



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 6ZJB / pdb_00006zjb
Title : Crystal structure of human adenylate kinase 3, AK3, in complex with inhibitor Gp5A
Authors : Grundstrom, C.; Rogne, P.; Wolf-Watz, M.; Sauer-Eriksson, A.E.
Deposited on : 2020-06-28
Resolution : 1.82 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

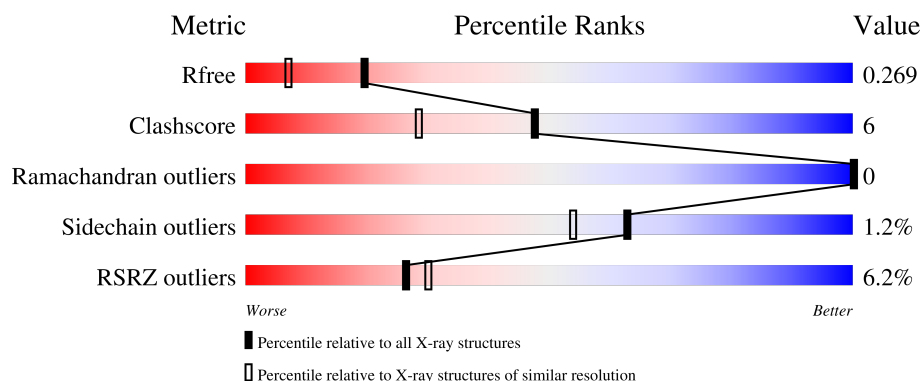
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	227	5% 82% 11% • •
1	B	227	7% 81% 14% •
1	C	227	13% 77% 18% 5%
1	D	227	3% 85% 10% •
1	E	227	3% 82% 11% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	

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	G5P	C	301	X	-	-	-

2 Entry composition [i](#)

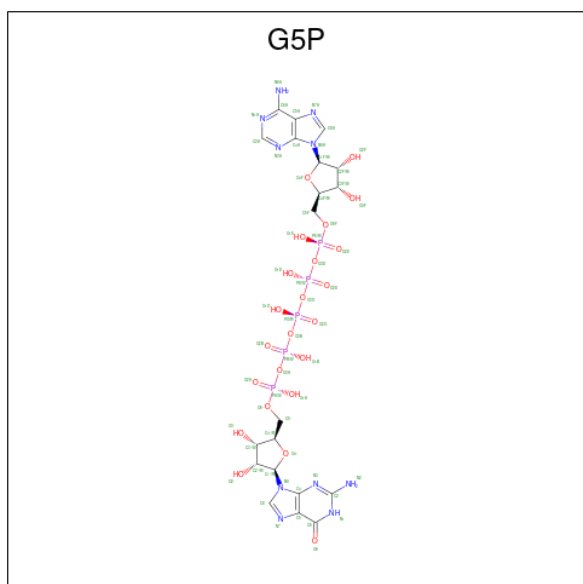
There are 4 unique types of molecules in this entry. The entry contains 11581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GTP:AMP phosphotransferase AK3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1736	1110	302	321	3			
1	B	217	Total	C	N	O	S	0	0	0
			1736	1110	302	321	3			
1	C	216	Total	C	N	O	S	0	0	0
			1730	1107	301	319	3			
1	D	218	Total	C	N	O	S	0	1	0
			1750	1118	305	324	3			
1	E	216	Total	C	N	O	S	0	1	0
			1738	1113	302	320	3			
1	F	216	Total	C	N	O	S	0	1	0
			1739	1112	303	321	3			

- Molecule 2 is P1-(5'-ADENOSYL)-P5-(5'-GUANOSYL) PENTAPHOSPHATE (CCD ID: G5P) (formula: $C_{20}H_{29}N_{10}O_{23}P_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			58	20	10	23	5		
2	B	1	Total	C	N	O	P	0	0
			58	20	10	23	5		
2	C	1	Total	C	N	O	P	0	0
			58	20	10	23	5		
2	D	1	Total	C	N	O	P	0	0
			58	20	10	23	5		
2	E	1	Total	C	N	O	P	0	0
			58	20	10	23	5		
2	F	1	Total	C	N	O	P	0	0
			58	20	10	23	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

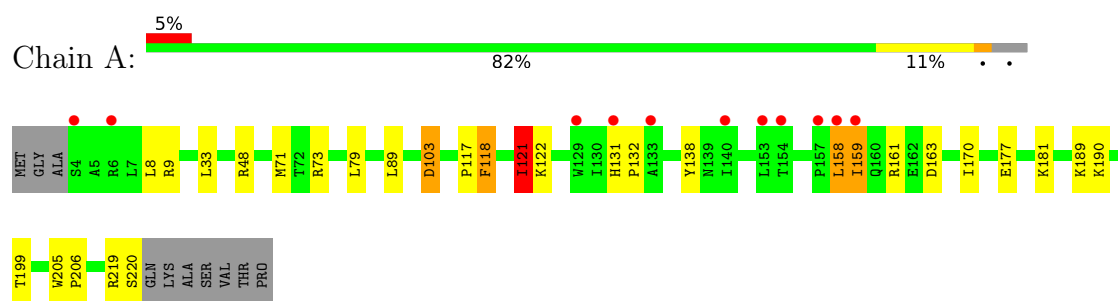
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	4
			130	130		
4	B	126	Total	O	0	3
			128	128		
4	C	66	Total	O	0	2
			68	68		
4	D	152	Total	O	0	6
			158	158		
4	E	148	Total	O	0	6
			154	154		
4	F	155	Total	O	0	6
			160	160		

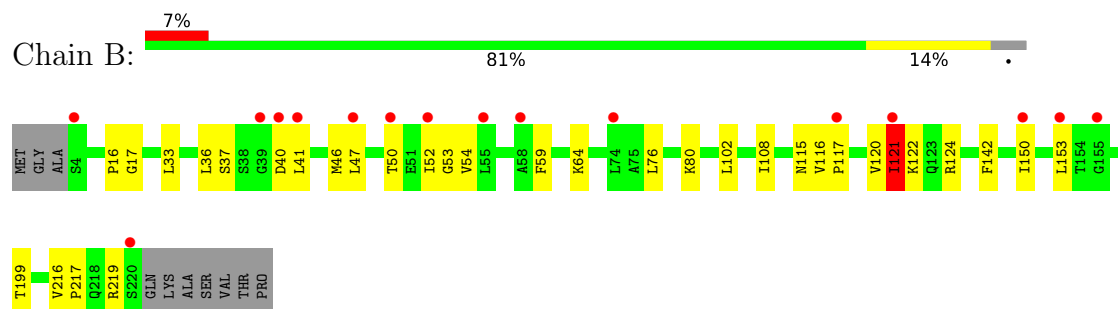
3 Residue-property plots [i](#)

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.

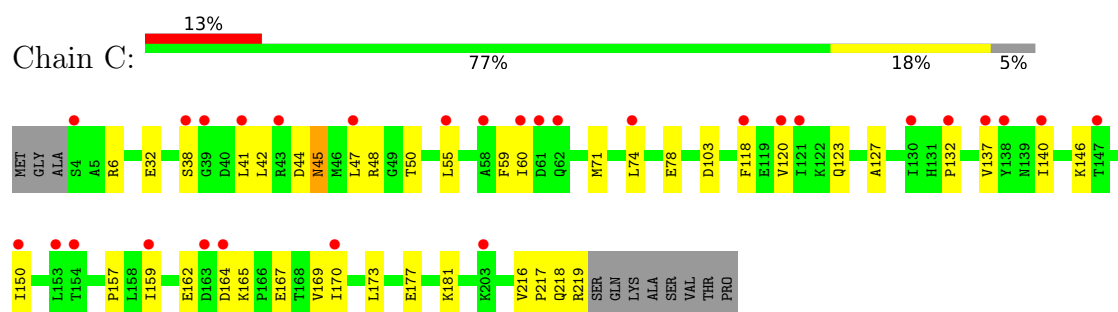
- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial



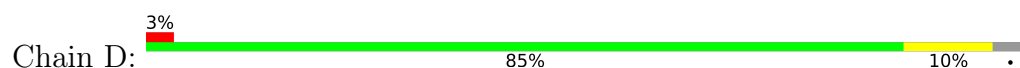
- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial



- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial

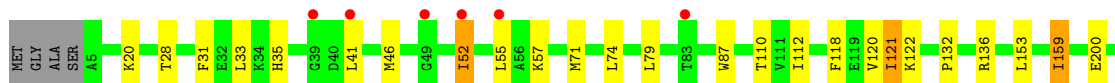
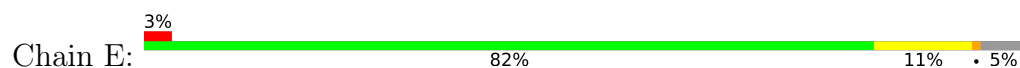


- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial

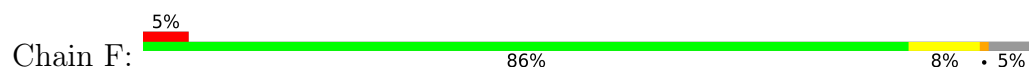




- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial



- Molecule 1: GTP:AMP phosphotransferase AK3, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.47Å 66.76Å 105.91Å 93.79° 93.95° 89.71°	Depositor
Resolution (Å)	45.36 – 1.82 45.36 – 1.82	Depositor EDS
% Data completeness (in resolution range)	93.0 (45.36-1.82) 93.0 (45.36-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.82Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.192 , 0.257 (Not available) , 0.269	Depositor DCC
R_{free} test set	5308 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.388	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11581	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1168e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: G5P, MG

