



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2021 – 04:03 PM EST

PDB ID : 7RMW  
Title : Crystal structure of B. subtilis PurR bound to ppGpp  
Authors : Schumacher, M.A.  
Deposited on : 2021-07-28  
Resolution : 2.45 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](mailto: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.

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

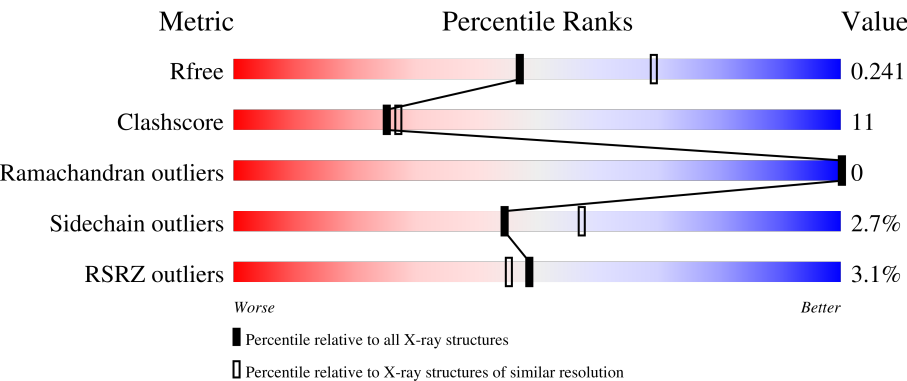
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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 <sub>free</sub>	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	285	<div><div>2%</div><div><div></div><div>80%</div><div>14%</div><div>• 5%</div></div></div>
1	B	285	<div><div>2%</div><div><div></div><div>74%</div><div>19%</div><div>• 6%</div></div></div>
1	C	285	<div><div>4%</div><div><div></div><div>66%</div><div>22%</div><div>• 10%</div></div></div>
1	D	285	<div><div>5%</div><div><div></div><div>71%</div><div>17%</div><div>• 8%</div></div></div>
1	E	285	<div><div>2%</div><div><div></div><div>68%</div><div>22%</div><div>• 9%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	285	

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	G4P	B	301	-	-	X	-
2	G4P	C	301	-	-	X	-

## 2 Entry composition [i](#)

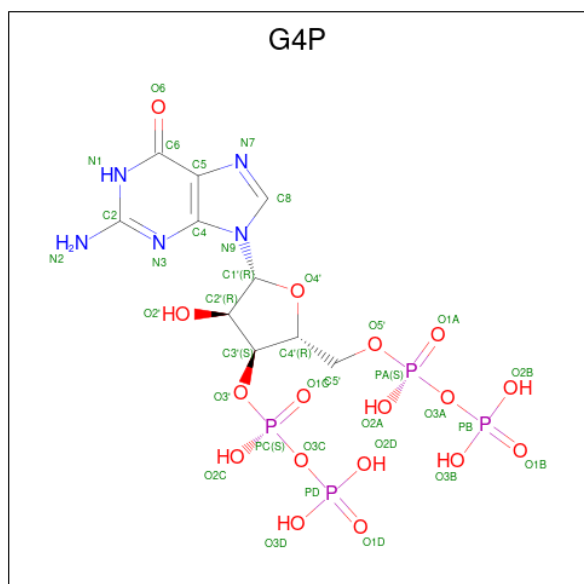
There are 3 unique types of molecules in this entry. The entry contains 12414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pur operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2075	1326	344	397	8			
1	B	269	Total	C	N	O	S	0	0	0
			2062	1318	342	394	8			
1	C	256	Total	C	N	O	S	0	0	0
			1972	1266	324	374	8			
1	D	261	Total	C	N	O	S	0	0	0
			2011	1291	333	379	8			
1	E	260	Total	C	N	O	S	0	0	0
			2006	1287	333	378	8			
1	F	265	Total	C	N	O	S	0	0	0
			2048	1311	341	388	8			

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula:  $C_{10}H_{17}N_5O_{17}P_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	B	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	C	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	F	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

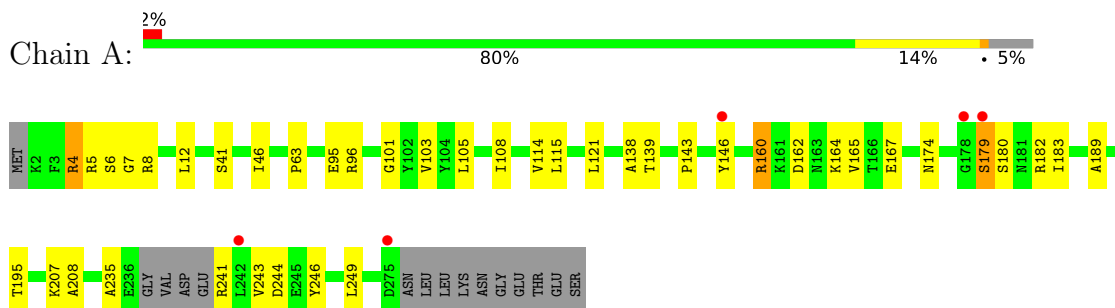
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	30	Total	O	0	0
			30	30		
3	C	9	Total	O	0	0
			9	9		
3	D	17	Total	O	0	0
			17	17		
3	E	12	Total	O	0	0
			12	12		
3	F	10	Total	O	0	0
			10	10		

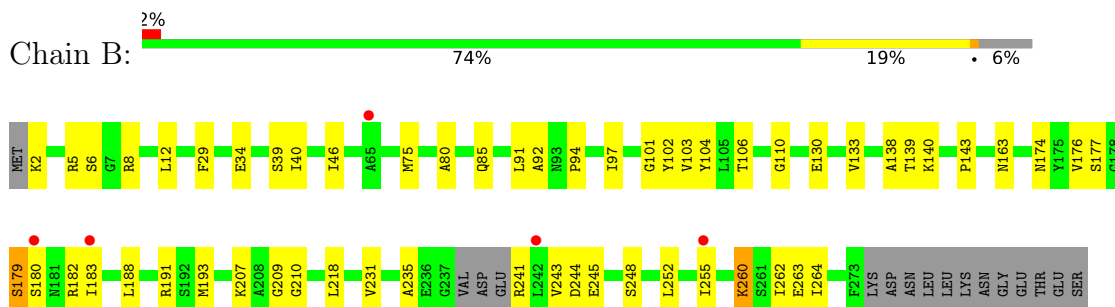
### 3 Residue-property plots [i](#)

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.

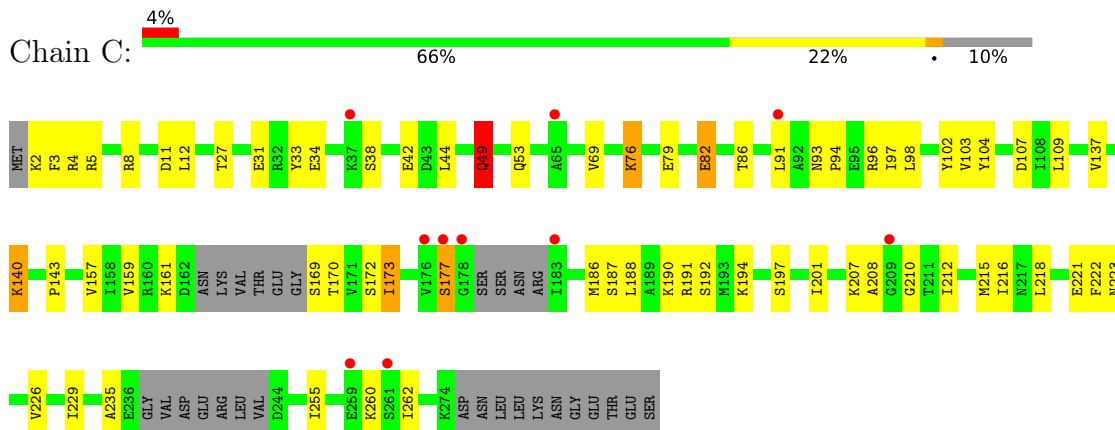
- Molecule 1: Pur operon repressor



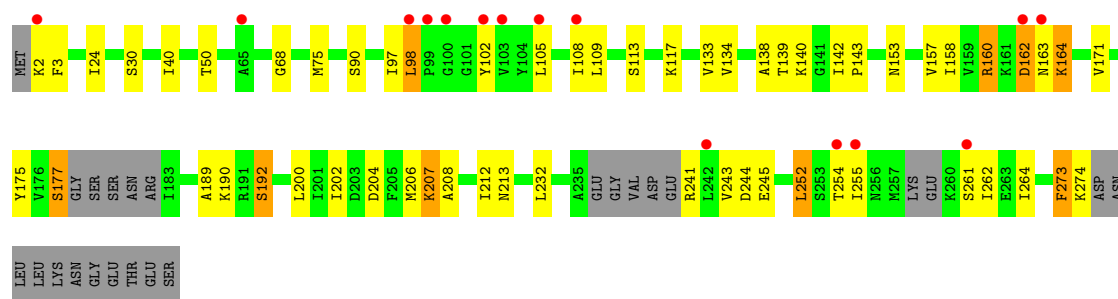
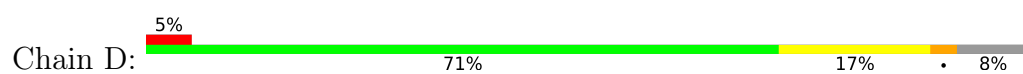
- Molecule 1: Pur operon repressor



