Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 10:19 PM EST

PDB ID	:	4RHT
Title	:	Crystal structures of Mycobacterium tuberculosis 6-oxopurine phosphoribosyltransferase which is a potential target for drug development against this disease
Authors	:	Eng, W.S.; Hockova, D.; Spacek, P.; West, N.P.; Woods, K.; Naesens, L.M.J.; Keough, D.T.; Guddat, L.W.
Deposited on	:	2014-10-03
Resolution	:	2.76 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

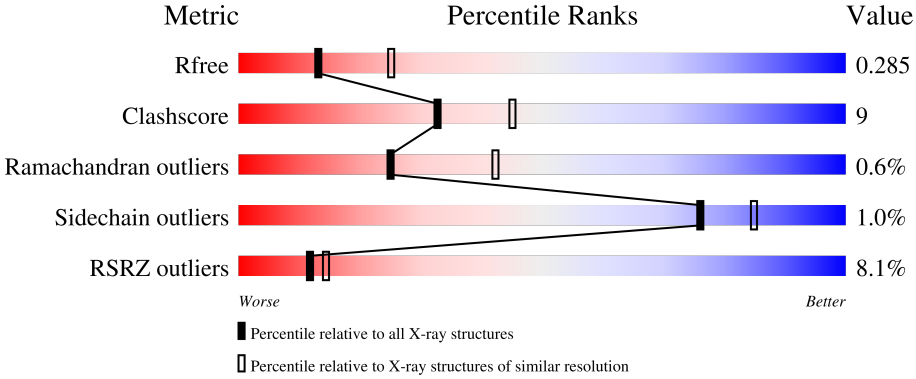
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	201	2%, 71%, 12%, 17%
1	B	201	%, 75%, 7%, 17%
1	C	201	12%, 56%, 23%, •, 20%
1	D	201	11%, 59%, 21%, 19%

2 Entry composition (i)

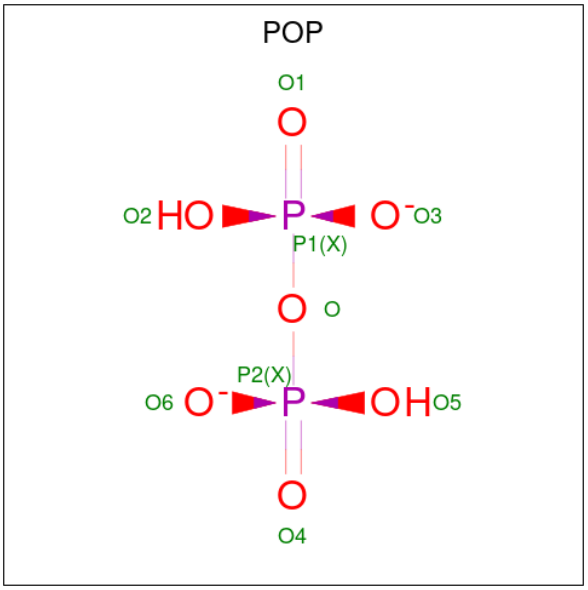
There are 5 unique types of molecules in this entry. The entry contains 5151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hypoxanthine-guanine phosphoribosyltransferase Hpt.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1286	821	221	242	2	0	0	0
1	B	166	1271	816	214	239	2	0	0	0
1	C	161	1196	766	202	226	2	0	0	0
1	D	162	1214	778	204	230	2	0	0	0

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	9	7	2	0	0
2	B	1	9	7	2	0	0

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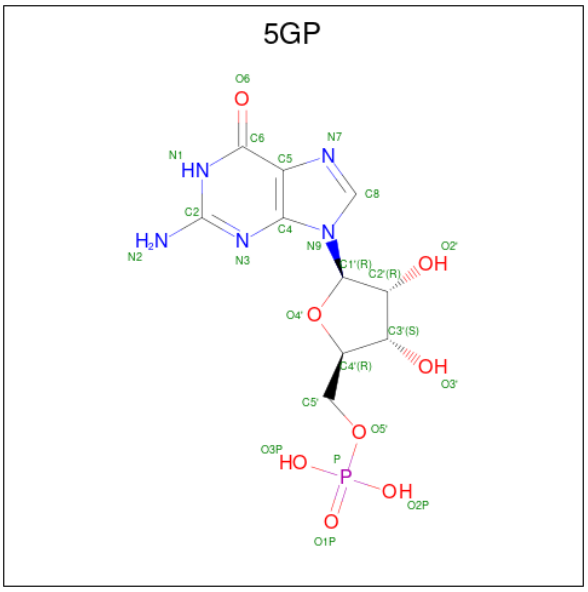
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
2	C	1	9	7	2		0	0
			Total	O	P			
2	D	1	9	7	2		0	0

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	24	10	5	8	1	0	0
			Total	C	N	O	P		
3	B	1	24	10	5	8	1	0	0
			Total	C	N	O	P		
3	C	1	24	10	5	8	1	0	0
			Total	C	N	O	P		
3	D	1	24	10	5	8	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0
			Total	Mg		
4	B	2	2	2	0	0
			Total	Mg		
4	C	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	D	2	2	2	0	0

- Molecule 5 is water.

