Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 04:45 AM EDT

PDB ID	:	6XRS
Title	:	Crystal structure of a GTP-binding protein EngA (Der homolog) from Neisseria gonorrhoeae bound to GDP
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2020-07-13
Resolution	:	2.80 Å(reported)

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

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

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

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

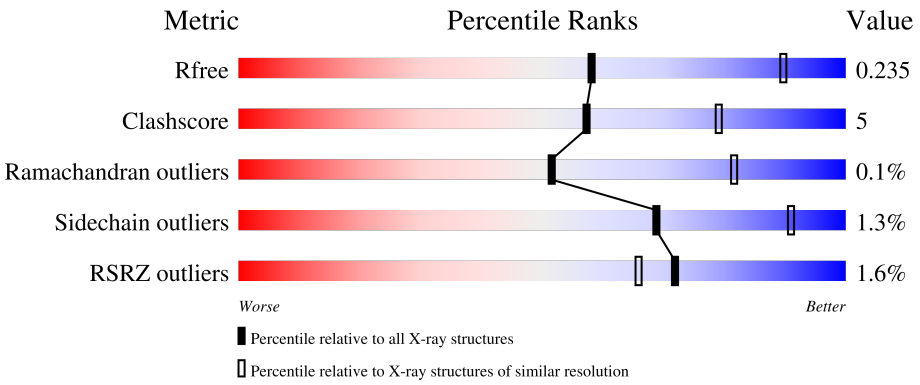
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	458	.% 75% 10% 15%
1	B	458	.% 75% 11% 14%
1	C	458	.% 74% 10% 15%
1	D	458	2% 75% 10% 14%

2 Entry composition (i)

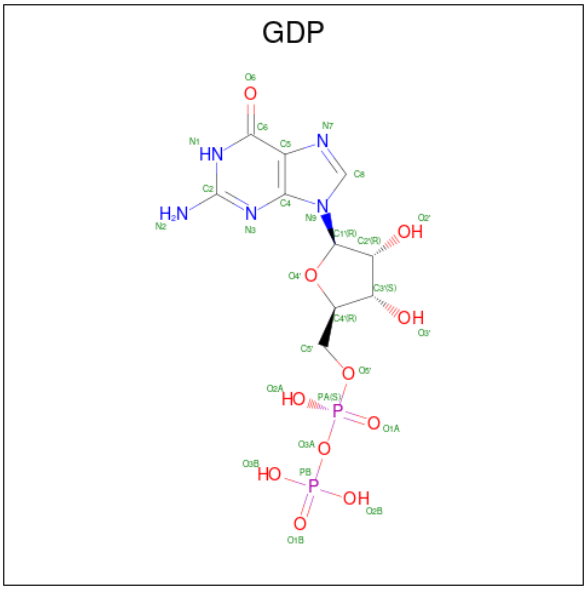
There are 5 unique types of molecules in this entry. The entry contains 11956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GTPase Der.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2887	1839	513	528	7	0	0	0
1	B	392	2928	1865	519	537	7	0	1	0
1	C	388	2891	1839	520	526	6	0	0	0
1	D	392	2909	1852	521	529	7	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0
2	B	1	28	10	5	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	56	20	10	22	4	0	1
2	C	1	56	20	10	22	4	0	1
2	C	1	28	10	5	11	2	0	0
2	D	1	28	10	5	11	2	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	2	2	2	0	0
4	D	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	16	16	16	0	0
5	B	32	32	32	0	0
5	C	29	29	29	0	0

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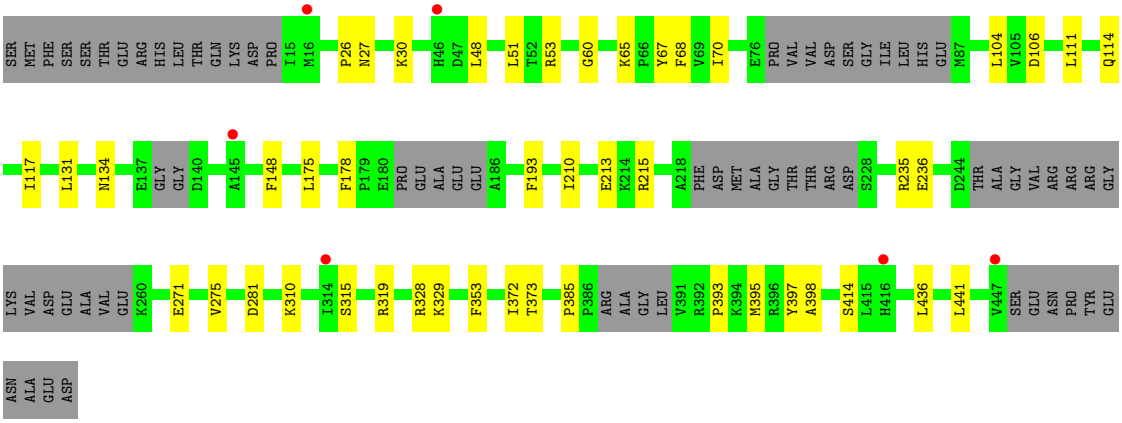
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	31	31	31	0	0

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.

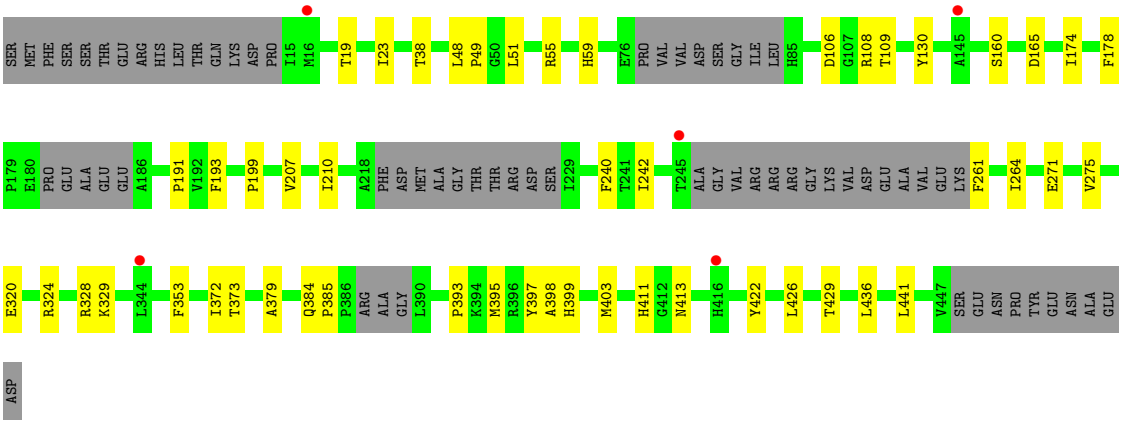
• Molecule 1: GTPase Der

Chain A:



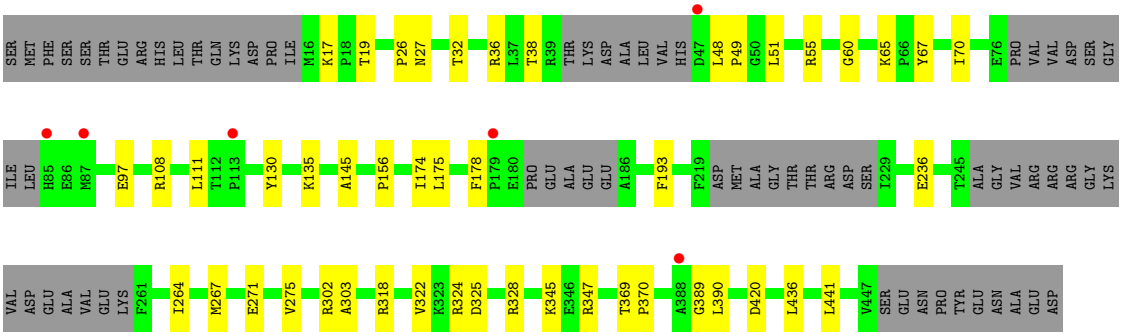
• Molecule 1: GTPase Der

Chain B:



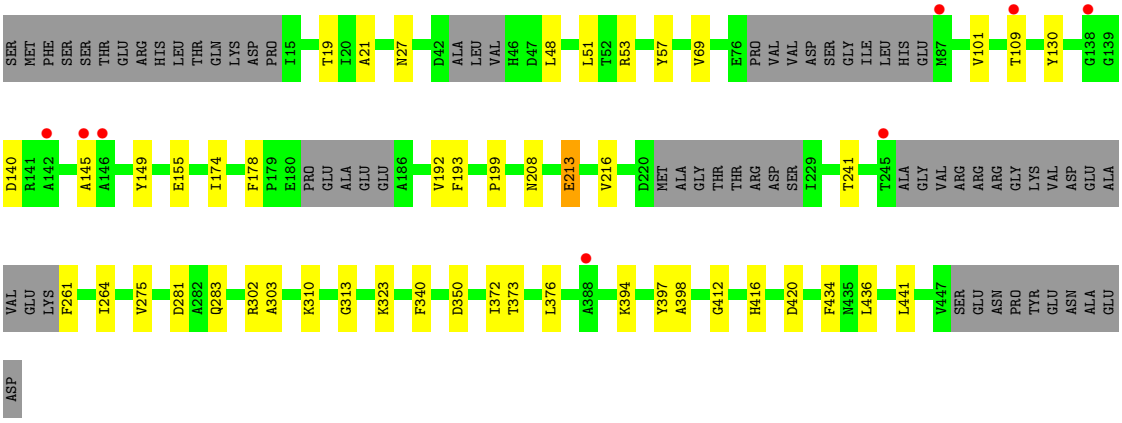
• Molecule 1: GTPase Der

Chain C:



- Molecule 1: GTPase Der

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.16Å 139.64Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 2.80 46.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.98-2.80) 99.9 (46.98-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.203 , 0.235 0.203 , 0.235	Depositor DCC
R_{free} test set	3121 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11956	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 44.61 % 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 1.4890e-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: GDP, CL, IOD

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	0.41	0/2942	0.57	0/3999
1	B	0.45	0/2987	0.61	0/4060
1	C	0.45	0/2947	0.65	1/4003 (0.0%)
1	D	0.44	0/2964	0.62	0/4026
All	All	0.44	0/11840	0.61	1/16088 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	36	ARG	NE-CZ-NH1	7.55	124.07	120.30

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	2887	0	2775	31	0
1	B	2928	0	2829	29	0
1	C	2891	0	2788	31	1
1	D	2909	0	2813	28	1
2	A	28	0	12	0	0
2	B	84	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	36	5	0
2	D	28	0	12	0	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	1	0
4	D	1	0	0	0	0
5	A	16	0	0	0	0
5	B	32	0	0	1	0
5	C	29	0	0	0	0
5	D	31	0	0	0	0
All	All	11956	0	11301	113	1

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 5.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:HZ	1:A:271:GLU:HG3	1.36	0.91
1:B:59:HIS:ND1	5:B:701:HOH:O	2.13	0.80
1:C:325:ASP:OD1	1:C:328:ARG:NH2	2.25	0.69
1:A:68:PHE:CZ	1:A:271:GLU:HG3	2.25	0.69
1:C:32:THR:OG1	2:C:601[A]:GDP:O2A	2.11	0.68
1:B:51:LEU:HD13	1:D:51:LEU:HD13	1.77	0.66
1:A:48:LEU:HB2	1:A:51:LEU:HD12	1.78	0.66
1:D:149:TYR:OH	1:D:155:GLU:OE1	2.16	0.64
1:A:51:LEU:HD13	1:C:51:LEU:HD13	1.80	0.64
1:C:345:LYS:HD3	1:C:347:ARG:NH2	2.14	0.63
1:B:193:PHE:HA	1:B:275:VAL:O	2.00	0.61
1:B:320:GLU:HB3	1:B:324[B]:ARG:NH1	2.18	0.58
1:B:373:THR:HG23	1:B:397:TYR:HA	1.86	0.58
1:D:48:LEU:HB2	1:D:51:LEU:HD12	1.86	0.58
1:B:399:HIS:CD2	1:B:411:HIS:HE2	2.22	0.58
1:D:192:VAL:HG22	1:D:241:THR:HB	1.86	0.57
1:B:384:GLN:HG3	1:B:385:PRO:HD2	1.87	0.57
1:D:199:PRO:HG3	1:D:261:PHE:HB2	1.87	0.56
1:C:65:LYS:HD2	1:C:175:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TYR:CE1	1:B:174:ILE:HG12	2.42	0.55
1:D:130:TYR:CE1	1:D:174:ILE:HG12	2.42	0.55
1:C:145:ALA:HB1	1:C:156:PRO:HG2	1.89	0.54
1:C:38:THR:HB	1:C:55:ARG:HH22	1.72	0.54
1:D:436:LEU:HD12	1:D:441:LEU:HD22	1.89	0.54
1:C:271:GLU:HG3	4:C:605:CL:CL	2.45	0.54
1:B:59:HIS:NE2	1:B:271:GLU:OE2	2.39	0.53
1:B:320:GLU:HB3	1:B:324[B]:ARG:HH11	1.73	0.53
1:C:65:LYS:HB2	1:C:175:LEU:HD13	1.91	0.53
1:A:385:PRO:HB2	1:A:393:PRO:HG2	1.90	0.53
1:A:193:PHE:HA	1:A:275:VAL:O	2.09	0.53
1:D:302:ARG:HA	1:D:302:ARG:HH11	1.73	0.53
2:B:602[B]:GDP:O2'	1:D:27:ASN:HA	2.09	0.53
1:A:215:ARG:HB2	1:A:235:ARG:NH1	2.23	0.53
1:C:60:GLY:HA3	1:C:67:TYR:CE2	2.45	0.52
1:B:108:ARG:NH1	1:D:109:THR:OG1	2.42	0.52
1:B:395:MET:HE1	1:B:422:TYR:HE2	1.74	0.52
1:A:213:GLU:OE1	1:A:215:ARG:N	2.39	0.51
1:A:53:ARG:HA	1:C:51:LEU:HD23	1.92	0.51
1:B:210:ILE:HG23	1:B:353:PHE:HZ	1.76	0.51
1:C:436:LEU:HD12	1:C:441:LEU:HD22	1.93	0.51
1:B:106:ASP:HB3	1:B:109:THR:HB	1.91	0.51
1:A:393:PRO:HB3	1:A:414:SER:O	2.12	0.49
1:C:135:LYS:HG2	2:C:601[A]:GDP:C6	2.46	0.49
1:B:48:LEU:HB2	1:B:51:LEU:HD12	1.94	0.49
1:B:207:VAL:HG22	1:B:242:ILE:HD11	1.93	0.49
1:C:27:ASN:HB3	2:C:601[B]:GDP:N3	2.28	0.49
1:A:26:PRO:O	1:A:27:ASN:HB2	2.13	0.49
1:C:302:ARG:HG3	1:C:303:ALA:O	2.13	0.49
1:D:213:GLU:HG2	1:D:216:VAL:HG23	1.94	0.48
1:A:328:ARG:NH2	1:A:329:LYS:HE3	2.27	0.48
1:A:235:ARG:HG2	1:A:236:GLU:HG3	1.96	0.48
1:C:27:ASN:HA	2:C:601[B]:GDP:O2'	2.14	0.48
1:D:376:LEU:HD22	1:D:398:ALA:HB2	1.96	0.48
1:A:114:GLN:O	1:A:117:ILE:HG12	2.14	0.47
1:C:48:LEU:HB3	1:C:49:PRO:HD2	1.95	0.47
1:A:436:LEU:HD12	1:A:441:LEU:HD22	1.96	0.47
1:B:160:SER:HB3	1:B:165:ASP:HB2	1.97	0.47
1:D:193:PHE:HA	1:D:275:VAL:O	2.14	0.47
1:A:65:LYS:HB2	1:A:175:LEU:HD13	1.96	0.47
1:D:323:LYS:HE2	1:D:340:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:THR:HG21	1:C:264:ILE:HG12	1.98	0.46
1:D:19:THR:HG21	1:D:264:ILE:HG12	1.96	0.46
1:B:19:THR:HG21	1:B:264:ILE:HG12	1.97	0.46
1:B:328:ARG:NH2	1:B:329:LYS:HE3	2.30	0.46
1:A:372:ILE:HG22	1:A:398:ALA:HB3	1.98	0.45
1:B:372:ILE:HG22	1:B:398:ALA:HB3	1.98	0.45
1:C:193:PHE:HA	1:C:275:VAL:O	2.16	0.45
1:B:385:PRO:HB2	1:B:393:PRO:HG2	1.98	0.45
1:A:27:ASN:HA	2:C:601[A]:GDP:O2'	2.16	0.45
1:D:302:ARG:HA	1:D:302:ARG:NH1	2.30	0.45
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.77	0.45
1:B:395:MET:HE1	1:B:426:LEU:HD11	1.99	0.45
1:A:131:LEU:HD21	1:A:148:PHE:HB3	1.98	0.45
1:D:283:GLN:HE21	1:D:313:GLY:HA3	1.81	0.45
1:C:264:ILE:HA	1:C:267:MET:HE2	1.98	0.44
1:D:21:ALA:HB3	1:D:101:VAL:HG22	2.00	0.44
1:D:434:PHE:HB2	1:D:436:LEU:HG	1.99	0.44
1:C:130:TYR:CE1	1:C:174:ILE:HG12	2.52	0.44
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.73	0.44
1:D:57:TYR:HA	1:D:69:VAL:O	2.18	0.43
1:A:104:LEU:HD11	1:A:134:ASN:HB2	1.99	0.43
1:B:38:THR:HB	1:B:55:ARG:HH22	1.83	0.43
1:B:436:LEU:HD12	1:B:441:LEU:HD22	1.99	0.43
1:A:210:ILE:HG23	1:A:353:PHE:CZ	2.53	0.43
1:D:394:LYS:O	1:D:412:GLY:HA3	2.18	0.43
1:B:379:ALA:HB2	1:B:429:THR:HG21	2.01	0.43
1:D:281:ASP:OD1	1:D:310:LYS:HD2	2.19	0.43
1:A:30:LYS:HB2	1:A:30:LYS:HE2	1.85	0.43
1:D:373:THR:HG23	1:D:397:TYR:HA	2.00	0.43
1:D:302:ARG:HG3	1:D:303:ALA:O	2.19	0.42
1:C:70:ILE:HD11	1:C:264:ILE:CG1	2.49	0.42
1:C:318:ARG:O	1:C:322:VAL:HG23	2.19	0.42
1:B:199:PRO:HG3	1:B:261:PHE:CB	2.49	0.42
1:C:60:GLY:HA3	1:C:67:TYR:CZ	2.55	0.42
1:D:372:ILE:HG22	1:D:398:ALA:HB3	2.02	0.42
1:B:48:LEU:HB3	1:B:49:PRO:HD2	2.01	0.41
1:A:213:GLU:OE2	1:A:235:ARG:NH1	2.52	0.41
1:A:385:PRO:HG3	1:A:395:MET:HE3	2.02	0.41
1:B:191:PRO:HG2	1:B:240:PHE:CD1	2.54	0.41
1:C:97:GLU:HB2	1:C:264:ILE:HD12	2.01	0.41
1:A:281:ASP:OD1	1:A:310:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD2	1:C:108:ARG:NH2	2.53	0.41
1:B:51:LEU:HD23	1:D:53:ARG:HA	2.02	0.41
1:A:70:ILE:HG21	1:A:70:ILE:HD13	1.82	0.41
1:C:302:ARG:HH11	1:C:302:ARG:HA	1.86	0.41
1:C:302:ARG:HA	1:C:302:ARG:NH1	2.35	0.41
1:A:60:GLY:HA3	1:A:67:TYR:CE2	2.56	0.40
1:C:26:PRO:O	1:C:27:ASN:HB2	2.22	0.40
1:C:369:THR:HB	1:C:370:PRO:HD3	2.04	0.40
1:D:145:ALA:O	1:D:149:TYR:CD2	2.74	0.40
1:D:130:TYR:CD1	1:D:174:ILE:HG12	2.56	0.40
1:A:315:SER:O	1:A:319:ARG:HG3	2.22	0.40
1:A:373:THR:HG23	1:A:397:TYR:HA	2.02	0.40