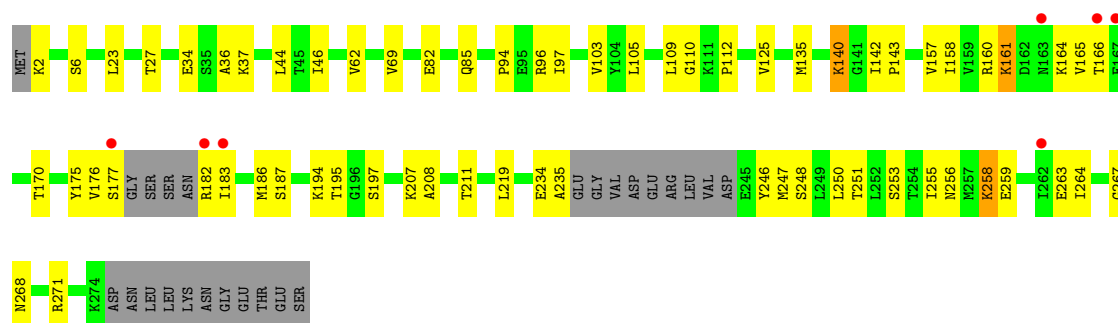
- Molecule 1: Pur operon repressor



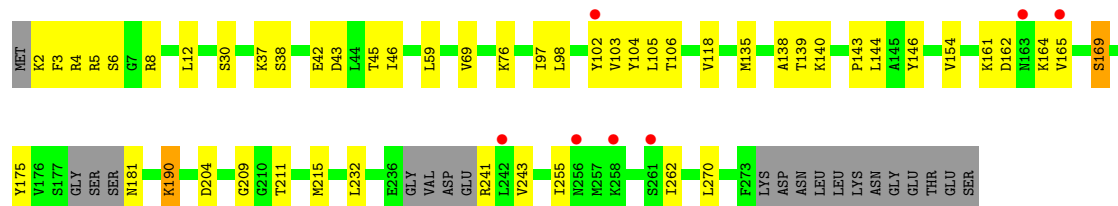
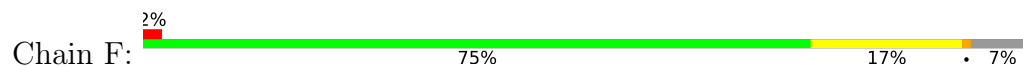
- Molecule 1: Pur operon repressor



• Molecule 1: Pur operon repressor



• Molecule 1: Pur operon repressor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.26Å 90.97Å 98.71Å 62.75° 75.36° 78.53°	Depositor
Resolution (Å)	80.49 – 2.45 80.49 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.2 (80.49-2.45) 85.6 (80.49-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.195 , 0.240 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	2000 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: G4P

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	0.37	0/2105	0.55	0/2843
1	B	0.43	1/2092 (0.0%)	0.58	0/2826
1	C	0.39	1/2000 (0.1%)	0.55	0/2698
1	D	0.46	2/2039 (0.1%)	0.59	0/2752
1	E	0.39	1/2035 (0.0%)	0.57	0/2746
1	F	0.36	0/2077	0.54	0/2804
All	All	0.40	5/12348 (0.0%)	0.56	0/16669

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	D	0	4
1	E	0	1
1	F	0	2
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	GLU	C-N	7.71	1.51	1.34
1	D	254	THR	C-N	7.55	1.51	1.34
1	D	160	ARG	C-N	7.39	1.51	1.34
1	E	258	LYS	CE-NZ	5.58	1.62	1.49
1	C	49	GLN	CD-OE1	-5.11	1.12	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	LYS	Peptide
1	A	179	SER	Peptide
1	A	246	TYR	Mainchain
1	B	179	SER	Peptide
1	D	162	ASP	Peptide
1	D	164	LYS	Peptide
1	D	273	PHE	Peptide
1	D	98	LEU	Peptide
1	E	164	LYS	Peptide
1	F	162	ASP	Peptide
1	F	164	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2075	0	2132	41	0
1	B	2062	0	2118	58	5
1	C	1972	0	2032	63	0
1	D	2011	0	2081	43	5
1	E	2006	0	2077	53	0
1	F	2048	0	2113	34	0
2	A	36	0	10	5	0
2	B	36	0	11	9	0
2	C	36	0	9	11	0
2	F	36	0	8	1	0
3	A	18	0	0	0	0
3	B	30	0	0	2	0
3	C	9	0	0	0	0
3	D	17	0	0	1	0
3	E	12	0	0	1	0
3	F	10	0	0	0	0
All	All	12414	0	12591	267	5