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	0.65	2/1773 (0.1%)	0.76	2/2405 (0.1%)
1	B	0.81	5/1773 (0.3%)	0.80	4/2405 (0.2%)
1	C	0.62	0/1767	0.76	0/2397
1	D	0.78	4/1787 (0.2%)	0.73	0/2424
1	E	0.74	3/1775 (0.2%)	0.78	0/2408
1	F	0.77	1/1776 (0.1%)	0.92	5/2409 (0.2%)
All	All	0.73	15/10651 (0.1%)	0.79	11/14448 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	119	GLU	C-O	-7.18	1.15	1.24
1	A	118	PHE	C-O	-6.73	1.16	1.24
1	D	159	ILE	C-O	-6.54	1.15	1.23
1	D	121	ILE	C-O	-6.45	1.16	1.24
1	B	122	LYS	C-O	-6.34	1.16	1.24
1	E	120	VAL	C-O	-6.29	1.17	1.24
1	F	159	ILE	C-O	-6.28	1.15	1.23
1	B	150	ILE	C-O	-6.14	1.18	1.24
1	A	121	ILE	C-O	-5.57	1.17	1.24
1	E	159	ILE	C-O	-5.52	1.17	1.23
1	E	122	LYS	C-O	-5.43	1.17	1.24
1	B	120	VAL	C-O	-5.41	1.17	1.24
1	B	17	GLY	C-O	-5.36	1.16	1.24
1	D	120	VAL	C-O	-5.10	1.18	1.24
1	B	16	PRO	C-O	-5.06	1.16	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	ASP	N-CA-C	10.53	122.51	111.14
1	B	153	LEU	N-CA-C	8.56	120.39	111.14
1	F	219	ARG	N-CA-C	8.03	120.03	111.28
1	F	183	VAL	CA-C-N	-7.29	110.51	120.28
1	F	183	VAL	C-N-CA	-7.29	110.51	120.28
1	B	124	ARG	N-CA-C	6.09	117.59	111.07
1	F	180	THR	N-CA-C	6.07	117.97	111.36
1	A	131	HIS	N-CA-C	-5.55	100.61	109.04
1	A	158	LEU	N-CA-C	-5.46	102.41	110.48
1	B	219	ARG	N-CA-C	5.27	118.32	110.52
1	B	121	ILE	N-CA-CB	5.09	117.46	110.54

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	1736	0	1770	20	0
1	B	1736	0	1770	17	0
1	C	1730	0	1765	33	0
1	D	1750	0	1782	14	0
1	E	1738	0	1775	20	0
1	F	1739	0	1772	19	0
2	A	58	0	21	2	0
2	B	58	0	22	1	0
2	C	58	0	22	2	0
2	D	58	0	21	0	0
2	E	58	0	21	1	0
2	F	58	0	22	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	130	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	128	0	0	0	0
4	C	68	0	0	0	0
4	D	158	0	0	0	0
4	E	154	0	0	0	0
4	F	160	0	0	0	0
All	All	11581	0	10763	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (121) 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:C:44:ASP:HA	1:C:47:LEU:HD12	1.50	0.93
1:C:55:LEU:HG	1:C:59:PHE:HE1	1.44	0.82
1:D:33:LEU:HD12	1:D:33:LEU:C	2.13	0.72
1:E:132:PRO:HG3	1:E:159:ILE:HG12	1.76	0.68
1:C:55:LEU:HG	1:C:59:PHE:CE1	2.29	0.67
1:E:136:ARG:NH2	1:E:153:LEU:HD23	2.10	0.66
1:C:32:GLU:HG3	1:C:219:ARG:HA	1.80	0.64
1:C:42:LEU:HD21	1:C:71:MET:SD	2.38	0.63
1:E:41[B]:LEU:CD2	1:E:74:LEU:HD21	2.29	0.63
1:C:41:LEU:HD21	1:C:78:GLU:HG3	1.79	0.62
1:B:33:LEU:C	1:B:33:LEU:HD12	2.25	0.62
1:B:50:THR:HG23	1:B:53:GLY:H	1.64	0.62
1:B:37:SER:OG	1:B:40:ASP:CG	2.45	0.60
1:A:132:PRO:HG3	1:A:159:ILE:HG12	1.84	0.60
1:F:216:VAL:CG2	1:F:217:PRO:HD2	2.32	0.60
1:D:127:ALA:HB1	1:D:140:ILE:HG12	1.85	0.59
1:B:121:ILE:C	1:B:121:ILE:HD12	2.28	0.59
1:D:33:LEU:HD12	1:D:33:LEU:O	2.01	0.59
1:A:118:PHE:HA	1:A:121:ILE:HD13	1.85	0.58
1:C:55:LEU:O	1:C:59:PHE:HD1	1.87	0.58
1:E:41[B]:LEU:HD22	1:E:74:LEU:HD21	1.86	0.58
1:F:33:LEU:C	1:F:33:LEU:HD12	2.29	0.57
1:F:179:GLN:O	1:F:182:PRO:HD2	2.05	0.57
1:F:121:ILE:C	1:F:121:ILE:HD12	2.30	0.56
1:A:118:PHE:HA	1:A:121:ILE:CD1	2.35	0.56
1:C:132:PRO:HG3	1:C:159:ILE:HD13	1.87	0.56
1:C:118:PHE:CD2	1:C:173:LEU:HD22	2.41	0.56
1:F:52:ILE:HA	1:F:55:LEU:CD2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ASN:ND2	1:C:74:LEU:HD21	2.21	0.55
1:B:52:ILE:HD12	1:B:52:ILE:H	1.71	0.54
1:A:103:ASP:OD2	1:A:190:LYS:NZ	2.38	0.54
1:A:177:GLU:HA	1:A:181:LYS:HG3	1.90	0.54
1:B:36:LEU:HD11	1:B:41:LEU:HD11	1.89	0.54
1:D:50:THR:HG22	1:D:52:ILE:H	1.73	0.54
1:A:8:LEU:HG	1:A:9:ARG:N	2.24	0.53
1:E:136:ARG:HH22	1:E:153:LEU:HD23	1.73	0.53
1:C:42:LEU:HD13	1:C:60:ILE:HD11	1.89	0.52
1:E:46:MET:HE3	1:E:57:LYS:HG3	1.91	0.52
1:C:55:LEU:O	1:C:59:PHE:CD1	2.62	0.52
1:F:52:ILE:HA	1:F:55:LEU:HG	1.91	0.51
1:A:73:ARG:HB2	1:C:6:ARG:HD3	1.93	0.51
1:C:164:ASP:O	1:C:165:LYS:C	2.54	0.51
1:F:216:VAL:HG23	1:F:217:PRO:HD2	1.92	0.51
1:C:41:LEU:HD11	1:C:78:GLU:HG3	1.91	0.51
1:D:32:GLU:HG3	1:D:217:PRO:HB2	1.93	0.50
1:B:33:LEU:HD12	1:B:33:LEU:O	2.12	0.50
1:A:189:LYS:N	1:A:189:LYS:HD3	2.25	0.50
1:A:71:MET:HG3	2:A:301:G5P:N1A	2.26	0.50
1:C:48:ARG:HG2	1:C:48:ARG:HH11	1.76	0.49
1:A:122:LYS:HE2	1:A:170:ILE:CD1	2.42	0.49
1:D:4:SER:OG	1:D:6:ARG:O	2.29	0.49
1:E:118:PHE:HA	1:E:121:ILE:HD13	1.95	0.49
1:B:50:THR:O	1:B:54:VAL:HG23	2.11	0.49
1:B:117:PRO:HG2	1:B:199:THR:HG22	1.93	0.49
1:A:122:LYS:HE2	1:A:170:ILE:HD13	1.95	0.49
1:B:116:VAL:HG13	1:B:117:PRO:HD2	1.93	0.49
1:A:161:ARG:HB3	1:A:163:ASP:OD1	2.13	0.49