All (1) 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:C:390:LEU:O	1:D:208:ASN:ND2[1_556]	2.19	0.01

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	374/458 (82%)	366 (98%)	8 (2%)	0	100	100
1	B	381/458 (83%)	373 (98%)	8 (2%)	0	100	100
1	C	376/458 (82%)	367 (98%)	8 (2%)	1 (0%)	41	72
1	D	380/458 (83%)	370 (97%)	9 (2%)	1 (0%)	41	72
All	All	1511/1832 (82%)	1476 (98%)	33 (2%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	ASP
1	C	389	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	280/375 (75%)	279 (100%)	1 (0%)	91 97
1	B	286/375 (76%)	282 (99%)	4 (1%)	67 90
1	C	279/375 (74%)	274 (98%)	5 (2%)	59 86
1	D	281/375 (75%)	276 (98%)	5 (2%)	59 86
All	All	1126/1500 (75%)	1111 (99%)	15 (1%)	69 91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	PHE
1	B	23	ILE
1	B	178	PHE
1	B	403	MET
1	B	413	ASN
1	C	17	LYS
1	C	178	PHE
1	C	236	GLU
1	C	324	ARG
1	C	420	ASP
1	D	178	PHE
1	D	213	GLU
1	D	350	ASP
1	D	416	HIS
1	D	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	GLN
1	C	93	GLN
1	C	283	GLN
1	D	27	ASN
1	D	283	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 17 ligands modelled in this entry, 9 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	$\#\|Z\| > 2$
2	GDP	B	601	-	24,30,30	0.98	1 (4%)	30,47,47	1.24	3 (10%)
2	GDP	C	601[A]	-	24,30,30	1.03	1 (4%)	30,47,47	1.44	5 (16%)
2	GDP	C	602	-	24,30,30	1.00	1 (4%)	30,47,47	1.44	6 (20%)
2	GDP	D	601	-	24,30,30	1.02	1 (4%)	30,47,47	1.10	2 (6%)
2	GDP	C	601[B]	-	24,30,30	1.13	1 (4%)	30,47,47	1.41	5 (16%)
2	GDP	B	602[B]	-	24,30,30	1.14	1 (4%)	30,47,47	1.38	6 (20%)
2	GDP	A	601	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	3 (10%)
2	GDP	B	602[A]	-	24,30,30	1.14	2 (8%)	30,47,47	1.70	9 (30%)