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 11.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:CD1	1:D:255:ILE:HG21	1.45	1.45
1:E:176:VAL:HG12	1:E:183:ILE:HA	1.36	1.05
1:B:97:ILE:CG2	1:B:255:ILE:HG21	1.87	1.04
1:D:97:ILE:HD12	1:D:255:ILE:HG21	1.40	1.03
1:D:97:ILE:CD1	1:D:255:ILE:CG2	2.40	0.99
1:A:195:THR:HG1	1:C:2:LYS:N	1.62	0.96
1:B:255:ILE:HD12	1:B:262:ILE:HG12	1.47	0.95
1:B:97:ILE:HG21	1:B:255:ILE:HG21	1.45	0.95
1:D:97:ILE:HD13	1:D:255:ILE:HG21	1.47	0.94
1:D:97:ILE:HD11	1:D:255:ILE:HG21	1.49	0.92
1:E:256:ASN:HB3	1:E:259:GLU:OE2	1.72	0.89
1:C:103:VAL:H	2:C:301:G4P:HN1	1.17	0.89
1:A:207:LYS:O	1:A:241:ARG:NH1	2.08	0.86
1:D:98:LEU:HG	1:D:102:TYR:HB2	1.59	0.83
1:B:97:ILE:HG23	1:B:255:ILE:HG21	1.60	0.82
1:E:176:VAL:CG1	1:E:183:ILE:HA	2.14	0.77
1:B:103:VAL:H	2:B:301:G4P:HN1	1.32	0.76
1:A:179:SER:HB2	2:A:301:G4P:O2C	1.86	0.74
1:D:97:ILE:HD12	1:D:255:ILE:CG2	2.10	0.74
1:B:133:VAL:HG11	1:B:193:MET:HE1	1.70	0.74
1:A:195:THR:HG23	1:C:2:LYS:HB2	1.70	0.74
1:C:94:PRO:HB3	1:C:260:LYS:HG2	1.69	0.73
1:B:252:LEU:HD12	1:B:264:ILE:CG2	2.19	0.72
1:B:252:LEU:HA	1:B:264:ILE:HG22	1.72	0.72
1:E:194:LYS:NZ	3:E:301:HOH:O	2.23	0.71
1:B:2:LYS:HD3	1:E:195:THR:HG21	1.72	0.71
1:D:274:LYS:HD2	1:E:37:LYS:HG3	1.74	0.70
1:E:234:GLU:OE2	1:E:246:TYR:OH	2.08	0.70
1:E:256:ASN:CB	1:E:259:GLU:OE2	2.40	0.69
1:A:160:ARG:HD3	1:A:165:VAL:HG11	1.75	0.68
1:B:263:GLU:OE2	1:B:263:GLU:N	2.28	0.67
1:B:130:GLU:OE1	3:B:401:HOH:O	2.13	0.66
1:C:221:GLU:OE2	1:C:221:GLU:N	2.29	0.66
1:D:207:LYS:HG2	1:D:208:ALA:H	1.60	0.65
1:C:11:ASP:OD2	1:C:33:TYR:OH	2.09	0.65
1:B:133:VAL:HG11	1:B:193:MET:CE	2.27	0.64
1:D:153:ASN:ND2	3:D:301:HOH:O	2.25	0.64
1:E:251:THR:HG23	1:E:267:GLY:HA2	1.80	0.64
1:A:101:GLY:O	2:A:301:G4P:N2	2.32	0.62
1:A:4:ARG:HD2	1:A:7:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HG13	1:D:202:ILE:HD13	1.80	0.62
1:B:235:ALA:O	1:B:241:ARG:NH2	2.32	0.62
1:F:175:TYR:HE1	1:F:211:THR:HG22	1.65	0.61
1:D:206:MET:HE3	1:D:212:ILE:HD12	1.81	0.61
1:C:93:ASN:HD22	1:C:94:PRO:HD2	1.65	0.60
1:E:253:SER:OG	1:E:263:GLU:O	2.20	0.60
1:C:103:VAL:HG12	2:C:301:G4P:HN1	1.66	0.60
1:E:142:ILE:HG12	1:E:158:ILE:HD12	1.84	0.60
1:F:98:LEU:HD11	1:F:102:TYR:HB2	1.82	0.60
1:B:91:LEU:HB3	1:B:264:ILE:CD1	2.32	0.59
1:D:105:LEU:HD12	1:D:109:LEU:HG	1.84	0.59
1:C:201:ILE:HB	1:C:229:ILE:HG12	1.84	0.59
1:B:97:ILE:HG21	1:B:255:ILE:CG2	2.28	0.59
1:A:207:LYS:HG3	1:A:235:ALA:HB3	1.85	0.58
1:C:76:LYS:HD2	1:C:79:GLU:H	1.68	0.58
1:C:137:VAL:HG12	1:C:159:VAL:HB	1.85	0.58
1:B:255:ILE:CD1	1:B:262:ILE:HG12	2.28	0.58
1:D:274:LYS:HE2	1:E:36:ALA:HA	1.84	0.58
1:C:38:SER:O	1:C:42:GLU:HG3	2.03	0.58
1:E:194:LYS:HG3	1:E:197:SER:OG	2.03	0.58
1:C:177:SER:HB2	2:C:301:G4P:O3B	2.03	0.58
1:C:5:ARG:HG3	1:C:8:ARG:HH21	1.69	0.57
1:B:179:SER:HB2	2:B:301:G4P:O2C	2.05	0.57
1:D:138:ALA:HB1	1:D:139:THR:HG22	1.86	0.57
1:F:97:ILE:HG23	1:F:255:ILE:HG21	1.85	0.57
1:A:179:SER:HB2	2:A:301:G4P:PC	2.44	0.57
1:E:256:ASN:OD1	1:E:258:LYS:HB3	2.04	0.57
1:C:76:LYS:HE3	1:C:79:GLU:HB2	1.87	0.57
1:F:118:VAL:HG11	1:F:144:LEU:HD22	1.87	0.56
1:F:103:VAL:HG23	1:F:105:LEU:HG	1.87	0.56
1:A:103:VAL:HG23	2:A:301:G4P:HN1	1.69	0.56
1:C:170:THR:HG1	1:C:187:SER:HG	1.51	0.56
1:C:27:THR:O	1:C:31:GLU:HG3	2.05	0.56
1:E:97:ILE:HG12	1:E:255:ILE:HD13	1.86	0.56
1:E:6:SER:HB3	1:F:46:ILE:HG21	1.88	0.56
1:B:207:LYS:O	1:B:241:ARG:NH1	2.40	0.55
1:D:206:MET:HE1	1:D:243:VAL:HG21	1.89	0.55
1:F:135:MET:HG2	1:F:215:MET:HE2	1.89	0.55
1:A:5:ARG:HH21	1:A:46:ILE:HD13	1.71	0.55
1:B:210:GLY:H	2:B:301:G4P:PB	2.29	0.55
1:C:102:TYR:HA	2:C:301:G4P:C2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LEU:HD13	1:E:264:ILE:HD11	1.89	0.55
1:D:160:ARG:HG2	1:D:160:ARG:HH11	1.71	0.55
1:D:262:ILE:HD11	1:D:264:ILE:HD11	1.89	0.55
1:B:91:LEU:HB3	1:B:264:ILE:HD11	1.89	0.54
1:B:92:ALA:HB2	1:B:264:ILE:HG12	1.89	0.54
1:C:103:VAL:HG12	2:C:301:G4P:N1	2.21	0.54
1:C:212:ILE:O	1:C:216:ILE:HG13	2.07	0.54
1:C:49:GLN:OE1	1:C:53:GLN:OE1	2.26	0.54
1:E:177:SER:OG	1:E:208:ALA:HB3	2.08	0.54
1:D:171:VAL:HG23	1:D:190:LYS:HG2	1.90	0.54
1:A:162:ASP:OD2	1:A:165:VAL:HG13	2.07	0.53
1:B:209:GLY:N	2:B:301:G4P:O3A	2.40	0.53
1:A:96:ARG:NH2	1:A:108:ILE:HD11	2.23	0.53
1:D:252:LEU:HD12	1:D:264:ILE:HG12	1.90	0.53
1:D:175:TYR:HE1	1:D:177:SER:HG	1.56	0.53
1:D:105:LEU:O	1:D:108:ILE:HG13	2.08	0.53
1:E:161:LYS:HA	1:E:186:MET:HA	1.90	0.53
1:C:109:LEU:HD13	1:C:140:LYS:HB3	1.91	0.53
1:C:12:LEU:HD13	1:C:33:TYR:HE1	1.72	0.53
1:F:30:SER:HB3	1:F:37:LYS:HG2	1.91	0.53
1:E:143:PRO:HG3	1:F:146:TYR:CE1	2.44	0.52
1:B:104:TYR:CZ	1:B:106:THR:HB	2.44	0.52
1:A:146:TYR:CE2	1:B:143:PRO:HG3	2.44	0.52
1:F:103:VAL:HG22	2:F:301:G4P:O6	2.09	0.52
1:C:3:PHE:CZ	1:D:50:THR:HG23	2.45	0.52
1:D:204:ASP:O	1:D:232:LEU:HB3	2.10	0.52
1:A:208:ALA:HB3	2:A:301:G4P:O2B	2.10	0.52
1:F:98:LEU:CD1	1:F:102:TYR:HB2	2.41	0.50
1:C:208:ALA:H	2:C:301:G4P:PB	2.33	0.50
1:E:170:THR:HG21	1:E:187:SER:HB3	1.93	0.50
1:C:159:VAL:HG22	1:C:188:LEU:HD12	1.94	0.50
1:B:140:LYS:O	1:B:143:PRO:HD2	2.12	0.50
1:D:142:ILE:HG12	1:D:158:ILE:HD12	1.94	0.49
1:B:235:ALA:O	1:B:241:ARG:NH1	2.45	0.49
1:D:162:ASP:HB3	1:D:164:LYS:HB2	1.94	0.49
1:E:140:LYS:HE2	1:F:165:VAL:HG21	1.95	0.49
1:E:207:LYS:HA	1:E:235:ALA:HB3	1.94	0.49
1:C:44:LEU:HD13	1:C:69:VAL:HG11	1.92	0.49
1:D:207:LYS:HG2	1:D:208:ALA:N	2.27	0.49
1:A:46:ILE:HG21	1:B:6:SER:HB3	1.95	0.49
1:B:207:LYS:HD3	2:B:301:G4P:O1C	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:N	2:C:301:G4P:HN1	1.99	0.49
1:D:133:VAL:HG21	1:D:157:VAL:CG2	2.42	0.49
1:D:274:LYS:HD2	1:E:37:LYS:CG	2.43	0.48
1:E:268:ASN:O	1:E:271:ARG:HG3	2.13	0.48
1:F:204:ASP:O	1:F:232:LEU:HB3	2.14	0.48
1:A:4:ARG:NH2	1:B:46:ILE:HG23	2.29	0.48
1:C:207:LYS:HB2	2:C:301:G4P:O5'	2.14	0.48
1:E:44:LEU:HD13	1:E:69:VAL:HG11	1.96	0.48
1:B:174:ASN:HB3	1:B:183:ILE:CG2	2.44	0.48
1:E:140:LYS:O	1:E:143:PRO:HD2	2.14	0.48
1:C:96:ARG:NH1	1:C:104:TYR:O	2.47	0.48
1:E:112:PRO:HG3	1:F:154:VAL:O	2.14	0.48
