Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 06:13 pm BST

PDB ID	:	2CNW / pdb_00002cnw
Title	:	GDPALF4 complex of the SRP GTPases Ffh and FtsY
Authors	:	Focia, P.J.; Gawronski-Salerno, J.; Coon V, J.S.; Freymann, D.M.
Deposited on	:	2006-05-24
Resolution	:	2.39 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:

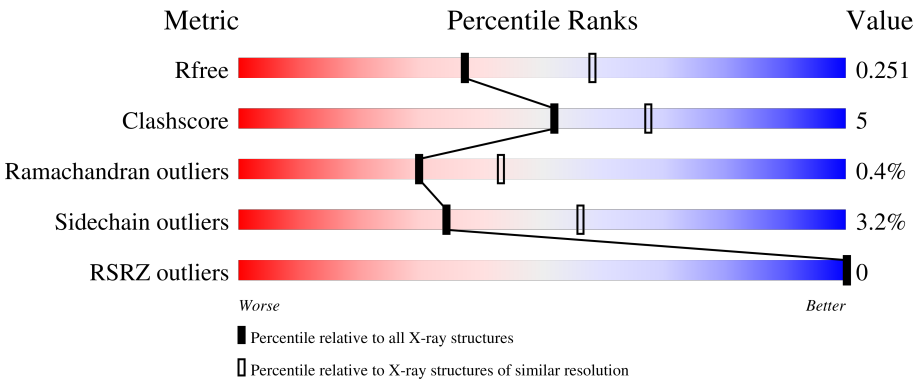
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	294	82% 15% • •
1	B	294	90% 8% • •
1	C	294	87% 11% • •
2	D	284	86% 12% • •
2	E	284	84% 13% • •

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Mol	Chain	Length	Quality of chain
2	F	284	78% 12% • 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13912 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.

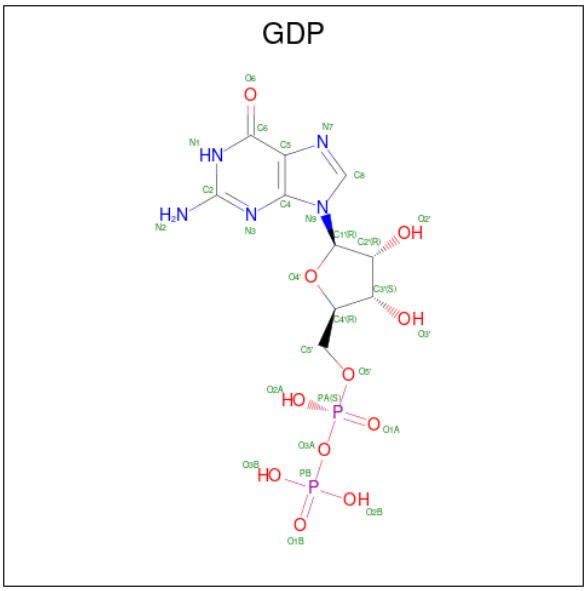
- Molecule 1 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2239	1405	409	421	4	22	1	0
1	B	290	2241	1406	412	419	4	0	1	0
1	C	290	2252	1412	416	420	4	14	2	0

- Molecule 2 is a protein called CELL DIVISION PROTEIN FTSY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	281	2175	1387	377	405	6	3	4	0
2	E	279	2143	1366	372	399	6	8	2	0
2	F	260	1965	1254	334	371	6	4	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

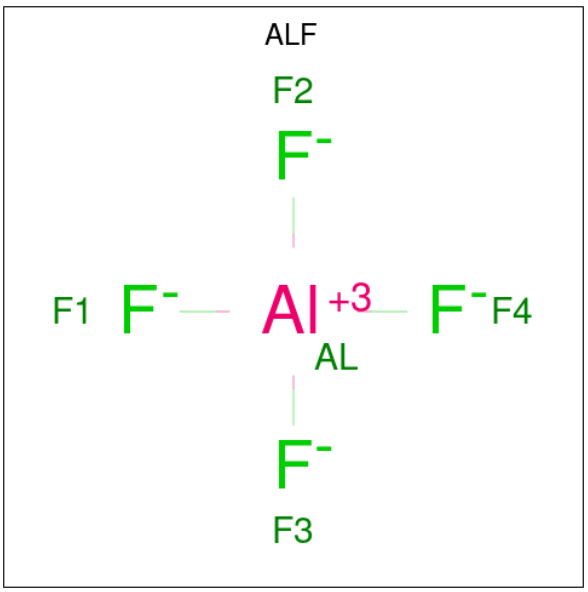


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	28	10	5	11	2	0	0
3	B	1	28	10	5	11	2	0	0
3	C	1	28	10	5	11	2	0	0
3	D	1	28	10	5	11	2	0	0
3	E	1	28	10	5	11	2	0	0
3	F	1	28	10	5	11	2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

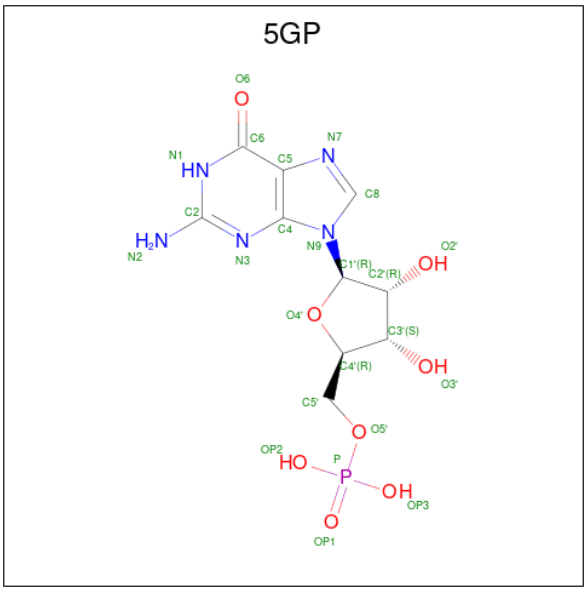
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0
4	F	1	1	1	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
5	A	1	5	1	4	0	0
5	B	1	5	1	4	0	0
5	C	1	5	1	4	0	0
5	D	1	5	1	4	0	0
5	E	1	5	1	4	0	0
5	F	1	5	1	4	0	0

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	D	1	24	10	5	8	1	0	0
			Total	C	N	O	P		
6	E	1	24	10	5	8	1	0	0
			Total	C	N	O	P		
6	F	1	24	10	5	8	1	0	0

- Molecule 7 is water.

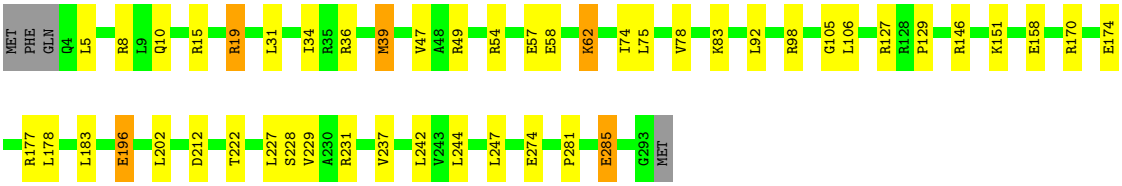
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	124	124	124	0	0
			Total	O		
7	B	104	104	104	0	0
			Total	O		
7	C	118	118	118	0	0
			Total	O		
7	D	104	104	104	0	0
			Total	O		
7	E	97	97	97	0	0
			Total	O		
7	F	74	74	74	0	0

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: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain A:

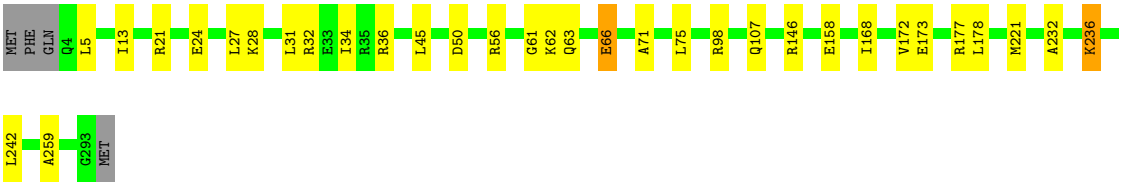


• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain B:

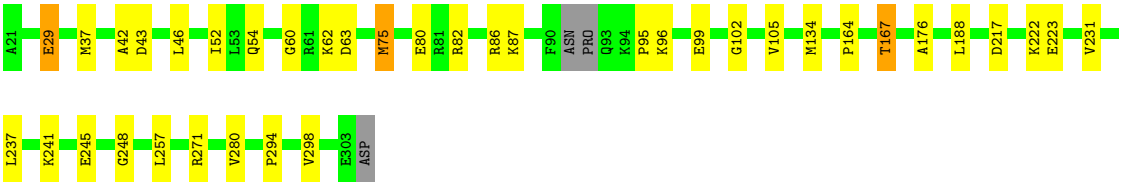
• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain C:



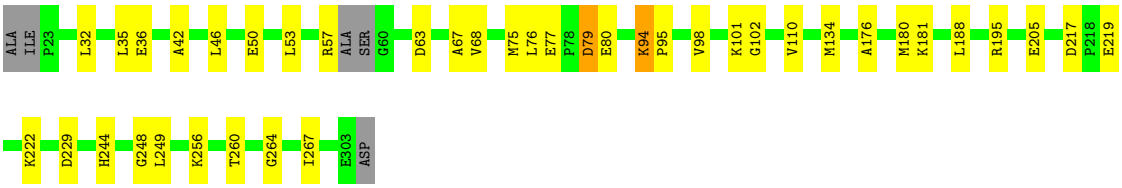
• Molecule 2: CELL DIVISION PROTEIN FTSY

Chain D:



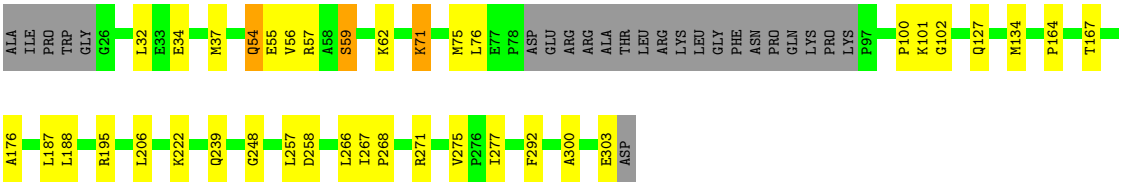
• Molecule 2: CELL DIVISION PROTEIN FTSY

Chain E:



- Molecule 2: CELL DIVISION PROTEIN FTSY

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	188.69Å 188.69Å 44.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.68 – 2.39 14.68 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.68-2.39) 100.0 (14.68-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.253 0.183 , 0.251	Depositor DCC
R_{free} test set	3522 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l 0.044 for h,-h-k,-l 0.130 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13912	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 27.32 % 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 2.2453e-03. 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, ALF, MG, 5GP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.65	0/2263	0.88	1/3050 (0.0%)
1	B	0.62	0/2265	0.88	0/3052
1	C	0.61	0/2276	0.88	0/3066
2	D	0.66	0/2209	0.90	2/2982 (0.1%)
2	E	0.60	0/2178	0.93	6/2941 (0.2%)
2	F	0.62	0/1994	0.89	0/2693
All	All	0.63	0/13185	0.89	9/17784 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	80	GLU	N-CA-C	-8.82	102.93	114.31
2	E	94	LYS	CA-C-N	8.48	128.54	119.89
2	E	94	LYS	C-N-CA	8.48	128.54	119.89
2	D	217	ASP	CA-C-N	6.58	127.11	119.47
2	D	217	ASP	C-N-CA	6.58	127.11	119.47
1	A	105	GLY	N-CA-C	5.19	117.03	110.38
2	E	217	ASP	CA-C-N	5.15	125.44	119.47
2	E	217	ASP	C-N-CA	5.15	125.44	119.47
2	E	79	ASP	N-CA-C	5.13	117.66	109.81

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	2239	0	2336	37	0
1	B	2241	0	2343	16	0
1	C	2252	0	2355	21	0
2	D	2175	0	2253	21	0
2	E	2143	0	2214	27	0
2	F	1965	0	2037	22	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
3	E	28	0	12	1	0
3	F	28	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	D	24	0	12	1	0
6	E	24	0	12	0	0
6	F	24	0	12	0	0
7	A	124	0	0	5	0
7	B	104	0	0	4	0
7	C	118	0	0	3	0
7	D	104	0	0	0	0
7	E	97	0	0	2	0
7	F	74	0	0	0	0
All	All	13912	0	13646	138	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 5.

