



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 AM UTC

PDB ID : 4KQ1 / pdb_00004kq1
Title : Crystal structure of yeast glycogen synthase in complex with uridine-5'-mono phosphate
Authors : Chikwana, V.M.; Hurley, T.D.
Deposited on : 2013-05-14
Resolution : 2.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

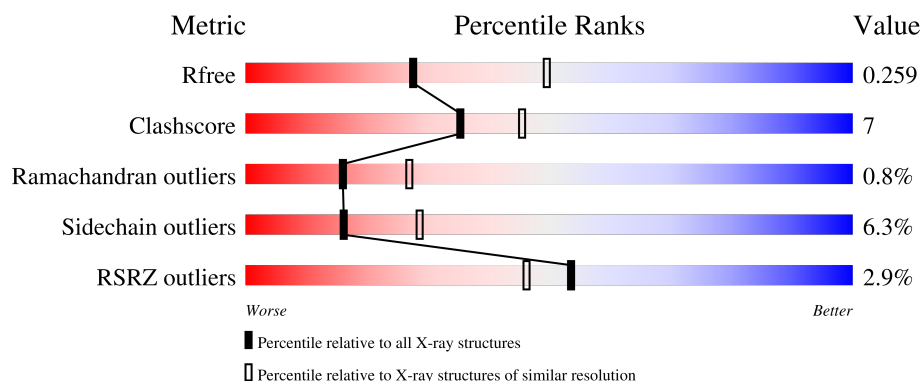
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	724	 2% 70% 17% 12%
1	B	724	 3% 68% 18% 12%
1	C	724	 2% 68% 18% 12%
1	D	724	 3% 67% 19% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20739 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	C	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	D	636	Total	C	N	O	S	0	0	0
			5128	3274	894	941	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP E7NKU1
A	-17	GLY	-	expression tag	UNP E7NKU1
A	-16	SER	-	expression tag	UNP E7NKU1
A	-15	SER	-	expression tag	UNP E7NKU1
A	-14	HIS	-	expression tag	UNP E7NKU1
A	-13	HIS	-	expression tag	UNP E7NKU1
A	-12	HIS	-	expression tag	UNP E7NKU1
A	-11	HIS	-	expression tag	UNP E7NKU1
A	-10	HIS	-	expression tag	UNP E7NKU1
A	-9	HIS	-	expression tag	UNP E7NKU1
A	-8	SER	-	expression tag	UNP E7NKU1
A	-7	SER	-	expression tag	UNP E7NKU1
A	-6	GLY	-	expression tag	UNP E7NKU1
A	-5	LEU	-	expression tag	UNP E7NKU1
A	-4	VAL	-	expression tag	UNP E7NKU1
A	-3	PRO	-	expression tag	UNP E7NKU1
A	-2	ARG	-	expression tag	UNP E7NKU1
A	-1	GLY	-	expression tag	UNP E7NKU1
A	0	SER	-	expression tag	UNP E7NKU1
A	589	ALA	ARG	engineered mutation	UNP E7NKU1
A	592	ALA	ARG	engineered mutation	UNP E7NKU1

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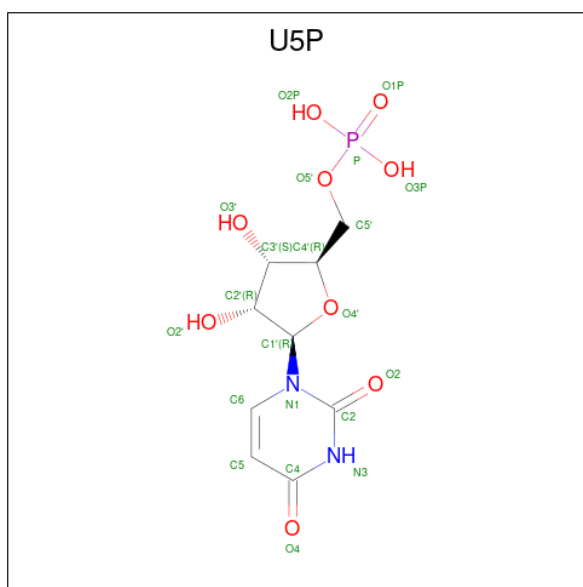
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP E7NKU1
B	-17	GLY	-	expression tag	UNP E7NKU1
B	-16	SER	-	expression tag	UNP E7NKU1
B	-15	SER	-	expression tag	UNP E7NKU1
B	-14	HIS	-	expression tag	UNP E7NKU1
B	-13	HIS	-	expression tag	UNP E7NKU1
B	-12	HIS	-	expression tag	UNP E7NKU1
B	-11	HIS	-	expression tag	UNP E7NKU1
B	-10	HIS	-	expression tag	UNP E7NKU1
B	-9	HIS	-	expression tag	UNP E7NKU1
B	-8	SER	-	expression tag	UNP E7NKU1
B	-7	SER	-	expression tag	UNP E7NKU1
B	-6	GLY	-	expression tag	UNP E7NKU1
B	-5	LEU	-	expression tag	UNP E7NKU1
B	-4	VAL	-	expression tag	UNP E7NKU1
B	-3	PRO	-	expression tag	UNP E7NKU1
B	-2	ARG	-	expression tag	UNP E7NKU1
B	-1	GLY	-	expression tag	UNP E7NKU1
B	0	SER	-	expression tag	UNP E7NKU1
B	589	ALA	ARG	engineered mutation	UNP E7NKU1
B	592	ALA	ARG	engineered mutation	UNP E7NKU1
C	-18	MET	-	initiating methionine	UNP E7NKU1
C	-17	GLY	-	expression tag	UNP E7NKU1
C	-16	SER	-	expression tag	UNP E7NKU1
C	-15	SER	-	expression tag	UNP E7NKU1
C	-14	HIS	-	expression tag	UNP E7NKU1
C	-13	HIS	-	expression tag	UNP E7NKU1
C	-12	HIS	-	expression tag	UNP E7NKU1
C	-11	HIS	-	expression tag	UNP E7NKU1
C	-10	HIS	-	expression tag	UNP E7NKU1
C	-9	HIS	-	expression tag	UNP E7NKU1
C	-8	SER	-	expression tag	UNP E7NKU1
C	-7	SER	-	expression tag	UNP E7NKU1
C	-6	GLY	-	expression tag	UNP E7NKU1
C	-5	LEU	-	expression tag	UNP E7NKU1
C	-4	VAL	-	expression tag	UNP E7NKU1
C	-3	PRO	-	expression tag	UNP E7NKU1
C	-2	ARG	-	expression tag	UNP E7NKU1
C	-1	GLY	-	expression tag	UNP E7NKU1
C	0	SER	-	expression tag	UNP E7NKU1
C	589	ALA	ARG	engineered mutation	UNP E7NKU1
C	592	ALA	ARG	engineered mutation	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP E7NKU1
D	-17	GLY	-	expression tag	UNP E7NKU1
D	-16	SER	-	expression tag	UNP E7NKU1
D	-15	SER	-	expression tag	UNP E7NKU1
D	-14	HIS	-	expression tag	UNP E7NKU1
D	-13	HIS	-	expression tag	UNP E7NKU1
D	-12	HIS	-	expression tag	UNP E7NKU1
D	-11	HIS	-	expression tag	UNP E7NKU1
D	-10	HIS	-	expression tag	UNP E7NKU1
D	-9	HIS	-	expression tag	UNP E7NKU1
D	-8	SER	-	expression tag	UNP E7NKU1
D	-7	SER	-	expression tag	UNP E7NKU1
D	-6	GLY	-	expression tag	UNP E7NKU1
D	-5	LEU	-	expression tag	UNP E7NKU1
D	-4	VAL	-	expression tag	UNP E7NKU1
D	-3	PRO	-	expression tag	UNP E7NKU1
D	-2	ARG	-	expression tag	UNP E7NKU1
D	-1	GLY	-	expression tag	UNP E7NKU1
D	0	SER	-	expression tag	UNP E7NKU1
D	589	ALA	ARG	engineered mutation	UNP E7NKU1
D	592	ALA	ARG	engineered mutation	UNP E7NKU1

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).



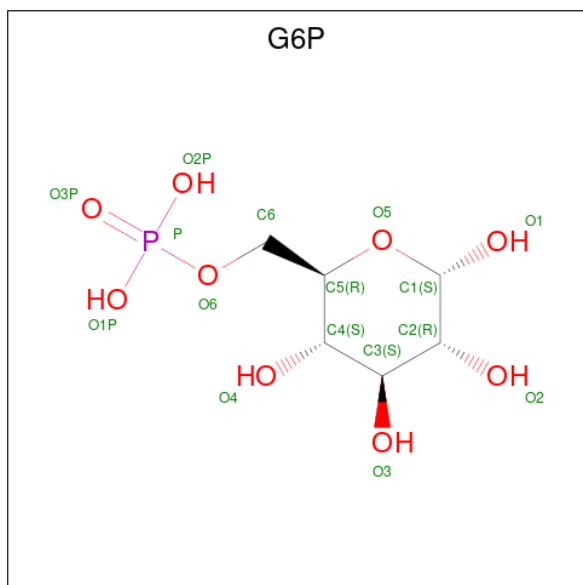
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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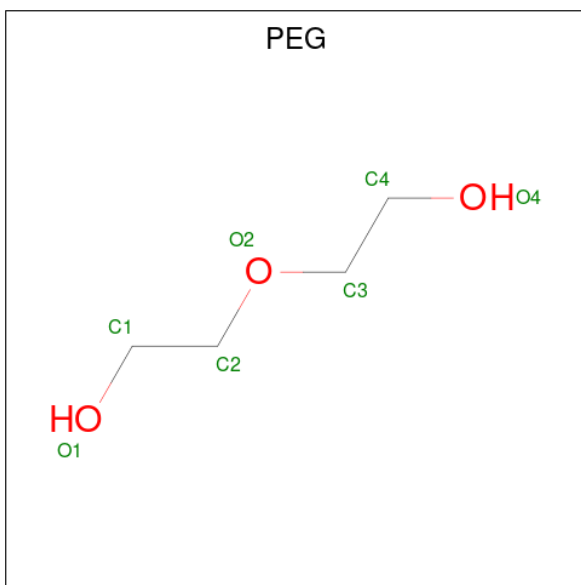
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).



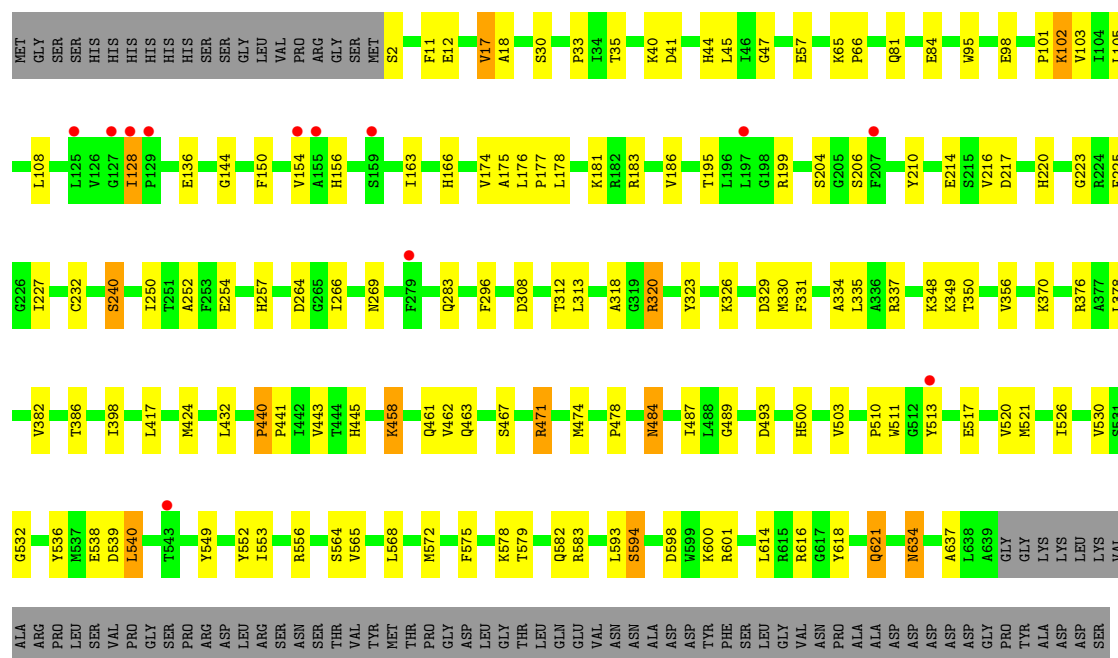
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