1:A:146:TYR:OH	1:B:110:GLY:HA2	2.14	0.48
1:C:207:LYS:HA	1:C:235:ALA:HB3	1.96	0.47
1:A:63:PRO:HG2	1:E:27:THR:HG21	1.97	0.47
1:A:195:THR:OG1	1:C:2:LYS:N	2.37	0.47
1:D:244:ASP:OD2	1:D:245:GLU:N	2.47	0.47
1:E:94:PRO:O	1:E:97:ILE:HD12	2.14	0.47
1:A:174:ASN:HB3	1:A:183:ILE:CG2	2.44	0.47
1:D:24:ILE:O	1:D:68:GLY:HA3	2.14	0.47
1:D:75:MET:O	1:D:273:PHE:HE1	1.97	0.47
1:E:256:ASN:CG	1:E:259:GLU:OE2	2.52	0.47
1:B:8:ARG:O	1:B:12:LEU:HB2	2.15	0.47
1:F:169:SER:OG	1:F:190:LYS:HG2	2.14	0.47
1:F:241:ARG:NH1	1:F:243:VAL:HG23	2.30	0.47
1:A:5:ARG:NH2	1:B:6:SER:OG	2.48	0.47
1:B:2:LYS:HD3	1:E:195:THR:CG2	2.44	0.47
1:C:82:GLU:OE2	1:C:86:THR:OG1	2.33	0.47
1:F:2:LYS:HG2	1:F:3:PHE:H	1.80	0.46
1:F:138:ALA:HA	1:F:139:THR:HA	1.60	0.46
1:B:252:LEU:HD12	1:B:264:ILE:HG22	1.97	0.46
1:C:93:ASN:HD22	1:C:94:PRO:CD	2.28	0.46
1:C:98:LEU:N	1:C:102:TYR:O	2.39	0.46
1:E:105:LEU:HB3	1:E:109:LEU:HD13	1.98	0.46
1:C:2:LYS:HG2	1:C:3:PHE:H	1.80	0.46
1:B:101:GLY:O	2:B:301:G4P:N2	2.49	0.46
1:A:95:GLU:O	1:B:191:ARG:NH2	2.48	0.46
1:B:103:VAL:N	2:B:301:G4P:HN1	2.05	0.46
1:A:96:ARG:HH22	1:A:108:ILE:HD11	1.81	0.46
1:C:2:LYS:HE2	1:C:34:GLU:HB3	1.97	0.46
1:D:189:ALA:HB3	1:D:192:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LYS:HE2	1:D:117:LYS:HA	1.98	0.46
1:A:63:PRO:HG2	1:E:27:THR:CG2	2.45	0.45
1:A:235:ALA:O	1:A:241:ARG:NH1	2.44	0.45
1:C:188:LEU:HD13	1:C:218:LEU:HD21	1.99	0.45
1:D:200:LEU:HG	1:D:202:ILE:HD11	1.97	0.45
1:E:110:GLY:HA2	1:F:146:TYR:OH	2.16	0.45
1:A:115:LEU:HD11	1:A:143:PRO:HB3	1.98	0.45
1:B:94:PRO:HB3	1:B:260:LYS:HG2	1.99	0.45
1:D:140:LYS:O	1:D:143:PRO:HD2	2.16	0.45
1:B:2:LYS:HG3	1:B:34:GLU:OE2	2.16	0.45
1:A:167:GLU:N	1:A:167:GLU:OE2	2.50	0.44
1:E:176:VAL:HG12	1:E:182:ARG:O	2.17	0.44
1:F:8:ARG:O	1:F:12:LEU:HB2	2.17	0.44
1:A:121:LEU:HD22	1:A:249:LEU:HD21	1.98	0.44
1:A:180:SER:C	1:A:182:ARG:H	2.21	0.44
1:C:91:LEU:HD23	1:C:96:ARG:HD3	1.99	0.44
1:C:98:LEU:HB2	1:C:102:TYR:HB2	1.99	0.44
1:E:109:LEU:HD23	1:E:140:LYS:HB3	1.98	0.44
1:C:172:SER:HA	1:C:186:MET:O	2.17	0.44
1:C:207:LYS:HB3	1:C:208:ALA:H	1.42	0.44
1:C:212:ILE:HG12	1:C:215:MET:HE3	1.99	0.44
1:E:135:MET:HA	1:E:157:VAL:O	2.18	0.44
1:E:256:ASN:OD1	1:E:259:GLU:OE2	2.35	0.44
1:A:160:ARG:NH1	1:A:162:ASP:OD1	2.50	0.44
1:B:138:ALA:HA	1:B:139:THR:HA	1.80	0.44
1:E:248:SER:OG	1:E:268:ASN:ND2	2.51	0.44
1:E:2:LYS:HD3	1:E:34:GLU:HB2	1.99	0.44
1:E:140:LYS:H	1:E:140:LYS:HD2	1.82	0.44
1:C:2:LYS:HA	1:C:34:GLU:CD	2.38	0.44
1:C:190:LYS:HD2	1:C:190:LYS:O	2.18	0.44
1:E:161:LYS:HD3	1:E:161:LYS:H	1.83	0.44
1:A:180:SER:C	1:A:182:ARG:N	2.71	0.43
1:C:102:TYR:HA	2:C:301:G4P:N1	2.33	0.43
1:B:180:SER:C	1:B:182:ARG:N	2.71	0.43
1:C:157:VAL:HG11	1:C:192:SER:O	2.17	0.43
1:C:161:LYS:O	1:C:161:LYS:HG2	2.19	0.43
1:C:97:ILE:HD11	1:C:262:ILE:HB	2.00	0.43
1:F:5:ARG:HD2	1:F:43:ASP:OD2	2.18	0.43
1:B:180:SER:C	1:B:182:ARG:H	2.21	0.43
1:E:165:VAL:HG12	1:E:166:THR:H	1.84	0.43
1:F:42:GLU:O	1:F:45:THR:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ALA:HA	1:D:139:THR:HA	1.53	0.43
1:A:167:GLU:HG2	1:A:189:ALA:HB2	2.00	0.43
1:B:241:ARG:HG3	1:B:243:VAL:HG22	2.01	0.43
1:B:102:TYR:HA	2:B:301:G4P:N2	2.33	0.43
1:C:207:LYS:CG	2:C:301:G4P:H4'	2.49	0.43
1:D:30:SER:HA	1:D:40:ILE:HD11	2.00	0.43
1:F:140:LYS:O	1:F:143:PRO:HD2	2.18	0.43
1:B:163:ASN:OD1	1:B:163:ASN:N	2.52	0.42
1:E:23:LEU:HD11	1:E:62:VAL:HG22	2.01	0.42
1:F:5:ARG:HD3	1:F:8:ARG:NH2	2.34	0.42
1:F:270:LEU:HD12	1:F:270:LEU:HA	1.86	0.42
1:B:2:LYS:CD	1:E:195:THR:HG21	2.46	0.42
1:E:125:VAL:HG21	1:E:247:MET:SD	2.58	0.42
1:A:167:GLU:HG2	1:A:167:GLU:O	2.19	0.42
1:B:102:TYR:HA	2:B:301:G4P:C2	2.48	0.42
1:C:173:ILE:HG22	1:C:218:LEU:HD12	2.02	0.42
1:D:97:ILE:HG13	1:D:102:TYR:O	2.20	0.42
1:C:97:ILE:HD13	1:C:255:ILE:CG2	2.49	0.42
1:C:216:ILE:HG23	1:C:226:VAL:HG21	2.01	0.42
1:F:135:MET:HB2	1:F:135:MET:HE3	1.95	0.42
1:B:133:VAL:CG1	1:B:193:MET:HE1	2.45	0.42
1:C:140:LYS:O	1:C:143:PRO:HD2	2.19	0.42
1:E:175:TYR:HE1	1:E:211:THR:HG22	1.85	0.42
1:A:5:ARG:HH21	1:A:46:ILE:CD1	2.33	0.42
1:A:138:ALA:HA	1:A:139:THR:HA	1.73	0.42
1:A:8:ARG:O	1:A:12:LEU:HB2	2.19	0.42
1:F:59:LEU:HD22	1:F:69:VAL:HG22	2.02	0.42
1:F:209:GLY:HA3	1:F:243:VAL:HG13	2.02	0.42
1:F:4:ARG:HA	1:F:4:ARG:HD2	1.74	0.41
1:B:176:VAL:HG22	1:B:177:SER:O	2.20	0.41
1:B:260:LYS:HE3	1:B:260:LYS:HB3	1.92	0.41
1:E:96:ARG:O	1:E:103:VAL:HA	2.20	0.41
1:A:179:SER:OG	1:A:180:SER:N	2.52	0.41
1:A:241:ARG:HG3	1:A:243:VAL:HG22	2.01	0.41
1:C:210:GLY:N	2:C:301:G4P:O3B	2.47	0.41
1:A:108:ILE:HG22	1:A:114:VAL:HG11	2.02	0.41
1:B:231:VAL:O	1:B:248:SER:HA	2.20	0.41
1:E:219:LEU:HA	1:E:219:LEU:HD23	1.83	0.41
1:A:6:SER:HB3	1:B:46:ILE:HG21	2.00	0.41
1:B:75:MET:HE3	1:B:80:ALA:HA	2.02	0.41
1:C:97:ILE:HD13	1:C:255:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ASN:ND2	1:F:181:ASN:O	2.54	0.41
1:F:161:LYS:HE2	1:F:175:TYR:OH	2.21	0.41
1:B:191:ARG:NH1	3:B:404:HOH:O	2.54	0.41
1:D:134:VAL:HG13	1:D:202:ILE:CD1	2.50	0.41
1:C:97:ILE:CG2	1:C:255:ILE:HG21	2.51	0.41
1:C:201:ILE:HG21	1:C:212:ILE:HG23	2.02	0.41
1:D:105:LEU:HD12	1:D:109:LEU:CG	2.50	0.41
1:E:82:GLU:O	1:E:85:GLN:HG3	2.20	0.41
1:E:175:TYR:CE1	1:E:211:THR:HG22	2.56	0.41
1:F:76:LYS:HA	1:F:76:LYS:HD2	1.81	0.41
1:B:29:PHE:HB3	1:B:40:ILE:HD13	2.02	0.41
1:D:133:VAL:CG2	1:D:157:VAL:HG23	2.51	0.40
1:B:179:SER:OG	1:B:180:SER:N	2.52	0.40
1:C:188:LEU:HD22	1:C:222:PHE:CZ	2.56	0.40
1:F:104:TYR:CZ	1:F:106:THR:HB	2.56	0.40
1:B:188:LEU:HB2	1:B:218:LEU:HD21	2.03	0.40
1:C:107:ASP:OD1	1:C:107:ASP:N	2.54	0.40
1:C:191:ARG:O	1:C:191:ARG:HG3	2.21	0.40
1:E:46:ILE:HG21	1:F:6:SER:HB3	2.02	0.40
1:C:96:ARG:NH2	1:C:107:ASP:OD2	2.52	0.40
1:C:194:LYS:O	1:C:197:SER:OG	2.33	0.40
1:D:200:LEU:HG	1:D:202:ILE:CD1	2.51	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:CG	1:D:163:ASN:ND2[1_465]	1.58	0.62
1:B:163:ASN:ND2	1:D:163:ASN:OD1[1_465]	1.95	0.25
1:B:163:ASN:ND2	1:D:163:ASN:ND2[1_465]	2.01	0.19
1:B:163:ASN:ND2	1:D:163:ASN:CG[1_465]	2.15	0.05
1:B:163:ASN:OD1	1:D:163:ASN:ND2[1_465]	2.16	0.04