All (138) 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)
2:D:164:PRO:O	2:D:167:THR:HG22	1.54	1.07
1:C:177:ARG:NH2	1:C:178:LEU:HD23	1.88	0.89
1:A:19:ARG:HH11	1:A:19:ARG:HG2	1.39	0.88
1:A:170:ARG:HD2	7:A:2073:HOH:O	1.76	0.85
2:E:32:LEU:HD21	2:E:57:ARG:HB2	1.57	0.85
2:E:134:MET:CE	2:E:180:MET:HB2	2.12	0.79
1:A:19:ARG:HH11	1:A:19:ARG:CG	1.95	0.78
1:C:177:ARG:HH21	1:C:178:LEU:HD23	1.46	0.77
1:C:13:ILE:HD11	1:C:75:LEU:HD13	1.68	0.75
1:B:146:ARG:HD3	1:B:158:GLU:OE2	1.87	0.74
2:E:134:MET:HE2	2:E:180:MET:HB2	1.70	0.73
1:A:196:GLU:OE1	1:A:196:GLU:HA	1.89	0.72
2:E:134:MET:HE3	2:E:188:LEU:HD13	1.72	0.72
2:D:164:PRO:O	2:D:167:THR:CG2	2.38	0.69
2:E:102:GLY:HA3	2:E:222:LYS:HG3	1.73	0.69
1:C:221:MET:HG2	7:C:2094:HOH:O	1.93	0.68
2:F:102:GLY:HA3	2:F:222:LYS:HG3	1.74	0.68
2:D:29:GLU:OE2	2:D:29:GLU:HA	1.96	0.65
1:C:177:ARG:HH21	1:C:178:LEU:CD2	2.10	0.64
2:E:134:MET:HE1	2:E:180:MET:HB2	1.79	0.64
1:C:13:ILE:HD12	1:C:71:ALA:HB1	1.79	0.64
2:E:134:MET:HE1	2:E:176:ALA:O	1.98	0.63
2:F:266:LEU:HD22	2:F:277:ILE:HD12	1.81	0.63
2:F:134:MET:HE1	2:F:176:ALA:O	1.98	0.63
2:E:134:MET:CE	2:E:188:LEU:HD13	2.28	0.62
2:F:134:MET:HE2	2:F:188:LEU:HD13	1.81	0.61
2:E:101:LYS:HB3	2:E:222:LYS:HB3	1.82	0.61
1:A:146:ARG:HD3	1:A:158:GLU:OE2	2.00	0.61
1:A:39:MET:HE3	2:D:46:LEU:HD21	1.83	0.60
1:C:232:ALA:O	1:C:236:LYS:HD3	2.02	0.60
2:D:257:LEU:CD2	2:D:280:VAL:HG21	2.32	0.59
1:B:244:LEU:HD23	1:B:247:LEU:HD11	1.84	0.59
1:A:170:ARG:CD	7:A:2073:HOH:O	2.44	0.58
1:B:17:ARG:HA	7:B:2003:HOH:O	2.06	0.56
2:F:75:MET:HE2	2:F:271:ARG:HD3	1.88	0.56
2:F:134:MET:CE	2:F:176:ALA:O	2.55	0.55
2:E:195:ARG:NH1	2:E:205:GLU:OE2	2.31	0.54
2:D:52:ILE:HG12	2:D:75:MET:HE1	1.90	0.53
2:D:257:LEU:HD22	2:D:280:VAL:HG21	1.88	0.53
1:A:8:ARG:HH21	1:A:36:ARG:NH1	2.07	0.53
1:A:222:THR:HG23	2:D:231[B]:VAL:HG12	1.90	0.53
1:A:49:ARG:HH22	2:D:37:MET:CE	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:GLU:HG3	2:E:53:LEU:HD11	1.91	0.52
1:A:58:GLU:O	1:A:62:LYS:HD3	2.11	0.51
1:A:47:VAL:HG23	1:A:227:LEU:HD12	1.93	0.51
2:F:277:ILE:HB	2:F:292:PHE:CD2	2.46	0.50
1:C:5:LEU:HD11	1:C:75:LEU:HD21	1.92	0.50
1:B:22:ILE:HB	1:B:26:ASP:HB2	1.92	0.50
2:F:300:ALA:O	2:F:303:GLU:HG2	2.12	0.50
2:E:50:GLU:HG3	7:E:2011:HOH:O	2.12	0.50
2:F:100:PRO:HG2	2:F:187:LEU:HD21	1.94	0.50
2:E:35:LEU:HD23	2:E:53:LEU:HD23	1.93	0.50
2:F:267:ILE:HB	2:F:268:PRO:CD	2.42	0.50
1:A:31:LEU:HD23	1:A:34:ILE:HD12	1.95	0.49
1:A:129:PRO:HA	1:A:183:LEU:O	2.13	0.49
2:D:102:GLY:HA3	2:D:222:LYS:HG3	1.93	0.49
2:F:101:LYS:HB3	2:F:222:LYS:HB3	1.95	0.49
2:D:134:MET:HE1	2:D:176:ALA:O	2.13	0.48
1:C:61:GLY:C	1:C:63:GLN:H	2.22	0.48
1:A:74:ILE:O	1:A:78:VAL:HG23	2.13	0.48
2:E:244:HIS:HA	2:E:249:LEU:HG	1.95	0.48
2:F:54:GLN:HG2	2:F:57:ARG:HH12	1.78	0.48
2:E:102:GLY:HA3	2:E:222:LYS:CG	2.43	0.47
2:F:76:LEU:HD21	2:F:267:ILE:HD13	1.97	0.47
1:C:173:GLU:HB3	7:C:2078:HOH:O	2.15	0.47
2:D:82:ARG:HD2	2:D:86:ARG:NH2	2.30	0.47
2:D:42:ALA:O	2:D:43:ASP:HB2	2.15	0.47
1:A:92:LEU:HD21	1:A:281:PRO:HB3	1.96	0.47
1:C:21:ARG:HD3	1:C:66:GLU:HA	1.97	0.46
2:E:32:LEU:HB3	7:E:2002:HOH:O	2.15	0.46
2:F:164:PRO:HD2	2:F:167:THR:HG21	1.97	0.46
1:A:83:LYS:HD2	1:A:285:GLU:HB2	1.98	0.46
2:D:257:LEU:HD23	2:D:280:VAL:HG21	1.98	0.46
1:B:39:MET:HE3	2:E:46:LEU:HD21	1.98	0.46
2:D:134:MET:HE2	2:D:188:LEU:HD13	1.97	0.46
1:C:28:LYS:HA	1:C:31:LEU:HD12	1.98	0.46
2:E:94:LYS:HA	2:E:95:PRO:HD2	1.77	0.45
1:A:106:LEU:HD11	1:A:229:VAL:HG21	1.98	0.45