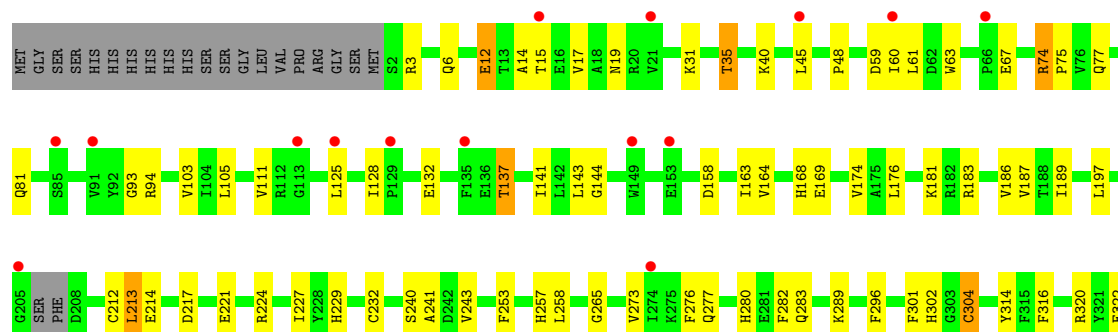


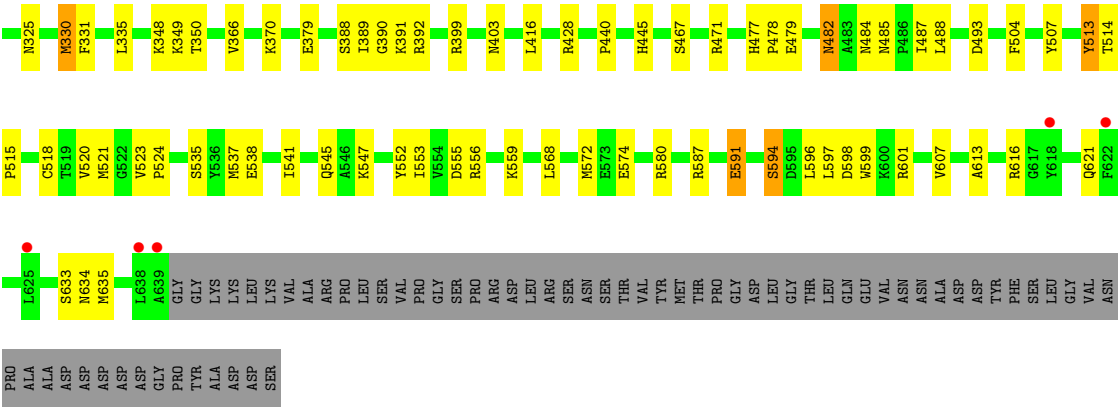
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 1: Gsy2p



- Molecule 1: Gsy2p





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.09Å 204.37Å 206.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.66 48.46 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.46-2.66) 95.1 (48.46-2.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.208 , 0.260 0.207 , 0.259	Depositor DCC
R_{free} test set	5574 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20739	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 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G6P, U5P, PEG

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	0.53	0/5270	0.92	6/7141 (0.1%)
1	B	0.68	1/5270 (0.0%)	0.96	2/7141 (0.0%)
1	C	0.56	0/5270	0.90	4/7141 (0.1%)
1	D	0.59	1/5251 (0.0%)	0.90	2/7114 (0.0%)
All	All	0.59	2/21061 (0.0%)	0.92	14/28537 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	THR	N-CA	5.17	1.52	1.46
1	D	314	TYR	CA-C	-5.02	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-C-N	7.70	127.42	119.56
1	A	485	ASN	C-N-CA	7.70	127.42	119.56
1	A	442	ILE	N-CA-C	-7.52	105.23	113.43
1	D	17	VAL	N-CA-C	6.48	118.01	110.62
1	C	128	ILE	N-CA-C	6.38	113.86	107.55
1	A	634	ASN	N-CA-C	6.31	118.14	108.42
1	B	93	GLY	N-CA-C	6.08	119.02	110.38
1	D	316	PHE	N-CA-C	5.54	118.48	109.06
1	A	40	LYS	CB-CA-C	-5.38	110.36	116.54
1	C	440	PRO	CA-C-N	5.33	125.62	119.92
1	C	440	PRO	C-N-CA	5.33	125.62	119.92
1	C	240	SER	N-CA-C	5.21	117.04	111.36
1	A	55	GLN	N-CA-C	5.17	117.00	111.36
1	B	463	GLN	N-CA-C	5.00	118.50	111.74

There are no chirality outliers.

There are no planarity outliers.