1:C:55:LEU:CG	1:C:59:PHE:HE1	2.20	0.49
1:C:38:SER:OG	2:C:301:G5P:O2E	2.31	0.48
1:A:117:PRO:HG2	1:A:199:THR:HG22	1.94	0.48
1:C:132:PRO:HG3	1:C:159:ILE:CD1	2.42	0.48
1:E:79:LEU:HD22	1:E:87:TRP:CE2	2.49	0.48
1:C:137:VAL:HG11	2:C:301:G5P:H7	1.94	0.48
1:F:52:ILE:O	1:F:55:LEU:HG	2.13	0.48
1:C:48:ARG:HG2	1:C:48:ARG:NH1	2.28	0.48
1:C:162:GLU:HA	1:C:162:GLU:OE1	2.12	0.48
1:D:51:GLU:HA	1:D:54:VAL:HG23	1.96	0.48
1:F:32:GLU:HG2	1:F:219:ARG:HA	1.96	0.48
1:B:46:MET:C	1:B:47:LEU:HD23	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PRO:HG3	1:D:159:ILE:HG12	1.96	0.47
1:C:216:VAL:HG22	1:C:217:PRO:HD2	1.97	0.47
1:F:177:GLU:O	1:F:181:LYS:HB2	2.15	0.47
1:E:33:LEU:C	1:E:33:LEU:HD12	2.40	0.47
1:E:110:THR:HG21	1:E:211:PHE:HE2	1.79	0.47
1:C:48:ARG:HD3	1:C:50:THR:HG23	1.97	0.46
1:A:138:TYR:CE2	1:A:158:LEU:HD21	2.50	0.46
1:A:219:ARG:O	1:A:220:SER:C	2.58	0.46
1:F:71:MET:HG3	2:F:301:G5P:N1A	2.31	0.46
1:E:118:PHE:HA	1:E:121:ILE:CD1	2.46	0.46
1:D:79:LEU:HD22	1:D:87:TRP:CE2	2.50	0.46
1:F:32:GLU:HB2	1:F:217:PRO:HG2	1.97	0.45
1:D:33:LEU:C	1:D:33:LEU:CD1	2.87	0.45
1:E:31:PHE:CE1	1:E:218:GLN:HG2	2.52	0.45
1:C:177:GLU:HA	1:C:181:LYS:HD3	1.98	0.44
1:D:216:VAL:HG22	1:D:217:PRO:HD2	1.98	0.44
1:A:48:ARG:HA	1:B:115:ASN:ND2	2.33	0.44
1:C:74:LEU:HD12	1:C:74:LEU:O	2.17	0.44
1:F:132:PRO:HG3	1:F:159:ILE:HG12	1.98	0.44
1:A:205:TRP:N	1:A:206:PRO:CD	2.81	0.44
1:B:59:PHE:CE2	1:B:64:LYS:HD3	2.52	0.44
1:E:112:ILE:HD11	1:E:212:LEU:HD21	1.98	0.44
1:F:52:ILE:HA	1:F:55:LEU:CG	2.48	0.43
1:F:46:MET:SD	1:F:57:LYS:HB2	2.58	0.43
1:B:102:LEU:HD21	1:B:108:ILE:HD11	2.00	0.43
1:C:127:ALA:HB1	1:C:140:ILE:HG12	2.00	0.43
1:F:55:LEU:HD12	1:F:56:ALA:N	2.34	0.43
1:C:150:ILE:HD13	1:C:157:PRO:HA	2.00	0.43
1:D:11:VAL:HB	1:D:111:VAL:HG22	2.00	0.43
1:C:41:LEU:HD21	1:C:78:GLU:CG	2.47	0.43
1:E:46:MET:CE	1:E:57:LYS:HG3	2.49	0.43
1:E:52:ILE:HD12	1:E:52:ILE:HA	1.67	0.42
1:D:118:PHE:HA	1:D:121:ILE:CD1	2.49	0.42
1:A:79:LEU:HD11	1:A:89:LEU:HD11	2.00	0.42
1:F:55:LEU:HD12	1:F:55:LEU:C	2.44	0.42
1:C:120:VAL:O	1:C:123:GLN:HB3	2.20	0.42
1:B:216:VAL:HG22	1:B:217:PRO:HD2	2.01	0.42
1:C:165:LYS:O	1:C:169:VAL:HG23	2.19	0.42
1:C:167:GLU:O	1:C:170:ILE:HG12	2.19	0.42
1:E:110:THR:HG21	1:E:211:PHE:CE2	2.55	0.42
1:B:76:LEU:O	1:B:80:LYS:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLN:O	1:C:219:ARG:C	2.62	0.41
1:E:28:THR:OG1	1:E:35:HIS:HB2	2.19	0.41
1:A:71:MET:HG3	2:A:301:G5P:C2A	2.50	0.41
1:E:71:MET:HG3	2:E:301:G5P:N1A	2.35	0.41
1:E:55:LEU:HA	1:E:55:LEU:HD23	1.86	0.41
1:A:33:LEU:C	1:A:33:LEU:HD12	2.45	0.41
1:D:52:ILE:HD11	1:D:70:VAL:HG13	2.03	0.41
1:F:179:GLN:C	1:F:182:PRO:HD2	2.46	0.41
1:F:216:VAL:HG22	1:F:217:PRO:HD2	2.03	0.40
1:E:200:GLU:CD	1:E:203:LYS:HD2	2.47	0.40
1:B:142:PHE:HB2	2:B:301:G5P:C2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/227 (95%)	214 (100%)	1 (0%)	0	100	100
1	B	215/227 (95%)	213 (99%)	2 (1%)	0	100	100
1	C	214/227 (94%)	211 (99%)	3 (1%)	0	100	100
1	D	217/227 (96%)	215 (99%)	2 (1%)	0	100	100
1	E	215/227 (95%)	215 (100%)	0	0	100	100
1	F	215/227 (95%)	211 (98%)	4 (2%)	0	100	100
All	All	1291/1362 (95%)	1279 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	190/197 (96%)	187 (98%)	3 (2%)	55	44
1	B	190/197 (96%)	189 (100%)	1 (0%)	81	77
1	C	189/197 (96%)	186 (98%)	3 (2%)	55	44
1	D	191/197 (97%)	188 (98%)	3 (2%)	55	44
1	E	190/197 (96%)	187 (98%)	3 (2%)	55	44
1	F	190/197 (96%)	189 (100%)	1 (0%)	81	77
All	All	1140/1182 (96%)	1126 (99%)	14 (1%)	63	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	121	ILE
1	A	159	ILE
1	B	121	ILE
1	C	45	ASN
1	C	103	ASP
1	C	146	LYS
1	D	103	ASP
1	D	121	ILE
1	D	219	ARG
1	E	20	LYS
1	E	52	ILE
1	E	121	ILE
1	F	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	143	ASN
1	B	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	113	ASN
1	B	115	ASN
1	B	143	ASN
1	B	179	GLN
1	C	30	HIS
1	C	113	ASN
1	C	115	ASN
1	C	123	GLN
1	C	143	ASN
1	D	30	HIS
1	D	113	ASN
1	E	113	ASN
1	F	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	G5P	A	301	3	63,63,63	1.86	15 (23%)	91,100,100	2.35	35 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G5P	C	301	3	63,63,63	1.92	16 (25%)	91,100,100	2.59	27 (29%)
2	G5P	E	301	3	63,63,63	1.88	13 (20%)	91,100,100	2.31	24 (26%)
2	G5P	B	301	3	63,63,63	1.80	15 (23%)	91,100,100	2.26	29 (31%)
2	G5P	F	301	3	63,63,63	1.95	16 (25%)	91,100,100	2.16	34 (37%)
2	G5P	D	301	3	63,63,63	1.78	13 (20%)	91,100,100	2.22	33 (36%)