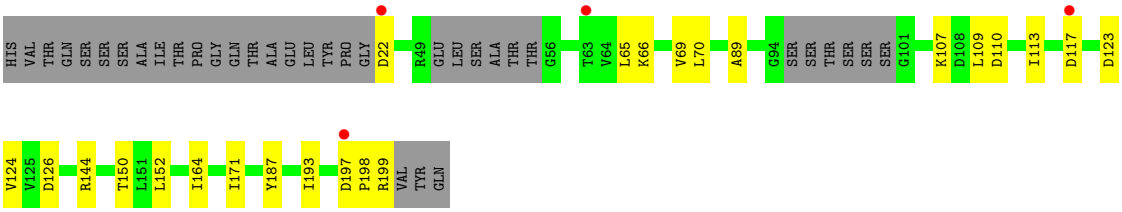
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	17	17	17	0	0
			Total	O		
5	B	16	16	16	0	0
			Total	O		
5	C	5	5	5	0	0
			Total	O		
5	D	6	6	6	0	0

3 Residue-property plots (i)

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

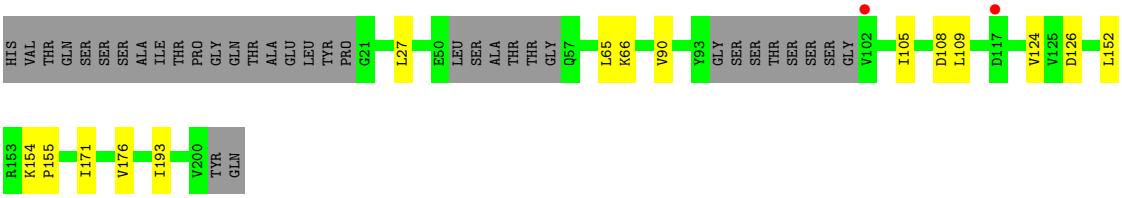
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase Hpt

Chain A:



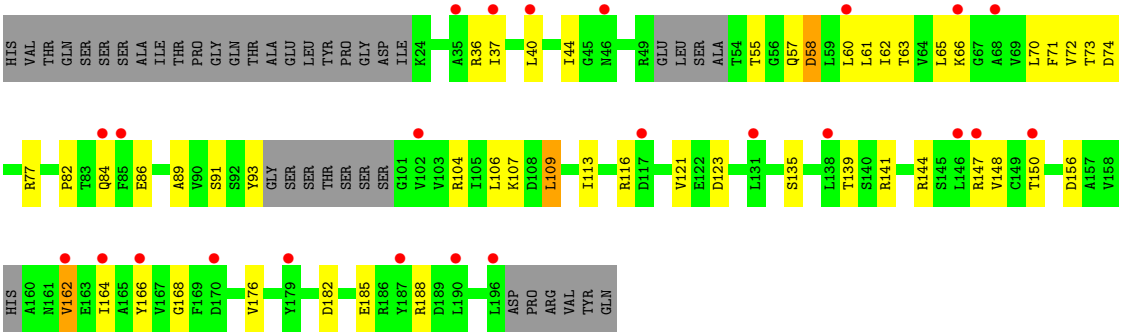
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase Hpt

Chain B:



• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase Hpt

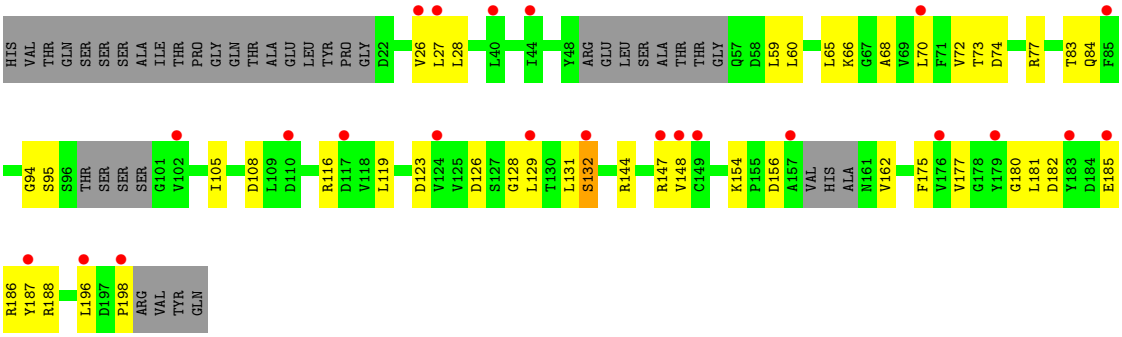
Chain C:



• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase Hpt

Chain D:

11%
59%
21%
19%


HIS VAL THR GLN SER SER SER ALA ILE THR PRO GLY GLN THR ALA GLU LEU TYR PRO GLY D22 V26 L27 L28 L40 I44 Y48 ARG GLU LEU SER ALA THR THR GLY Q57 D58 L59 L60 L65 K66 G67 A68 V69 L70 F71 V72 T73 D74 R77 T83 Q84 F85
G94 S95 S96 THR SER SER SER G101 V102 I105 D108 L109 D110 R116 D117 V118 L119 D123 V124 V125 D126 S127 G128 L129 T130 L131 S132 R144 R147 V148 C149 K154 P155 D156 A157 VAL HIS ALA N161 V162 F175 V176 V177 G178 Y179 G180 L181 D182 Y183 D184 E185
R186 Y187 R188 L196 D197 P198 ARG VAL TYR GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.42Å 85.58Å 156.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.76 47.10 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.10-2.76) 93.7 (47.10-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.225 , 0.284 0.226 , 0.285	Depositor DCC
R_{free} test set	1998 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5151	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.24 % 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 9.7035e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, MG, POP

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	0.23	0/1305	0.40	0/1774
1	B	0.22	0/1290	0.37	0/1758
1	C	0.25	0/1212	0.41	0/1652
1	D	0.29	0/1230	0.48	0/1675
All	All	0.25	0/5037	0.41	0/6859