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	5145	0	5054	74	0
1	B	5145	0	5054	71	0
1	C	5145	0	5054	78	0
1	D	5128	0	5039	84	0
2	A	21	0	11	0	0
2	B	21	0	11	0	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
3	A	16	0	11	2	0
3	B	16	0	11	0	0
3	C	16	0	11	2	0
3	D	16	0	11	2	0
4	B	14	0	20	1	0
4	C	7	0	10	0	0
4	D	7	0	10	1	0
All	All	20739	0	20329	302	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 (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:HH11	1:A:180:ARG:HG3	1.29	0.97
1:C:579:THR:H	1:C:582:GLN:HE21	1.10	0.95
1:D:482:ASN:HD22	1:D:484:ASN:H	1.21	0.89
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.12	0.84
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.12	0.83
1:D:493:ASP:HB2	1:D:521:MET:HE1	1.62	0.81
1:A:521:MET:HE2	1:A:521:MET:HA	1.63	0.81
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ARG:NH2	1:B:158:ASP:O	2.17	0.78
1:D:507:TYR:HB2	1:D:556:ARG:NH2	1.98	0.78
1:C:579:THR:H	1:C:582:GLN:NE2	1.81	0.77
1:D:513:TYR:HD1	1:D:513:TYR:H	1.30	0.77
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.66	0.76
1:D:3:ARG:NH2	1:D:158:ASP:O	2.21	0.74
1:B:445:HIS:ND1	1:B:478:PRO:HD2	2.03	0.74
1:C:458:LYS:O	1:C:462:VAL:HG22	1.89	0.73
1:C:484:ASN:N	1:C:484:ASN:HD22	1.89	0.70
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.73	0.70
1:C:296:PHE:HE1	1:C:487:ILE:HD12	1.56	0.70
1:D:591:GLU:O	1:D:594:SER:HB3	1.92	0.70
1:A:492:TYR:O	1:A:496:VAL:HG23	1.91	0.69
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.75	0.68
1:D:31:LYS:NZ	1:D:35:THR:HG21	2.09	0.68
1:D:513:TYR:CD1	1:D:513:TYR:N	2.60	0.67
1:A:379:GLU:HG2	4:B:1004:PEG:H41	1.75	0.67
1:B:8:HIS:HA	1:B:161:HIS:HB3	1.77	0.66
1:C:330:MET:HG3	1:C:565:VAL:HG22	1.77	0.66
1:B:339:ASN:O	1:B:343:LYS:HG3	1.96	0.66
1:D:74:ARG:N	1:D:75:PRO:HD2	2.10	0.66
1:C:634:ASN:ND2	1:C:637:ALA:H	1.96	0.64
1:A:283:GLN:HG3	3:A:802:G6P:O1	1.97	0.64
1:A:92:TYR:OH	1:A:102:LYS:HD3	1.97	0.64
1:C:335:LEU:HD13	1:C:474:MET:HE1	1.79	0.63
1:D:493:ASP:HB2	1:D:521:MET:CE	2.28	0.63
1:D:399:ARG:HG3	1:D:399:ARG:HH11	1.62	0.63
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.63	0.62
1:C:296:PHE:CE1	1:C:487:ILE:HD12	2.34	0.62
1:C:634:ASN:C	1:C:634:ASN:HD22	2.07	0.61
1:C:330:MET:HE1	1:C:564:SER:HB3	1.83	0.61
1:D:389:ILE:HG23	1:D:416:LEU:HB3	1.83	0.60
1:B:419:SER:O	1:B:423:VAL:HG23	2.03	0.59
1:A:283:GLN:HG2	1:D:280:HIS:HE1	1.67	0.58
1:B:295:ASP:CG	1:B:376:ARG:HH22	2.12	0.58
1:C:174:VAL:O	1:C:177:PRO:HD2	2.04	0.57
1:D:59:ASP:HB3	1:D:94:ARG:HB2	1.86	0.57
1:A:323:TYR:OH	1:A:458:LYS:HG3	2.04	0.57
1:A:634:ASN:HB3	1:A:637:ALA:H	1.70	0.57
1:B:634:ASN:HB2	1:B:637:ALA:H	1.69	0.57
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASP:OD2	1:A:460:ARG:NH2	2.38	0.57
1:D:399:ARG:HD3	1:D:403:ASN:HD22	1.69	0.57
1:C:503:VAL:HG11	1:C:572:MET:HE3	1.87	0.57
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.87	0.56
1:A:327:GLY:HA3	1:A:505:PRO:O	2.04	0.56
1:A:348:LYS:HE3	1:A:348:LYS:HA	1.84	0.56
1:D:547:LYS:HE3	1:D:574:GLU:OE2	2.05	0.56
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.38	0.56
1:B:95:TRP:HB3	1:B:101:PRO:HD2	1.88	0.56
1:C:445:HIS:ND1	1:C:478:PRO:HD2	2.21	0.56
1:D:214:GLU:HG3	1:D:257:HIS:CD2	2.41	0.55
1:B:463:GLN:HG2	1:B:465:PHE:CE2	2.42	0.55
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.86	0.55
1:D:176:LEU:HD22	1:D:241:ALA:HB2	1.88	0.55
1:B:214:GLU:HG2	1:B:257:HIS:CD2	2.41	0.55
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.40	0.54
1:D:265:GLY:HA3	1:D:635:MET:HE2	1.88	0.54
1:A:513:TYR:N	1:A:513:TYR:CD2	2.74	0.54
1:C:150:PHE:O	1:C:154:VAL:HG23	2.08	0.54
1:D:3:ARG:H	1:D:621:GLN:HE22	1.56	0.54
1:A:357:MET:O	1:A:478:PRO:HA	2.06	0.54
1:B:187:VAL:HG11	1:B:613:ALA:O	2.08	0.54
1:C:536:TYR:OH	1:C:601:ARG:NH1	2.41	0.53
1:A:517:GLU:O	1:A:521:MET:HG2	2.08	0.53
1:B:540:LEU:C	1:B:541:ILE:HG13	2.33	0.53
1:B:490:LEU:HD13	1:B:495:PHE:HA	1.89	0.53
1:C:549:TYR:HB3	1:C:593:LEU:HD11	1.89	0.53
1:B:59:ASP:HB3	1:B:94:ARG:HB2	1.90	0.53
1:B:488:LEU:O	1:B:490:LEU:N	2.36	0.53
1:D:164:VAL:HA	1:D:187:VAL:HG23	1.90	0.53
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.90	0.53
1:A:374:GLU:HB3	1:A:432:LEU:HD23	1.90	0.53
1:B:187:VAL:HG21	1:B:614:LEU:HD23	1.90	0.53
1:C:177:PRO:HA	1:C:240:SER:OG	2.09	0.53
1:C:598:ASP:OD2	1:C:600:LYS:HB2	2.09	0.53
1:B:337:ARG:NH1	1:B:566:GLU:OE2	2.41	0.53
1:A:195:THR:OG1	1:A:254:GLU:OE1	2.16	0.52
1:A:180:ARG:HH11	1:A:180:ARG:CG	2.12	0.52
1:C:312:THR:HG22	1:C:350:THR:HB	1.92	0.52
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.44	0.52
1:D:482:ASN:ND2	1:D:484:ASN:H	1.99	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ALA:O	1:A:332:ILE:HG13	2.10	0.52
1:A:330:MET:HE2	1:A:568:LEU:HD12	1.92	0.52
1:D:217:ASP:O	1:D:221:GLU:HG2	2.09	0.52
1:D:282:PHE:CE2	1:D:591:GLU:HG3	2.45	0.52
1:C:17:VAL:HG12	1:C:18:ALA:N	2.24	0.51
1:D:485:ASN:OD1	1:D:487:ILE:HG13	2.10	0.51
1:A:180:ARG:HG3	1:A:180:ARG:NH1	2.08	0.51
1:A:510:PRO:O	1:A:532:GLY:HA3	2.10	0.51
1:A:520:VAL:HG12	1:A:521:MET:HE3	1.93	0.51
1:D:283:GLN:HG3	3:D:802:G6P:O1	2.11	0.51
1:A:355:ILE:HD11	1:A:474:MET:CE	2.41	0.51
1:D:213:LEU:HD21	1:D:253:PHE:HE2	1.75	0.51
1:D:273:VAL:HG13	1:D:520:VAL:HG13	1.93	0.51
1:C:283:GLN:O	3:C:802:G6P:H1	2.11	0.51
1:A:521:MET:HE2	1:A:521:MET:CA	2.36	0.51
1:D:616:ARG:HH21	1:D:633:SER:HA	1.76	0.51
1:C:510:PRO:O	1:C:532:GLY:HA3	2.11	0.50
1:D:391:LYS:HG2	4:D:803:PEG:H42	1.93	0.50
1:B:82:THR:O	1:B:85:SER:HB2	2.12	0.50
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.44	0.50
1:D:227:ILE:O	1:D:227:ILE:HG22	2.11	0.50
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.77	0.49
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.94	0.49
1:D:197:LEU:HD12	1:D:258:LEU:HB3	1.95	0.49
1:D:63:TRP:H	1:D:63:TRP:CD1	2.30	0.49
1:A:319:GLY:HA3	1:A:326:LYS:HE3	1.93	0.49
1:C:30:SER:O	1:C:33:PRO:HD2	2.13	0.49
1:C:217:ASP:HB3	1:C:220:HIS:HB2	1.95	0.49
1:B:606:TYR:HB3	1:B:610:ARG:NH1	2.27	0.49
1:D:568:LEU:HG	1:D:572:MET:HE3	1.93	0.49
1:B:580:ARG:O	1:B:584:ILE:HG13	2.14	0.48
1:C:252:ALA:HB2	1:C:266:ILE:HD11	1.95	0.48
1:D:61:LEU:HB2	1:D:93:GLY:HA2	1.95	0.48
1:A:526:ILE:HA	1:A:552:TYR:HB2	1.95	0.48
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.95	0.48
1:C:593:LEU:O	1:C:594:SER:C	2.56	0.48
1:D:320:ARG:NH1	1:D:322:GLU:OE1	2.47	0.48
1:A:175:ALA:HA	1:A:178:LEU:HD12	1.94	0.48
1:C:382:VAL:O	1:C:386:THR:HG23	2.13	0.48
1:C:484:ASN:N	1:C:484:ASN:ND2	2.58	0.48
1:D:596:LEU:HA	1:D:601:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLU:O	1:B:157:LEU:HG	2.13	0.48
1:B:269:ASN:HD22	1:B:511:TRP:CG	2.32	0.48
1:B:352:VAL:CG1	1:B:475:ILE:HD12	2.43	0.48
1:C:308:ASP:O	1:C:312:THR:HG23	2.13	0.48
1:C:583:ARG:NH1	3:C:802:G6P:O1P	2.47	0.48
1:A:269:ASN:HB2	1:A:511:TRP:CD1	2.49	0.48
1:B:55:GLN:HA	1:B:55:GLN:HE21	1.79	0.48
1:D:137:THR:HG21	1:D:229:HIS:HD2	1.79	0.48
1:D:213:LEU:HD21	1:D:253:PHE:CE2	2.48	0.48
1:D:538:GLU:HB3	1:D:553:ILE:HD13	1.96	0.48
1:A:513:TYR:H	1:A:513:TYR:HD2	1.59	0.48
1:D:322:GLU:HB3	1:D:325:ASN:HB2	1.95	0.48
1:A:213:LEU:C	1:A:215:SER:H	2.21	0.47
1:A:335:LEU:HB3	1:A:472:VAL:HG11	1.96	0.47
1:B:192:THR:HG22	1:B:246:THR:HG22	1.95	0.47
1:C:618:TYR:HB3	1:C:621:GLN:HG3	1.95	0.47
1:A:264:ASP:CG	1:A:616:ARG:HH12	2.22	0.47
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.14	0.47
1:D:183:ARG:O	1:D:183:ARG:HG3	2.14	0.47
1:B:593:LEU:O	1:B:594:SER:C	2.56	0.47
1:A:330:MET:HE3	1:A:565:VAL:HA	1.95	0.47
1:B:330:MET:HG2	1:B:565:VAL:HG22	1.96	0.47
1:B:479:GLU:HA	1:B:479:GLU:OE1	2.15	0.47
1:C:102:LYS:H	1:C:102:LYS:HG2	1.54	0.47
1:C:144:GLY:HA3	1:C:174:VAL:HB	1.96	0.47
1:B:485:ASN:OD1	1:B:488:LEU:N	2.42	0.47
1:A:576:VAL:O	1:A:576:VAL:HG12	2.15	0.47
1:D:283:GLN:NE2	1:D:587:ARG:HH21	2.12	0.47
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.97	0.47
1:A:634:ASN:HB2	1:A:637:ALA:CB	2.45	0.46
1:B:61:LEU:HB2	1:B:93:GLY:HA2	1.96	0.46
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.96	0.46
1:A:312:THR:HG22	1:A:313:LEU:N	2.30	0.46
1:A:29:LYS:HG3	1:A:97:ILE:HD13	1.98	0.46
1:A:30:SER:O	1:A:33:PRO:HD2	2.16	0.46
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.98	0.46
1:D:399:ARG:HG3	1:D:399:ARG:NH1	2.27	0.46
1:C:458:LYS:O	1:C:458:LYS:HD3	2.15	0.46
1:C:214:GLU:HG3	1:C:257:HIS:CD2	2.49	0.46
1:D:31:LYS:HZ2	1:D:35:THR:HG21	1.80	0.46
1:D:301:PHE:O	1:D:302:HIS:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HG23	1:D:243:VAL:HB	1.97	0.46
1:B:542:GLU:OE1	1:B:545:GLN:HG3	2.16	0.46
1:A:269:ASN:HB2	1:A:511:TRP:NE1	2.30	0.46
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.97	0.46
1:C:181:LYS:C	1:C:183:ARG:H	2.23	0.46
1:C:318:ALA:HA	1:C:356:VAL:O	2.16	0.46
1:C:443:VAL:HG22	1:C:445:HIS:H	1.81	0.46
1:C:175:ALA:HA	1:C:178:LEU:HD12	1.97	0.46
1:D:366:VAL:O	1:D:370:LYS:HB2	2.16	0.46
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.99	0.45
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.98	0.45
1:A:333:GLU:O	1:A:337:ARG:HG3	2.15	0.45
1:C:195:THR:OG1	1:C:254:GLU:OE2	2.33	0.45
1:B:326:LYS:HD2	1:B:326:LYS:HA	1.69	0.45
1:A:108:LEU:HD22	1:A:142:LEU:HB3	1.99	0.45
1:B:174:VAL:O	1:B:177:PRO:HD2	2.15	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.99	0.45
1:A:323:TYR:CE2	1:A:329:ASP:HB3	2.51	0.45
1:C:227:ILE:HG22	1:C:227:ILE:O	2.17	0.45
1:C:440:PRO:HA	1:C:441:PRO:HD3	1.77	0.45
1:D:547:LYS:HG2	1:D:552:TYR:CD2	2.51	0.45
1:B:176:LEU:HD22	1:B:241:ALA:HB2	1.99	0.45
1:C:128:ILE:HG12	1:C:232:CYS:HB3	1.98	0.45
1:D:301:PHE:CD2	1:D:440:PRO:HG2	2.52	0.45
1:B:74:ARG:N	1:B:75:PRO:CD	2.80	0.44
1:A:555:ASP:HB3	1:A:559:LYS:HD2	1.99	0.44
1:B:55:GLN:HA	1:B:55:GLN:NE2	2.32	0.44
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.99	0.44
1:D:330:MET:HE3	1:D:330:MET:HB3	1.78	0.44
1:A:19:ASN:OD1	1:A:21:VAL:HG23	2.18	0.44
1:B:3:ARG:H	1:B:621:GLN:HE22	1.66	0.44
1:D:282:PHE:CD2	1:D:591:GLU:HG3	2.53	0.44
1:A:214:GLU:HG3	1:A:257:HIS:CD2	2.53	0.44
1:A:634:ASN:CB	1:A:637:ALA:H	2.31	0.44
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.47	0.44
1:B:184:ILE:HG22	1:B:186:VAL:HG23	2.00	0.44
1:C:199:ARG:HH22	1:C:320:ARG:HH22	1.63	0.44
1:A:213:LEU:CD1	1:A:257:HIS:HB2	2.48	0.44
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.53	0.44
1:B:214:GLU:HG2	1:B:257:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASP:CG	1:C:616:ARG:HH12	2.26	0.44
1:C:41:ASP:OD1	1:C:41:ASP:N	2.50	0.44
1:D:514:THR:HB	1:D:515:PRO:CD	2.48	0.44
1:B:357:MET:O	1:B:478:PRO:HA	2.18	0.43
1:D:103:VAL:HG12	1:D:105:LEU:HG	1.99	0.43
1:A:269:ASN:HD22	1:A:511:TRP:CD1	2.36	0.43
1:B:299:GLY:O	1:B:302:HIS:HD2	2.00	0.43
1:C:269:ASN:HD22	1:C:511:TRP:CD1	2.36	0.43
1:C:323:TYR:CE2	1:C:329:ASP:HB3	2.53	0.43
1:C:47:GLY:O	1:C:105:LEU:HA	2.19	0.43
1:A:92:TYR:HH	1:A:102:LYS:HD3	1.83	0.43
1:B:114:TYR:N	1:B:114:TYR:CD1	2.87	0.43
1:B:382:VAL:O	1:B:386:THR:HG23	2.18	0.43
1:B:38:GLN:OE1	1:B:39:TYR:CE1	2.72	0.43
1:D:221:GLU:OE2	1:D:224:ARG:NH1	2.52	0.43
1:A:392:ARG:HD2	1:A:415:GLU:O	2.18	0.43
1:B:144:GLY:HA3	1:B:174:VAL:HB	2.00	0.43
1:D:48:PRO:HG3	1:D:143:LEU:HD22	2.01	0.43
1:A:31:LYS:HB3	1:A:31:LYS:HE3	1.90	0.43
1:B:435:PRO:HD2	1:B:438:GLN:NE2	2.34	0.43
1:D:428:ARG:HA	1:D:428:ARG:HD3	1.71	0.43
1:D:445:HIS:ND1	1:D:478:PRO:HD2	2.34	0.43
1:A:14:ALA:O	1:A:17:VAL:HG23	2.19	0.43
1:C:95:TRP:HB3	1:C:101:PRO:HD2	2.00	0.42
1:D:14:ALA:HB2	1:D:168:HIS:HB2	2.01	0.42
1:D:520:VAL:HA	1:D:594:SER:HB2	2.01	0.42
1:A:322:GLU:O	1:A:326:LYS:HB2	2.18	0.42
1:C:12:GLU:HG3	1:C:166:HIS:HB3	2.01	0.42
1:A:634:ASN:HB2	1:A:637:ALA:HB3	2.01	0.42
1:C:538:GLU:HB2	1:C:553:ILE:HD13	2.01	0.42
1:A:287:ALA:HB2	3:A:802:G6P:H2	2.00	0.42
1:B:522:GLY:HA2	1:B:590:THR:HG22	2.01	0.42
1:D:276:PHE:O	1:D:277:GLN:C	2.62	0.42
1:A:16:GLU:HB3	1:A:25:TYR:HB2	2.02	0.42
1:A:503:VAL:HG21	1:A:572:MET:HE2	2.00	0.42
1:C:176:LEU:HB2	1:C:177:PRO:HD3	2.00	0.42
1:C:349:LYS:O	1:C:471:ARG:HG3	2.20	0.42
1:D:598:ASP:OD1	1:D:599:TRP:N	2.52	0.42
1:B:110:SER:O	1:B:111:VAL:HG13	2.20	0.42
1:C:378:LEU:HD22	1:C:432:LEU:HD11	2.01	0.42
1:C:575:PHE:O	1:C:578:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:HIS:O	1:D:479:GLU:N	2.46	0.42
1:A:95:TRP:HB3	1:A:101:PRO:HD2	2.02	0.42
1:A:117:GLU:H	1:A:117:GLU:HG3	1.66	0.42
1:B:213:LEU:C	1:B:215:SER:H	2.28	0.42
1:C:334:ALA:HB2	1:C:568:LEU:HD23	2.02	0.42
1:D:349:LYS:O	1:D:471:ARG:HD3	2.19	0.42
1:B:32:ALA:O	1:B:33:PRO:C	2.64	0.41
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.55	0.41
1:B:301:PHE:O	1:B:302:HIS:C	2.62	0.41
1:A:458:LYS:O	1:A:462:VAL:HG22	2.21	0.41
1:A:366:VAL:O	1:A:370:LYS:HB2	2.21	0.41
1:B:39:TYR:CB	1:B:43:TYR:HB2	2.51	0.41
1:C:513:TYR:O	1:C:517:GLU:HG2	2.21	0.41
1:D:181:LYS:C	1:D:183:ARG:H	2.28	0.41
1:D:523:VAL:HA	1:D:524:PRO:HD2	1.89	0.41
1:B:248:SER:HA	1:B:266:ILE:HG23	2.03	0.41
1:B:357:MET:HA	1:B:358:PRO:HD3	1.83	0.41
1:B:399:ARG:HH11	1:B:399:ARG:HB3	1.85	0.41
1:C:204:SER:C	1:C:206:SER:H	2.29	0.41
1:C:621:GLN:HE21	1:C:621:GLN:HB3	1.70	0.41
1:B:80:LEU:HD22	1:B:90:PHE:CE2	2.56	0.41
1:B:113:GLY:C	1:B:115:SER:H	2.28	0.41
1:B:268:PRO:HB2	1:B:602:MET:CE	2.49	0.41
1:B:319:GLY:O	1:B:357:MET:HG2	2.20	0.41
1:B:518:CYS:O	1:B:519:THR:C	2.64	0.41
1:C:11:PHE:HA	1:C:44:HIS:O	2.21	0.41
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.56	0.41
1:C:540:LEU:HD13	1:C:540:LEU:HA	1.83	0.41
1:D:12:GLU:HB3	1:D:45:LEU:HD23	2.02	0.41
1:D:580:ARG:HE	3:D:802:G6P:H62	1.86	0.41
1:B:474:MET:C	1:B:475:ILE:HG13	2.46	0.41
1:A:542:GLU:O	1:A:545:GLN:HB2	2.21	0.40
1:C:223:GLY:C	1:C:225:PHE:H	2.29	0.40
1:C:458:LYS:HE3	1:C:461:GLN:OE1	2.21	0.40
1:D:296:PHE:CB	1:D:488:LEU:HD13	2.51	0.40
1:D:482:ASN:HD22	1:D:482:ASN:C	2.29	0.40
1:D:504:PHE:CE1	1:D:514:THR:HG22	2.56	0.40
1:B:83:MET:HE1	1:B:150:PHE:HA	2.03	0.40
1:C:65:LYS:HA	1:C:66:PRO:HD3	1.90	0.40
1:D:555:ASP:HB3	1:D:559:LYS:HD2	2.03	0.40
1:A:431:ALA:HB2	1:C:484:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:CZ	1:C:530:VAL:HB	2.57	0.40
1:C:313:LEU:HA	1:C:500:HIS:ND1	2.36	0.40
1:C:386:THR:HG21	1:D:390:GLY:CA	2.51	0.40
1:A:322:GLU:HB3	1:A:325:ASN:HB2	2.04	0.40
1:C:634:ASN:ND2	1:C:634:ASN:C	2.78	0.40
1:D:187:VAL:HG11	1:D:613:ALA:O	2.22	0.40
1:D:388:SER:HB3	1:D:392:ARG:NH2	2.37	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	636/724 (88%)	588 (92%)	42 (7%)	6 (1%)	14 24
1	B	636/724 (88%)	585 (92%)	42 (7%)	9 (1%)	9 14
1	C	636/724 (88%)	597 (94%)	37 (6%)	2 (0%)	36 52
1	D	632/724 (87%)	592 (94%)	36 (6%)	4 (1%)	21 34
All	All	2540/2896 (88%)	2362 (93%)	157 (6%)	21 (1%)	16 27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	VAL
1	C	17	VAL
1	D	111	VAL
1	B	115	SER
1	B	304	CYS
1	B	483	ALA
1	A	169	GLU
1	A	183	ARG