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	G5P	A	301	3	-	5/44/76/76	0/6/6/6
2	G5P	C	301	3	1/1/13/13	9/44/76/76	0/6/6/6
2	G5P	E	301	3	-	4/44/76/76	0/6/6/6
2	G5P	B	301	3	-	4/44/76/76	0/6/6/6
2	G5P	F	301	3	-	8/44/76/76	0/6/6/6
2	G5P	D	301	3	-	7/44/76/76	0/6/6/6

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	G5P	C2'-C1'	-5.83	1.35	1.53
2	E	301	G5P	C2F-C1F	-5.74	1.35	1.53
2	C	301	G5P	C2F-C1F	-5.61	1.35	1.53
2	B	301	G5P	C2F-C1F	-5.46	1.36	1.53
2	F	301	G5P	C2'-C1'	-5.35	1.36	1.53
2	A	301	G5P	C4-N3	5.32	1.46	1.34
2	A	301	G5P	C2F-C1F	-5.32	1.36	1.53
2	D	301	G5P	C2'-C1'	-5.32	1.36	1.53
2	B	301	G5P	C2'-C1'	-5.28	1.36	1.53
2	D	301	G5P	C2F-C1F	-5.26	1.36	1.53
2	F	301	G5P	C4-N3	5.25	1.46	1.34
2	F	301	G5P	C2F-C1F	-5.25	1.37	1.53
2	A	301	G5P	C2'-C1'	-5.13	1.37	1.53
2	C	301	G5P	C4-N3	5.07	1.45	1.34
2	B	301	G5P	C4-N3	4.96	1.45	1.34
2	E	301	G5P	C4-N3	4.92	1.45	1.34
2	D	301	G5P	C4-N3	4.67	1.44	1.34
2	C	301	G5P	C2'-C1'	-4.33	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	G5P	O2'-C2'	-4.25	1.32	1.43
2	E	301	G5P	O2'-C2'	-4.09	1.32	1.43
2	C	301	G5P	O3'-C3'	-3.85	1.33	1.43
2	F	301	G5P	PB-O3B	3.72	1.63	1.59
2	B	301	G5P	O2'-C2'	-3.71	1.33	1.43
2	D	301	G5P	C6-N1	3.66	1.45	1.38
2	C	301	G5P	PG-O3G	3.56	1.63	1.59
2	C	301	G5P	C6-N1	3.51	1.45	1.38
2	F	301	G5P	PD-O3D	-3.49	1.55	1.59
2	E	301	G5P	O3'-C3'	-3.45	1.34	1.43
2	E	301	G5P	C6-N1	3.44	1.45	1.38
2	F	301	G5P	O2'-C2'	-3.44	1.34	1.43
2	C	301	G5P	PD-O3G	3.31	1.63	1.59
2	A	301	G5P	O3'-C3'	-3.31	1.34	1.43
2	D	301	G5P	O2'-C2'	-3.28	1.34	1.43
2	A	301	G5P	C6-N1	3.18	1.44	1.38
2	A	301	G5P	O2'-C2'	-3.16	1.35	1.43
2	C	301	G5P	C2-N2	3.16	1.41	1.34
2	F	301	G5P	C6-N1	3.07	1.44	1.38
2	D	301	G5P	O3'-C3'	-3.03	1.35	1.43
2	B	301	G5P	C3'-C4'	3.02	1.60	1.53
2	C	301	G5P	C2-N3	2.92	1.40	1.33
2	E	301	G5P	C8A-N9A	-2.88	1.32	1.37
2	A	301	G5P	PE-O3D	-2.83	1.56	1.59
2	E	301	G5P	C2-N3	2.81	1.40	1.33
2	A	301	G5P	C2-N3	2.81	1.40	1.33
2	E	301	G5P	C5-C6	-2.80	1.34	1.44
2	A	301	G5P	C2-N2	2.78	1.40	1.34
2	B	301	G5P	C5-C6	-2.78	1.34	1.44
2	B	301	G5P	C6-N1	2.76	1.44	1.38
2	C	301	G5P	C8A-N9A	-2.67	1.33	1.37
2	E	301	G5P	C2-N2	2.66	1.40	1.34
2	D	301	G5P	PB-O3B	2.65	1.62	1.59
2	D	301	G5P	C3'-C4'	2.63	1.59	1.53
2	F	301	G5P	C4A-N3A	2.63	1.39	1.34
2	D	301	G5P	C2-N3	2.57	1.39	1.33
2	F	301	G5P	C4-N9	-2.55	1.31	1.38
2	D	301	G5P	C8A-N9A	-2.55	1.33	1.37
2	E	301	G5P	C3'-C4'	2.55	1.59	1.53
2	F	301	G5P	C5-C6	-2.53	1.35	1.44
2	F	301	G5P	C3'-C4'	2.48	1.59	1.53
2	B	301	G5P	C4-N9	-2.46	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	G5P	PB-O3B	2.43	1.62	1.59
2	C	301	G5P	C5-C6	-2.39	1.35	1.44
2	A	301	G5P	C5-C6	-2.38	1.35	1.44
2	E	301	G5P	C5-N7	-2.38	1.34	1.39
2	B	301	G5P	PD-O3D	-2.38	1.56	1.59
2	B	301	G5P	C8A-N9A	-2.38	1.33	1.37
2	C	301	G5P	C3'-C4'	2.35	1.58	1.53
2	B	301	G5P	C2-N2	2.28	1.39	1.34
2	E	301	G5P	C4-N9	-2.25	1.32	1.38
2	F	301	G5P	C4A-N9A	-2.24	1.33	1.37
2	C	301	G5P	C5-N7	-2.24	1.34	1.39
2	F	301	G5P	O3'-C3'	-2.24	1.37	1.43
2	B	301	G5P	C5-N7	-2.22	1.34	1.39
2	A	301	G5P	C8A-N9A	-2.22	1.33	1.37
2	D	301	G5P	C2-N2	2.20	1.39	1.34
2	D	301	G5P	C5-C6	-2.17	1.36	1.44
2	A	301	G5P	O5F-C5F	-2.15	1.36	1.44
2	B	301	G5P	PA-O3A	-2.13	1.57	1.59
2	F	301	G5P	C5'-C4'	2.12	1.57	1.51
2	D	301	G5P	PG-O3G	-2.10	1.57	1.59
2	A	301	G5P	PB-O1B	-2.08	1.45	1.55
2	B	301	G5P	C2-N3	2.08	1.38	1.33
2	A	301	G5P	PB-O3B	2.07	1.61	1.59
2	F	301	G5P	PA-O2A	2.07	1.58	1.50
2	C	301	G5P	C4A-N3A	2.05	1.38	1.34
2	A	301	G5P	C4A-N9A	-2.04	1.33	1.37
2	F	301	G5P	C2-N3	2.01	1.38	1.33
2	B	301	G5P	O3'-C3'	-2.01	1.38	1.43