## 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	266/285 (93%)	254 (96%)	12 (4%)	0	100	100
1	B	265/285 (93%)	250 (94%)	15 (6%)	0	100	100
1	C	248/285 (87%)	242 (98%)	6 (2%)	0	100	100
1	D	253/285 (89%)	241 (95%)	12 (5%)	0	100	100
1	E	254/285 (89%)	247 (97%)	7 (3%)	0	100	100
1	F	259/285 (91%)	252 (97%)	7 (3%)	0	100	100
All	All	1545/1710 (90%)	1486 (96%)	59 (4%)	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	230/244 (94%)	225 (98%)	5 (2%)	52	64
1	B	228/244 (93%)	223 (98%)	5 (2%)	52	64
1	C	218/244 (89%)	209 (96%)	9 (4%)	30	40
1	D	223/244 (91%)	212 (95%)	11 (5%)	25	32
1	E	222/244 (91%)	219 (99%)	3 (1%)	67	77
1	F	227/244 (93%)	223 (98%)	4 (2%)	59	71
All	All	1348/1464 (92%)	1311 (97%)	37 (3%)	44	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	41	SER
1	A	105	LEU
1	A	160	ARG

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Mol	Chain	Res	Type
1	A	244	ASP
1	B	5	ARG
1	B	39	SER
1	B	85	GLN
1	B	244	ASP
1	B	260	LYS
1	C	4	ARG
1	C	49	GLN
1	C	76	LYS
1	C	82	GLU
1	C	140	LYS
1	C	169	SER
1	C	173	ILE
1	C	177	SER
1	C	223	ASN
1	D	2	LYS
1	D	3	PHE
1	D	90	SER
1	D	113	SER
1	D	177	SER
1	D	192	SER
1	D	207	LYS
1	D	213	ASN
1	D	241	ARG
1	D	252	LEU
1	D	261	SER
1	E	140	LYS
1	E	160	ARG
1	E	161	LYS
1	F	38	SER
1	F	169	SER
1	F	190	LYS
1	F	262	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	B	85	GLN
1	B	265	GLN
1	C	93	ASN
1	C	217	ASN

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Mol	Chain	Res	Type
1	D	85	GLN
1	D	265	GLN
1	E	53	GLN
1	E	268	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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	G4P	B	301	-	30,38,38	4.38	13 (43%)	43,61,61	1.68	8 (18%)
2	G4P	C	301	-	30,38,38	4.41	13 (43%)	43,61,61	1.92	9 (20%)
2	G4P	F	301	-	30,38,38	4.33	13 (43%)	43,61,61	2.07	12 (27%)
2	G4P	A	301	-	30,38,38	4.39	13 (43%)	43,61,61	1.76	9 (20%)

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	G4P	B	301	-	-	10/23/43/43	0/3/3/3
2	G4P	C	301	-	-	10/23/43/43	0/3/3/3
2	G4P	F	301	-	-	9/23/43/43	0/3/3/3
2	G4P	A	301	-	-	8/23/43/43	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	G4P	C2'-C3'	-13.78	1.22	1.52
2	B	301	G4P	C2'-C3'	-13.24	1.23	1.52
2	C	301	G4P	C2'-C3'	-13.12	1.23	1.52
2	F	301	G4P	C2'-C3'	-13.01	1.23	1.52
2	C	301	G4P	C4-N3	9.12	1.50	1.35
2	B	301	G4P	C4-N3	8.71	1.49	1.35
2	A	301	G4P	C4-N3	8.60	1.49	1.35
2	F	301	G4P	C5-C6	8.07	1.55	1.41
2	A	301	G4P	O4'-C1'	7.33	1.51	1.41
2	B	301	G4P	O4'-C1'	7.22	1.51	1.41
2	B	301	G4P	C5-C6	7.22	1.53	1.41
2	F	301	G4P	O4'-C1'	7.21	1.51	1.41
2	C	301	G4P	O4'-C1'	7.10	1.51	1.41
2	A	301	G4P	C5-C6	6.88	1.53	1.41
2	C	301	G4P	C5-C6	6.86	1.53	1.41
2	F	301	G4P	C4-N3	6.76	1.46	1.35
2	F	301	G4P	O4'-C4'	-6.60	1.30	1.45
2	C	301	G4P	C2-N2	6.36	1.46	1.33
2	A	301	G4P	O4'-C4'	-6.36	1.30	1.45
2	F	301	G4P	C6-N1	6.30	1.44	1.33
2	B	301	G4P	O4'-C4'	-6.18	1.31	1.45
2	C	301	G4P	O4'-C4'	-6.03	1.31	1.45
2	B	301	G4P	C6-N1	5.98	1.43	1.33
2	C	301	G4P	C6-N1	5.97	1.43	1.33
2	A	301	G4P	C6-N1	5.91	1.43	1.33
2	B	301	G4P	C2-N2	5.88	1.45	1.33
2	A	301	G4P	C2-N2	5.84	1.45	1.33
2	C	301	G4P	C3'-C4'	5.59	1.67	1.52
2	B	301	G4P	C3'-C4'	5.29	1.67	1.52
2	A	301	G4P	C3'-C4'	5.19	1.66	1.52
2	C	301	G4P	C2-N1	5.19	1.44	1.35
2	A	301	G4P	C2-N1	5.17	1.44	1.35
2	F	301	G4P	C2-N2	5.13	1.44	1.33
2	F	301	G4P	C2-N1	5.13	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	G4P	C2-N1	5.11	1.44	1.35
2	F	301	G4P	C3'-C4'	5.11	1.66	1.52
2	F	301	G4P	C2'-C1'	4.75	1.61	1.53
2	C	301	G4P	C2'-C1'	4.61	1.60	1.53
2	B	301	G4P	C2'-C1'	4.51	1.60	1.53
2	A	301	G4P	C2'-C1'	4.02	1.59	1.53
2	F	301	G4P	O2'-C2'	3.33	1.50	1.43
2	C	301	G4P	O2'-C2'	3.25	1.50	1.43
2	B	301	G4P	O2'-C2'	3.22	1.50	1.43
2	A	301	G4P	O2'-C2'	3.19	1.50	1.43
2	F	301	G4P	C8-N7	2.78	1.39	1.34
2	F	301	G4P	O6-C6	-2.59	1.18	1.24
2	C	301	G4P	C2-N3	2.50	1.46	1.34
2	B	301	G4P	C2-N3	2.43	1.46	1.34
2	A	301	G4P	C2-N3	2.37	1.45	1.34
2	A	301	G4P	O6-C6	-2.29	1.18	1.24
2	B	301	G4P	O6-C6	-2.28	1.18	1.24
2	C	301	G4P	O6-C6	-2.22	1.19	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	G4P	C4-C5-C6	-6.55	114.54	120.80
2	C	301	G4P	N3-C2-N1	-6.46	118.60	127.22
2	A	301	G4P	N3-C2-N1	-5.85	119.42	127.22
2	B	301	G4P	N3-C2-N1	-5.69	119.64	127.22
2	F	301	G4P	N2-C2-N1	5.56	125.90	117.25
2	F	301	G4P	N3-C2-N1	-5.02	120.53	127.22
2	C	301	G4P	O3C-PC-O3'	4.49	111.54	102.48
2	C	301	G4P	O4'-C1'-C2'	-4.36	100.55	106.93
2	C	301	G4P	C2-N3-C4	4.03	119.95	115.36
2	B	301	G4P	C2-N3-C4	3.97	119.89	115.36
2	B	301	G4P	O3C-PC-O3'	3.57	109.68	102.48
2	F	301	G4P	C1'-N9-C4	-3.53	120.43	126.64
2	C	301	G4P	C2-N1-C6	3.52	121.52	115.93
2	A	301	G4P	O3C-PC-O3'	3.34	109.21	102.48
2	A	301	G4P	C2-N3-C4	3.32	119.15	115.36
2	A	301	G4P	C2-N1-C6	3.19	120.99	115.93
2	F	301	G4P	PC-O3C-PD	-3.16	121.97	132.83
2	C	301	G4P	C5-C6-N1	-3.07	119.24	123.43
2	A	301	G4P	C5-C6-N1	-3.00	119.33	123.43
2	A	301	G4P	O3B-PB-O3A	2.79	114.00	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	G4P	C1'-N9-C4	2.73	131.44	126.64
2	F	301	G4P	O3C-PC-O3'	2.71	107.95	102.48
2	F	301	G4P	C2-N3-C4	2.70	118.44	115.36
2	B	301	G4P	C2-N1-C6	2.70	120.21	115.93
2	A	301	G4P	O4'-C1'-C2'	-2.65	103.05	106.93
2	B	301	G4P	C5-C6-N1	-2.63	119.84	123.43
2	F	301	G4P	N2-C2-N3	-2.59	113.57	117.79
2	F	301	G4P	PA-O3A-PB	-2.54	124.10	132.83
2	B	301	G4P	O4'-C1'-C2'	-2.40	103.42	106.93
2	B	301	G4P	PC-O3C-PD	-2.35	124.77	132.83
2	F	301	G4P	C2-N1-C6	2.31	119.59	115.93
2	B	301	G4P	N2-C2-N1	2.27	120.78	117.25
2	F	301	G4P	C4-C5-N7	-2.22	107.08	109.40
2	C	301	G4P	N2-C2-N1	2.17	120.62	117.25
2	A	301	G4P	N2-C2-N1	2.15	120.60	117.25
2	A	301	G4P	PC-O3'-C3'	-2.14	111.63	119.41
2	F	301	G4P	O2B-PB-O3A	2.09	111.63	104.64
2	C	301	G4P	PC-O3C-PD	-2.00	125.95	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	G4P	C5'-O5'-PA-O3A
2	A	301	G4P	C3'-C4'-C5'-O5'
2	A	301	G4P	C3'-O3'-PC-O2C
2	A	301	G4P	PD-O3C-PC-O3'
2	B	301	G4P	C5'-O5'-PA-O1A
2	B	301	G4P	C5'-O5'-PA-O2A
2	B	301	G4P	C3'-C4'-C5'-O5'
2	C	301	G4P	C5'-O5'-PA-O1A
2	C	301	G4P	C5'-O5'-PA-O2A
2	F	301	G4P	C5'-O5'-PA-O1A
2	F	301	G4P	C5'-O5'-PA-O2A
2	C	301	G4P	C3'-C4'-C5'-O5'
2	A	301	G4P	C3'-O3'-PC-O3C
2	A	301	G4P	O4'-C4'-C5'-O5'
2	B	301	G4P	C4'-C3'-O3'-PC
2	B	301	G4P	C2'-C3'-O3'-PC
2	B	301	G4P	O4'-C4'-C5'-O5'
2	F	301	G4P	C3'-C4'-C5'-O5'
2	C	301	G4P	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	F	301	G4P	O4'-C4'-C5'-O5'
2	A	301	G4P	C3'-O3'-PC-O1C
2	F	301	G4P	C4'-C5'-O5'-PA
2	B	301	G4P	PD-O3C-PC-O3'
2	C	301	G4P	PD-O3C-PC-O3'
2	F	301	G4P	PD-O3C-PC-O3'
2	B	301	G4P	PB-O3A-PA-O2A
2	A	301	G4P	C5'-O5'-PA-O1A
2	B	301	G4P	C4'-C5'-O5'-PA
2	F	301	G4P	C3'-O3'-PC-O3C
2	F	301	G4P	PB-O3A-PA-O2A
2	C	301	G4P	O4'-C4'-C5'-O5'
2	B	301	G4P	C5'-O5'-PA-O3A
2	C	301	G4P	C5'-O5'-PA-O3A
2	F	301	G4P	C5'-O5'-PA-O3A
2	C	301	G4P	PB-O3A-PA-O2A
2	C	301	G4P	PD-O3C-PC-O1C
2	C	301	G4P	PD-O3C-PC-O2C