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Mol	Chain	Res	Type
1	D	40	LYS
1	B	48	PRO
1	D	304	CYS
1	B	194	ALA
1	D	169	GLU
1	A	112	ARG
1	A	194	ALA
1	B	111	VAL
1	C	489	GLY
1	A	561	PRO
1	B	489	GLY
1	B	626	VAL
1	A	512	GLY

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	551/622 (89%)	514 (93%)	37 (7%)	15	25
1	B	551/622 (89%)	519 (94%)	32 (6%)	18	31
1	C	551/622 (89%)	514 (93%)	37 (7%)	15	25
1	D	549/622 (88%)	516 (94%)	33 (6%)	17	30
All	All	2202/2488 (88%)	2063 (94%)	139 (6%)	16	29

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	34	ILE
1	A	51	LYS
1	A	60	ILE
1	A	61	LEU
1	A	111	VAL
1	A	117	GLU
1	A	180	ARG

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Mol	Chain	Res	Type
1	A	213	LEU
1	A	218	VAL
1	A	249	GLN
1	A	272	ASN
1	A	288	LEU
1	A	304	CYS
1	A	310	ASP
1	A	322	GLU
1	A	324	LYS
1	A	348	LYS
1	A	363	SER
1	A	376	ARG
1	A	398	ILE
1	A	406	THR
1	A	458	LYS
1	A	461	GLN
1	A	471	ARG
1	A	485	ASN
1	A	513	TYR
1	A	520	VAL
1	A	521	MET
1	A	539	ASP
1	A	540	LEU
1	A	541	ILE
1	A	556	ARG
1	A	568	LEU
1	A	591	GLU
1	A	595	ASP
1	A	601	ARG
1	B	16	GLU
1	B	17	VAL
1	B	56	ASN
1	B	71	ASP
1	B	83	MET
1	B	111	VAL
1	B	114	TYR
1	B	124	SER
1	B	125	LEU
1	B	176	LEU
1	B	180	ARG
1	B	187	VAL
1	B	192	THR

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Mol	Chain	Res	Type
1	B	199	ARG
1	B	227	ILE
1	B	254	GLU
1	B	288	LEU
1	B	310	ASP
1	B	324	LYS
1	B	363	SER
1	B	376	ARG
1	B	399	ARG
1	B	407	THR
1	B	458	LYS
1	B	518	CYS
1	B	521	MET
1	B	540	LEU
1	B	543	THR
1	B	556	ARG
1	B	564	SER
1	B	568	LEU
1	B	581	ARG
1	C	2	SER
1	C	35	THR
1	C	40	LYS
1	C	45	LEU
1	C	57	GLU
1	C	81	GLN
1	C	84	GLU
1	C	98	GLU
1	C	102	LYS
1	C	103	VAL
1	C	108	LEU
1	C	136	GLU
1	C	156	HIS
1	C	216	VAL
1	C	250	ILE
1	C	320	ARG
1	C	326	LYS
1	C	337	ARG
1	C	348	LYS
1	C	370	LYS
1	C	376	ARG
1	C	398	ILE
1	C	417	LEU

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Mol	Chain	Res	Type
1	C	424	MET
1	C	458	LYS
1	C	463	GLN
1	C	467	SER
1	C	471	ARG
1	C	484	ASN
1	C	520	VAL
1	C	539	ASP
1	C	540	LEU
1	C	556	ARG
1	C	594	SER
1	C	614	LEU
1	C	621	GLN
1	C	634	ASN
1	D	6	GLN
1	D	12	GLU
1	D	15	THR
1	D	19	ASN
1	D	35	THR
1	D	60	ILE
1	D	67	GLU
1	D	74	ARG
1	D	81	GLN
1	D	125	LEU
1	D	132	GLU
1	D	137	THR
1	D	212	CYS
1	D	213	LEU
1	D	240	SER
1	D	289	LYS
1	D	304	CYS
1	D	330	MET
1	D	348	LYS
1	D	379	GLU
1	D	467	SER
1	D	482	ASN
1	D	513	TYR
1	D	518	CYS
1	D	535	SER
1	D	537	MET
1	D	541	ILE
1	D	545	GLN

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Mol	Chain	Res	Type
1	D	591	GLU
1	D	594	SER
1	D	597	LEU
1	D	607	VAL
1	D	634	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	160	GLN
1	A	277	GLN
1	A	461	GLN
1	B	55	GLN
1	B	116	ASN
1	B	249	GLN
1	B	269	ASN
1	B	403	ASN
1	B	484	ASN
1	B	621	GLN
1	B	634	ASN
1	C	38	GLN
1	C	44	HIS
1	C	133	ASN
1	C	161	HIS
1	C	257	HIS
1	C	452	ASN
1	C	484	ASN
1	C	582	GLN
1	C	585	ASN
1	C	621	GLN
1	C	634	ASN
1	D	6	GLN
1	D	19	ASN
1	D	50	ASN
1	D	211	ASN
1	D	229	HIS
1	D	280	HIS
1	D	283	GLN
1	D	403	ASN
1	D	482	ASN
1	D	621	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	U5P	B	1002	-	22,22,22	1.02	1 (4%)	32,33,33	1.84	7 (21%)
3	G6P	B	1003	-	16,16,16	0.58	0	23,24,24	1.41	2 (8%)
3	G6P	D	802	-	16,16,16	0.52	0	23,24,24	1.30	2 (8%)
4	PEG	B	1004	-	6,6,6	0.54	0	5,5,5	0.14	0
3	G6P	C	802	-	16,16,16	0.48	0	23,24,24	0.88	1 (4%)
4	PEG	B	1001	-	6,6,6	0.42	0	5,5,5	0.48	0
4	PEG	D	803	-	6,6,6	0.47	0	5,5,5	0.33	0
3	G6P	A	802	-	16,16,16	0.48	0	23,24,24	1.18	4 (17%)
2	U5P	A	801	-	22,22,22	1.14	4 (18%)	32,33,33	1.86	7 (21%)
4	PEG	C	803	-	6,6,6	0.51	0	5,5,5	0.19	0
2	U5P	D	801	-	22,22,22	0.98	1 (4%)	32,33,33	1.85	6 (18%)
2	U5P	C	801	-	22,22,22	1.19	4 (18%)	32,33,33	1.89	4 (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	U5P	B	1002	-	-	1/10/26/26	0/2/2/2
3	G6P	B	1003	-	-	1/6/26/26	0/1/1/1
3	G6P	D	802	-	-	2/6/26/26	0/1/1/1
4	PEG	B	1004	-	-	3/4/4/4	-
3	G6P	C	802	-	-	1/6/26/26	0/1/1/1
4	PEG	B	1001	-	-	4/4/4/4	-
4	PEG	D	803	-	-	3/4/4/4	-
3	G6P	A	802	-	-	5/6/26/26	0/1/1/1
2	U5P	A	801	-	-	2/10/26/26	0/2/2/2
4	PEG	C	803	-	-	2/4/4/4	-
2	U5P	D	801	-	-	4/10/26/26	0/2/2/2
2	U5P	C	801	-	-	6/10/26/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	U5P	C6-C5	2.42	1.40	1.35
2	C	801	U5P	C2-N1	2.39	1.42	1.38
2	D	801	U5P	C6-C5	2.32	1.40	1.35
2	C	801	U5P	C2-N3	-2.29	1.34	1.38
2	A	801	U5P	C4-N3	-2.29	1.34	1.38
2	A	801	U5P	C2-N1	2.12	1.41	1.38
2	C	801	U5P	C4-N3	-2.09	1.35	1.38
2	A	801	U5P	C2-N3	-2.06	1.34	1.38
2	C	801	U5P	C5-C4	-2.06	1.39	1.43
2	A	801	U5P	C6-C5	2.01	1.39	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	U5P	C4-N3-C2	-5.43	119.87	126.61
2	A	801	U5P	C4-N3-C2	-5.10	120.28	126.61
2	B	1002	U5P	C4-N3-C2	-5.06	120.33	126.61
2	B	1002	U5P	N3-C2-N1	4.97	121.37	114.89
2	D	801	U5P	C4-N3-C2	-4.89	120.54	126.61
2	A	801	U5P	N3-C2-N1	4.69	120.99	114.89
3	B	1003	G6P	C1-O5-C5	4.54	122.43	113.65
2	C	801	U5P	C5-C4-N3	4.37	120.92	114.80
2	D	801	U5P	N3-C2-N1	4.37	120.58	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	U5P	N3-C2-N1	4.36	120.57	114.89
2	D	801	U5P	O2-C2-N1	-3.79	117.86	122.80
2	A	801	U5P	C5-C4-N3	3.77	120.08	114.80
2	C	801	U5P	O4-C4-C5	-3.75	118.70	125.16
2	D	801	U5P	C5-C4-N3	3.62	119.87	114.80
2	B	1002	U5P	O2-C2-N1	-3.49	118.25	122.80
2	B	1002	U5P	C5-C4-N3	3.16	119.22	114.80
3	D	802	G6P	C1-O5-C5	3.12	119.70	113.65
2	D	801	U5P	O4-C4-C5	-2.88	120.19	125.16
3	A	802	G6P	C3-C4-C5	-2.62	105.47	110.23
2	B	1002	U5P	O4-C4-C5	-2.61	120.67	125.16
2	A	801	U5P	O4-C4-C5	-2.56	120.75	125.16
3	D	802	G6P	O6-P-O3P	-2.50	99.69	106.44
3	A	802	G6P	O2P-P-O1P	2.36	116.67	107.80
3	B	1003	G6P	O2P-P-O3P	2.33	119.91	110.83
2	B	1002	U5P	O3P-P-O2P	2.21	116.08	107.80
2	D	801	U5P	O3P-P-O2P	2.20	116.04	107.80
2	B	1002	U5P	O3P-P-O5'	-2.19	100.95	106.67
2	A	801	U5P	O2-C2-N1	-2.11	120.05	122.80
3	C	802	G6P	O2P-P-O1P	2.10	115.68	107.80
2	A	801	U5P	O3P-P-O5'	-2.07	101.27	106.67
3	A	802	G6P	O2P-P-O6	-2.06	101.29	106.67
2	A	801	U5P	C3'-C2'-C1'	2.03	105.31	101.46
3	A	802	G6P	O5-C5-C6	2.01	110.68	106.69