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1286	0	1290	15	0
1	B	1271	0	1261	8	0
1	C	1196	0	1156	44	0
1	D	1214	0	1188	27	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	1	0
2	D	9	0	0	0	0
3	A	24	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	12	0	0
3	C	24	0	12	2	0
3	D	24	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	17	0	0	0	0
5	B	16	0	0	0	0
5	C	5	0	0	1	0
5	D	6	0	0	0	0
All	All	5151	0	4943	87	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 9.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ASP:HB3	1:B:154:LYS:HB2	1.71	0.73
1:C:185:GLU:O	1:D:84:GLN:NE2	2.25	0.69
1:A:117:ASP:OD1	1:A:144:ARG:NH2	2.27	0.67
2:C:301:POP:O4	3:C:302:5GP:O2'	2.14	0.66
1:D:182:ASP:OD2	1:D:188:ARG:NH2	2.30	0.65
1:B:124:VAL:HG22	1:B:152:LEU:HB2	1.80	0.64
1:A:89:ALA:HB3	1:A:107:LYS:HB3	1.81	0.63
1:C:36:ARG:NH1	1:C:168:GLY:O	2.32	0.62
1:C:55:THR:HG22	1:C:57:GLN:H	1.64	0.61
1:D:74:ASP:OD1	1:D:77:ARG:NH2	2.34	0.60
1:A:152:LEU:HD11	1:A:193:ILE:HD13	1.82	0.60
1:C:185:GLU:OE2	1:C:188:ARG:NH2	2.35	0.60
1:C:84:GLN:HG2	1:D:185:GLU:OE1	2.02	0.60
1:C:150:THR:HG22	1:C:164:ILE:HG21	1.84	0.59
1:C:84:GLN:HG2	1:D:185:GLU:CD	2.23	0.58
1:C:84:GLN:HE22	1:C:116:ARG:NH2	2.03	0.57
1:C:84:GLN:HE22	1:C:116:ARG:HH22	1.51	0.57
1:C:66:LYS:NZ	5:C:405:HOH:O	2.36	0.56
1:A:126:ASP:OD2	1:A:126:ASP:N	2.40	0.55
1:A:197:ASP:O	1:A:199:ARG:N	2.40	0.55
1:C:63:THR:HG22	1:C:121:VAL:HB	1.89	0.55
1:C:147:ARG:NH2	1:C:166:TYR:OH	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ILE:HG12	1:C:86:GLU:HB3	1.89	0.54
1:C:74:ASP:OD1	1:C:77:ARG:NH2	2.41	0.54
1:C:89:ALA:HB3	1:C:107:LYS:HB3	1.89	0.54
1:C:63:THR:HG21	1:C:72:VAL:CG1	2.38	0.54
1:C:60:LEU:HD12	1:C:84:GLN:HB3	1.90	0.53
1:C:40:LEU:O	1:C:44:ILE:HG12	2.07	0.53
1:C:55:THR:OG1	1:C:144:ARG:NH1	2.42	0.53
1:A:109:LEU:HD13	1:A:113:ILE:HD11	1.90	0.53
1:C:36:ARG:HE	1:C:40:LEU:HD11	1.74	0.53
1:D:177:VAL:HG21	1:D:196:LEU:HD13	1.90	0.52
1:C:176:VAL:O	3:C:302:5GP:N2	2.32	0.52
1:C:91:SER:HB2	1:C:106:LEU:HD11	1.91	0.52
1:D:126:ASP:OD1	1:D:128:GLY:N	2.43	0.52
1:C:185:GLU:HB3	1:D:84:GLN:NE2	2.25	0.51
1:C:62:ILE:HD13	1:C:109:LEU:HD21	1.90	0.51
1:D:116:ARG:H	1:D:144:ARG:H	1.58	0.50
1:B:90:VAL:HG22	1:B:105:ILE:HA	1.96	0.48
1:C:182:ASP:OD1	1:C:188:ARG:NH1	2.46	0.47
1:C:113:ILE:HG12	1:C:141:ARG:HD3	1.97	0.47
1:C:84:GLN:HG2	1:D:185:GLU:OE2	2.14	0.47
1:D:123:ASP:HB2	1:D:181:LEU:HD21	1.97	0.47
1:D:65:LEU:HA	1:D:66:LYS:HA	1.60	0.47
1:B:108:ASP:OD1	1:B:109:LEU:N	2.42	0.46
1:D:105:ILE:HG21	1:D:108:ASP:HB2	1.97	0.46
1:D:123:ASP:OD1	1:D:123:ASP:N	2.46	0.46
1:D:129:LEU:HD21	1:D:132:SER:OG	2.16	0.46
1:C:123:ASP:OD1	1:C:123:ASP:N	2.47	0.45
1:A:123:ASP:OD1	1:A:123:ASP:N	2.41	0.45
1:D:154:LYS:O	1:D:156:ASP:N	2.46	0.45
1:C:185:GLU:HB3	1:D:84:GLN:HE21	1.80	0.45
1:A:152:LEU:HD13	1:A:171:ILE:HD13	1.98	0.45
1:C:135:SER:O	1:C:139:THR:HG23	2.17	0.45
1:D:131:LEU:HD21	1:D:148:VAL:HG11	2.00	0.44
1:D:186:ARG:HD3	1:D:187:TYR:CE2	2.52	0.44
1:A:124:VAL:HG22	1:A:152:LEU:HB2	2.00	0.44
1:A:144:ARG:HH21	1:A:144:ARG:HG2	1.82	0.44
1:B:65:LEU:HA	1:B:66:LYS:HA	1.59	0.44
1:C:63:THR:CG2	1:C:121:VAL:HB	2.48	0.44
1:C:73:THR:O	1:C:77:ARG:NE	2.47	0.43
1:C:148:VAL:HG13	1:C:164:ILE:HA	2.00	0.43
1:C:93:TYR:CZ	1:C:104:ARG:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HB3	1:D:28:LEU:HD12	2.00	0.43
1:B:27:LEU:HD22	1:B:176:VAL:HG11	1.99	0.43
1:C:58:ASP:HB3	1:C:82:PRO:O	2.19	0.43
1:A:69:VAL:HG23	1:A:70:LEU:HD12	2.00	0.42
1:B:152:LEU:HD11	1:B:193:ILE:HD13	2.01	0.42
1:C:70:LEU:HD12	1:D:73:THR:HB	2.01	0.42
1:A:22:ASP:OD2	1:A:187:TYR:OH	2.12	0.42
1:C:65:LEU:HA	1:C:66:LYS:HA	1.74	0.42
1:C:135:SER:OG	1:C:162:VAL:HG11	2.20	0.42
1:C:156:ASP:OD1	1:C:156:ASP:N	2.43	0.42
1:A:65:LEU:HA	1:A:66:LYS:HA	1.63	0.42
1:D:59:LEU:HD23	1:D:83:THR:HG22	2.01	0.42
1:B:155:PRO:HD3	1:B:171:ILE:O	2.20	0.42
1:D:175:PHE:CE2	1:D:198:PRO:HG3	2.55	0.42
1:D:60:LEU:HD23	1:D:84:GLN:HB3	2.01	0.42
1:A:110:ASP:OD1	1:C:104:ARG:NH1	2.53	0.41
1:C:37:ILE:HG12	1:C:71:PHE:HE1	1.85	0.41
1:C:58:ASP:N	1:C:58:ASP:OD1	2.51	0.41
1:D:70:LEU:HD23	1:D:180:GLY:N	2.35	0.41
1:C:60:LEU:CD1	1:C:84:GLN:HB3	2.50	0.41
1:C:61:LEU:N	1:C:84:GLN:O	2.45	0.41
1:D:119:LEU:HD12	1:D:147:ARG:O	2.21	0.41
1:A:150:THR:HG22	1:A:164:ILE:HG21	2.03	0.41
1:D:68:ALA:O	1:D:72:VAL:HG23	2.21	0.41