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	GDP	B	601	-	-	1/12/32/32	0/3/3/3
2	GDP	C	601[A]	-	-	6/12/32/32	0/3/3/3
2	GDP	C	602	-	-	1/12/32/32	0/3/3/3
2	GDP	D	601	-	-	1/12/32/32	0/3/3/3
2	GDP	C	601[B]	-	-	4/12/32/32	0/3/3/3
2	GDP	B	602[B]	-	-	5/12/32/32	0/3/3/3
2	GDP	A	601	-	-	2/12/32/32	0/3/3/3
2	GDP	B	602[A]	-	-	5/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602[B]	GDP	C6-N1	-3.10	1.33	1.37
2	C	601[B]	GDP	C6-N1	-2.93	1.33	1.37
2	D	601	GDP	C6-N1	-2.91	1.33	1.37
2	C	602	GDP	C6-N1	-2.90	1.33	1.37
2	B	601	GDP	C6-N1	-2.88	1.33	1.37
2	A	601	GDP	C6-N1	-2.65	1.33	1.37
2	C	601[A]	GDP	C6-N1	-2.62	1.34	1.37
2	B	602[A]	GDP	C6-N1	-2.45	1.34	1.37
2	B	602[A]	GDP	O4'-C1'	2.32	1.44	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602[A]	GDP	C3'-C2'-C1'	4.38	107.57	100.98
2	C	601[A]	GDP	O4'-C1'-C2'	-3.59	101.68	106.93
2	C	601[A]	GDP	PA-O3A-PB	-3.55	120.66	132.83
2	C	602	GDP	O4'-C1'-C2'	-3.40	101.96	106.93
2	C	602	GDP	PA-O3A-PB	-3.17	121.96	132.83
2	B	602[B]	GDP	O4'-C1'-C2'	-3.10	102.40	106.93
2	B	602[A]	GDP	PA-O3A-PB	-3.04	122.39	132.83
2	A	601	GDP	PA-O3A-PB	-2.94	122.73	132.83
2	A	601	GDP	C3'-C2'-C1'	2.90	105.34	100.98
2	B	602[B]	GDP	C3'-C2'-C1'	2.85	105.27	100.98
2	B	602[B]	GDP	PA-O3A-PB	-2.84	123.08	132.83
2	D	601	GDP	C8-N7-C5	2.82	108.36	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	602	GDP	C3'-C2'-C1'	2.80	105.20	100.98
2	B	602[A]	GDP	O2'-C2'-C3'	-2.75	102.92	111.82
2	C	601[B]	GDP	C3'-C2'-C1'	2.72	105.07	100.98
2	C	601[B]	GDP	C5-C6-N1	2.71	118.74	113.95
2	B	602[A]	GDP	O3'-C3'-C4'	2.69	118.82	111.05
2	B	602[A]	GDP	C8-N7-C5	2.68	108.09	102.99
2	B	601	GDP	C5-C6-N1	2.67	118.67	113.95
2	C	601[A]	GDP	C3'-C2'-C1'	2.64	104.95	100.98
2	B	601	GDP	PA-O3A-PB	-2.61	123.88	132.83
2	B	602[B]	GDP	C8-N7-C5	2.59	107.92	102.99
2	C	601[B]	GDP	PA-O3A-PB	-2.58	123.97	132.83
2	B	602[B]	GDP	C5-C6-N1	2.47	118.31	113.95
2	C	601[B]	GDP	C8-N7-C5	2.45	107.66	102.99
2	C	602	GDP	O2B-PB-O3A	2.43	112.79	104.64
2	B	602[A]	GDP	O3'-C3'-C2'	-2.42	104.01	111.82
2	C	602	GDP	C8-N7-C5	2.37	107.50	102.99
2	D	601	GDP	PA-O3A-PB	-2.35	124.75	132.83
2	C	601[A]	GDP	C5-C6-N1	2.32	118.04	113.95
2	C	601[A]	GDP	C8-N7-C5	2.29	107.35	102.99
2	B	601	GDP	C8-N7-C5	2.28	107.34	102.99
2	B	602[A]	GDP	C5-C6-N1	2.28	117.97	113.95
2	A	601	GDP	C8-N7-C5	2.26	107.30	102.99
2	C	602	GDP	C5-C6-N1	2.16	117.76	113.95
2	C	601[B]	GDP	C2-N1-C6	-2.13	121.17	125.10
2	B	602[A]	GDP	O6-C6-C5	-2.06	120.35	124.37
2	B	602[B]	GDP	C2-N1-C6	-2.03	121.36	125.10
2	B	602[A]	GDP	O3B-PB-O2B	2.02	115.36	107.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GDP	PA-O3A-PB-O3B
2	B	602[A]	GDP	PA-O3A-PB-O2B
2	B	602[B]	GDP	PA-O3A-PB-O2B
2	C	601[A]	GDP	C5'-O5'-PA-O1A
2	C	601[A]	GDP	O4'-C4'-C5'-O5'
2	C	601[B]	GDP	PA-O3A-PB-O3B
2	C	602	GDP	PA-O3A-PB-O3B
2	D	601	GDP	PA-O3A-PB-O3B
2	B	602[B]	GDP	O4'-C4'-C5'-O5'
2	C	601[A]	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	602[B]	GDP	C3'-C4'-C5'-O5'
2	C	601[B]	GDP	O4'-C4'-C5'-O5'
2	C	601[B]	GDP	C3'-C4'-C5'-O5'
2	B	601	GDP	PA-O3A-PB-O1B
2	B	602[B]	GDP	C5'-O5'-PA-O3A
2	C	601[A]	GDP	C5'-O5'-PA-O3A
2	C	601[A]	GDP	C5'-O5'-PA-O2A
2	B	602[A]	GDP	O4'-C4'-C5'-O5'
2	B	602[A]	GDP	PA-O3A-PB-O1B
2	C	601[A]	GDP	PA-O3A-PB-O1B
2	A	601	GDP	PA-O3A-PB-O1B
2	B	602[A]	GDP	C3'-C4'-C5'-O5'
2	C	601[B]	GDP	PA-O3A-PB-O1B
2	B	602[A]	GDP	C5'-O5'-PA-O3A
2	B	602[B]	GDP	C5'-O5'-PA-O1A

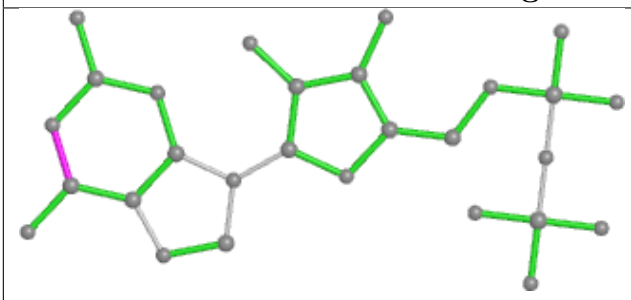
There are no ring outliers.

3 monomers are involved in 6 short contacts:

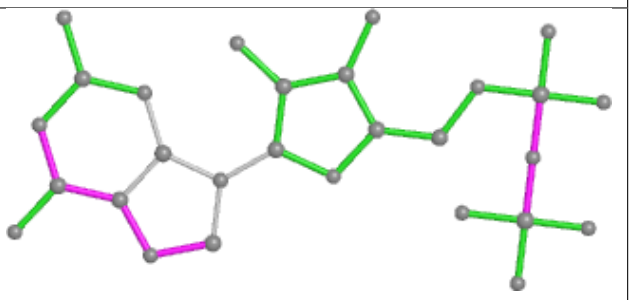
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601[A]	GDP	3	0
2	C	601[B]	GDP	2	0
2	B	602[B]	GDP	1	0

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.

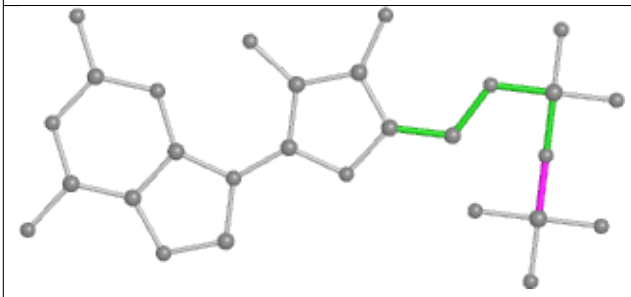
Ligand GDP B 601



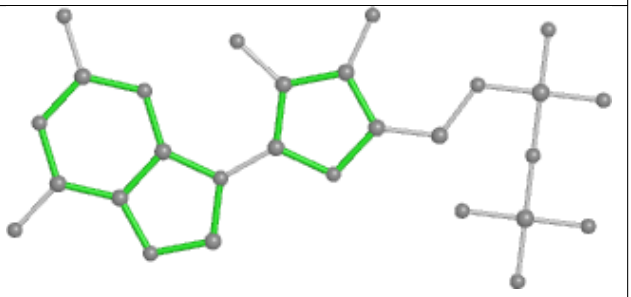
Bond lengths



Bond angles

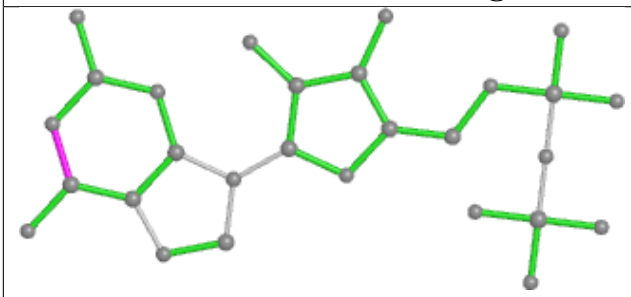


Torsions



Rings

Ligand GDP C 601 (A)



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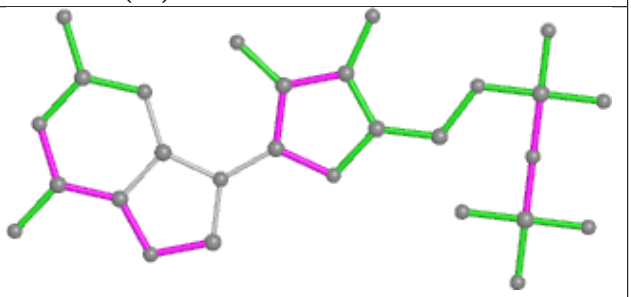

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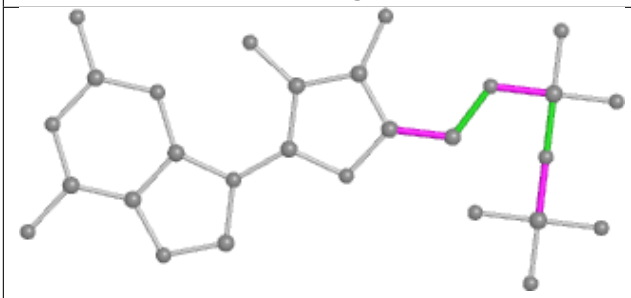

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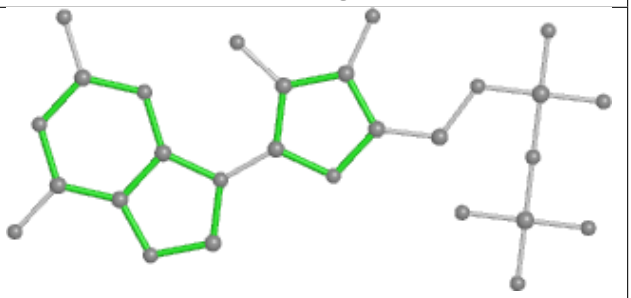
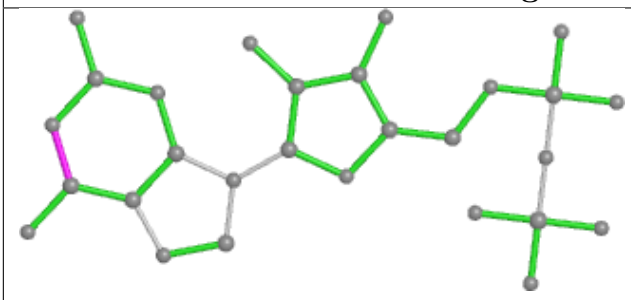