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	G5P	O4F-C1F-N9A	10.96	129.14	108.09
2	C	301	G5P	C2'-C3'-C4'	-8.48	86.23	102.61
2	C	301	G5P	O4F-C1F-N9A	8.15	123.74	108.09
2	B	301	G5P	O4F-C1F-N9A	7.94	123.34	108.09
2	E	301	G5P	C2F-C1F-N9A	-7.55	94.54	113.30
2	A	301	G5P	O1D-PD-O3D	7.45	127.41	107.27
2	B	301	G5P	C5A-C4A-N3A	-7.39	116.55	126.72
2	D	301	G5P	O4F-C1F-N9A	7.33	122.16	108.09
2	E	301	G5P	C5A-C4A-N3A	-6.70	117.49	126.72
2	C	301	G5P	C5A-C4A-N3A	-6.63	117.59	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	G5P	C4'-O4'-C1'	-6.31	95.54	109.47
2	A	301	G5P	O4F-C1F-N9A	5.91	119.43	108.09
2	C	301	G5P	O5'-C5'-C4'	-5.75	89.42	108.99
2	D	301	G5P	C5A-C4A-N3A	-5.68	118.90	126.72
2	A	301	G5P	O3D-PD-O2D	-5.59	93.89	110.70
2	F	301	G5P	C5A-C4A-N3A	-5.56	119.06	126.72
2	C	301	G5P	C2F-C1F-N9A	-5.52	99.58	113.30
2	F	301	G5P	O4F-C1F-N9A	5.44	118.54	108.09
2	A	301	G5P	C5A-C4A-N3A	-5.08	119.72	126.72
2	B	301	G5P	C4A-C5A-N7A	-5.00	104.86	110.58
2	A	301	G5P	C4A-C5A-N7A	-4.89	104.99	110.58
2	C	301	G5P	C5-C4-N3	-4.87	120.64	128.39
2	D	301	G5P	C5-C4-N3	-4.76	120.82	128.39
2	A	301	G5P	C5-C4-N3	-4.71	120.89	128.39
2	E	301	G5P	N3A-C4A-N9A	4.67	135.11	127.17
2	D	301	G5P	C4A-C5A-N7A	-4.60	105.33	110.58
2	C	301	G5P	N1A-C2A-N3A	-4.57	121.66	128.58
2	C	301	G5P	C4A-C5A-N7A	-4.56	105.37	110.58
2	B	301	G5P	N3A-C4A-N9A	4.54	134.88	127.17
2	F	301	G5P	O3D-PE-O2E	-4.51	97.15	110.70
2	C	301	G5P	N3A-C4A-N9A	4.46	134.75	127.17
2	E	301	G5P	C5-C4-N3	-4.42	121.36	128.39
2	A	301	G5P	O1E-PE-O3D	-4.35	95.53	107.27
2	A	301	G5P	N1A-C2A-N3A	-4.34	122.01	128.58
2	D	301	G5P	O1D-PD-O3G	-4.33	95.56	107.27
2	B	301	G5P	N1A-C2A-N3A	-4.31	122.05	128.58
2	A	301	G5P	C2F-C1F-N9A	-4.23	102.78	113.30
2	B	301	G5P	C2A-N3A-C4A	4.21	122.12	111.83
2	F	301	G5P	N3A-C4A-N9A	4.20	134.31	127.17
2	E	301	G5P	N1A-C2A-N3A	-4.20	122.23	128.58
2	C	301	G5P	C2-N3-C4	4.15	119.45	112.30
2	D	301	G5P	N1A-C2A-N3A	-4.14	122.31	128.58
2	F	301	G5P	N1A-C2A-N3A	-4.13	122.33	128.58
2	C	301	G5P	C2A-N3A-C4A	3.98	121.54	111.83
2	F	301	G5P	O6-C6-N1	-3.98	112.64	120.11
2	B	301	G5P	C5-C4-N3	-3.96	122.09	128.39
2	B	301	G5P	O1G-PG-O3G	3.94	117.92	107.27
2	F	301	G5P	C4A-N9A-C8A	3.93	109.86	105.74
2	E	301	G5P	C2A-N3A-C4A	3.92	121.42	111.83
2	E	301	G5P	C4A-C5A-N7A	-3.89	106.14	110.58
2	D	301	G5P	C2-N3-C4	3.87	118.97	112.30
2	E	301	G5P	C2-N3-C4	3.78	118.81	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	G5P	C1F-N9A-C8A	-3.74	118.79	127.09
2	F	301	G5P	C5-C4-N3	-3.71	122.49	128.39
2	F	301	G5P	C2-N1-C6	-3.68	118.43	125.11
2	A	301	G5P	C2-N3-C4	3.63	118.55	112.30
2	D	301	G5P	O1D-PD-O3D	3.59	116.98	107.27
2	D	301	G5P	C2F-C1F-N9A	-3.55	104.48	113.30
2	F	301	G5P	C4A-C5A-N7A	-3.55	106.52	110.58
2	A	301	G5P	C5A-N7A-C8A	3.51	108.97	103.45
2	F	301	G5P	C5-C6-N1	3.50	122.17	113.25
2	C	301	G5P	C5A-N7A-C8A	3.50	108.95	103.45
2	B	301	G5P	C2F-C3F-C4F	-3.48	95.89	102.61
2	D	301	G5P	C2-N1-C6	-3.46	118.84	125.11
2	A	301	G5P	N3A-C4A-N9A	3.40	132.94	127.17
2	C	301	G5P	O4'-C4'-C5'	3.39	120.20	109.33
2	D	301	G5P	O6-C6-N1	-3.38	113.75	120.11
2	D	301	G5P	C4-C5-N7	-3.36	105.35	110.67
2	D	301	G5P	C2A-N3A-C4A	3.36	120.03	111.83
2	A	301	G5P	C2'-C1'-N9	3.35	122.56	113.25
2	A	301	G5P	C2A-N3A-C4A	3.33	119.97	111.83
2	B	301	G5P	O1D-PD-O3D	-3.29	98.37	107.27
2	F	301	G5P	C2-N3-C4	3.29	117.97	112.30
2	D	301	G5P	N3A-C4A-N9A	3.28	132.75	127.17
2	F	301	G5P	C2'-C1'-N9	3.27	122.36	113.25
2	B	301	G5P	C2'-C1'-N9	3.27	122.35	113.25
2	A	301	G5P	C4A-N9A-C8A	3.26	109.17	105.74
2	E	301	G5P	C2-N1-C6	-3.24	119.23	125.11
2	B	301	G5P	C5A-N7A-C8A	3.23	108.52	103.45
2	B	301	G5P	C2F-C1F-N9A	-3.18	105.41	113.30
2	A	301	G5P	N9A-C8A-N7A	-3.17	109.44	113.94
2	E	301	G5P	C2'-C1'-N9	3.14	121.99	113.25
2	B	301	G5P	C2-N1-C6	-3.12	119.45	125.11
2	A	301	G5P	C2-N1-C6	-3.11	119.47	125.11
2	E	301	G5P	C5-C6-N1	3.09	121.12	113.25
2	B	301	G5P	C3F-C2F-C1F	3.09	107.30	101.46
2	C	301	G5P	O1D-PD-O3G	3.08	115.60	107.27
2	F	301	G5P	N9-C8-N7	-3.08	107.69	113.40
2	C	301	G5P	O4'-C4'-C3'	-3.07	99.06	105.15
2	F	301	G5P	O1B-PB-O3B	3.02	115.44	107.27
2	F	301	G5P	C2A-N3A-C4A	2.98	119.11	111.83
2	F	301	G5P	O4'-C1'-N9	-2.98	101.61	108.36
2	D	301	G5P	O4'-C1'-N9	-2.97	101.63	108.36
2	F	301	G5P	O1E-PE-O3D	2.95	115.26	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	G5P	C2'-C1'-N9	2.94	121.44	113.25
2	F	301	G5P	C4-C5-N7	-2.93	106.02	110.67
2	D	301	G5P	C1F-N9A-C8A	-2.92	120.61	127.09
2	F	301	G5P	C2F-C3F-C4F	-2.87	97.06	102.61
2	B	301	G5P	O3B-PB-O2B	-2.87	102.07	110.70
2	A	301	G5P	C5-C6-N1	2.84	120.48	113.25
2	D	301	G5P	C5-C6-N1	2.83	120.45	113.25
2	E	301	G5P	N9-C8-N7	-2.82	108.16	113.40
2	F	301	G5P	C5-C4-N9	2.81	110.69	105.66
2	C	301	G5P	N9A-C8A-N7A	-2.76	110.02	113.94
2	D	301	G5P	C5A-N7A-C8A	2.76	107.79	103.45
2	C	301	G5P	C2-N1-C6	-2.76	120.11	125.11
2	B	301	G5P	O3G-PG-O2G	-2.75	102.42	110.70
2	C	301	G5P	C5-C6-N1	2.73	120.21	113.25
2	E	301	G5P	O1G-PG-O3G	2.72	114.64	107.27
2	F	301	G5P	N9A-C8A-N7A	-2.72	110.08	113.94
2	F	301	G5P	C2F-C1F-N9A	-2.71	106.58	113.30
2	F	301	G5P	C6-C5-N7	2.70	135.21	130.29
2	D	301	G5P	C8-N7-C5	2.67	109.01	104.26
2	D	301	G5P	O1G-PG-O3G	2.66	114.45	107.27
2	A	301	G5P	O6-C6-N1	-2.65	115.13	120.11
2	B	301	G5P	C2-N3-C4	2.64	116.85	112.30
2	F	301	G5P	O3F-C3F-C2F	2.60	120.15	111.82
2	A	301	G5P	O1G-PG-O3G	2.60	114.29	107.27
2	C	301	G5P	N1-C2-N3	-2.59	118.58	123.32
2	B	301	G5P	O4'-C1'-N9	-2.57	102.53	108.36
2	A	301	G5P	O3D-PE-O2E	2.56	118.42	110.70
2	B	301	G5P	C5-C6-N1	2.56	119.76	113.25
2	D	301	G5P	N9-C8-N7	-2.56	108.66	113.40
2	A	301	G5P	C1F-N9A-C8A	-2.54	121.46	127.09
2	A	301	G5P	C4-C5-N7	-2.54	106.65	110.67
2	C	301	G5P	C4-C5-N7	-2.53	106.65	110.67
2	B	301	G5P	C5A-C4A-N9A	2.53	108.57	105.81
2	B	301	G5P	N9-C8-N7	-2.53	108.71	113.40
2	F	301	G5P	O2F-C2F-C3F	-2.51	103.76	111.82
2	C	301	G5P	C5-C4-N9	2.49	110.11	105.66
2	D	301	G5P	O3D-PD-O2D	2.48	118.16	110.70
2	E	301	G5P	C5A-N7A-C8A	2.47	107.33	103.45
2	D	301	G5P	O3F-C3F-C2F	2.47	119.72	111.82
2	B	301	G5P	C1F-N9A-C8A	-2.46	121.63	127.09
2	B	301	G5P	C4-C5-N7	-2.44	106.80	110.67
2	A	301	G5P	O2'-C2'-C3'	-2.44	103.99	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	G5P	N1-C2-N3	-2.40	118.93	123.32
2	E	301	G5P	C1F-N9A-C8A	-2.37	121.84	127.09
2	D	301	G5P	O1B-PB-O3B	2.37	113.67	107.27
2	D	301	G5P	C5-C4-N9	2.36	109.88	105.66
2	C	301	G5P	N2-C2-N1	2.35	121.72	116.76
2	A	301	G5P	C6A-C5A-N7A	2.34	136.61	132.09
2	E	301	G5P	O1B-PB-O3B	2.34	113.60	107.27
2	A	301	G5P	N9-C8-N7	-2.33	109.07	113.40
2	A	301	G5P	C3F-C2F-C1F	2.33	105.87	101.46
2	F	301	G5P	C3F-C2F-C1F	2.31	105.84	101.46
2	A	301	G5P	O2F-C2F-C3F	-2.31	104.43	111.82
2	B	301	G5P	O2F-C2F-C3F	-2.29	104.46	111.82
2	D	301	G5P	C5A-C4A-N9A	2.29	108.30	105.81
2	F	301	G5P	O1A-PA-O3A	2.28	113.43	107.27
2	D	301	G5P	C3F-C2F-C1F	2.27	105.76	101.46
2	D	301	G5P	N9A-C8A-N7A	-2.27	110.72	113.94
2	D	301	G5P	C2A-N1A-C6A	2.23	122.39	118.73
2	C	301	G5P	C3F-C2F-C1F	2.22	105.66	101.46
2	F	301	G5P	C5A-N7A-C8A	2.20	106.91	103.45
2	F	301	G5P	C8-N7-C5	2.20	108.19	104.26
2	B	301	G5P	C6A-C5A-C4A	2.20	120.18	117.18
2	E	301	G5P	N9-C4-N3	2.19	130.33	125.95
2	E	301	G5P	C4-C5-N7	-2.19	107.20	110.67
2	A	301	G5P	O1G-PG-O3B	-2.16	101.42	107.27
2	A	301	G5P	C2F-C3F-C4F	-2.16	98.43	102.61
2	C	301	G5P	C4A-N9A-C8A	2.15	108.00	105.74
2	D	301	G5P	O4'-C1'-C2'	2.15	111.21	106.62
2	A	301	G5P	C5-C4-N9	2.14	109.49	105.66
2	E	301	G5P	O6-C6-C5	-2.14	120.88	126.53
2	F	301	G5P	O3B-PB-O2B	-2.14	104.28	110.70
2	E	301	G5P	C8-N7-C5	2.13	108.05	104.26
2	B	301	G5P	C5-C4-N9	2.13	109.47	105.66
2	B	301	G5P	N9A-C8A-N7A	-2.13	110.92	113.94
2	A	301	G5P	N1-C2-N3	-2.10	119.47	123.32
2	F	301	G5P	O1D-PD-O3D	-2.10	101.59	107.27
2	B	301	G5P	O4'-C1'-C2'	2.10	111.10	106.62
2	C	301	G5P	O2'-C2'-C1'	2.09	117.30	110.10
2	F	301	G5P	O4'-C1'-C2'	2.09	111.08	106.62
2	D	301	G5P	C5F-C4F-C3F	-2.09	107.70	115.21
2	E	301	G5P	C4A-N9A-C8A	2.09	107.93	105.74
2	A	301	G5P	O1B-PB-O3A	2.07	112.87	107.27
2	A	301	G5P	O3F-C3F-C2F	2.06	118.41	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	G5P	O1G-PG-O3G	2.04	112.78	107.27
2	D	301	G5P	C6-C5-N7	2.02	133.97	130.29
2	A	301	G5P	O3'-C3'-C2'	-2.02	105.34	111.82
2	E	301	G5P	C2F-C3F-C4F	-2.01	98.73	102.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	301	G5P	C4'