2:D:105:VAL:HG22	2:D:223:GLU:HB2	1.98	0.45
2:D:294:PRO:O	2:D:298:VAL:HG23	2.17	0.45
2:F:34:GLU:OE2	2:F:37:MET:HE2	2.15	0.45
1:C:31:LEU:HA	1:C:34:ILE:HD12	1.98	0.45
2:E:110:VAL:HA	2:E:195:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.18	0.45
1:A:15:ARG:O	1:A:19:ARG:NH1	2.50	0.44
1:A:83:LYS:HE3	7:A:2027:HOH:O	2.17	0.44
2:F:37:MET:HE3	2:F:37:MET:HB3	1.80	0.44
1:A:174:GLU:O	1:A:178:LEU:HG	2.17	0.44
2:D:257:LEU:HD22	2:D:280:VAL:CG2	2.46	0.44
2:E:229:ASP:CG	2:E:256:LYS:HD2	2.42	0.44
1:A:274:GLU:OE2	6:D:3001:5GP:N1	2.51	0.44
1:A:151:LYS:NZ	7:A:2061:HOH:O	2.50	0.44
1:A:202:LEU:HD23	1:A:237:VAL:HG21	1.99	0.44
1:B:16:LEU:HB2	1:B:71:ALA:HB2	2.00	0.44
2:E:77:GLU:C	2:E:79:ASP:H	2.26	0.44
1:A:19:ARG:CG	1:A:19:ARG:NH1	2.65	0.43
1:A:177:ARG:HH21	1:A:178:LEU:CD2	2.31	0.43
1:A:244:LEU:HD23	1:A:247:LEU:HD11	2.00	0.43
2:F:56:VAL:HA	2:F:59:SER:HB2	2.00	0.43
1:C:168:ILE:O	1:C:172:VAL:HG23	2.19	0.43
1:C:32:ARG:O	1:C:36:ARG:HG3	2.19	0.43
1:B:194:ILE:HD13	2:E:260:THR:HG23	2.01	0.43
1:B:14:GLY:C	1:B:16:LEU:H	2.26	0.43
1:B:206:LYS:NZ	1:B:237:VAL:O	2.51	0.42
2:D:237:LEU:O	2:D:241:LYS:HG3	2.19	0.42
2:E:219:GLU:HB3	2:E:222:LYS:NZ	2.34	0.42
1:A:5:LEU:HD11	1:A:75:LEU:HD21	2.02	0.42
1:C:221:MET:SD	2:F:239:GLN:NE2	2.87	0.42
2:E:63:ASP:HB2	2:E:67:ALA:HB2	2.00	0.42
1:B:165:PRO:HD3	7:B:2056:HOH:O	2.18	0.42
1:A:227:LEU:C	1:A:227:LEU:HD23	2.44	0.42
1:B:45:LEU:HD22	7:B:2010:HOH:O	2.20	0.42
1:B:98:ARG:HG3	7:B:2080:HOH:O	2.19	0.42
1:C:146:ARG:HD3	1:C:158:GLU:OE2	2.20	0.42
1:C:242:LEU:HD21	1:C:259:ALA:HB1	2.02	0.42
2:E:42:ALA:O	2:E:264:GLY:HA3	2.20	0.42
2:F:267:ILE:HB	2:F:268:PRO:HD3	2.02	0.42
1:B:107:GLN:NE2	3:E:1001:GDP:HN22	2.18	0.42
1:B:174:GLU:HG2	1:B:177:ARG:NH2	2.34	0.42
1:C:107:GLN:HA	5:C:1007:ALF:F1	2.10	0.42
1:B:107:GLN:HA	5:B:1007:ALF:F1	2.10	0.41
1:A:98:ARG:NH1	1:A:212:ASP:OD1	2.53	0.41
2:F:54:GLN:HG2	2:F:57:ARG:NH1	2.34	0.41
2:F:55:GLU:OE1	2:F:71:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HD3	1:A:98:ARG:C	2.45	0.41
1:A:177:ARG:NH2	1:A:178:LEU:HD23	2.36	0.41
1:B:131:LEU:HB2	1:B:156:VAL:HG22	2.01	0.41
1:A:57:GLU:HG3	7:A:2017:HOH:O	2.21	0.41
2:F:195:ARG:HD2	2:F:206:LEU:HD22	2.02	0.41
1:A:39:MET:HE2	1:A:39:MET:HB2	1.90	0.41
1:A:177:ARG:HH21	1:A:178:LEU:HD23	1.86	0.41
2:E:76:LEU:HD21	2:E:267:ILE:HD13	2.03	0.41
1:C:24:GLU:HB3	7:C:2005:HOH:O	2.21	0.41
1:A:227:LEU:HD21	1:A:231:ARG:NH2	2.36	0.41
2:D:62:LYS:HG3	2:D:63:ASP:N	2.36	0.41
2:E:180:MET:HE2	2:E:181:LYS:HG3	2.02	0.41
1:C:31:LEU:HD11	1:C:56:ARG:HB3	2.03	0.41
2:D:134:MET:CE	2:D:176:ALA:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/294 (98%)	283 (98%)	6 (2%)	0	100	100
1	B	289/294 (98%)	280 (97%)	9 (3%)	0	100	100
1	C	290/294 (99%)	281 (97%)	9 (3%)	0	100	100
2	D	281/284 (99%)	266 (95%)	11 (4%)	4 (1%)	9	13
2	E	277/284 (98%)	259 (94%)	17 (6%)	1 (0%)	30	43
2	F	256/284 (90%)	243 (95%)	11 (4%)	2 (1%)	16	25
All	All	1682/1734 (97%)	1612 (96%)	63 (4%)	7 (0%)	30	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	PRO
2	D	96	LYS
2	E	248	GLY
2	F	59	SER
2	D	60	GLY
2	D	248	GLY
2	F	248	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	230/233 (99%)	220 (96%)	10 (4%)	26	44
1	B	230/233 (99%)	224 (97%)	6 (3%)	40	63
1	C	231/233 (99%)	224 (97%)	7 (3%)	36	58
2	D	227/226 (100%)	217 (96%)	10 (4%)	25	43
2	E	224/226 (99%)	221 (99%)	3 (1%)	61	80
2	F	206/226 (91%)	198 (96%)	8 (4%)	28	48
All	All	1348/1377 (98%)	1304 (97%)	44 (3%)	34	55