Rings

Ligand GDP C 602



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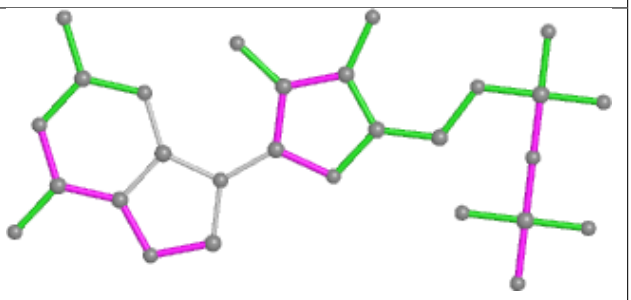

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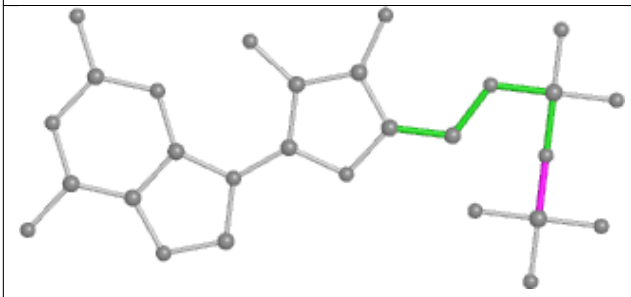
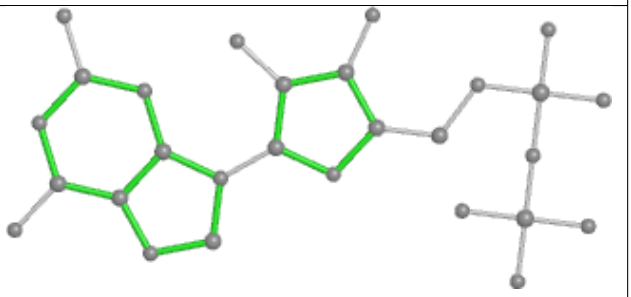
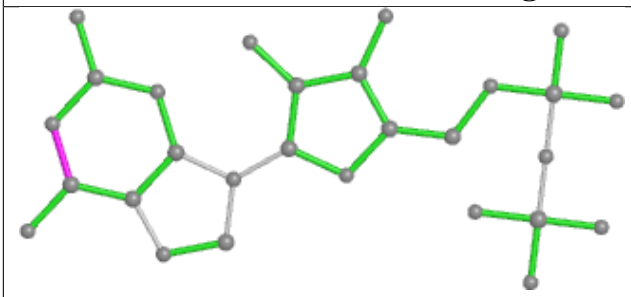


Torsions

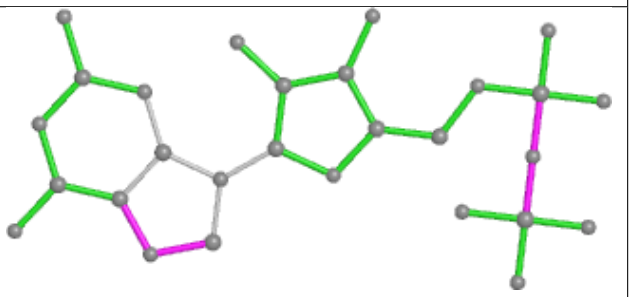


Rings

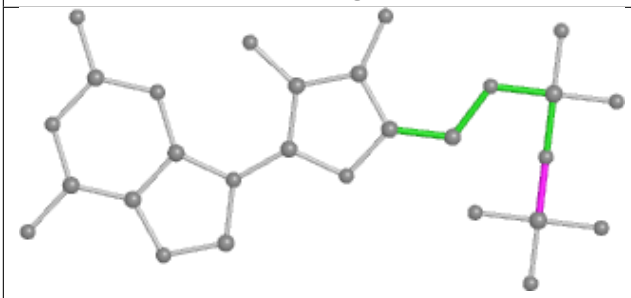
Ligand GDP D 601



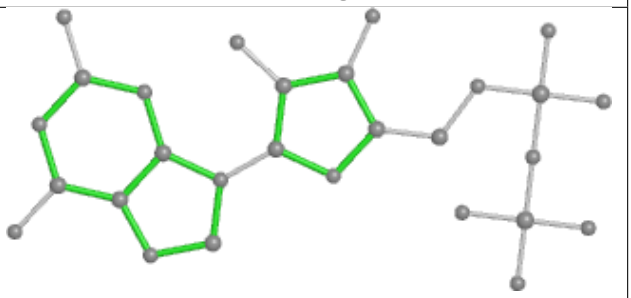
Bond lengths



Bond angles

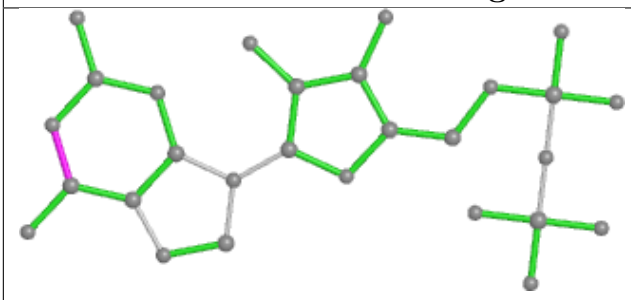


Torsions

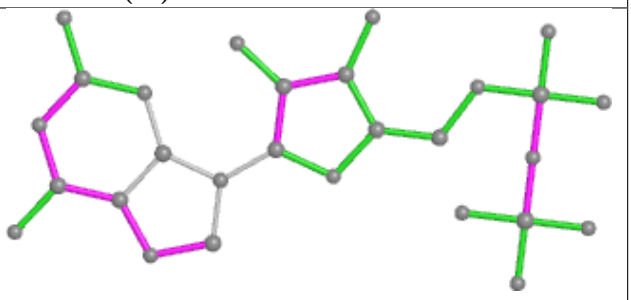


Rings

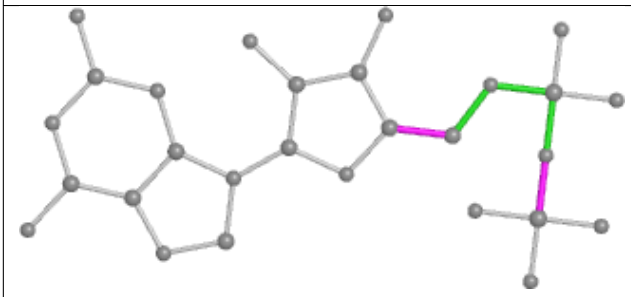
Ligand GDP C 601 (B)



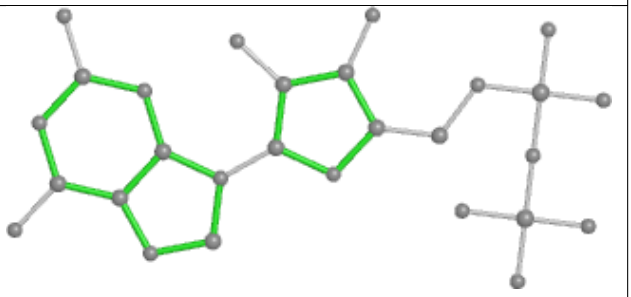
Bond lengths



Bond angles

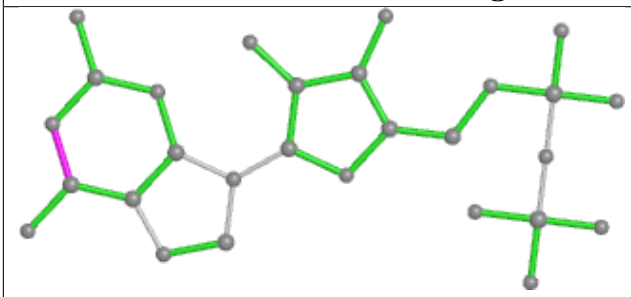


Torsions

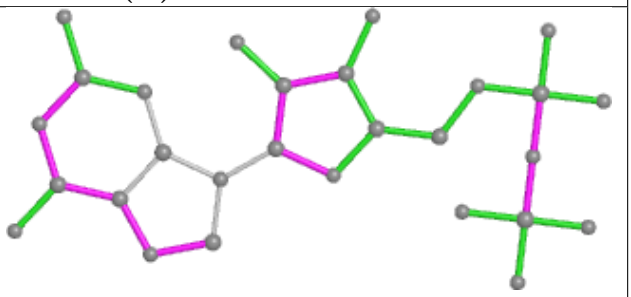


Rings

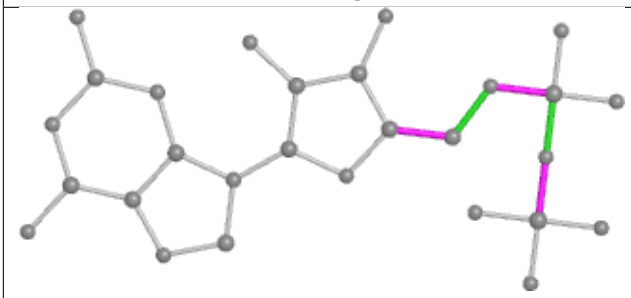
Ligand GDP B 602 (B)