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	G5P	C5F-O5F-PE-O2E
2	C	301	G5P	C5F-O5F-PE-O3D
2	C	301	G5P	O4'-C4'-C5'-O5'
2	F	301	G5P	C5F-O5F-PE-O1E
2	F	301	G5P	C5F-O5F-PE-O3D
2	C	301	G5P	C3'-C4'-C5'-O5'
2	C	301	G5P	C3F-C4F-C5F-O5F
2	B	301	G5P	PD-O3G-PG-O2G
2	D	301	G5P	PE-O3D-PD-O2D
2	E	301	G5P	PG-O3B-PB-O2B
2	F	301	G5P	PG-O3B-PB-O2B
2	B	301	G5P	PD-O3D-PE-O1E
2	D	301	G5P	PE-O3D-PD-O1D
2	E	301	G5P	PD-O3G-PG-O1G
2	F	301	G5P	C5F-O5F-PE-O2E
2	F	301	G5P	PG-O3B-PB-O1B
2	C	301	G5P	O4F-C4F-C5F-O5F
2	C	301	G5P	C4'-C5'-O5'-PA
2	A	301	G5P	PE-O3D-PD-O2D
2	D	301	G5P	PD-O3D-PE-O2E
2	D	301	G5P	PG-O3B-PB-O2B
2	D	301	G5P	PB-O3A-PA-O2A
2	A	301	G5P	PE-O3D-PD-O1D
2	A	301	G5P	PG-O3B-PB-O1B
2	A	301	G5P	PA-O3A-PB-O1B
2	C	301	G5P	PB-O3B-PG-O1G
2	C	301	G5P	PB-O3A-PA-O1A
2	D	301	G5P	PD-O3G-PG-O2G
2	D	301	G5P	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	301	G5P	PD-O3G-PG-O2G
2	E	301	G5P	PG-O3B-PB-O1B
2	F	301	G5P	PA-O3A-PB-O1B
2	F	301	G5P	PA-O3A-PB-O2B
2	A	301	G5P	PA-O3A-PB-O2B
2	B	301	G5P	PD-O3G-PG-O1G
2	B	301	G5P	PB-O3A-PA-O1A
2	F	301	G5P	PG-O3G-PD-O1D

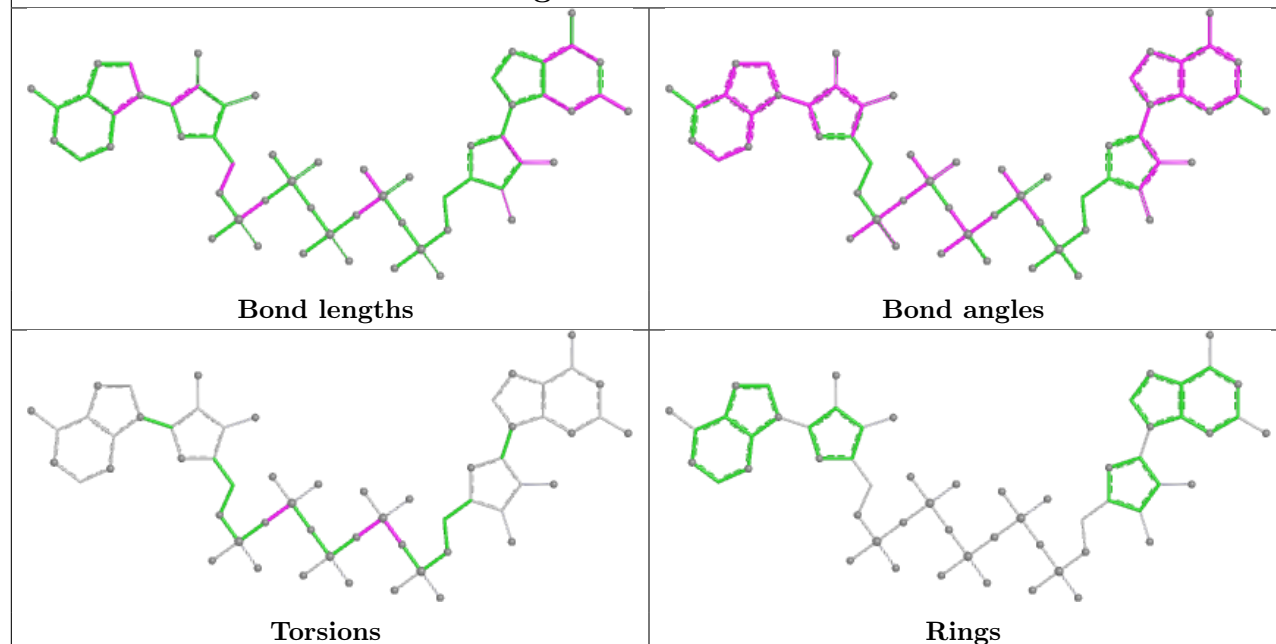
There are no ring outliers.

5 monomers are involved in 7 short contacts:

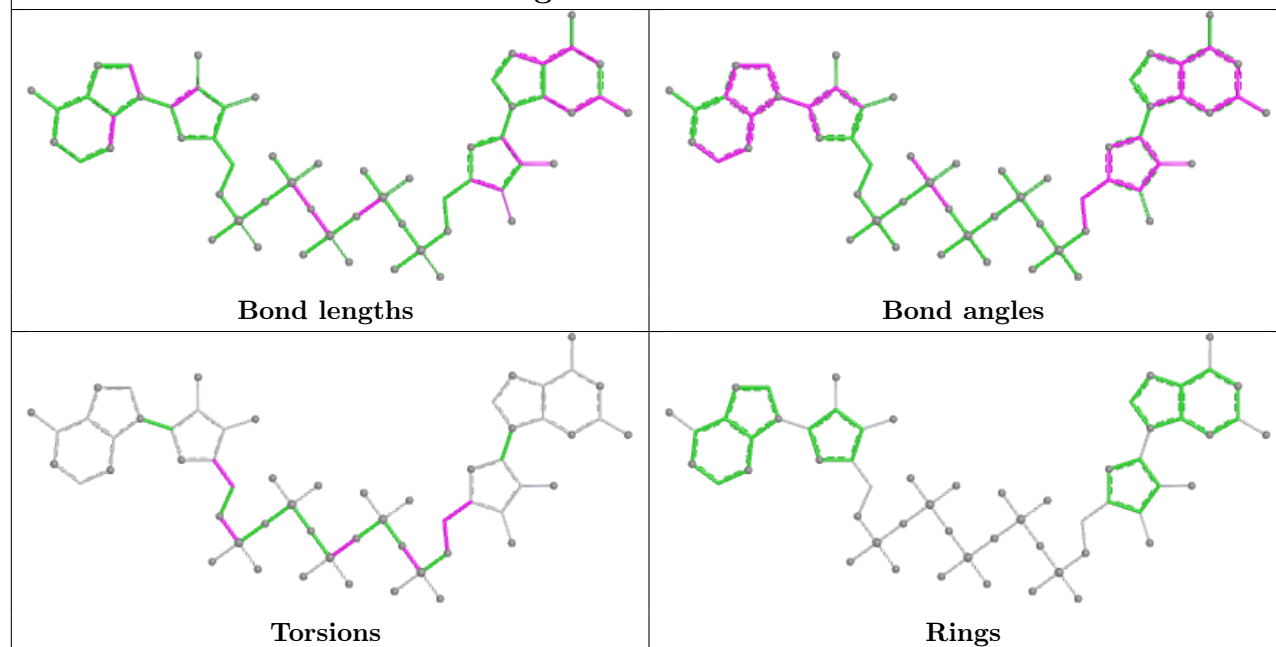
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	G5P	2	0
2	C	301	G5P	2	0
2	E	301	G5P	1	0
2	B	301	G5P	1	0
2	F	301	G5P	1	0

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.