There are no ring outliers.

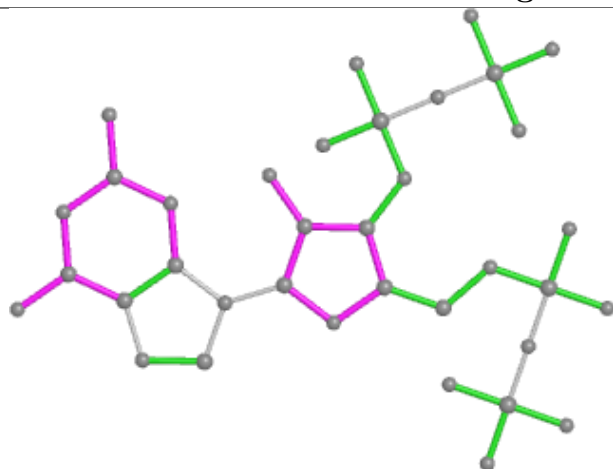
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	G4P	9	0
2	C	301	G4P	11	0
2	F	301	G4P	1	0
2	A	301	G4P	5	0

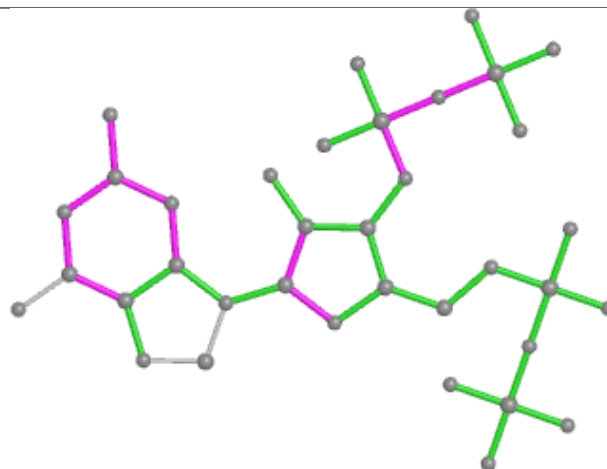
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