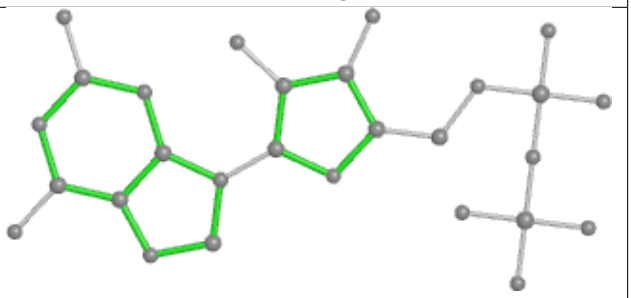
Bond lengths



Bond angles

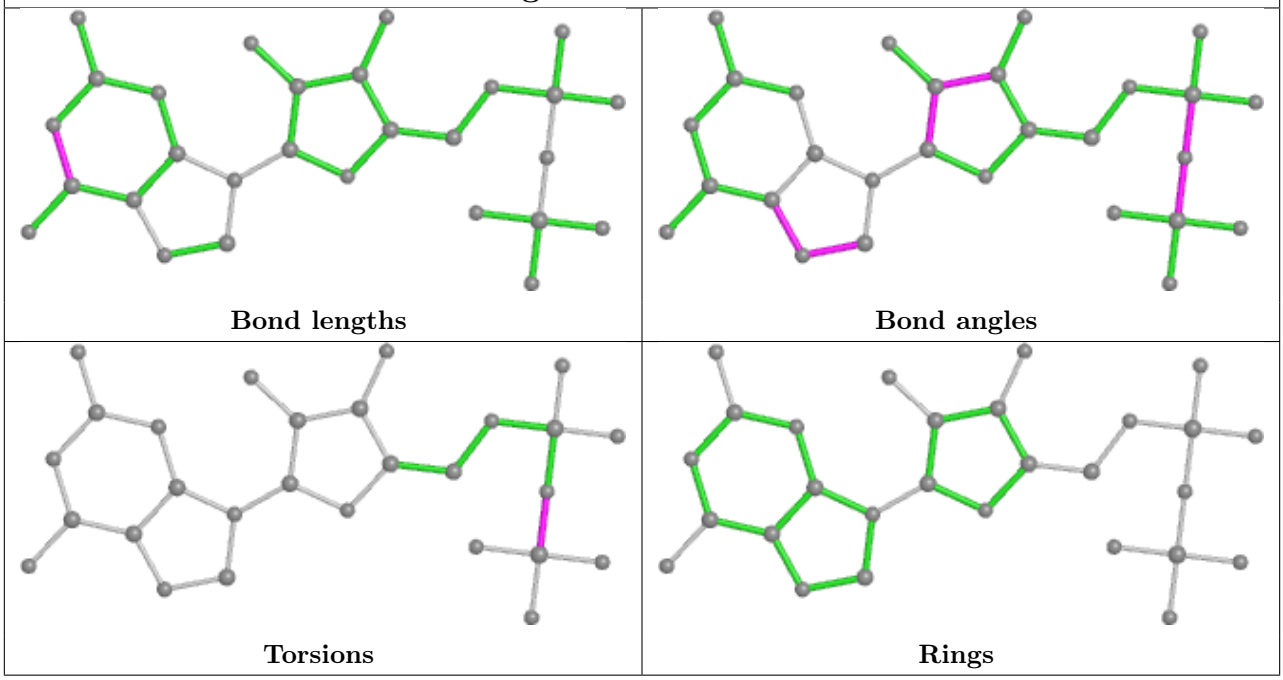


Torsions

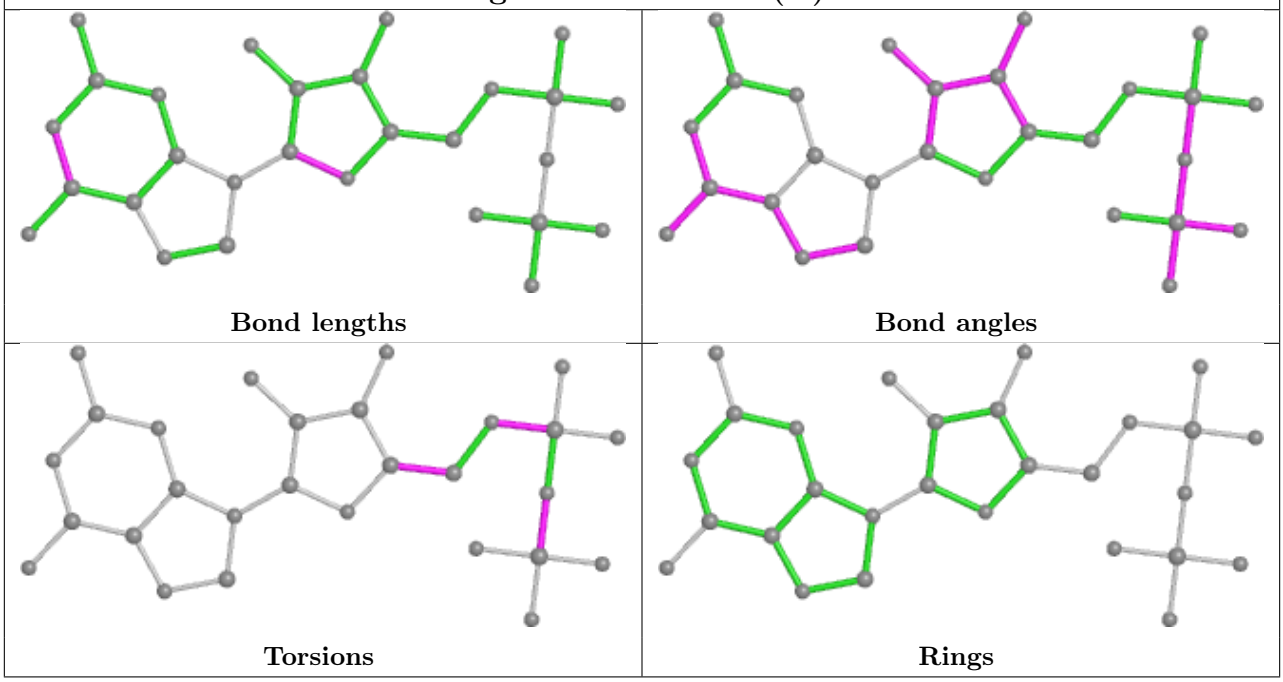


Rings

Ligand GDP A 601



Ligand GDP B 602 (A)



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	388/458 (84%)	-0.27	6 (1%)	73	68	36, 57, 108, 165	0
1	B	392/458 (85%)	-0.29	5 (1%)	77	72	31, 58, 108, 141	0
1	C	388/458 (84%)	-0.24	6 (1%)	73	68	27, 53, 104, 147	0
1	D	392/458 (85%)	-0.25	8 (2%)	65	56	30, 51, 106, 173	0
All	All	1560/1832 (85%)	-0.26	25 (1%)	72	66	27, 55, 108, 173	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	ALA	6.6
1	A	145	ALA	5.5
1	B	245	THR	5.3
1	D	145	ALA	5.0
1	D	142	ALA	3.9
1	D	245	THR	3.5
1	C	85	HIS	3.4
1	A	16	MET	3.1
1	A	447	VAL	2.8
1	C	113	PRO	2.8
1	D	138	GLY	2.7
1	C	87	MET	2.7
1	A	314	ILE	2.6
1	B	145	ALA	2.6
1	A	46	HIS	2.4
1	D	109	THR	2.3
1	D	87	MET	2.3
1	B	344	LEU	2.2
1	C	388	ALA	2.2
1	B	16	MET	2.2
1	A	416	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	416	HIS	2.1
1	C	179	PRO	2.1
1	D	388	ALA	2.0
1	C	47	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