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	160/201 (80%)	153 (96%)	6 (4%)	1 (1%)	25 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	160/201 (80%)	154 (96%)	6 (4%)	0	100	100
1	C	153/201 (76%)	143 (94%)	9 (6%)	1 (1%)	22	39
1	D	154/201 (77%)	136 (88%)	16 (10%)	2 (1%)	12	21
All	All	627/804 (78%)	586 (94%)	37 (6%)	4 (1%)	25	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	VAL
1	A	198	PRO
1	D	95	SER
1	D	94	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/174 (80%)	139 (100%)	0	100	100
1	B	135/174 (78%)	135 (100%)	0	100	100
1	C	121/174 (70%)	119 (98%)	2 (2%)	60	76
1	D	126/174 (72%)	123 (98%)	3 (2%)	49	68
All	All	521/696 (75%)	516 (99%)	5 (1%)	76	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	ASP
1	C	109	LEU
1	D	26	VAL
1	D	132	SER
1	D	162	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	84	GLN
1	D	84	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	5GP	C	302	-	22,26,26	1.20	2 (9%)	26,40,40	1.24	4 (15%)
3	5GP	A	302	-	22,26,26	1.21	2 (9%)	26,40,40	1.26	3 (11%)
3	5GP	D	302	-	22,26,26	1.23	2 (9%)	26,40,40	1.26	4 (15%)
2	POP	C	301	4	6,8,8	0.72	0	13,13,13	1.45	1 (7%)
2	POP	D	301	4	6,8,8	0.73	0	13,13,13	1.28	1 (7%)
2	POP	B	301	4	6,8,8	0.75	0	13,13,13	1.22	1 (7%)
2	POP	A	301	4	6,8,8	0.75	0	13,13,13	1.23	1 (7%)
3	5GP	B	302	-	22,26,26	1.21	2 (9%)	26,40,40	1.24	4 (15%)

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
3	5GP	C	302	-	-	5/6/26/26	0/3/3/3
3	5GP	A	302	-	-	6/6/26/26	0/3/3/3
3	5GP	D	302	-	-	2/6/26/26	0/3/3/3
2	POP	C	301	4	-	0/6/6/6	-
2	POP	D	301	4	-	0/6/6/6	-
2	POP	B	301	4	-	0/6/6/6	-
2	POP	A	301	4	-	0/6/6/6	-
3	5GP	B	302	-	-	1/6/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	5GP	C5-C6	-4.12	1.39	1.47
3	C	302	5GP	C5-C6	-4.00	1.39	1.47
3	A	302	5GP	C5-C6	-3.99	1.39	1.47
3	B	302	5GP	C5-C6	-3.96	1.39	1.47
3	B	302	5GP	C6-N1	-2.52	1.34	1.37
3	A	302	5GP	C6-N1	-2.45	1.34	1.37
3	D	302	5GP	C6-N1	-2.36	1.34	1.37
3	C	302	5GP	C6-N1	-2.33	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	POP	P2-O-P1	-4.06	118.89	132.83
2	D	301	POP	P2-O-P1	-3.38	121.23	132.83
2	A	301	POP	P2-O-P1	-3.33	121.42	132.83
3	D	302	5GP	C5-C6-N1	3.17	119.56	113.95
3	A	302	5GP	C5-C6-N1	3.16	119.53	113.95
3	B	302	5GP	C5-C6-N1	3.14	119.49	113.95
3	C	302	5GP	C5-C6-N1	3.07	119.38	113.95
2	B	301	POP	P2-O-P1	-2.72	123.49	132.83
3	C	302	5GP	C8-N7-C5	2.43	107.61	102.99
3	A	302	5GP	C8-N7-C5	2.41	107.58	102.99
3	D	302	5GP	C8-N7-C5	2.39	107.55	102.99
3	B	302	5GP	C8-N7-C5	2.36	107.48	102.99
3	B	302	5GP	C2-N1-C6	-2.29	120.89	125.10
3	D	302	5GP	C2-N1-C6	-2.28	120.90	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	5GP	C2-N1-C6	-2.26	120.94	125.10
3	D	302	5GP	O6-C6-C5	-2.21	120.06	124.37
3	A	302	5GP	C2-N1-C6	-2.10	121.23	125.10
3	C	302	5GP	O6-C6-C5	-2.02	120.42	124.37
3	B	302	5GP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	5GP	C5'-O5'-P-O1P
3	A	302	5GP	C5'-O5'-P-O2P
3	A	302	5GP	C5'-O5'-P-O3P
3	A	302	5GP	O4'-C4'-C5'-O5'
3	C	302	5GP	C5'-O5'-P-O1P
3	C	302	5GP	C5'-O5'-P-O2P
3	C	302	5GP	C5'-O5'-P-O3P
3	D	302	5GP	C3'-C4'-C5'-O5'
3	A	302	5GP	C3'-C4'-C5'-O5'
3	D	302	5GP	O4'-C4'-C5'-O5'
3	C	302	5GP	C4'-C5'-O5'-P
3	A	302	5GP	C4'-C5'-O5'-P
3	B	302	5GP	C4'-C5'-O5'-P
3	C	302	5GP	O4'-C4'-C5'-O5'

There are no ring outliers.