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	19	ARG
1	A	39	MET
1	A	54	ARG
1	A	62	LYS
1	A	127	ARG
1	A	196	GLU
1	A	228	SER
1	A	242	LEU
1	A	285	GLU
1	B	10	GLN
1	B	39	MET

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Mol	Chain	Res	Type
1	B	40	ASP
1	B	45	LEU
1	B	49	ARG
1	B	236	LYS
1	C	27	LEU
1	C	45	LEU
1	C	50	ASP
1	C	62	LYS
1	C	66	GLU
1	C	98	ARG
1	C	236	LYS
2	D	29	GLU
2	D	54[A]	GLN
2	D	54[B]	GLN
2	D	75	MET
2	D	80	GLU
2	D	87	LYS
2	D	99	GLU
2	D	167	THR
2	D	245	GLU
2	D	271	ARG
2	E	68	VAL
2	E	75	MET
2	E	98	VAL
2	F	32	LEU
2	F	54	GLN
2	F	62	LYS
2	F	71	LYS
2	F	127	GLN
2	F	257	LEU
2	F	258	ASP
2	F	275	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	261	HIS
1	C	137	GLN
1	C	144	GLN
2	D	27	ASN
2	E	91	ASN

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Mol	Chain	Res	Type
2	E	234	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	GDP	E	1001	5,4	28,30,30	1.15	3 (10%)	44,47,47	1.91	8 (18%)
5	ALF	C	1007	7,3	0,4,4	-	-	-		
3	GDP	A	1001	5,4	28,30,30	1.10	2 (7%)	44,47,47	1.84	9 (20%)
6	5GP	E	3001	-	26,26,26	1.18	3 (11%)	40,40,40	1.93	9 (22%)
3	GDP	B	1001	5,4	28,30,30	1.13	3 (10%)	44,47,47	1.74	7 (15%)
5	ALF	B	1007	7,3	0,4,4	-	-	-		
5	ALF	D	1007	7,3	0,4,4	-	-	-		
3	GDP	C	1001	5,4	28,30,30	1.18	3 (10%)	44,47,47	1.81	7 (15%)
5	ALF	F	1007	7,3	0,4,4	-	-	-		
5	ALF	E	1007	7,3	0,4,4	-	-	-		
6	5GP	F	3001	-	26,26,26	1.21	3 (11%)	40,40,40	1.90	9 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GDP	F	1001	5,4	28,30,30	1.13	3 (10%)	44,47,47	1.85	8 (18%)
5	ALF	A	1007	7,3	0,4,4	-	-	-		
3	GDP	D	1001	5,4	28,30,30	1.10	2 (7%)	44,47,47	1.86	8 (18%)
6	5GP	D	3001	-	26,26,26	1.14	3 (11%)	40,40,40	1.97	8 (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
3	GDP	E	1001	5,4	-	2/16/32/32	0/3/3/3
6	5GP	E	3001	-	-	1/10/26/26	0/3/3/3
3	GDP	A	1001	5,4	-	2/16/32/32	0/3/3/3
3	GDP	B	1001	5,4	-	3/16/32/32	0/3/3/3
3	GDP	C	1001	5,4	-	2/16/32/32	0/3/3/3
6	5GP	F	3001	-	-	2/10/26/26	0/3/3/3
3	GDP	F	1001	5,4	-	2/16/32/32	0/3/3/3
3	GDP	D	1001	5,4	-	2/16/32/32	0/3/3/3
6	5GP	D	3001	-	-	2/10/26/26	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3001	5GP	C5-C4	3.63	1.48	1.38
6	E	3001	5GP	C5-C4	3.37	1.48	1.38
6	D	3001	5GP	C5-C4	3.25	1.47	1.38
3	B	1001	GDP	C5-C4	3.10	1.47	1.38
3	E	1001	GDP	C5-C4	2.76	1.46	1.38
3	F	1001	GDP	C5-C4	2.76	1.46	1.38
3	A	1001	GDP	C5-C4	2.75	1.46	1.38
3	F	1001	GDP	C5-N7	-2.68	1.33	1.39
3	D	1001	GDP	C5-C4	2.67	1.46	1.38
3	C	1001	GDP	C5-C4	2.63	1.46	1.38
3	D	1001	GDP	C5-N7	-2.63	1.34	1.39
6	E	3001	5GP	C6-N1	-2.56	1.34	1.38
3	B	1001	GDP	C5-N7	-2.55	1.34	1.39
3	E	1001	GDP	C6-N1	-2.51	1.34	1.38
6	F	3001	5GP	C5-N7	-2.32	1.34	1.39
6	D	3001	5GP	C5-N7	-2.26	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3001	5GP	C5-N7	-2.23	1.34	1.39
6	F	3001	5GP	C6-N1	-2.21	1.34	1.38
3	B	1001	GDP	C6-N1	-2.18	1.34	1.38
3	C	1001	GDP	C4-N9	-2.16	1.32	1.38
3	C	1001	GDP	C6-N1	-2.15	1.34	1.38
3	A	1001	GDP	C5-N7	-2.14	1.34	1.39
3	E	1001	GDP	C5-N7	-2.12	1.35	1.39
3	F	1001	GDP	C6-N1	-2.09	1.35	1.38
6	D	3001	5GP	C6-N1	-2.03	1.35	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	3001	5GP	C5-C4-N3	-5.98	118.75	128.46
3	C	1001	GDP	C2-N3-C4	5.89	122.79	112.30
6	D	3001	5GP	C5-C4-N3	-5.88	118.92	128.46
3	F	1001	GDP	C5-C4-N3	-5.82	119.02	128.46
6	F	3001	5GP	C5-C4-N3	-5.70	119.21	128.46
3	D	1001	GDP	C2-N3-C4	5.57	122.22	112.30
3	E	1001	GDP	C2-N3-C4	5.53	122.16	112.30
3	D	1001	GDP	C5-C4-N3	-5.51	119.52	128.46
3	B	1001	GDP	C5-C4-N3	-5.49	119.56	128.46
3	E	1001	GDP	C5-C4-N3	-5.40	119.70	128.46
3	A	1001	GDP	C5-C4-N3	-5.39	119.71	128.46
3	F	1001	GDP	C2-N3-C4	5.22	121.61	112.30
6	D	3001	5GP	C2-N3-C4	5.19	121.55	112.30
3	C	1001	GDP	C5-C4-N3	-5.15	120.11	128.46
3	A	1001	GDP	C2-N3-C4	5.12	121.42	112.30
6	E	3001	5GP	C2-N3-C4	4.99	121.20	112.30
6	F	3001	5GP	C2-N3-C4	4.97	121.15	112.30
3	B	1001	GDP	C2-N3-C4	4.92	121.07	112.30
6	F	3001	5GP	N9-C4-N3	4.43	134.84	125.94
3	E	1001	GDP	C6-C5-N7	4.41	138.44	130.25
6	E	3001	5GP	N9-C4-N3	4.38	134.73	125.94
6	D	3001	5GP	N9-C4-N3	4.35	134.68	125.94
3	F	1001	GDP	N9-C4-N3	4.35	134.66	125.94
3	D	1001	GDP	N9-C4-N3	4.20	134.38	125.94
3	A	1001	GDP	N9-C4-N3	4.17	134.32	125.94
3	B	1001	GDP	N9-C4-N3	4.15	134.28	125.94
3	C	1001	GDP	C6-C5-N7	3.96	137.61	130.25
3	C	1001	GDP	N9-C4-N3	3.86	133.69	125.94
3	D	1001	GDP	C6-C5-N7	3.79	137.29	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	3001	5GP	C6-C5-N7	3.59	136.92	130.25
6	F	3001	5GP	C6-C5-N7	3.53	136.82	130.25
6	D	3001	5GP	C6-C5-N7	3.53	136.81	130.25
3	B	1001	GDP	C6-C5-N7	3.45	136.67	130.25
3	F	1001	GDP	C6-C5-N7	3.45	136.67	130.25
3	A	1001	GDP	C6-C5-N7	3.45	136.66	130.25
3	E	1001	GDP	N9-C4-N3	3.26	132.49	125.94
3	E	1001	GDP	O4'-C1'-N9	3.18	115.64	108.36
3	E	1001	GDP	C4-C5-N7	-3.13	105.76	110.72
6	F	3001	5GP	OP2-P-O5'	-3.10	98.49	106.73
6	D	3001	5GP	OP2-P-O5'	-2.97	98.83	106.73
6	E	3001	5GP	C4-C5-N7	-2.95	106.05	110.72
3	A	1001	GDP	O6-C6-C5	-2.84	119.08	126.60
3	C	1001	GDP	O6-C6-C5	-2.78	119.24	126.60
6	F	3001	5GP	C4-C5-N7	-2.77	106.34	110.72
6	D	3001	5GP	C4-C5-N7	-2.76	106.35	110.72
6	E	3001	5GP	OP3-P-OP1	2.74	121.41	110.68
3	F	1001	GDP	C4-C5-N7	-2.71	106.43	110.72
3	C	1001	GDP	C6-C5-C4	-2.68	114.65	118.77
3	A	1001	GDP	C4-C5-N7	-2.60	106.60	110.72
3	D	1001	GDP	O6-C6-C5	-2.56	119.80	126.60
3	D	1001	GDP	C4-C5-N7	-2.51	106.75	110.72
3	B	1001	GDP	O6-C6-C5	-2.48	120.03	126.60
3	B	1001	GDP	C4-C5-N7	-2.40	106.92	110.72
3	F	1001	GDP	O6-C6-C5	-2.35	120.36	126.60
3	C	1001	GDP	C5-C6-N1	2.33	119.11	113.19
6	E	3001	5GP	OP2-P-O5'	-2.24	100.78	106.73
3	A	1001	GDP	C8-N7-C5	2.22	108.26	104.24
6	D	3001	5GP	OP3-P-OP1	2.20	119.30	110.68
6	E	3001	5GP	C8-N7-C5	2.20	108.22	104.24
6	F	3001	5GP	O4'-C1'-N9	2.16	113.29	108.36
3	A	1001	GDP	C2-N1-C6	-2.15	121.18	125.10
3	D	1001	GDP	O2A-PA-O1A	2.14	122.82	112.24
6	E	3001	5GP	C2'-C1'-N9	-2.14	107.16	113.22
3	F	1001	GDP	C8-N7-C5	2.13	108.09	104.24
3	E	1001	GDP	N2-C2-N1	2.13	121.24	116.71
3	D	1001	GDP	C5-C6-N1	2.12	118.57	113.19
3	F	1001	GDP	O3'-C3'-C4'	-2.11	104.94	111.05
3	A	1001	GDP	N9-C8-N7	-2.10	109.43	113.39
6	F	3001	5GP	OP3-P-OP1	2.10	118.90	110.68
6	F	3001	5GP	C8-N7-C5	2.09	108.02	104.24
6	D	3001	5GP	C8-N7-C5	2.08	108.00	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1001	GDP	C8-N7-C5	2.07	107.98	104.24
3	B	1001	GDP	C5-C6-N1	2.03	118.34	113.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GDP	PA-O3A-PB-O3B
3	B	1001	GDP	PA-O3A-PB-O3B
3	C	1001	GDP	PA-O3A-PB-O3B
3	D	1001	GDP	PA-O3A-PB-O3B
3	E	1001	GDP	PA-O3A-PB-O3B
3	F	1001	GDP	PA-O3A-PB-O3B
6	D	3001	5GP	O4'-C4'-C5'-O5'
6	D	3001	5GP	C3'-C4'-C5'-O5'
6	F	3001	5GP	O4'-C4'-C5'-O5'
6	F	3001	5GP	C3'-C4'-C5'-O5'
3	E	1001	GDP	PA-O3A-PB-O1B
3	D	1001	GDP	PA-O3A-PB-O1B
6	E	3001	5GP	C5'-O5'-P-OP3
3	B	1001	GDP	PA-O3A-PB-O1B
3	C	1001	GDP	PA-O3A-PB-O1B
3	F	1001	GDP	PA-O3A-PB-O1B
3	A	1001	GDP	PA-O3A-PB-O2B
3	B	1001	GDP	PA-O3A-PB-O2B

There are no ring outliers.