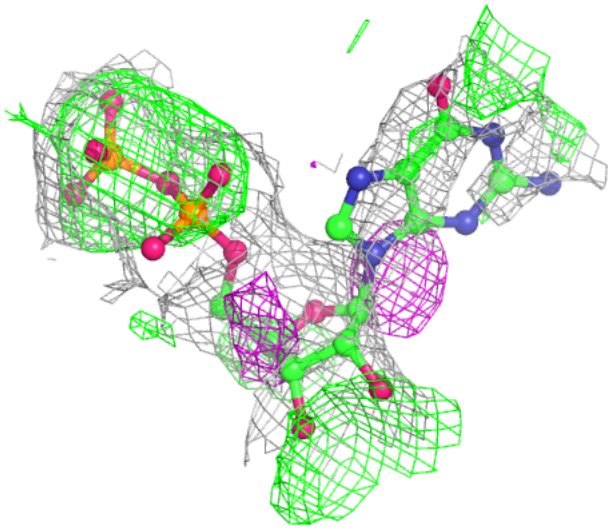
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GDP	B	602[A]	28/28	0.86	0.39	21,42,62,68	28
2	GDP	B	602[B]	28/28	0.86	0.39	20,39,44,47	28
2	GDP	C	601[A]	28/28	0.87	0.36	27,54,71,72	28
2	GDP	C	601[B]	28/28	0.87	0.36	27,54,65,71	28
3	IOD	B	603	1/1	0.94	0.07	91,91,91,91	1
4	CL	C	604	1/1	0.95	0.07	62,62,62,62	0
2	GDP	B	601	28/28	0.96	0.15	38,55,61,72	0
2	GDP	A	601	28/28	0.97	0.11	45,53,58,69	0
4	CL	A	603	1/1	0.97	0.13	52,52,52,52	0
2	GDP	C	602	28/28	0.97	0.14	38,44,51,58	0
4	CL	B	604	1/1	0.98	0.11	42,42,42,42	0
2	GDP	D	601	28/28	0.98	0.12	35,46,53,66	0
3	IOD	D	602	1/1	0.99	0.08	70,70,70,70	1
3	IOD	A	602	1/1	0.99	0.05	83,83,83,83	0
4	CL	C	605	1/1	0.99	0.12	47,47,47,47	0
4	CL	D	603	1/1	0.99	0.18	26,26,26,26	0
3	IOD	C	603	1/1	1.00	0.07	82,82,82,82	0

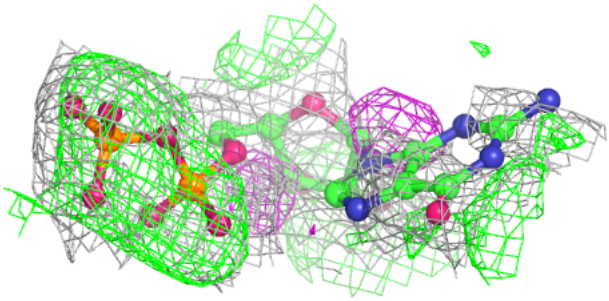
The following is a graphical depiction of the model fit to experimental electron density of all

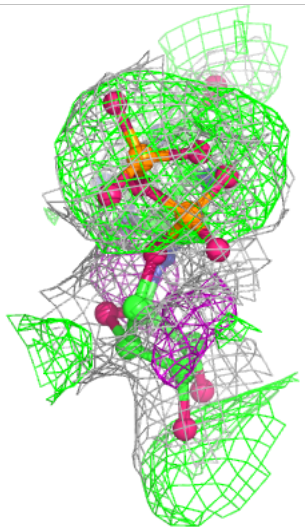
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP B 602 (A):

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

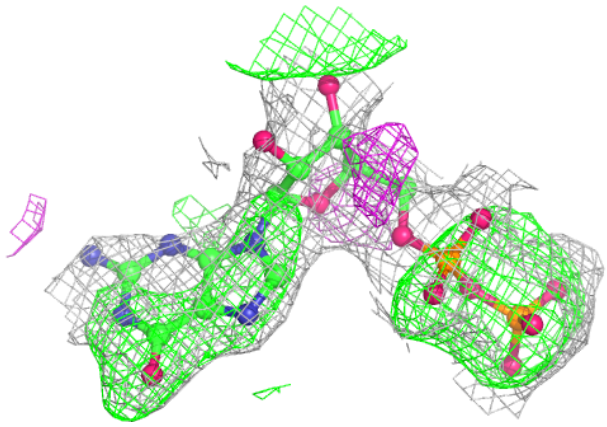


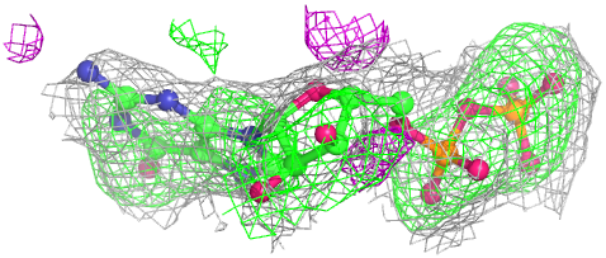


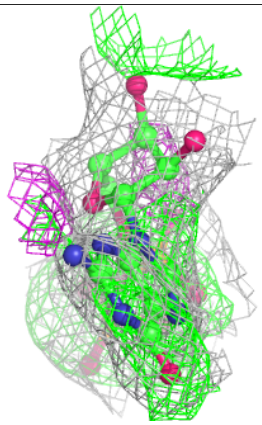


Electron density around GDP B 602 (B):

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

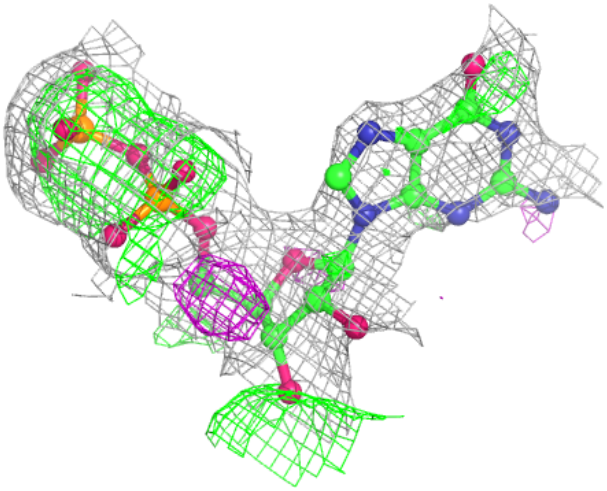


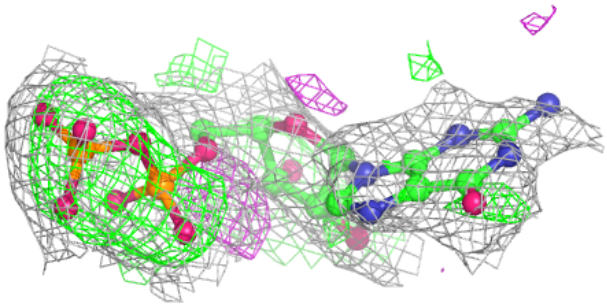


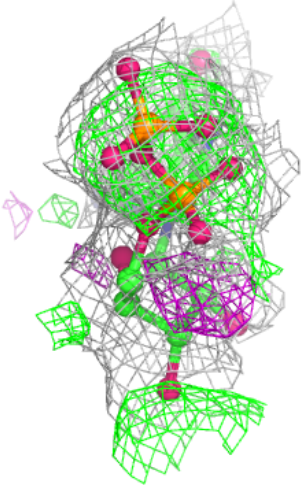


Electron density around GDP C 601 (A):

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







Electron density around GDP C 601 (B):

