	2.3
1	D	18	ALA	2.3
1	B	125	LEU	2.3
1	C	156	HIS	2.3
1	D	151	LEU	2.3
1	D	163	ILE	2.3
1	B	116	ASN	2.2
1	D	73	MET	2.2
1	C	14	ALA	2.2
1	B	544	ASN	2.2
1	D	56	ASN	2.2
1	D	406	THR	2.2
1	D	620	ASP	2.1
1	B	18	ALA	2.1
1	D	127	GLY	2.1
1	D	186	VAL	2.1
1	A	416	LEU	2.1
1	B	61	LEU	2.1
1	D	55	GLN	2.1
1	C	151	LEU	2.1
1	D	124	SER	2.1
1	D	222	ALA	2.1
1	B	419	SER	2.1
1	C	155	ALA	2.1
1	D	223	GLY	2.1
1	C	417	LEU	2.0
1	D	125	LEU	2.0
1	C	109	ASP	2.0
1	B	626	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

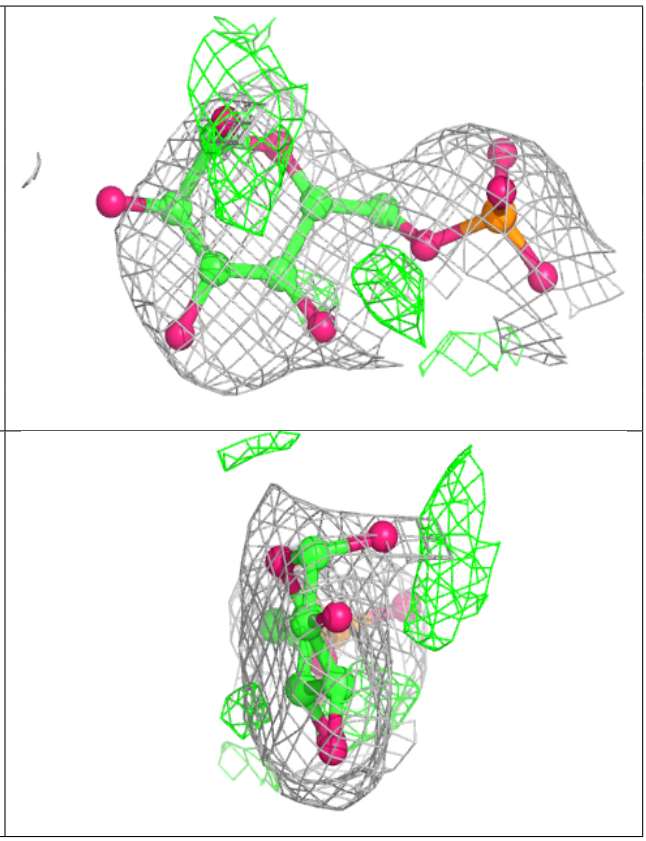
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G6P	A	902	16/16	0.90	0.32	54,63,66,68	16
2	G6P	B	902	16/16	0.92	0.23	76,85,94,94	0
2	G6P	B	901	16/16	0.98	0.15	50,60,64,66	0
2	G6P	A	901	16/16	0.98	0.18	42,49,54,54	0
2	G6P	C	901	16/16	0.98	0.17	46,61,69,70	0
2	G6P	D	901	16/16	0.98	0.14	41,45,49,51	0

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

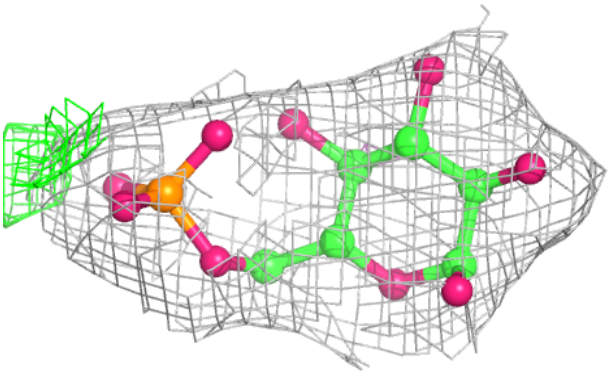
Electron density around G6P A 902:

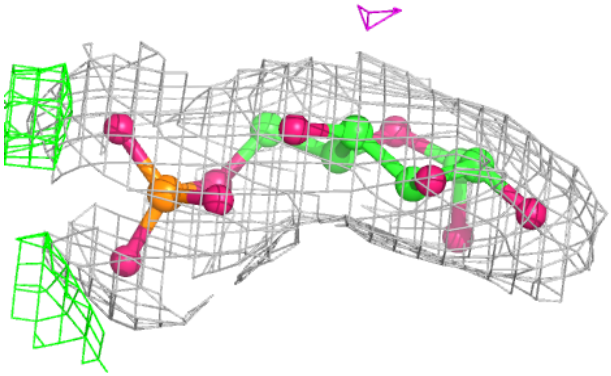
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

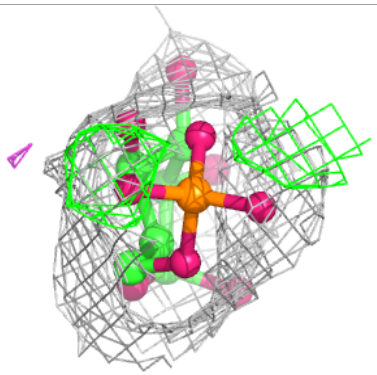


Electron density around G6P B 902:

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

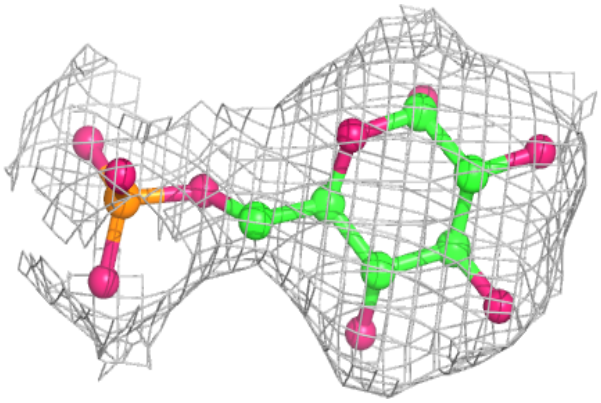


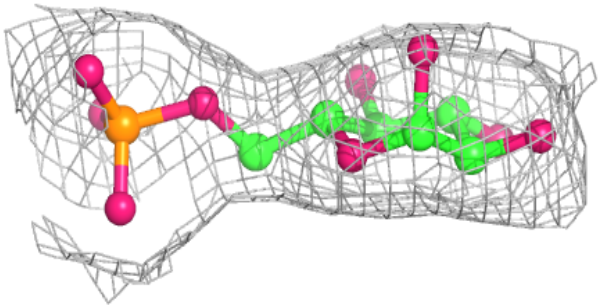


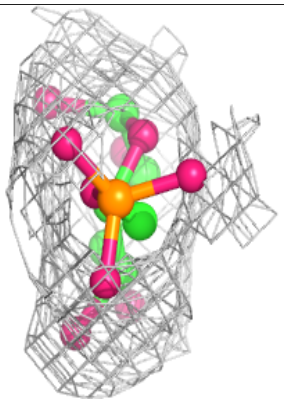


Electron density around G6P B 901:

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

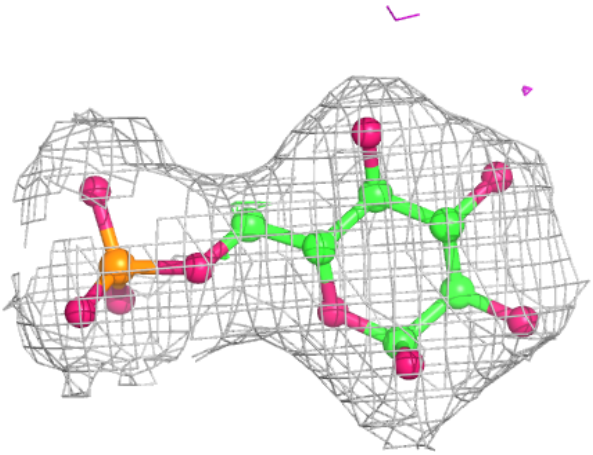


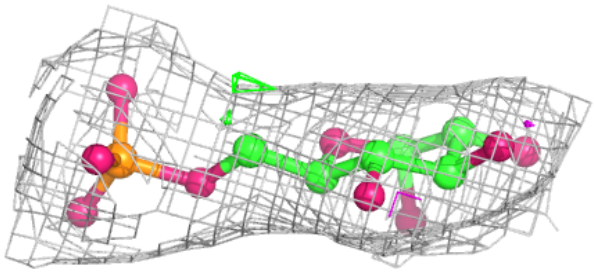


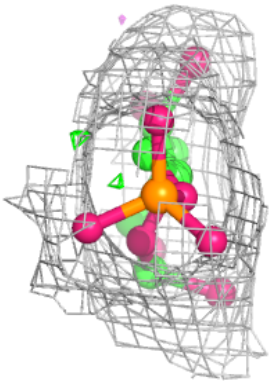


Electron density around G6P A 901:

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

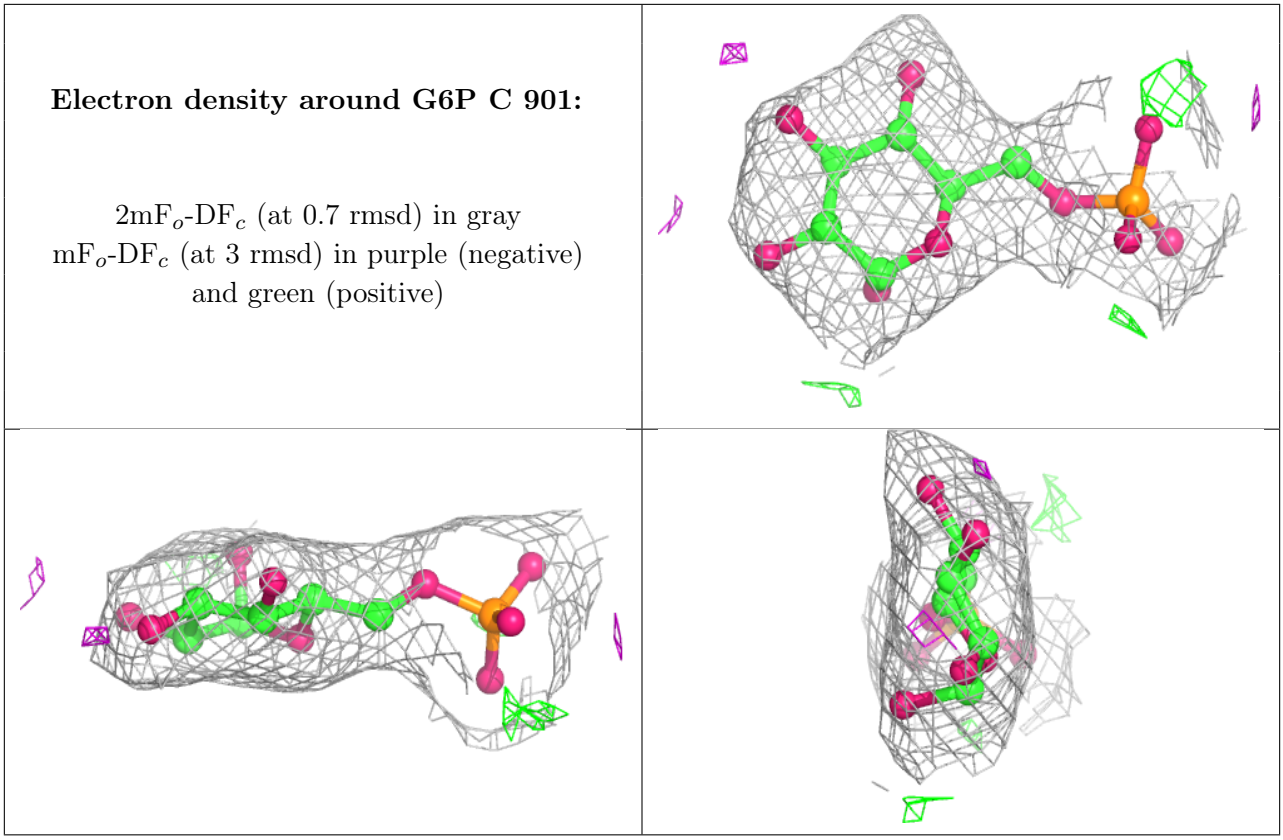






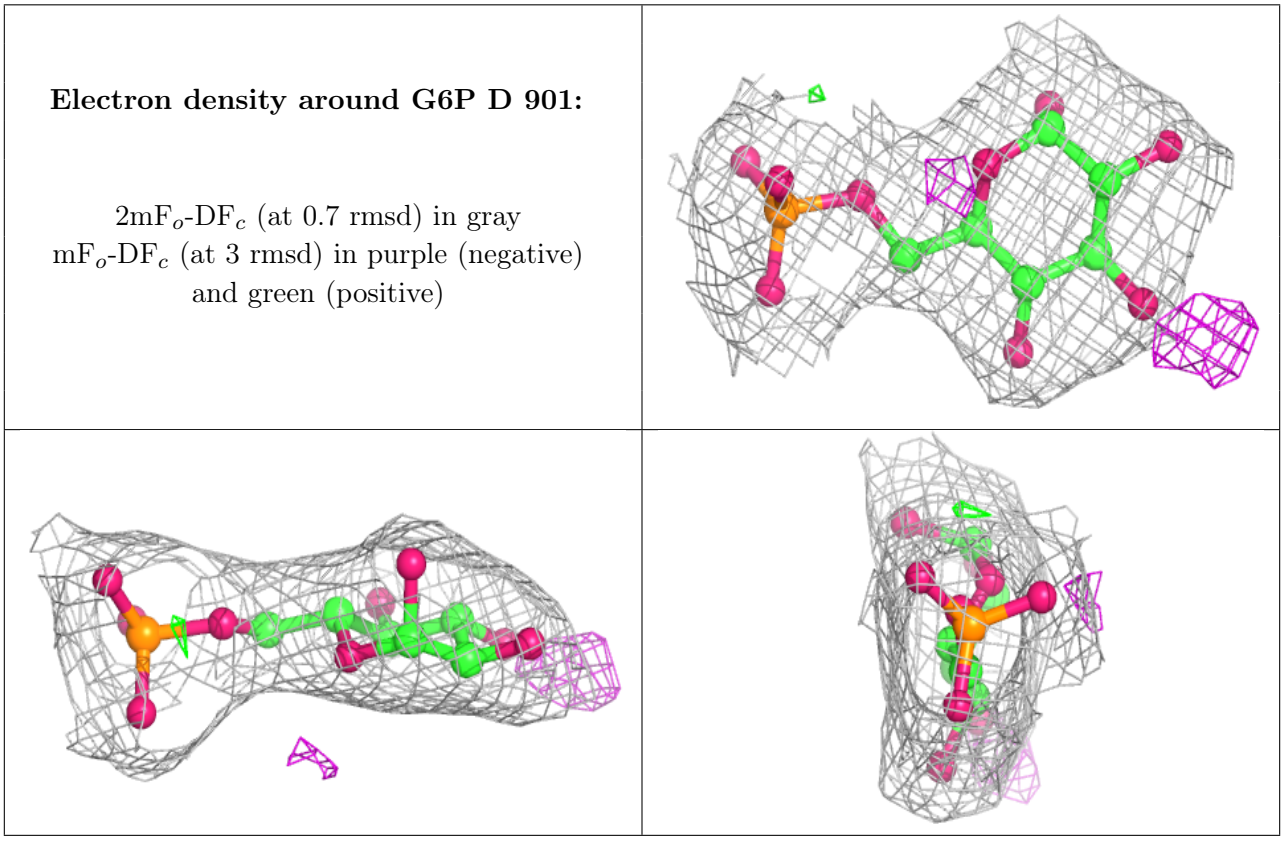
Electron density around G6P C 901:

$2mF_o$-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 901:

$2mF_o$-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.