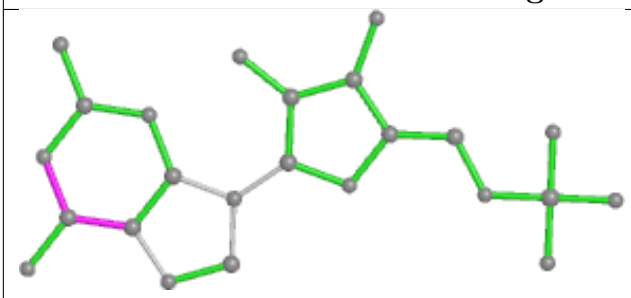
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	5GP	2	0
2	C	301	POP	1	0

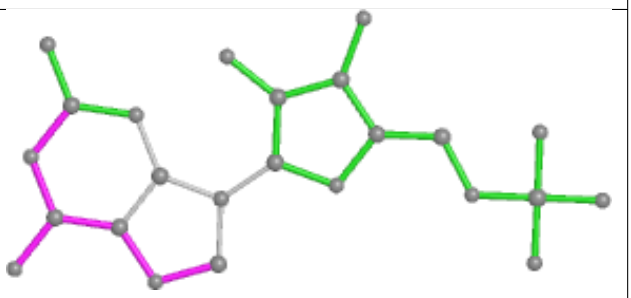
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