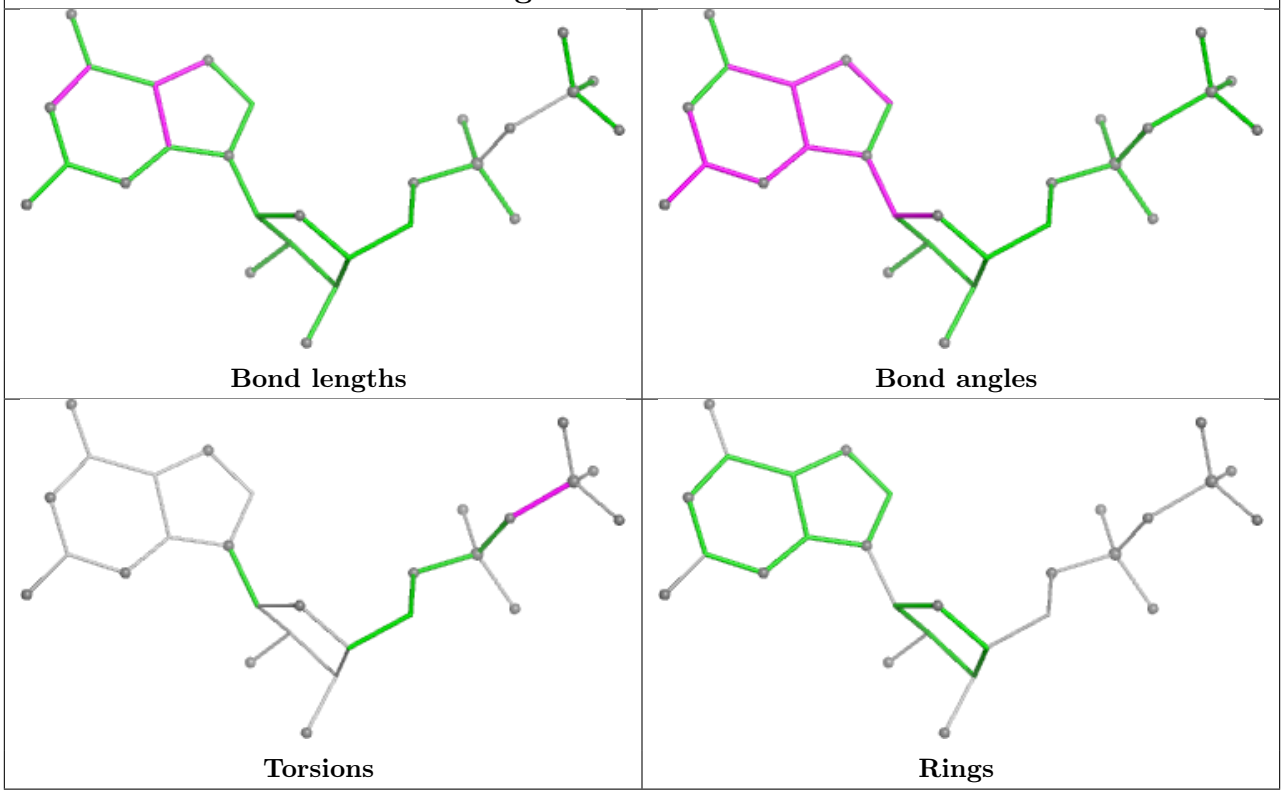
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1001	GDP	1	0
5	C	1007	ALF	1	0
5	B	1007	ALF	1	0
6	D	3001	5GP	1	0

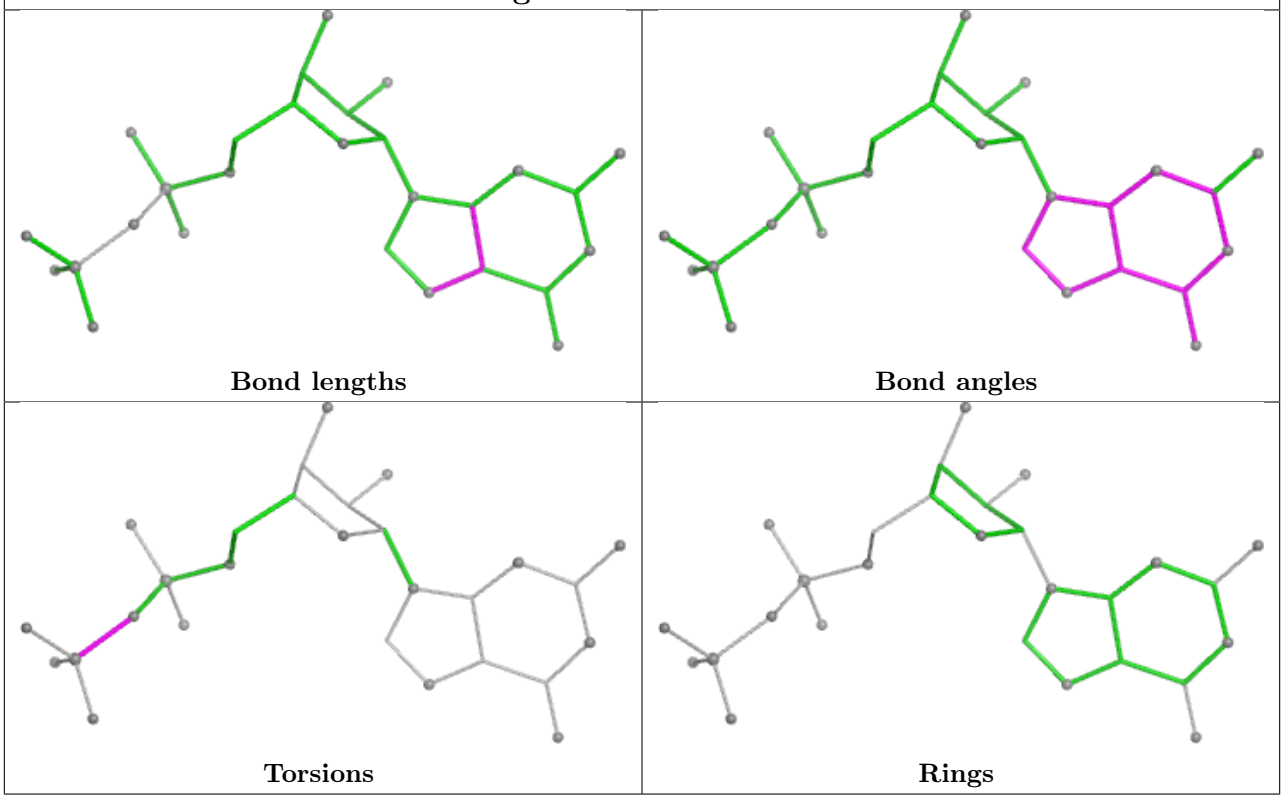
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