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	U5P	C5'-O5'-P-O1P
2	C	801	U5P	C5'-O5'-P-O2P
2	C	801	U5P	C5'-O5'-P-O3P
2	D	801	U5P	C5'-O5'-P-O2P
2	D	801	U5P	C5'-O5'-P-O3P
3	A	802	G6P	O5-C5-C6-O6
3	A	802	G6P	C6-O6-P-O1P
3	A	802	G6P	C6-O6-P-O2P
3	D	802	G6P	C6-O6-P-O3P
2	A	801	U5P	O4'-C4'-C5'-O5'
2	A	801	U5P	C3'-C4'-C5'-O5'
2	C	801	U5P	O4'-C4'-C5'-O5'
4	B	1001	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	C	801	U5P	C3'-C4'-C5'-O5'
4	C	803	PEG	O2-C3-C4-O4
4	D	803	PEG	O2-C3-C4-O4
2	D	801	U5P	C5'-O5'-P-O1P
3	A	802	G6P	C6-O6-P-O3P
3	C	802	G6P	C4-C5-C6-O6
4	B	1001	PEG	C4-C3-O2-C2
3	D	802	G6P	C6-O6-P-O2P
4	D	803	PEG	C4-C3-O2-C2
4	B	1001	PEG	C1-C2-O2-C3
4	C	803	PEG	C4-C3-O2-C2
4	D	803	PEG	C1-C2-O2-C3
4	B	1001	PEG	O1-C1-C2-O2
2	B	1002	U5P	O4'-C4'-C5'-O5'
4	B	1004	PEG	C1-C2-O2-C3
3	A	802	G6P	C4-C5-C6-O6
3	B	1003	G6P	C4-C5-C6-O6
4	B	1004	PEG	O1-C1-C2-O2
2	C	801	U5P	C4'-C5'-O5'-P
4	B	1004	PEG	C4-C3-O2-C2
2	D	801	U5P	O4'-C4'-C5'-O5'

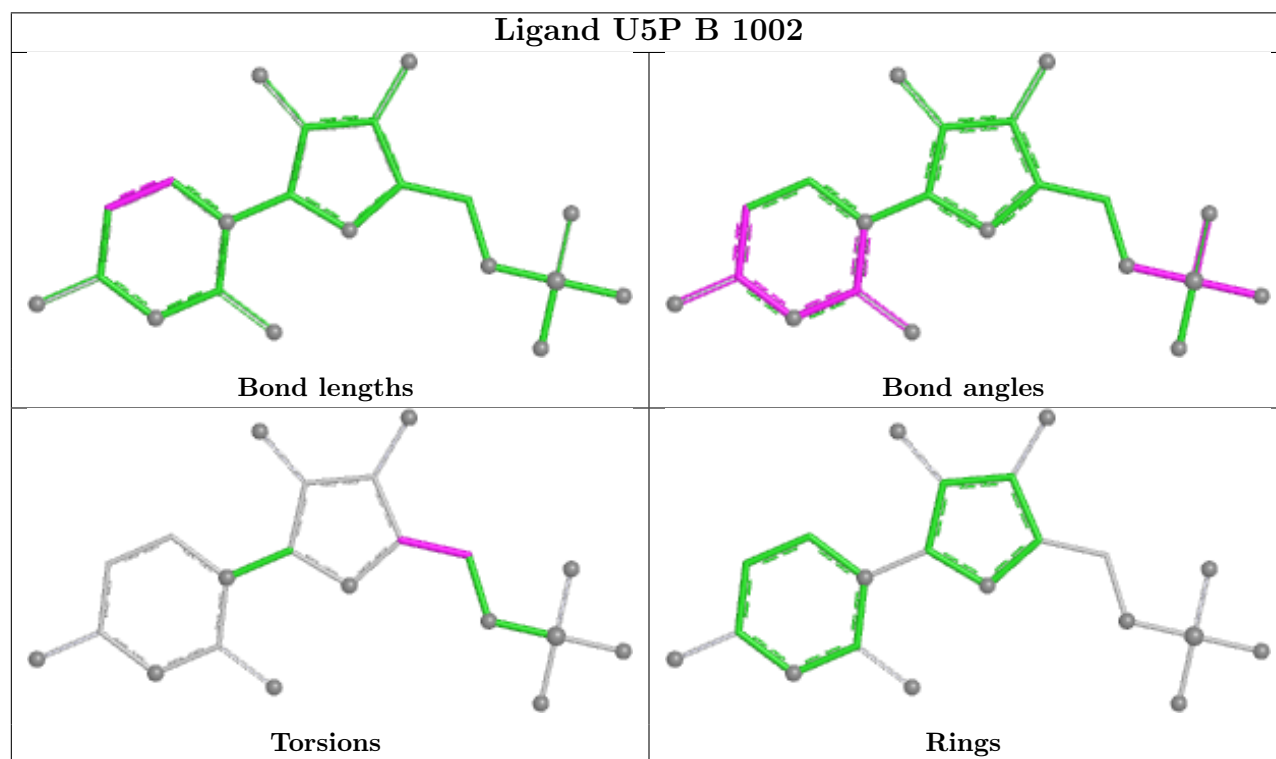
There are no ring outliers.

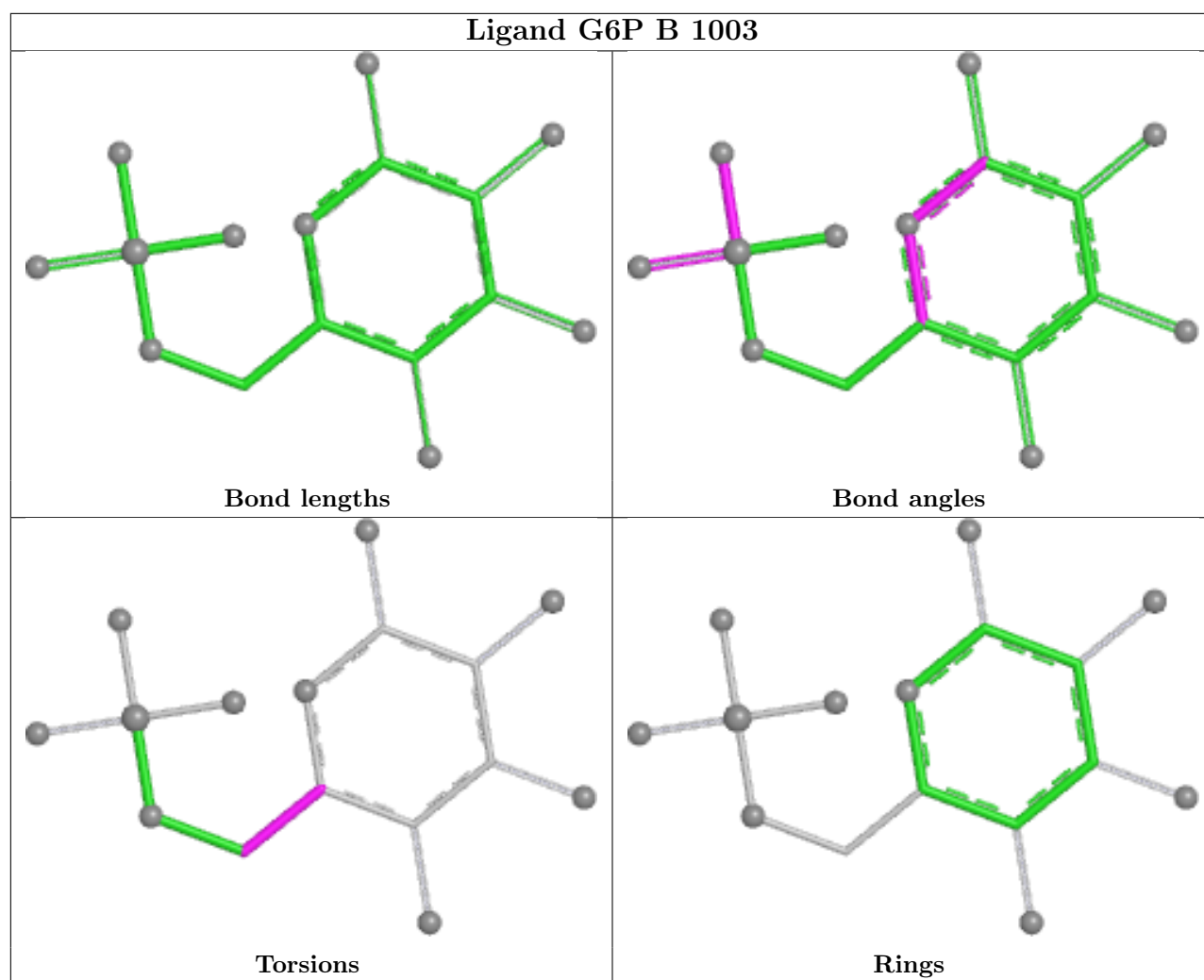
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	G6P	2	0
4	B	1004	PEG	1	0
3	C	802	G6P	2	0
4	D	803	PEG	1	0
3	A	802	G6P	2	0