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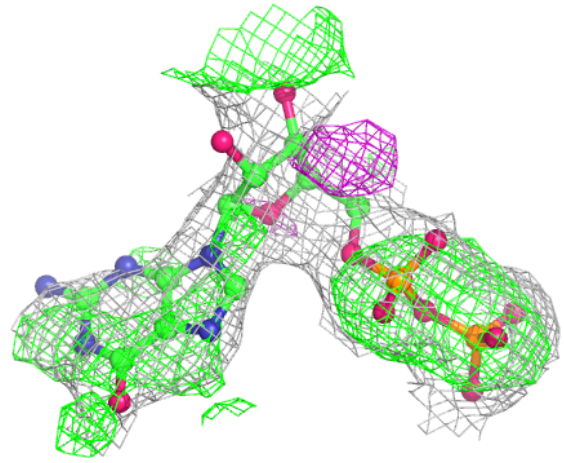
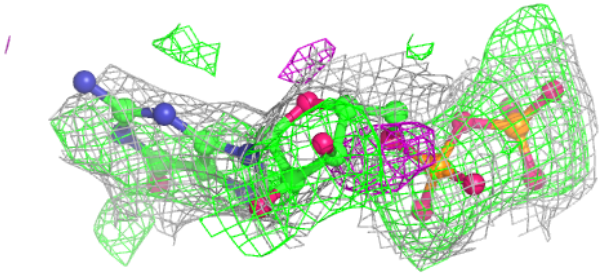
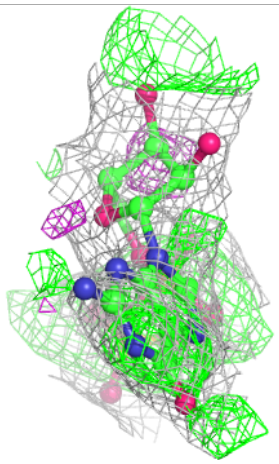
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

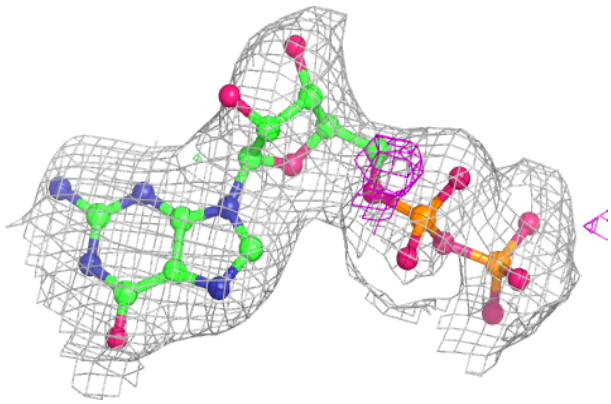


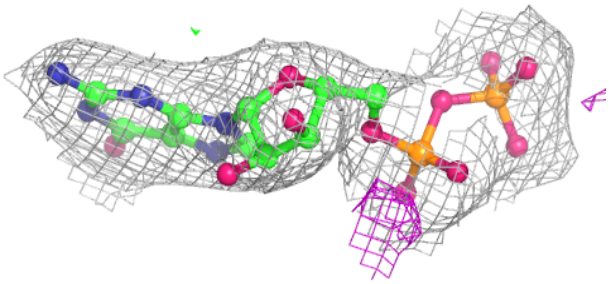


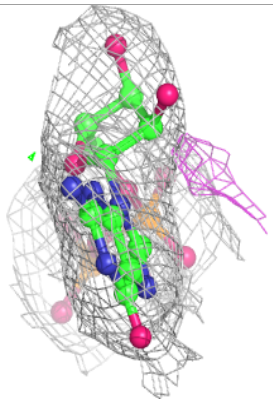


Electron density around GDP B 601:

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

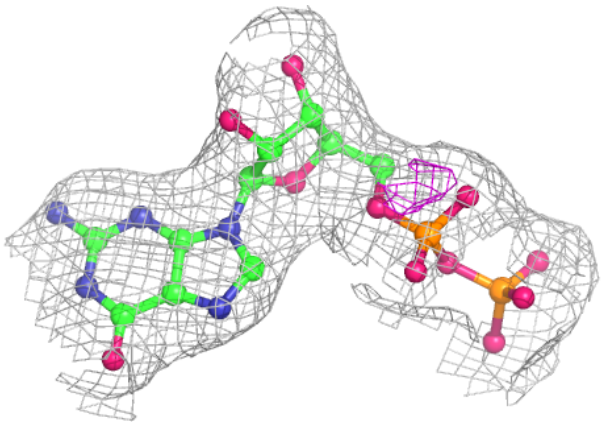


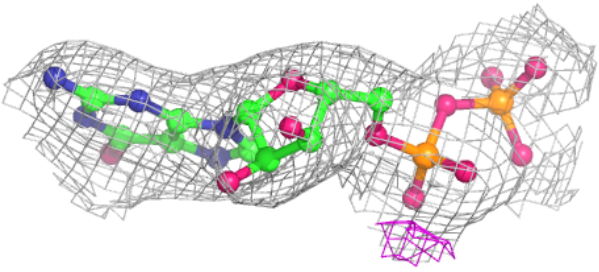


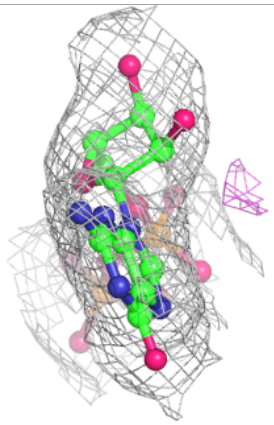


Electron density around GDP A 601:

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

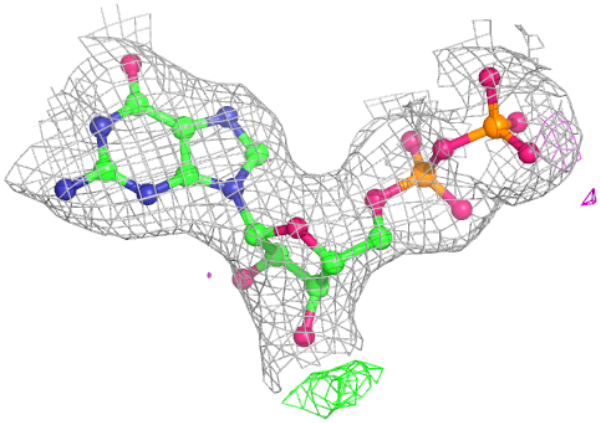


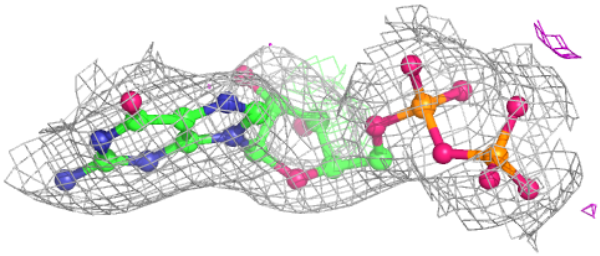


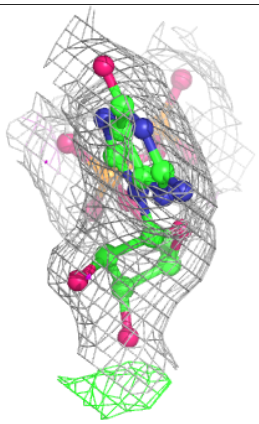


Electron density around GDP C 602:

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







Electron density around GDP D 601:

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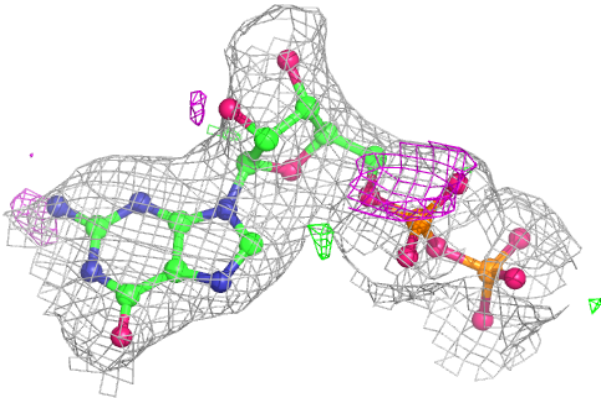
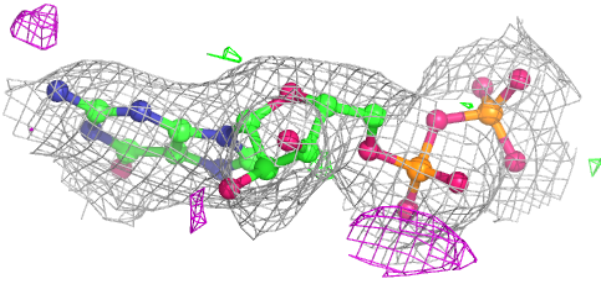
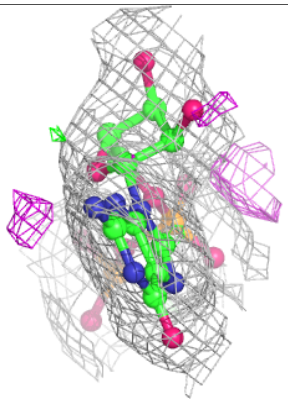
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.