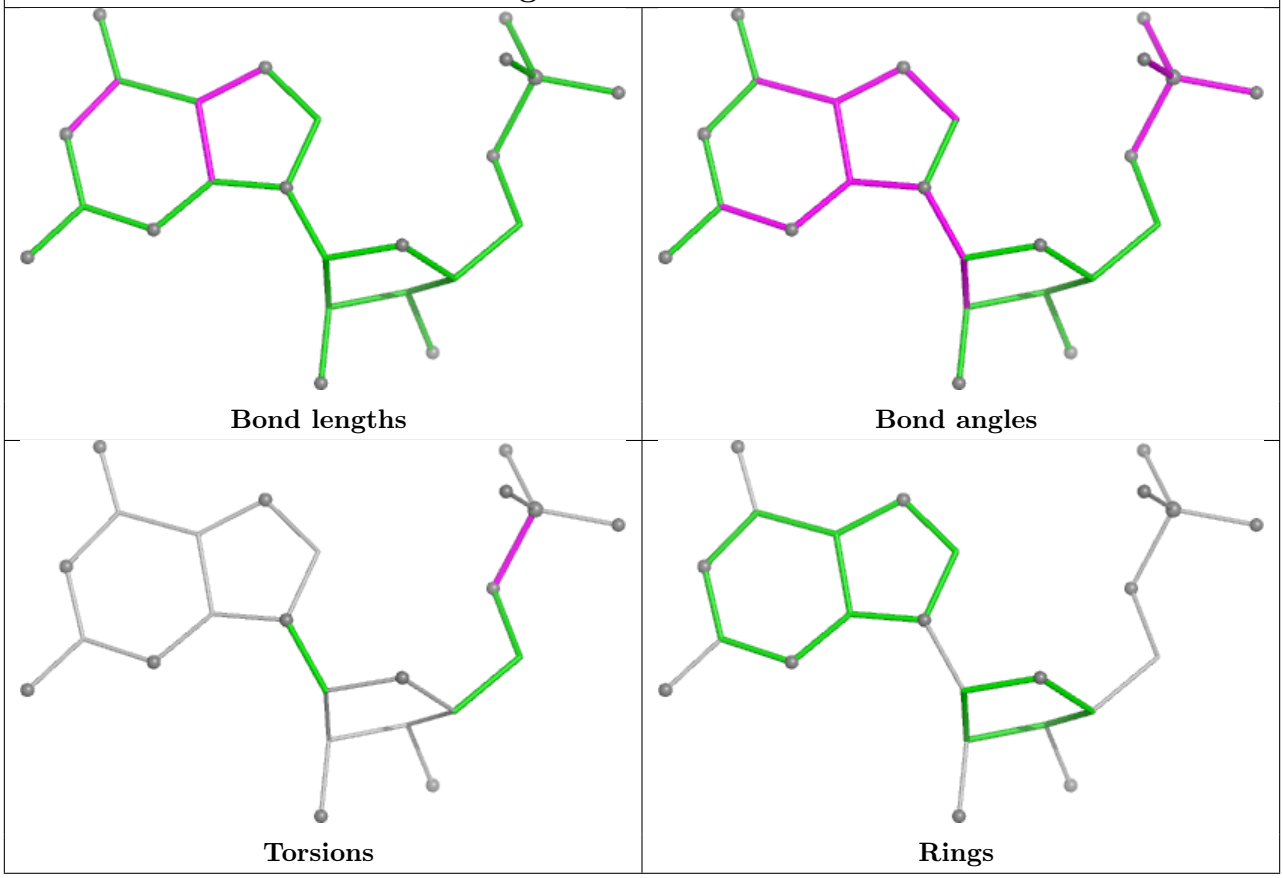
Ligand GDP E 1001



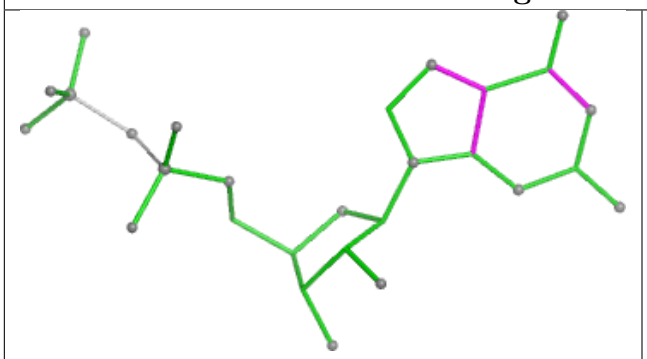
Ligand GDP A 1001



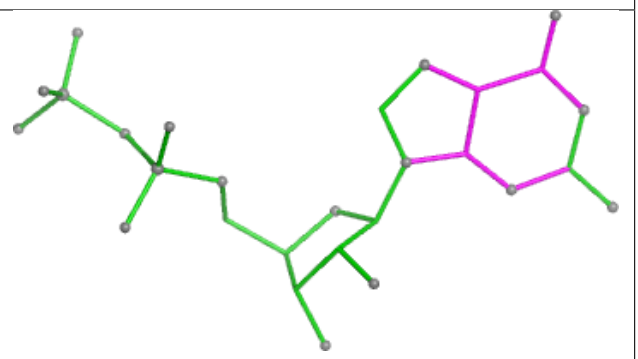
Ligand 5GP E 3001



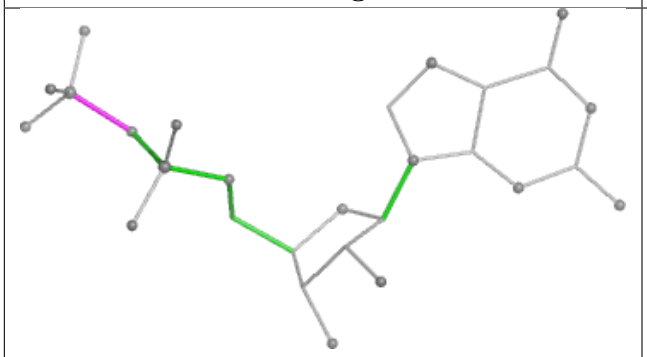
Ligand GDP B 1001



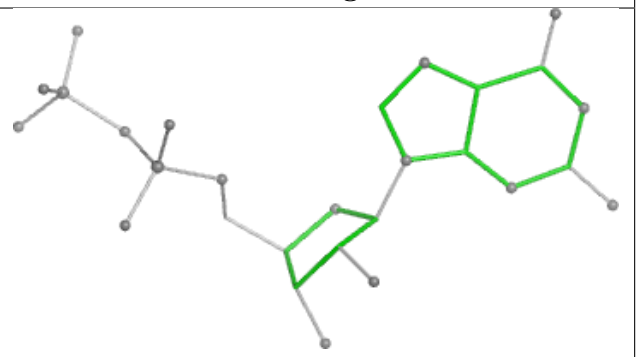
Bond lengths



Bond angles

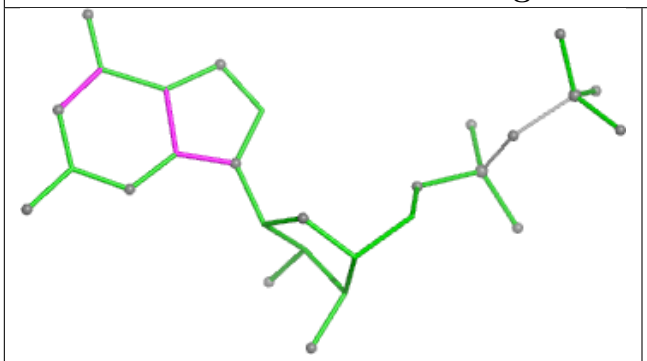


Torsions