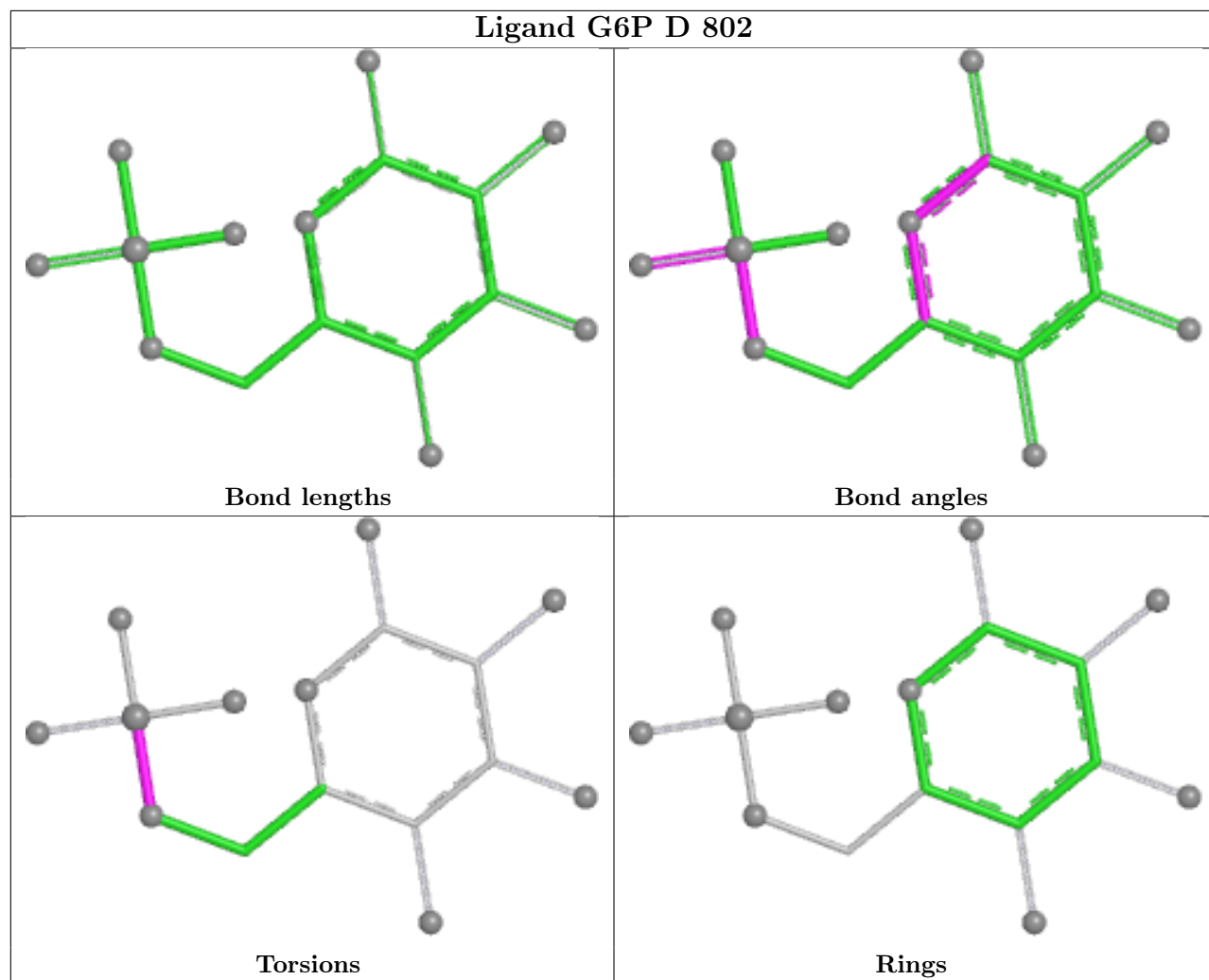
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