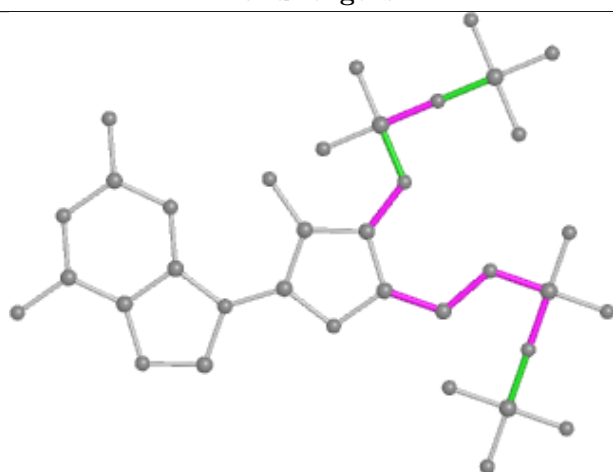
## Ligand G4P B 301



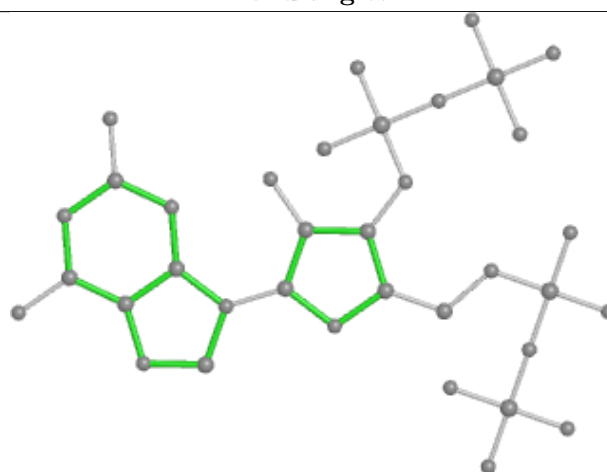
Bond lengths



Bond angles

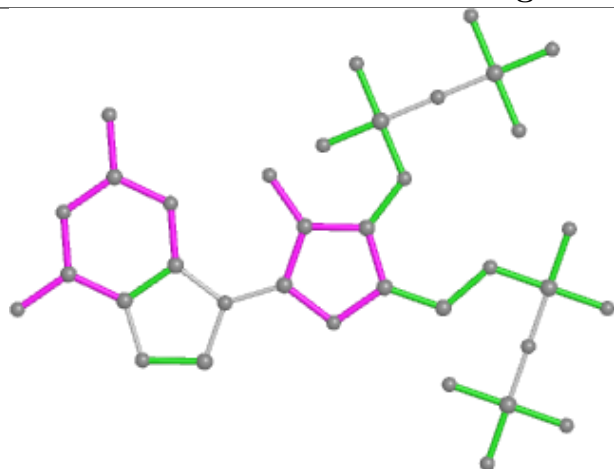


Torsions

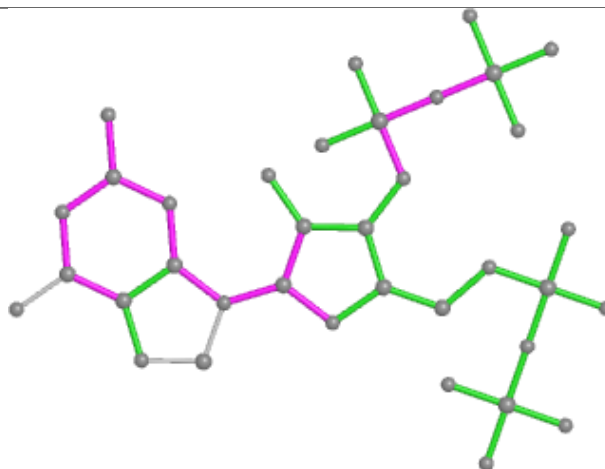


Rings

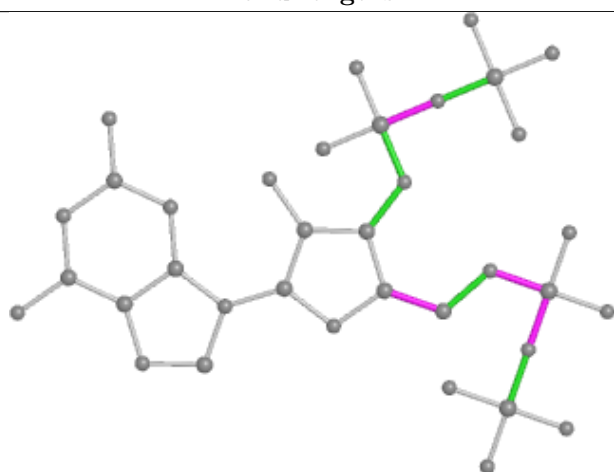
## Ligand G4P C 301



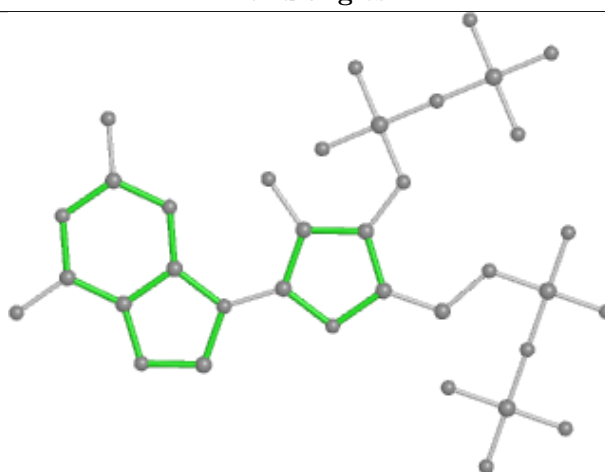
Bond lengths



Bond angles

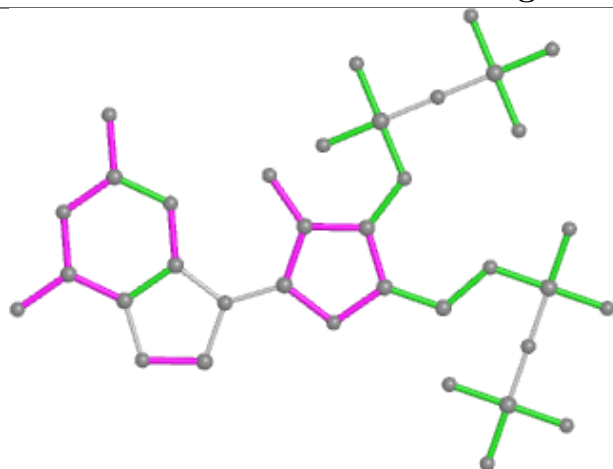


Torsions

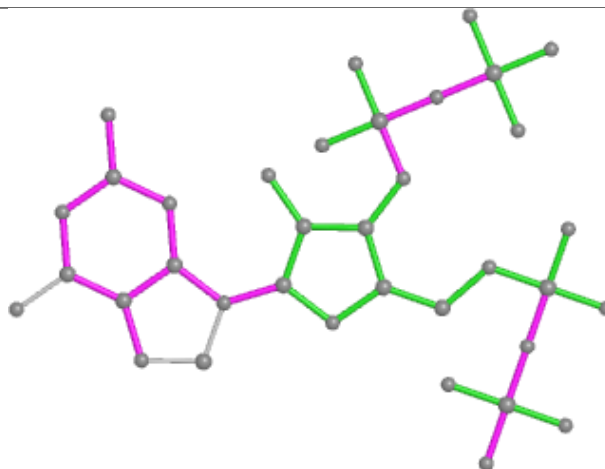


Rings

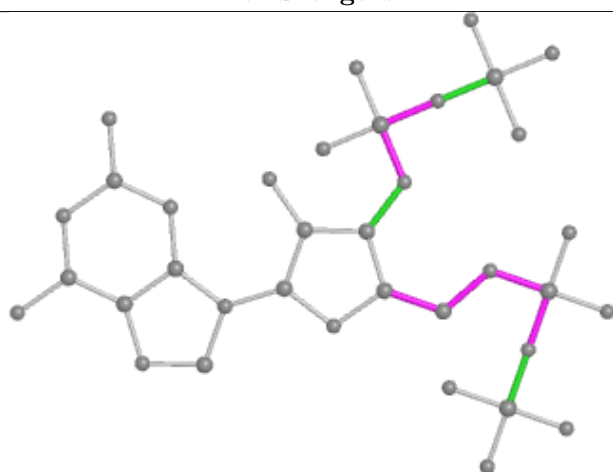
## Ligand G4P F 301



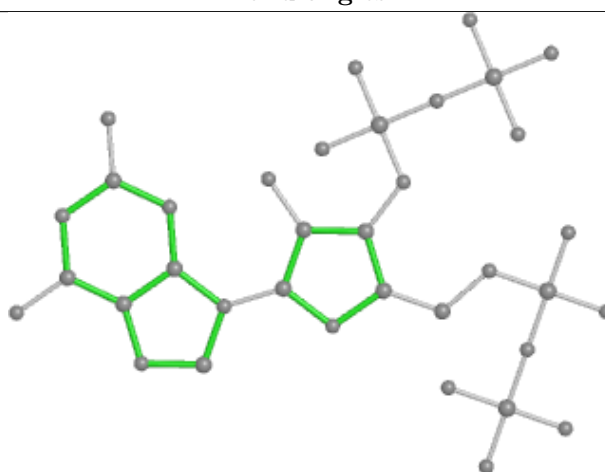
Bond lengths



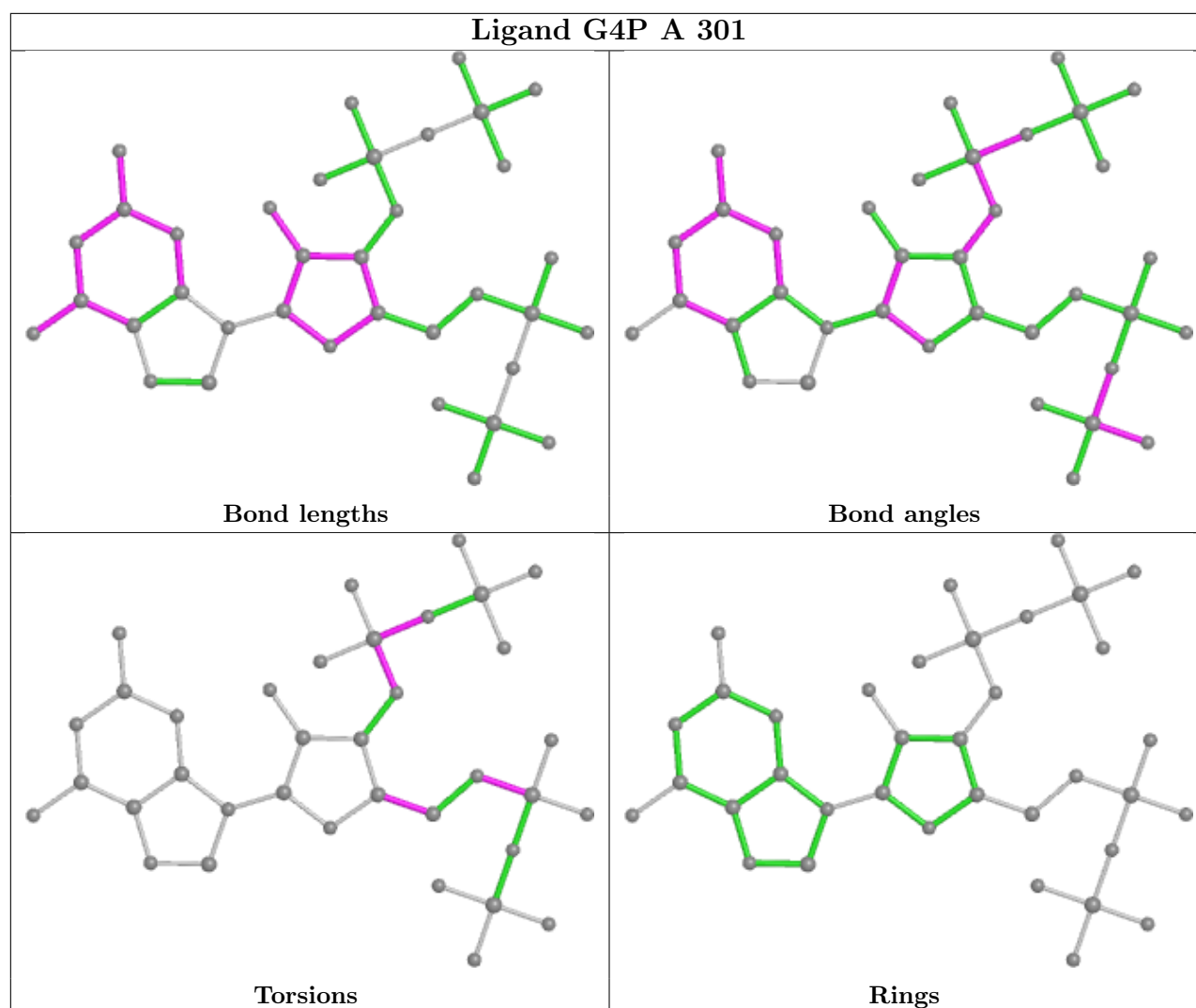
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	270/285 (94%)	-0.25	5 (1%)	66 64	32, 63, 118, 181	0
1	B	269/285 (94%)	-0.05	5 (1%)	66 64	38, 61, 140, 207	0
1	C	256/285 (89%)	0.14	10 (3%)	39 36	48, 84, 144, 316	0
1	D	261/285 (91%)	0.17	15 (5%)	23 20	39, 71, 159, 220	0
1	E	260/285 (91%)	-0.10	7 (2%)	54 50	43, 77, 145, 182	0
1	F	265/285 (92%)	-0.25	7 (2%)	56 52	40, 68, 148, 184	0
All	All	1581/1710 (92%)	-0.06	49 (3%)	49 45	32, 69, 145, 316	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	TYR	10.3
1	E	163	ASN	7.1
1	D	99	PRO	6.0
1	C	183	ILE	5.5
1	B	255	ILE	5.2
1	D	100	GLY	4.9
1	D	255	ILE	4.8
1	D	98	LEU	4.5
1	C	178	GLY	4.4
1	E	182	ARG	4.4
1	E	177	SER	4.2
1	D	103	VAL	4.2
1	D	254	THR	3.4
1	E	183	ILE	3.3
1	F	258	LYS	3.3
1	C	177	SER	3.2
1	D	242	LEU	3.2
1	F	256	ASN	3.1
1	C	176	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	65	ALA	3.0
1	C	259	GLU	3.0
1	F	242	LEU	2.9
1	A	275	ASP	2.8
1	F	165	VAL	2.7
1	F	261	SER	2.7
1	D	163	ASN	2.7
1	D	261	SER	2.6
1	D	65	ALA	2.5
1	B	180	SER	2.5
1	F	163	ASN	2.5
1	A	178	GLY	2.5
1	D	2	LYS	2.5
1	B	242	LEU	2.4
1	C	261	SER	2.4
1	A	242	LEU	2.4
1	B	183	ILE	2.4
1	C	91	LEU	2.4
1	D	108	ILE	2.4
1	E	166	THR	2.3
1	E	167	GLU	2.3
1	C	65	ALA	2.3
1	F	102	TYR	2.3
1	C	37	LYS	2.2
1	D	105	LEU	2.2
1	A	179	SER	2.2
1	C	209	GLY	2.2
1	E	262	ILE	2.1
1	D	162	ASP	2.1
1	A	146	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