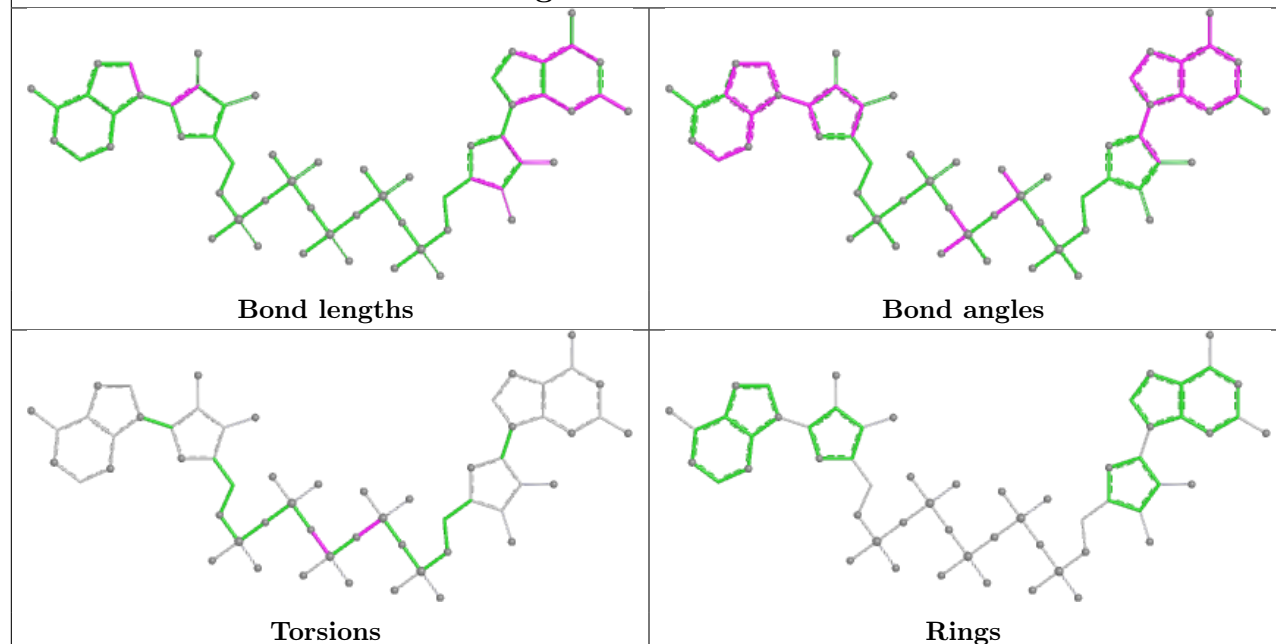
Ligand G5P A 301



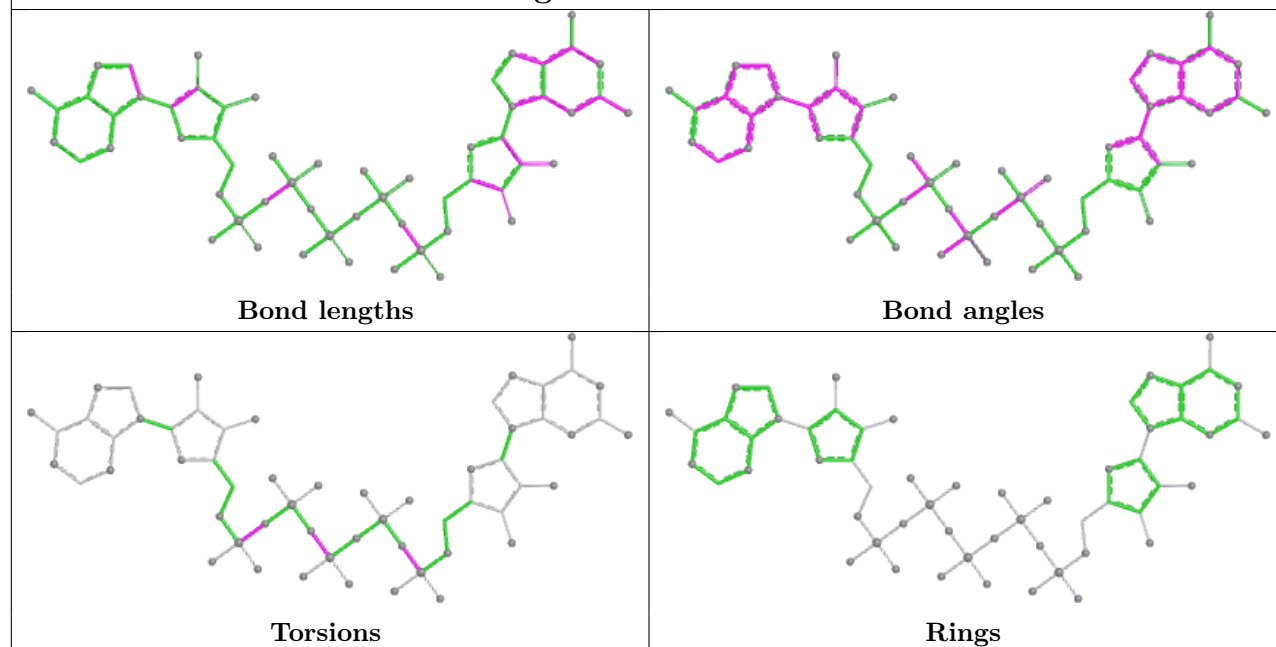
Ligand G5P C 301

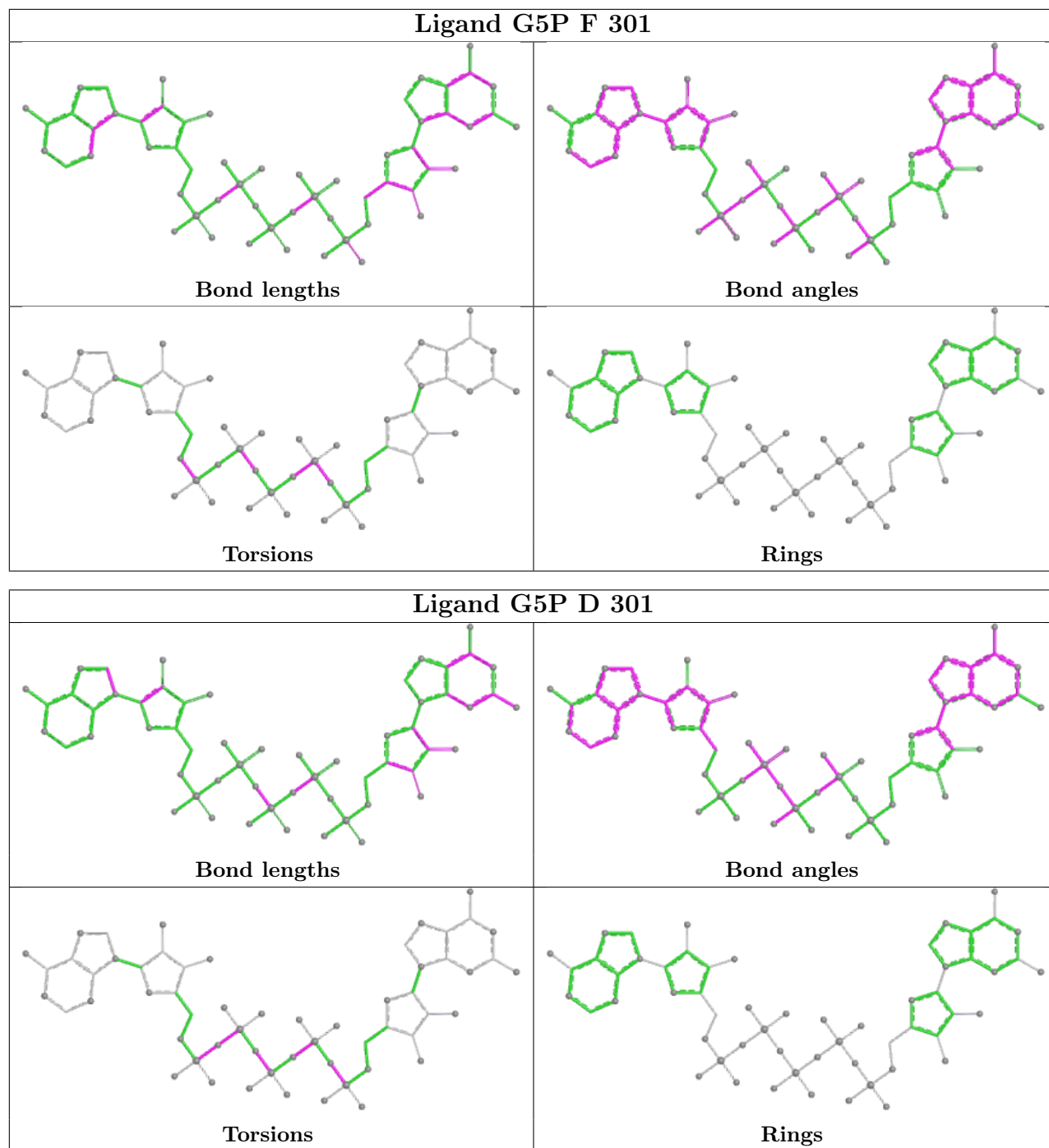


Ligand G5P E 301



Ligand G5P B 301





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	217/227 (95%)	0.41	11 (5%) 33 38	20, 34, 62, 77	0
1	B	217/227 (95%)	0.38	16 (7%) 20 23	22, 34, 63, 94	0
1	C	216/227 (95%)	1.01	29 (13%) 7 7	28, 48, 78, 90	0
1	D	218/227 (96%)	0.22	7 (3%) 50 57	14, 32, 56, 69	1 (0%)
1	E	216/227 (95%)	0.22	6 (2%) 55 60	20, 30, 58, 79	1 (0%)
1	F	216/227 (95%)	0.27	12 (5%) 30 34	17, 30, 58, 82	1 (0%)
All	All	1300/1362 (95%)	0.42	81 (6%) 26 30	14, 34, 68, 94	3 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	GLY	5.0
1	F	41	LEU	3.9
1	E	83	THR	3.9
1	D	220	SER	3.9
1	C	130	ILE	3.8
1	C	58	ALA	3.6
1	C	118	PHE	3.6
1	B	58	ALA	3.4
1	C	170	ILE	3.4
1	F	52	ILE	3.4
1	C	74	LEU	3.4
1	C	159	ILE	3.3
1	A	157	PRO	3.3
1	A	154	THR	3.3
1	A	158	LEU	3.1
1	A	153	LEU	3.1
1	E	55	LEU	3.0
1	B	153	LEU	3.0
1	A	129	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	50	THR	2.8
1	C	55	LEU	2.8
1	A	4	SER	2.8
1	B	220	SER	2.8
1	E	52	ILE	2.8
1	C	120	VAL	2.8
1	B	55	LEU	2.7
1	B	39	GLY	2.7
1	C	138	TYR	2.7
1	C	38	SER	2.7
1	C	132	PRO	2.7
1	A	133	ALA	2.6
1	F	47	LEU	2.6
1	B	50	THR	2.6
1	C	154	THR	2.6
1	C	140	ILE	2.6
1	F	49	GLY	2.6
1	B	52	ILE	2.6
1	C	41	LEU	2.5
1	E	39	GLY	2.5
1	C	150	ILE	2.5
1	C	163	ASP	2.5
1	B	4	SER	2.5
1	D	3	ALA	2.5
1	B	121	ILE	2.4
1	C	39	GLY	2.4
1	F	121	ILE	2.4
1	F	54	VAL	2.4
1	C	203	LYS	2.4
1	C	164	ASP	2.3
1	D	153	LEU	2.3
1	C	60	ILE	2.3
1	B	155	GLY	2.3
1	C	137	VAL	2.3
1	F	45	ASN	2.3
1	A	159	ILE	2.3
1	E	49	GLY	2.3
1	D	4	SER	2.3
1	C	43	ARG	2.3
1	B	47	LEU	2.3
1	C	153	LEU	2.3
1	C	121	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	47	LEU	2.3
1	B	74	LEU	2.2
1	B	117	PRO	2.2
1	B	150	ILE	2.2
1	B	41	LEU	2.2
1	B	40	ASP	2.2
1	C	62	GLN	2.2
1	C	61	ASP	2.2
1	F	55	LEU	2.2
1	A	131	HIS	2.1
1	F	46	MET	2.1
1	A	140	ILE	2.1
1	D	85	TYR	2.1
1	A	6	ARG	2.1
1	C	147	THR	2.1
1	D	39	GLY	2.1
1	C	4	SER	2.0
1	F	220	SER	2.0
1	E	41[A]	LEU	2.0
1	D	5	ALA	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
3	MG	B	302	1/1	0.86	0.13	42,42,42,42	0
3	MG	C	302	1/1	0.90	0.09	50,50,50,50	0
2	G5P	C	301	58/58	0.93	0.09	33,44,55,60	0