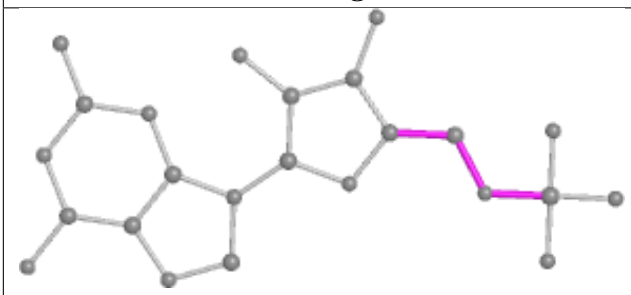
Ligand 5GP C 302



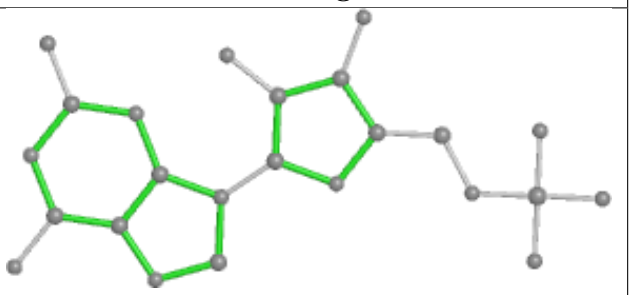
Bond lengths



Bond angles

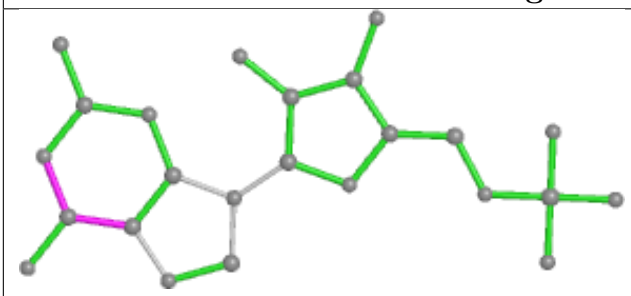


Torsions

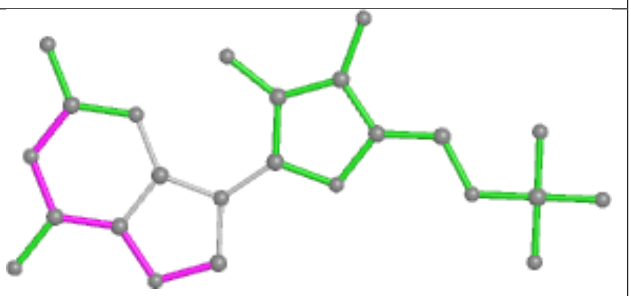


Rings

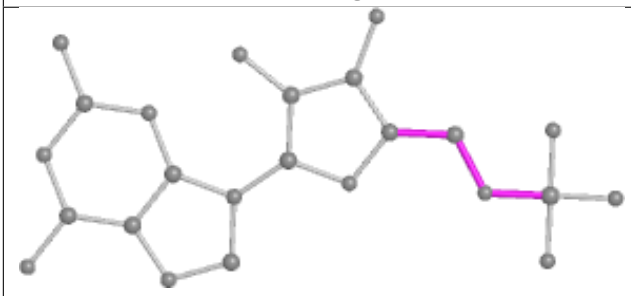
Ligand 5GP A 302



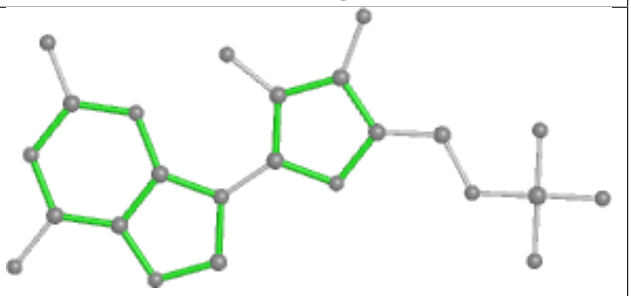
Bond lengths



Bond angles

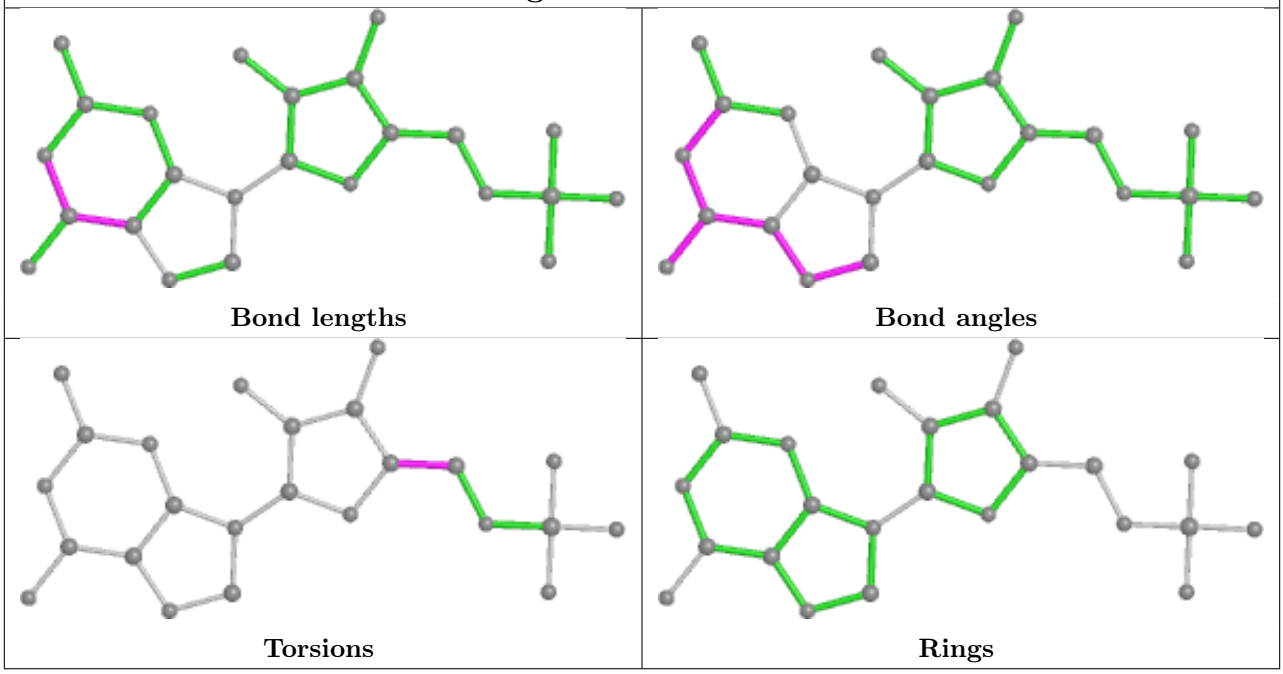


Torsions

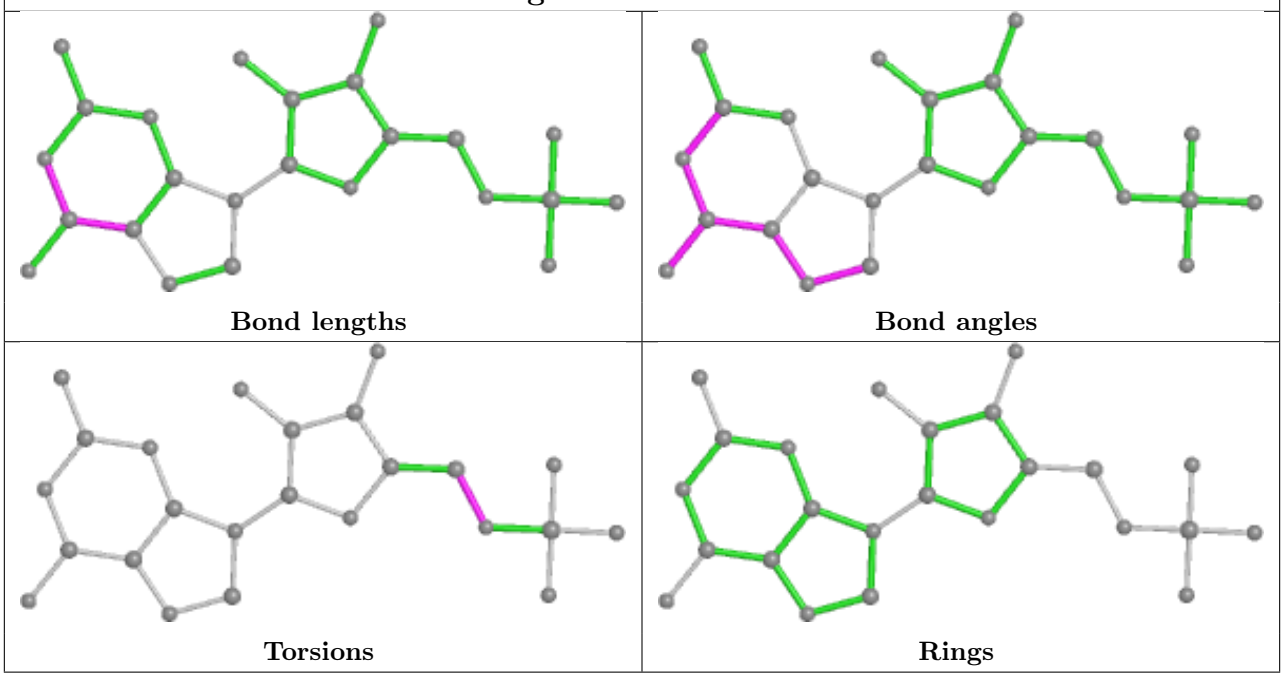


Rings

Ligand 5GP D 302



Ligand 5GP B 302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	166/201 (82%)	0.15	4 (2%)	59	68	33, 51, 92, 121	0
1	B	166/201 (82%)	0.18	2 (1%)	79	85	34, 55, 90, 117	0
1	C	161/201 (80%)	0.96	24 (14%)	2	2	51, 101, 131, 157	0
1	D	162/201 (80%)	1.00	23 (14%)	2	3	59, 102, 144, 173	0
All	All	655/804 (81%)	0.57	53 (8%)	12	14	33, 78, 131, 173	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	ILE	5.1
1	A	22	ASP	4.5
1	D	102	VAL	4.1
1	D	176	VAL	4.1
1	C	84	GLN	3.9
1	C	85	PHE	3.8
1	D	27	LEU	3.7
1	D	157	ALA	3.6
1	D	117	ASP	3.5
1	D	185	GLU	3.5
1	D	40	LEU	3.4
1	D	129	LEU	3.3
1	D	85	PHE	3.2
1	C	162	VAL	3.1
1	D	132	SER	3.1
1	C	35	ALA	3.1
1	D	179	TYR	3.0
1	C	179	TYR	3.0
1	C	117	ASP	2.9
1	C	46	ASN	2.9
1	C	68	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	198	PRO	2.8
1	C	147	ARG	2.8
1	B	102	VAL	2.7
1	C	170	ASP	2.7
1	C	131	LEU	2.7
1	C	102	VAL	2.7
1	D	183	TYR	2.6
1	D	26	VAL	2.5