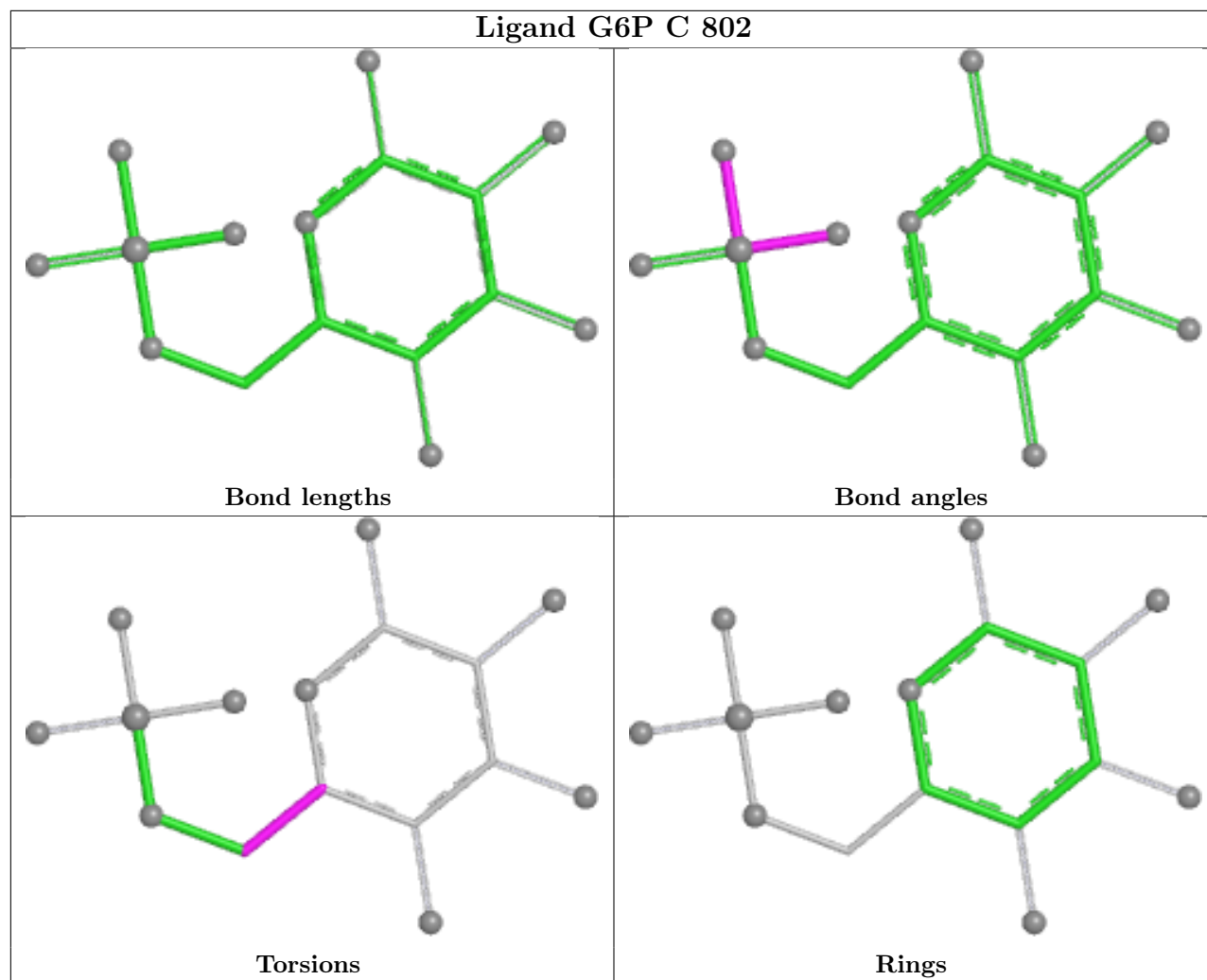




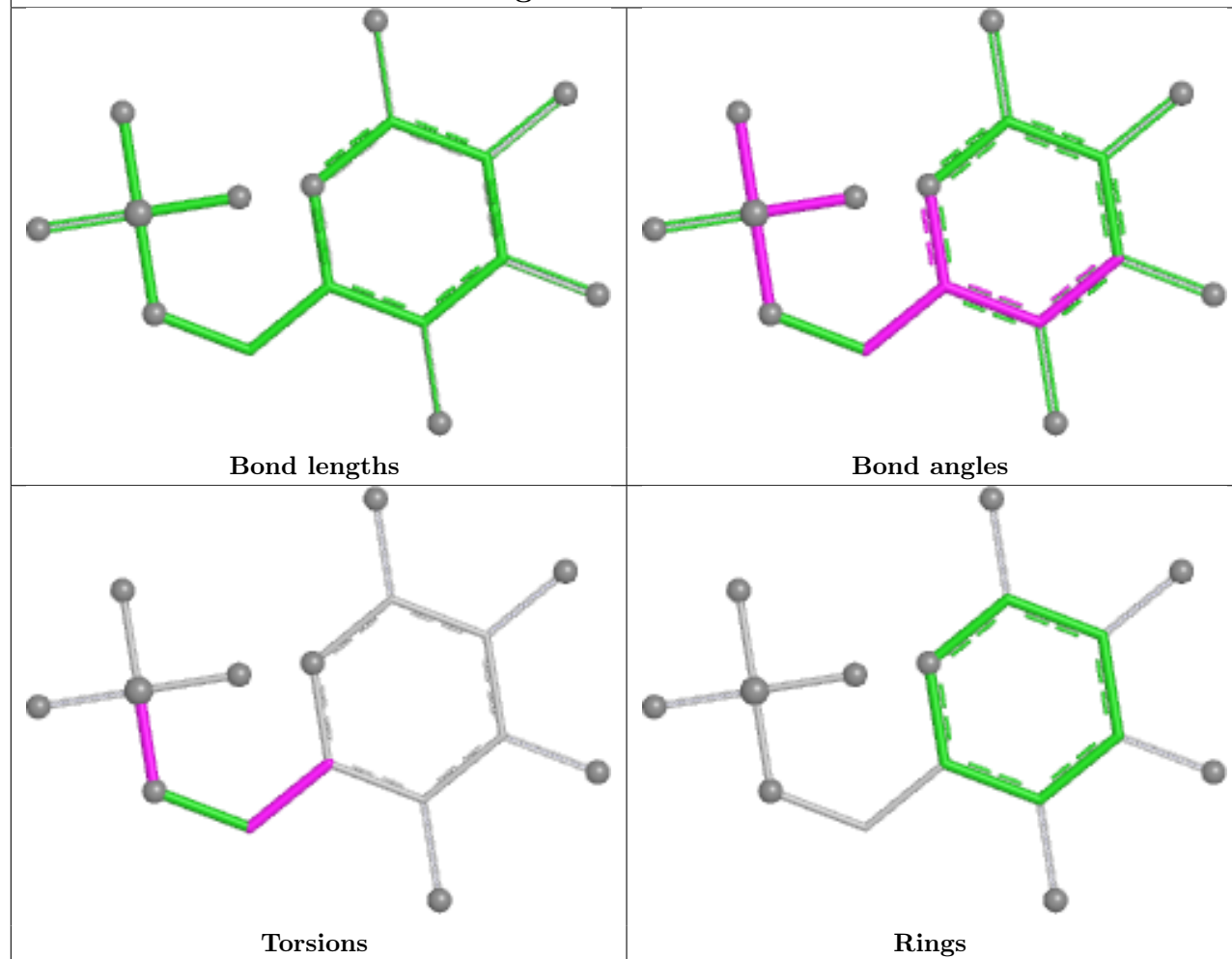
Ligand G6P D 802



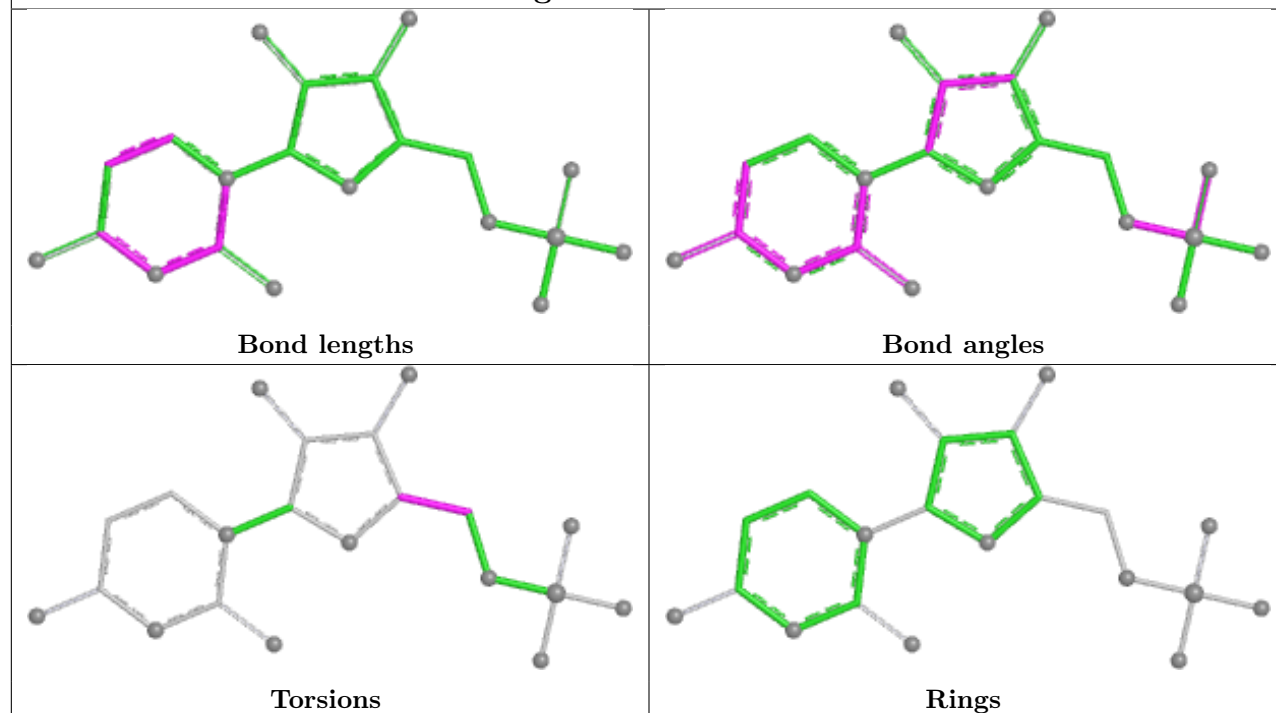
Ligand G6P C 802

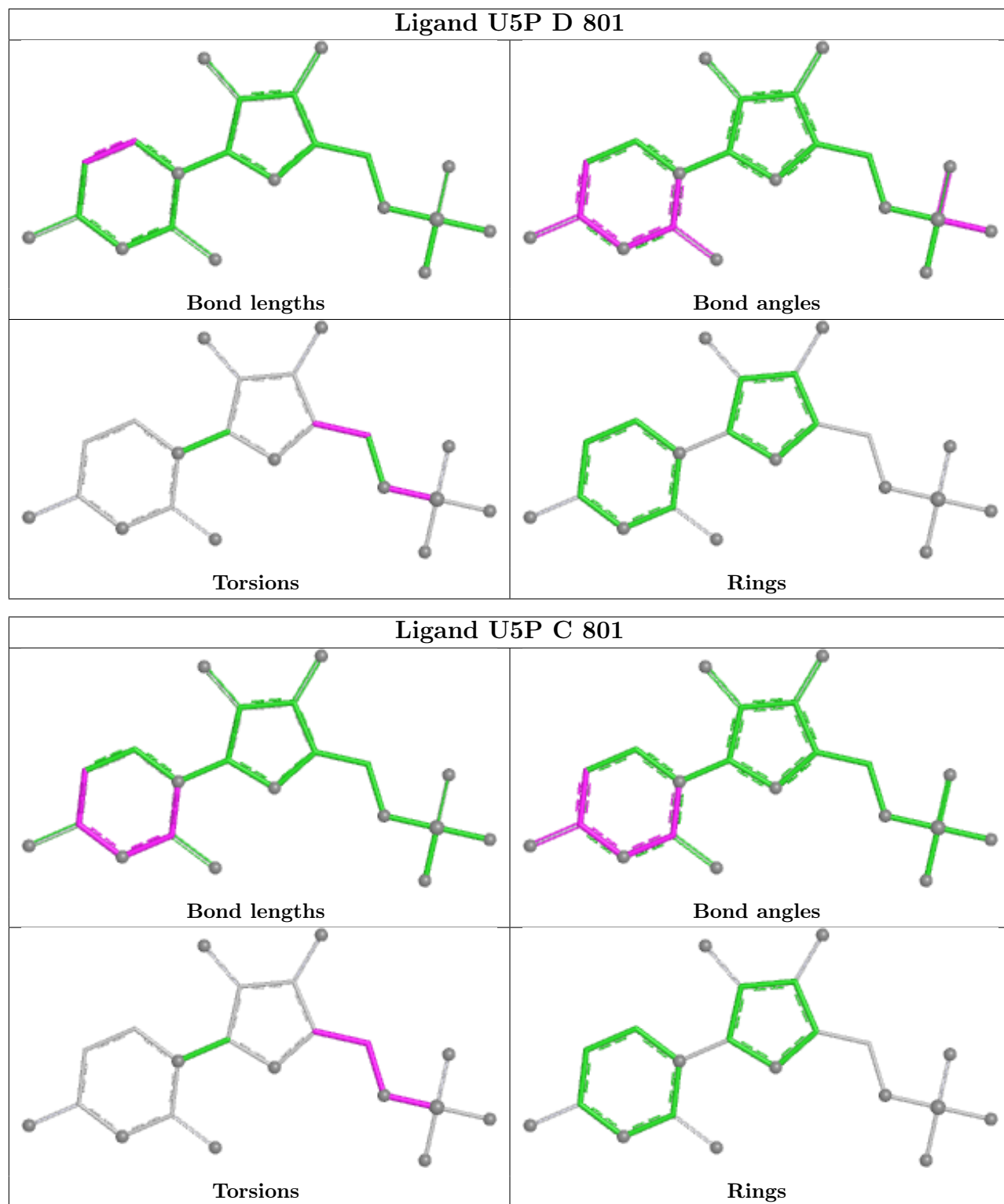


Ligand G6P A 802



Ligand U5P A 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	638/724 (88%)	0.11	18 (2%) 55 48	39, 76, 136, 163	0
1	B	638/724 (88%)	0.05	24 (3%) 44 36	24, 65, 126, 170	0
1	C	638/724 (88%)	0.11	12 (1%) 66 61	30, 74, 122, 182	0
1	D	636/724 (87%)	0.20	20 (3%) 51 43	32, 81, 152, 185	0
All	All	2550/2896 (88%)	0.12	74 (2%) 53 46	24, 73, 139, 185	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	PRO	4.6
1	D	149	TRP	3.7
1	D	60	ILE	3.6
1	D	125	LEU	3.4
1	D	205	GLY	3.4
1	A	129	PRO	3.4
1	D	625	LEU	3.4
1	B	625	LEU	3.3
1	D	66	PRO	3.1
1	D	618	TYR	3.0
1	C	125	LEU	3.0
1	B	135	PHE	2.9
1	A	149	TRP	2.9
1	D	85	SER	2.9
1	B	108	LEU	2.8
1	D	45	LEU	2.8
1	C	279	PHE	2.8
1	B	65	LYS	2.8
1	D	129	PRO	2.7
1	D	21	VAL	2.7
1	A	21	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	637	ALA	2.7
1	D	639	ALA	2.7
1	D	622	PHE	2.6
1	B	630	LEU	2.6
1	D	113	GLY	2.6
1	B	2	SER	2.6
1	A	274	ILE	2.6
1	B	639	ALA	2.6
1	C	159	SER	2.5
1	B	534	GLY	2.5
1	C	207	PHE	2.5
1	B	114	TYR	2.5
1	A	131	PRO	2.5
1	A	125	LEU	2.5
1	A	128	ILE	2.5
1	B	61	LEU	2.4
1	B	155	ALA	2.4
1	D	91	VAL	2.4
1	A	18	ALA	2.4
1	D	135	PHE	2.4
1	A	507	TYR	2.3
1	A	513	TYR	2.3
1	B	543	THR	2.3
1	C	154	VAL	2.3
1	A	108	LEU	2.3
1	C	197	LEU	2.3
1	D	638	LEU	2.3
1	C	128	ILE	2.3
1	B	81	GLN	2.3
1	A	106	PHE	2.2
1	C	543	THR	2.2
1	A	320	ARG	2.2
1	B	77	GLN	2.2
1	D	15	THR	2.2
1	A	123	TRP	2.2
1	A	207	PHE	2.2
1	A	155	ALA	2.2
1	B	79	ALA	2.2
1	B	632	ASP	2.2
1	B	160	GLN	2.1
1	B	635	MET	2.1
1	A	203	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	127	GLY	2.1
1	B	88	VAL	2.1
1	A	61	LEU	2.1
1	C	513	TYR	2.1
1	C	155	ALA	2.0
1	D	153	GLU	2.0
1	B	78	HIS	2.0
1	B	205	GLY	2.0
1	B	154	VAL	2.0
1	B	5	LEU	2.0
1	D	274	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

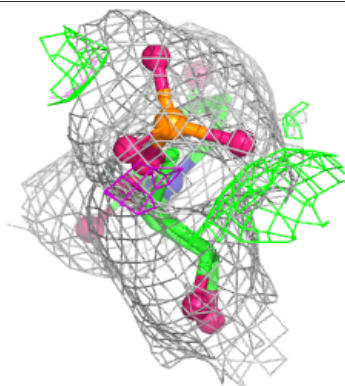
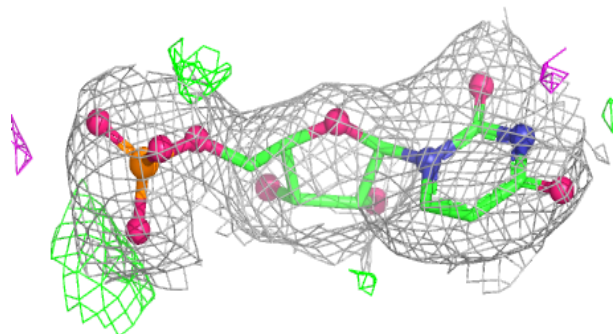
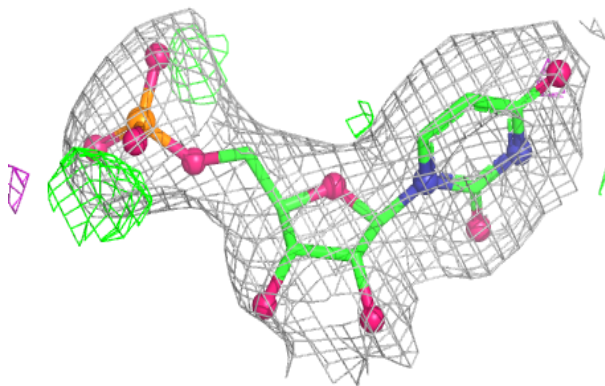
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	U5P	A	801	21/21	0.90	0.10	65,71,91,93	0
2	U5P	B	1002	21/21	0.91	0.10	66,80,86,87	0
4	PEG	B	1004	7/7	0.91	0.17	83,87,92,92	0
4	PEG	D	803	7/7	0.91	0.17	85,88,95,96	0
4	PEG	B	1001	7/7	0.92	0.13	68,69,72,81	0
2	U5P	D	801	21/21	0.93	0.09	66,80,99,105	0
2	U5P	C	801	21/21	0.93	0.10	63,68,91,98	0
4	PEG	C	803	7/7	0.95	0.10	66,67,78,78	0
3	G6P	C	802	16/16	0.96	0.06	51,54,56,61	0
3	G6P	B	1003	16/16	0.97	0.07	37,43,48,49	0
3	G6P	D	802	16/16	0.97	0.06	39,46,50,51	0
3	G6P	A	802	16/16	0.98	0.05	54,59,62,63	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.