Continued on next page...

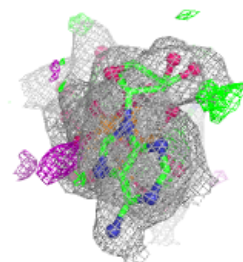
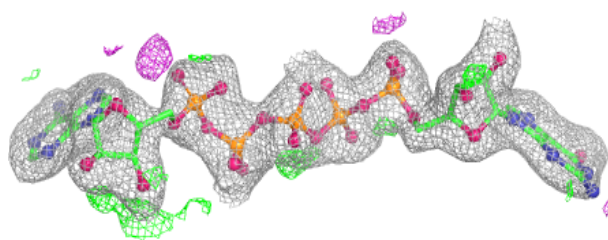
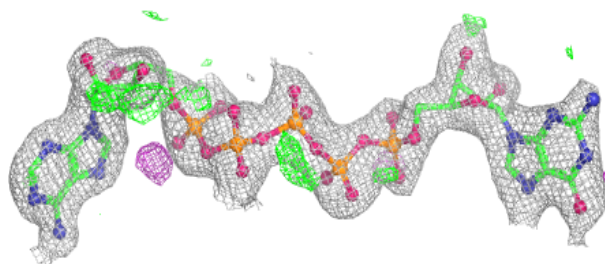
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	F	302	1/1	0.95	0.11	31,31,31,31	0
2	G5P	E	301	58/58	0.96	0.07	16,23,31,48	0
2	G5P	B	301	58/58	0.96	0.06	22,29,43,51	0
2	G5P	D	301	58/58	0.97	0.06	19,24,31,39	0
2	G5P	A	301	58/58	0.97	0.06	19,26,33,38	0
3	MG	D	302	1/1	0.97	0.05	28,28,28,28	0
3	MG	A	302	1/1	0.97	0.09	31,31,31,31	0
3	MG	E	302	1/1	0.98	0.08	27,27,27,27	0
2	G5P	F	301	58/58	0.98	0.05	16,23,35,39	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.

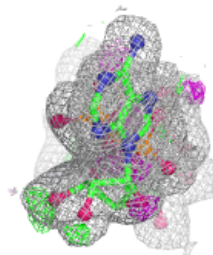
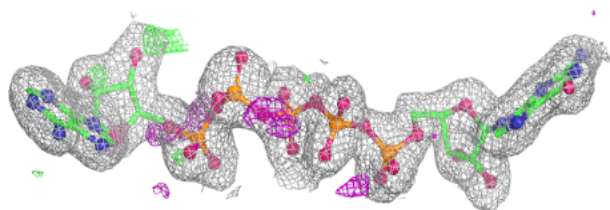
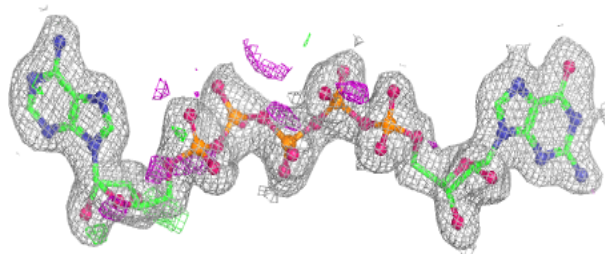
Electron density around G5P C 301:

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

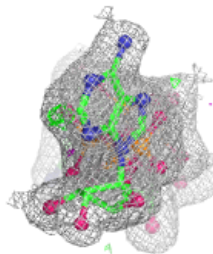
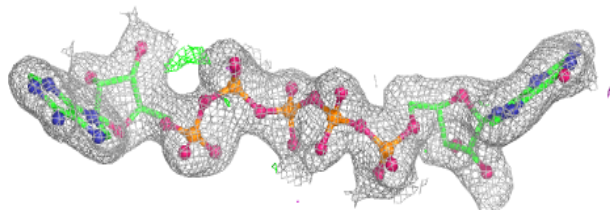
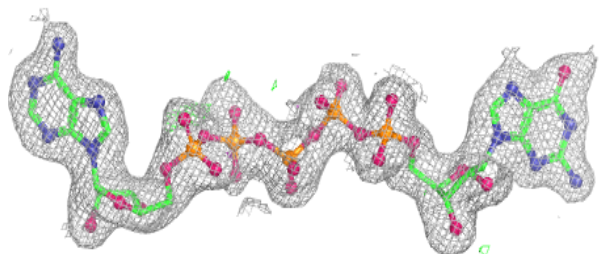


Electron density around G5P E 301:

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

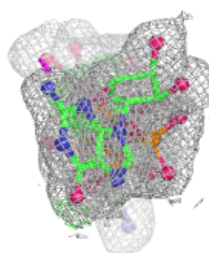
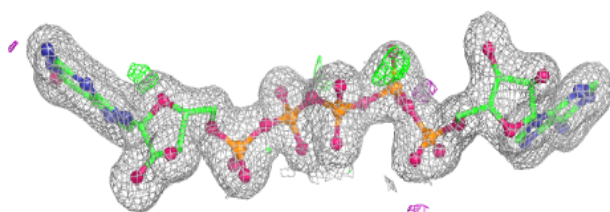
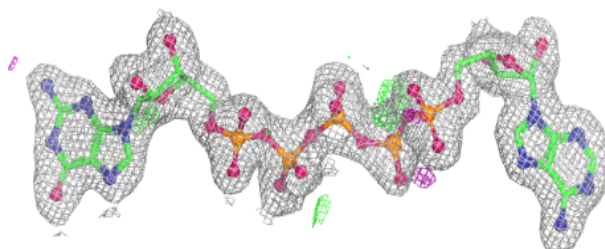
**Electron density around G5P B 301:**

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

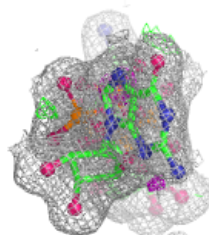
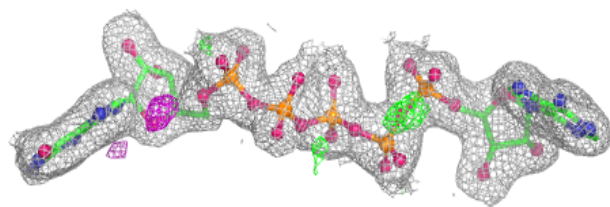
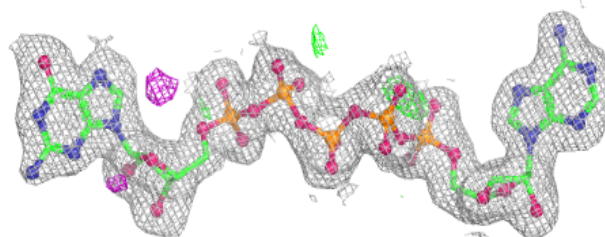


Electron density around G5P D 301:

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

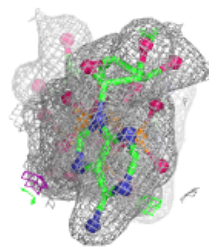
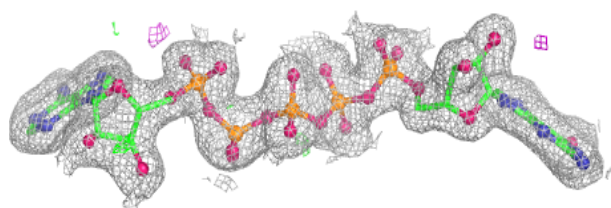
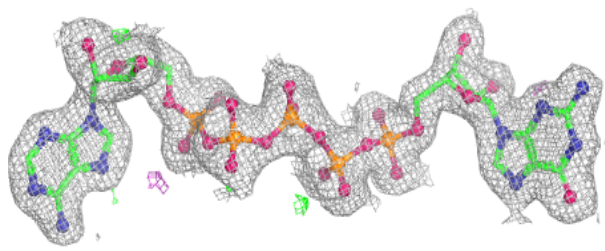
**Electron density around G5P A 301:**

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



Electron density around G5P F 301:

$2mF_o - DF_c$ (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.