1	D	149	CYS	2.5
1	D	147	ARG	2.4
1	D	148	VAL	2.4
1	C	196	LEU	2.4
1	D	110	ASP	2.3
1	D	44	ILE	2.3
1	D	196	LEU	2.3
1	C	146	LEU	2.3
1	C	40	LEU	2.3
1	C	150	THR	2.2
1	A	197	ASP	2.2
1	C	60	LEU	2.2
1	C	187	TYR	2.2
1	C	66	LYS	2.2
1	A	117	ASP	2.1
1	C	166	TYR	2.1
1	C	164	ILE	2.1
1	D	124	VAL	2.1
1	C	190	LEU	2.1
1	D	187	TYR	2.1
1	B	117	ASP	2.0
1	A	63	THR	2.0
1	C	138	LEU	2.0
1	D	70	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

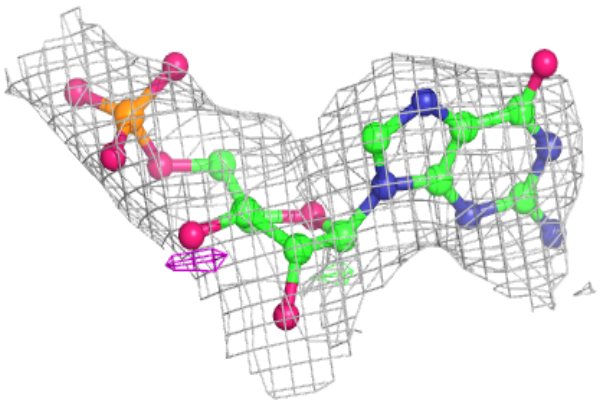
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

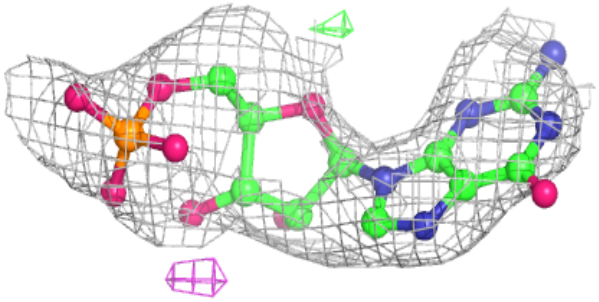
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	5GP	C	302	24/24	0.75	0.22	114,117,152,154	0
4	MG	A	304	1/1	0.81	0.18	63,63,63,63	0
4	MG	C	303	1/1	0.82	0.09	67,67,67,67	0
3	5GP	A	302	24/24	0.84	0.22	59,75,254,254	0
3	5GP	D	302	24/24	0.84	0.17	101,109,147,147	0
4	MG	D	303	1/1	0.88	0.14	96,96,96,96	0
3	5GP	B	302	24/24	0.89	0.20	57,76,167,168	0
4	MG	B	304	1/1	0.92	0.04	50,50,50,50	0
4	MG	A	303	1/1	0.92	0.30	65,65,65,65	0
2	POP	D	301	9/9	0.92	0.11	95,97,116,124	0
4	MG	C	304	1/1	0.94	0.11	83,83,83,83	0
2	POP	C	301	9/9	0.94	0.12	64,90,107,110	0
4	MG	D	304	1/1	0.95	0.10	78,78,78,78	0
2	POP	B	301	9/9	0.96	0.12	67,72,87,87	0
2	POP	A	301	9/9	0.96	0.12	64,69,82,172	0
4	MG	B	303	1/1	0.97	0.36	65,65,65,65	0

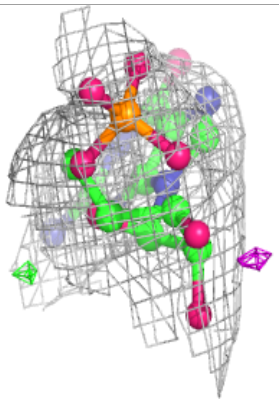
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP C 302:

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

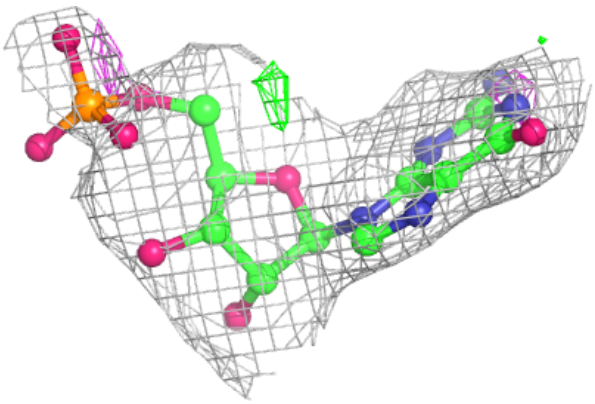


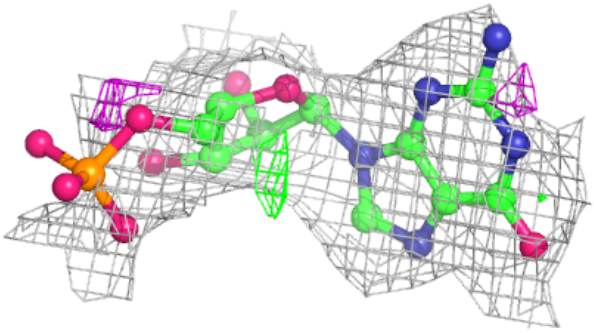


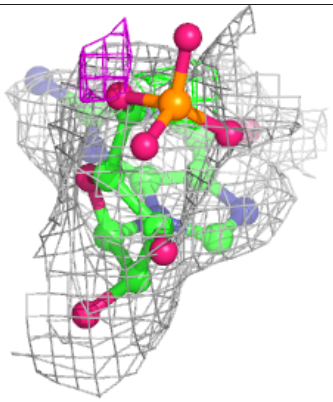


Electron density around 5GP A 302:

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

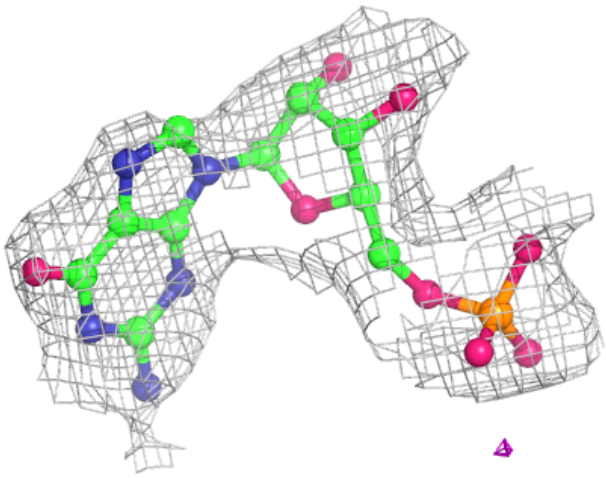


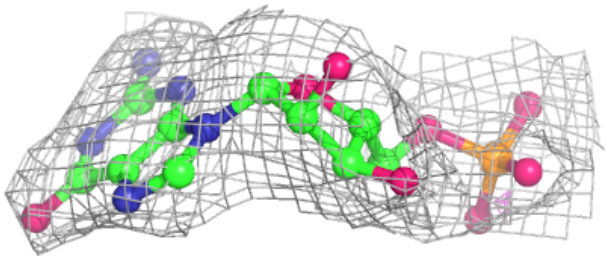


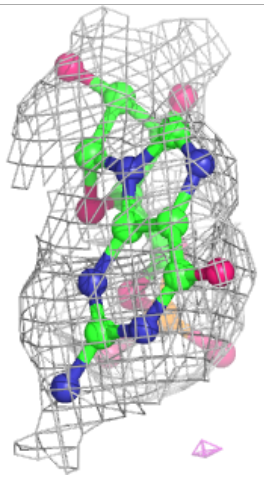


Electron density around 5GP D 302:

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







Electron density around 5GP B 302:

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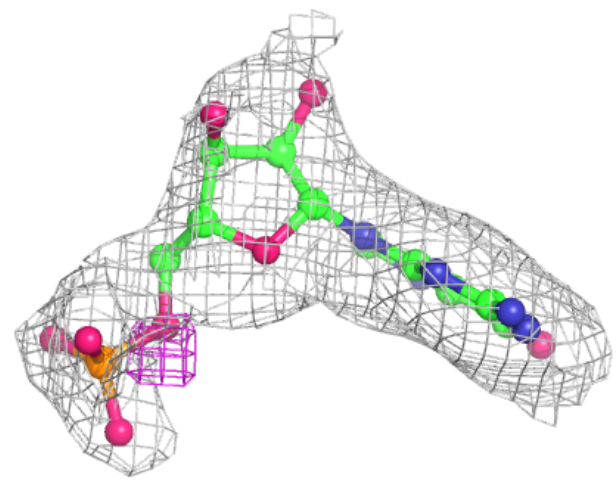
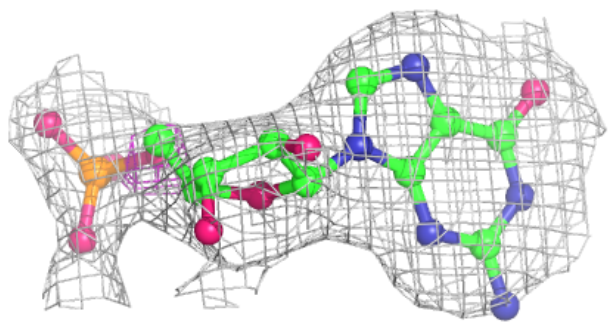
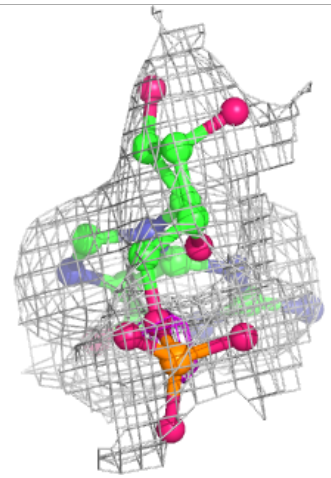
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.