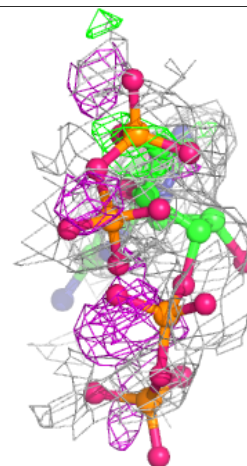
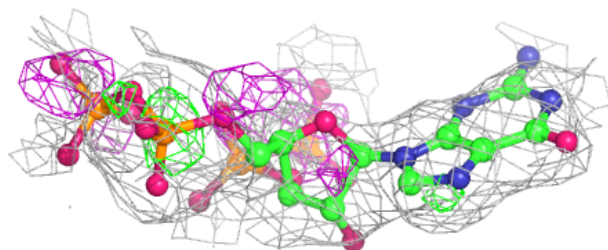
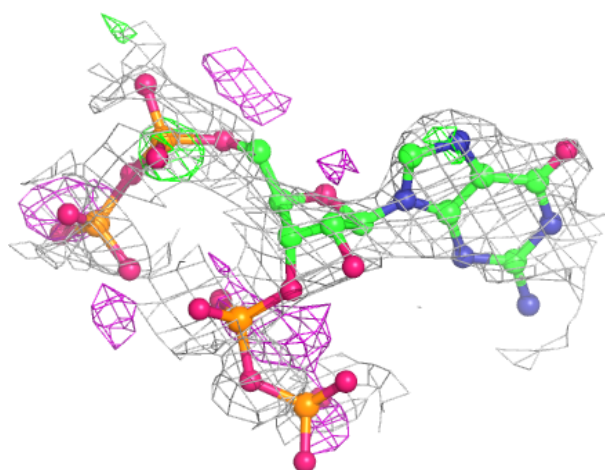
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	G4P	B	301	36/36	0.57	0.30	70,95,109,111	0
2	G4P	F	301	36/36	0.59	0.36	180,213,276,277	0
2	G4P	C	301	36/36	0.61	0.38	215,298,342,343	0
2	G4P	A	301	36/36	0.83	0.26	83,92,99,99	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.

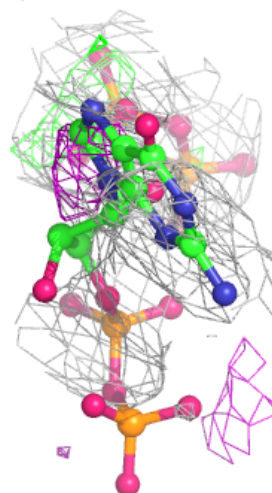
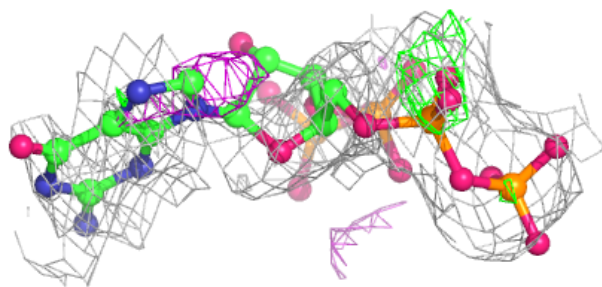
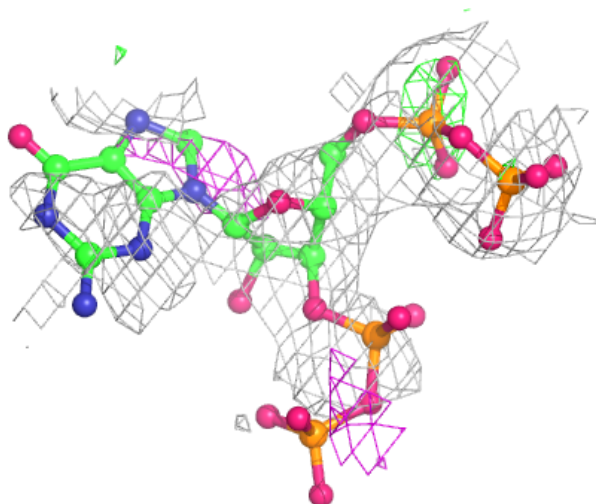
### Electron density around G4P B 301:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around G4P F 301:**

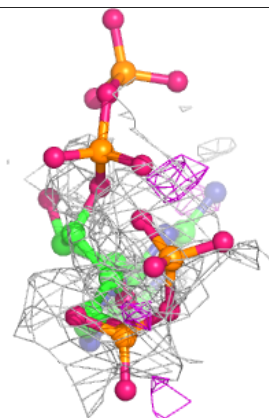
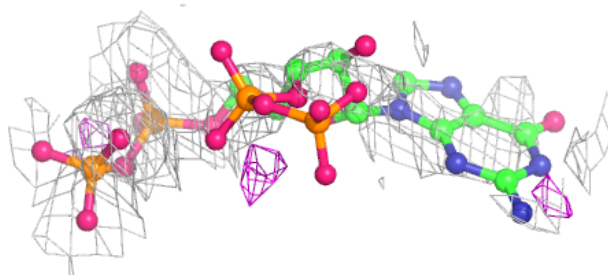
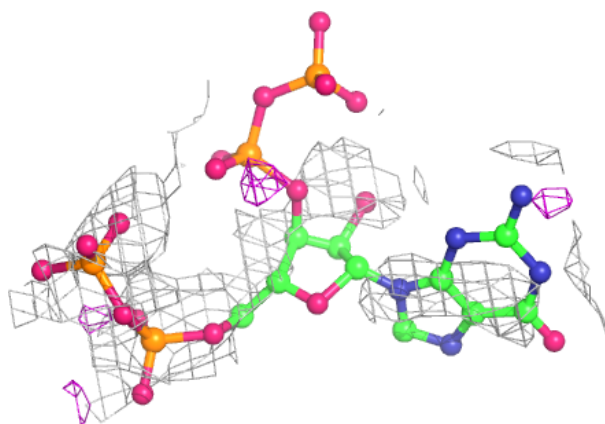
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





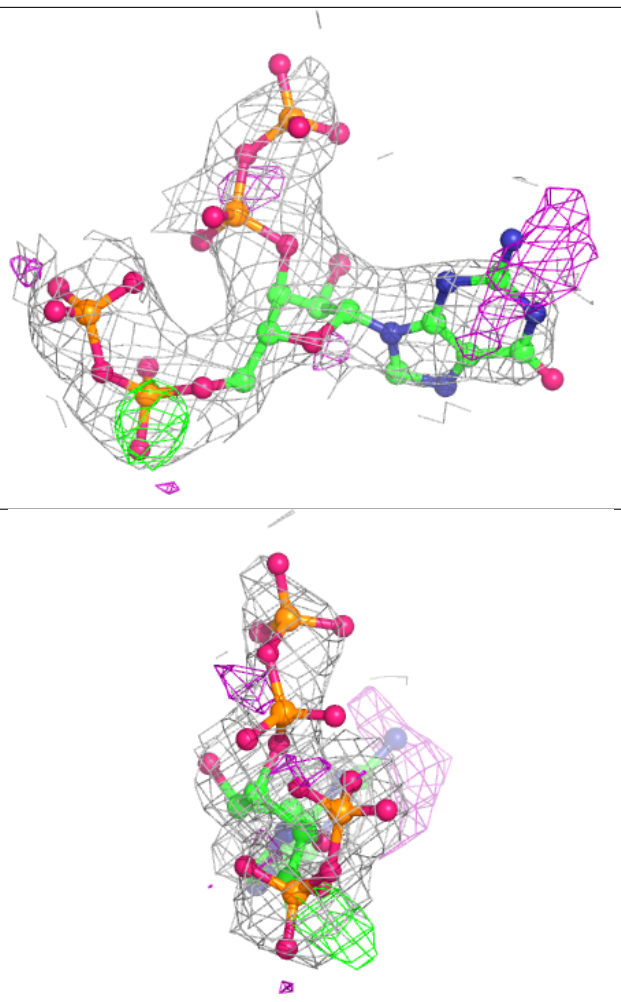
**Electron density around G4P C 301:**

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



**Electron density around G4P 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.