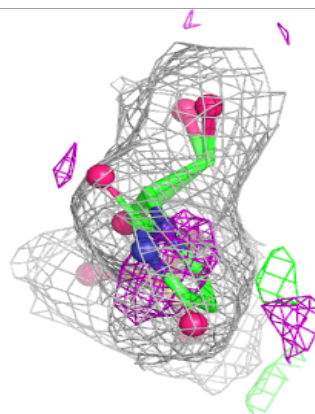
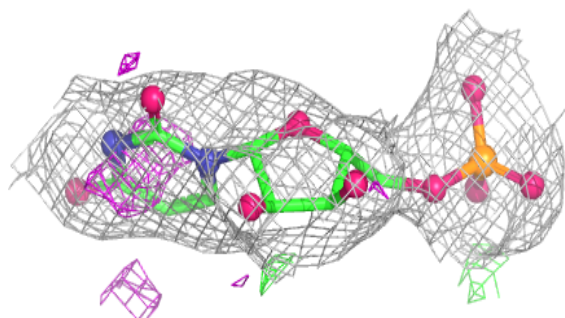
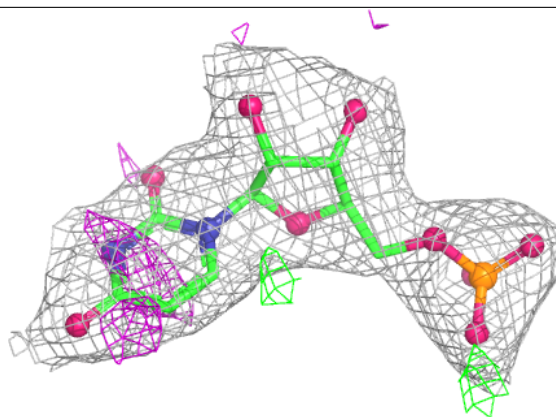
Electron density around U5P A 801:

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

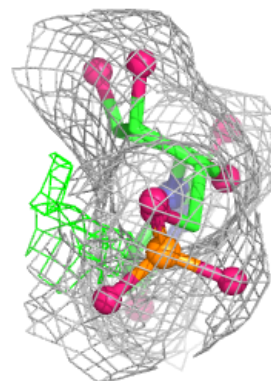
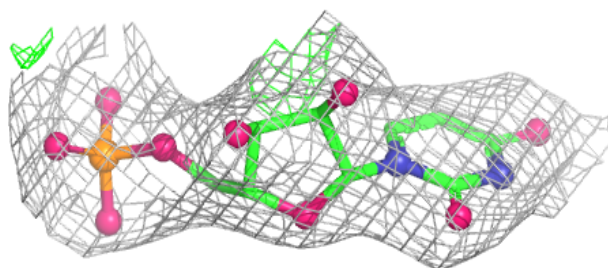
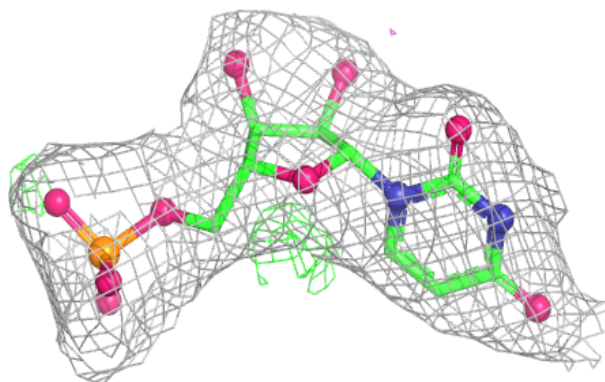


Electron density around U5P B 1002:

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

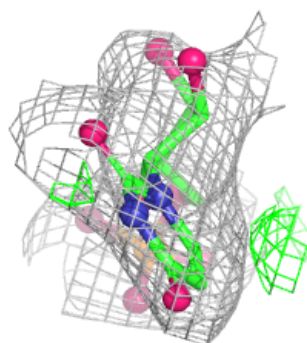
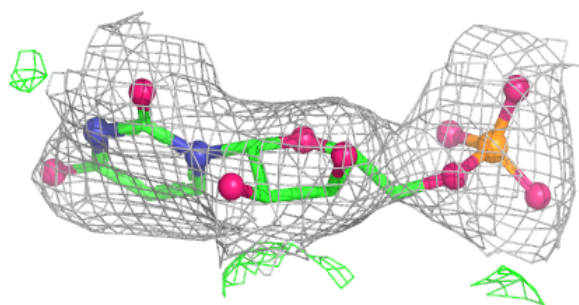
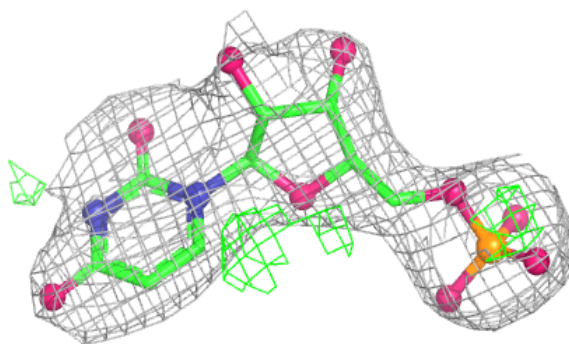
**Electron density around U5P D 801:**

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

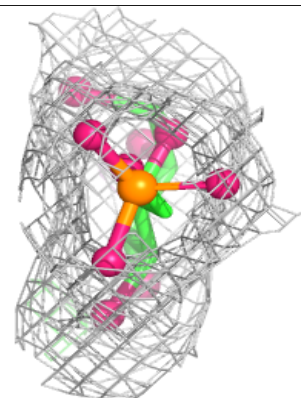
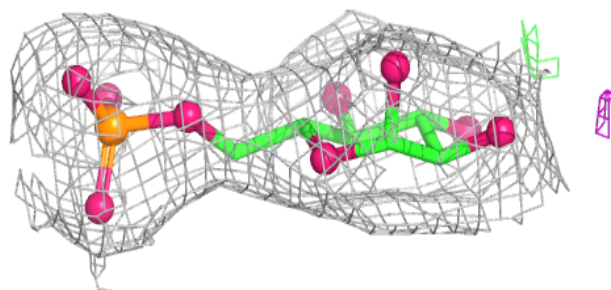
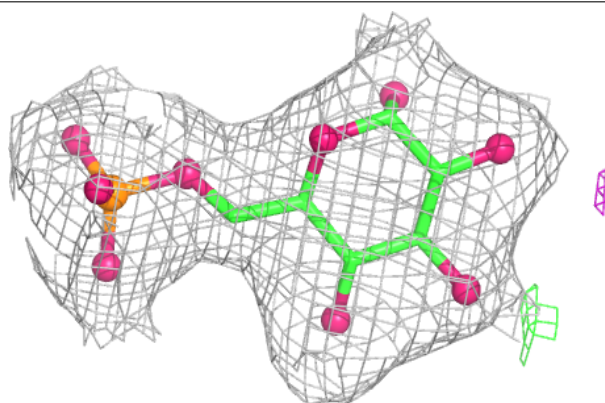


Electron density around U5P C 801:

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

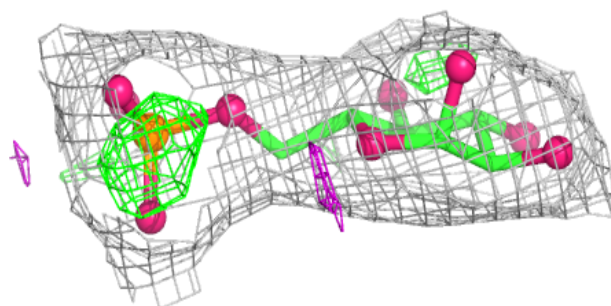
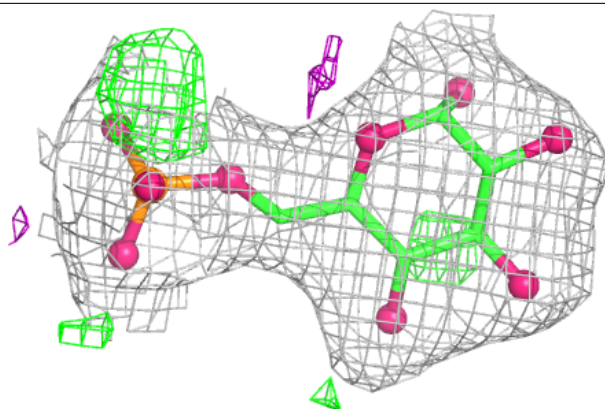
**Electron density around G6P C 802:**

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

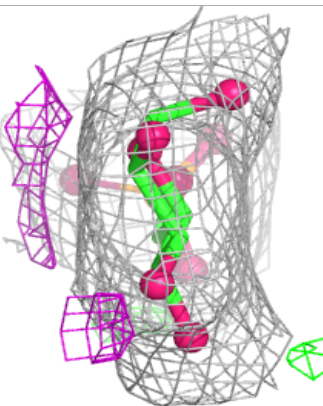
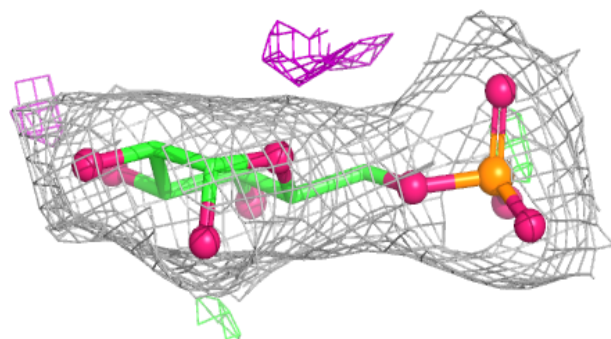
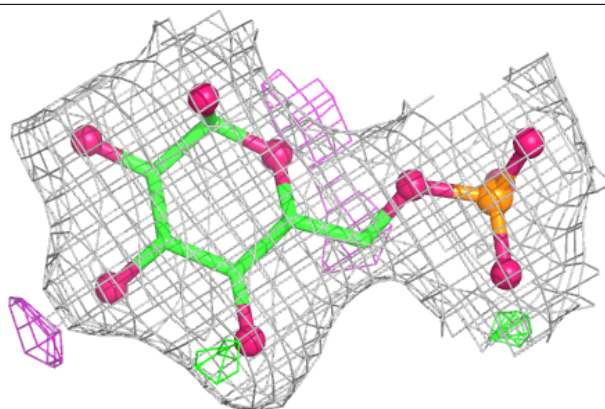


Electron density around G6P B 1003:

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

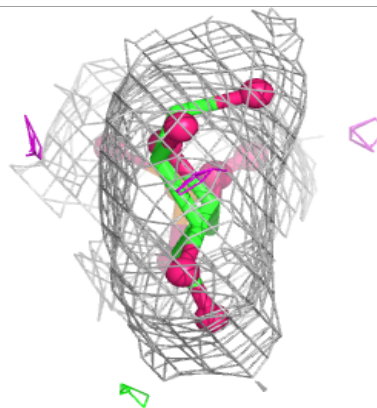
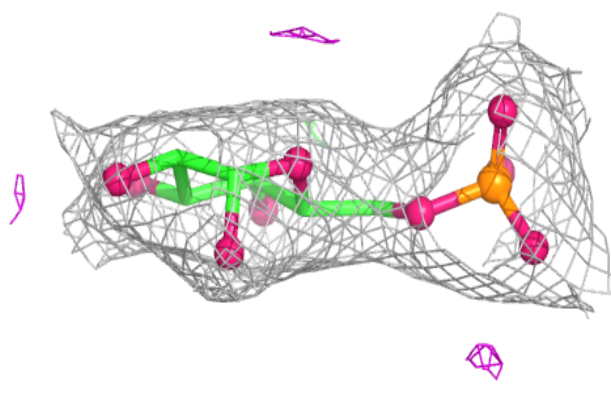
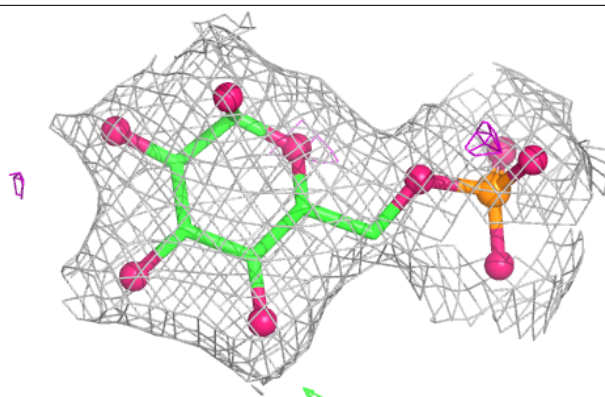
**Electron density around G6P D 802:**

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



Electron density around G6P A 802:

$2mF_o-DF_c$ (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.