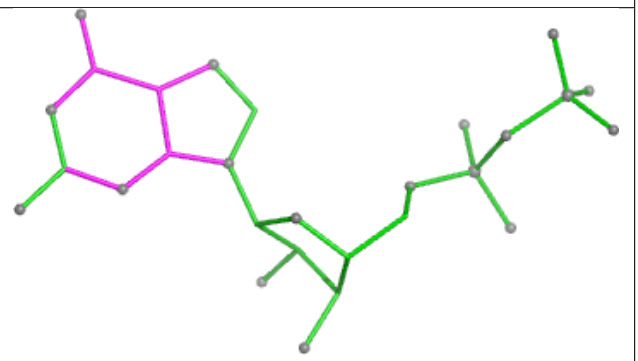


Rings

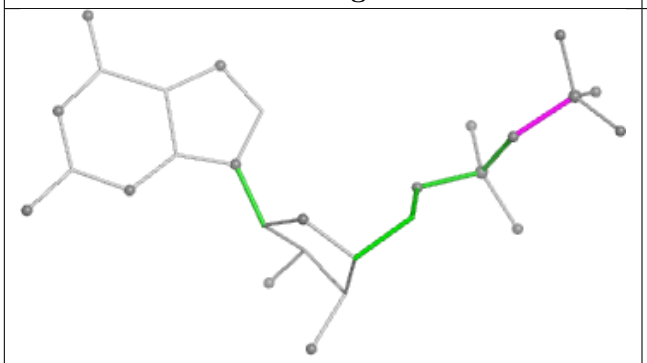
Ligand GDP C 1001



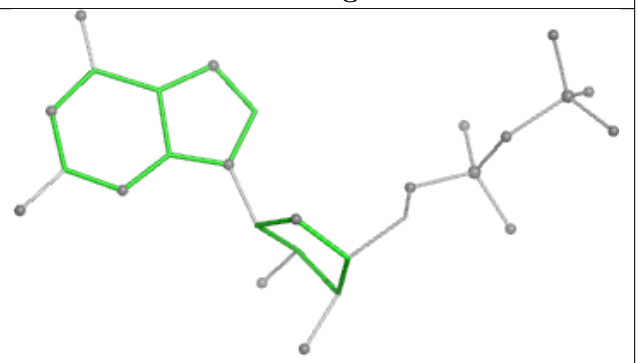
Bond lengths



Bond angles

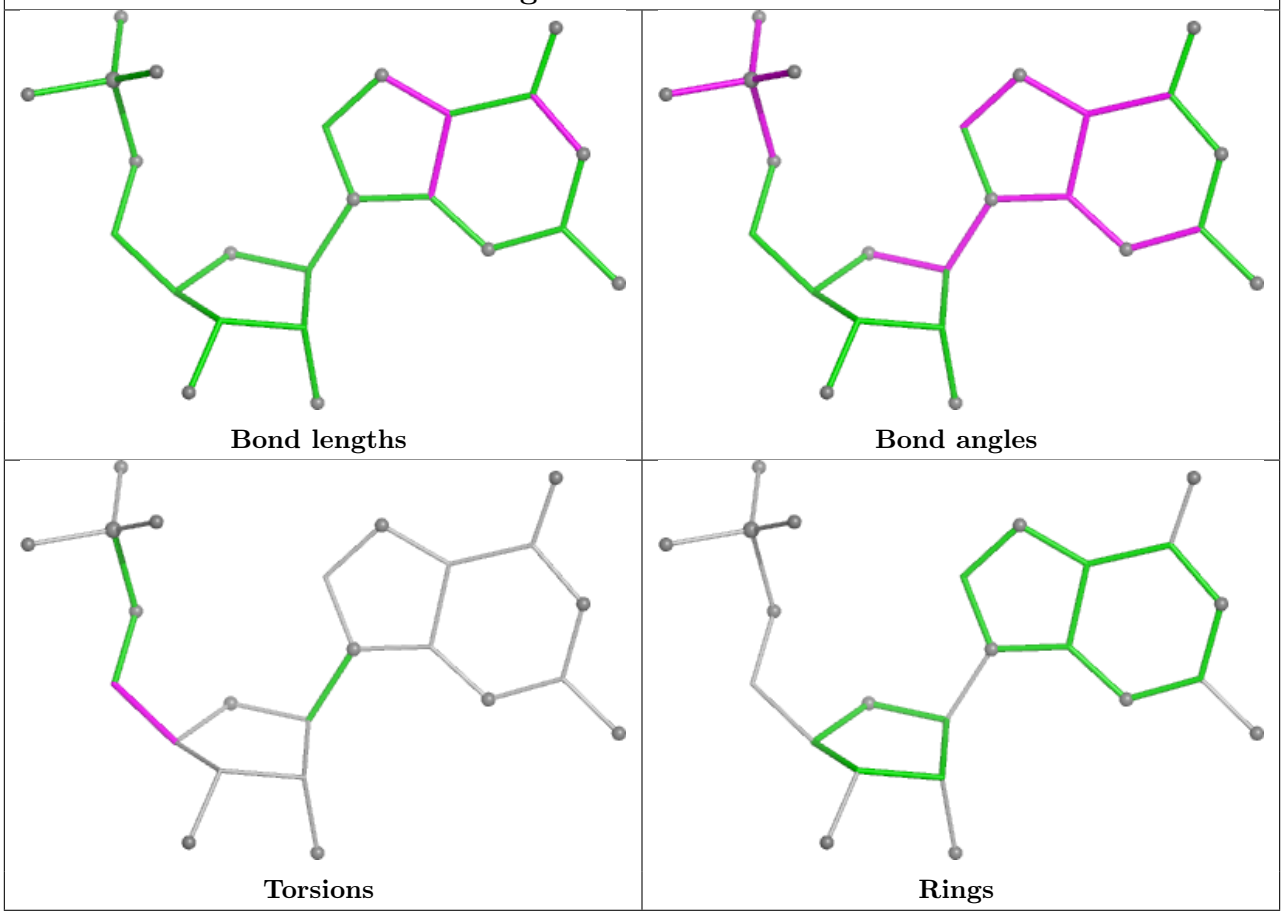


Torsions

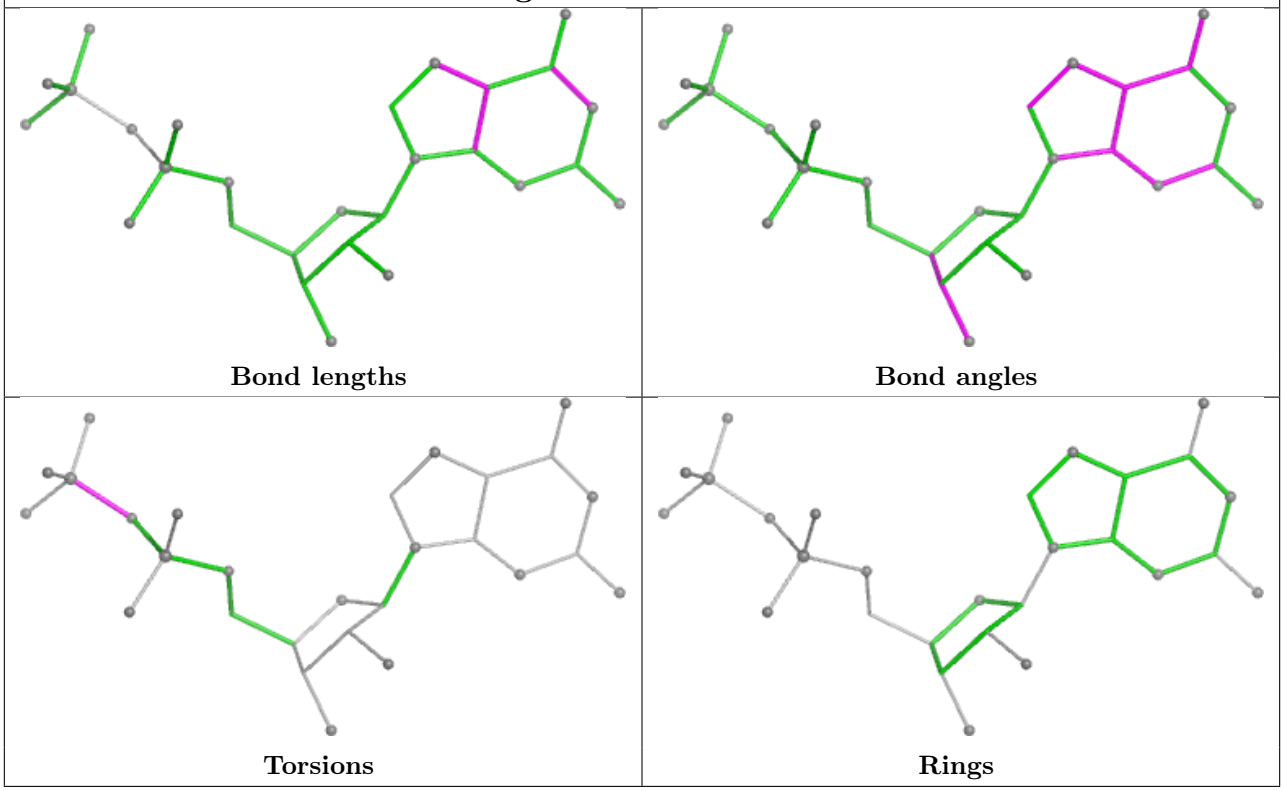


Rings

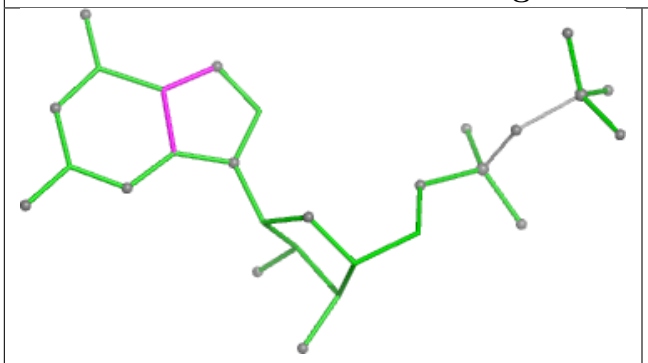
Ligand 5GP F 3001



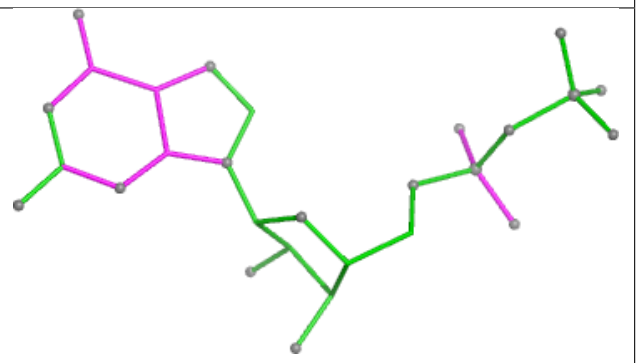
Ligand GDP F 1001



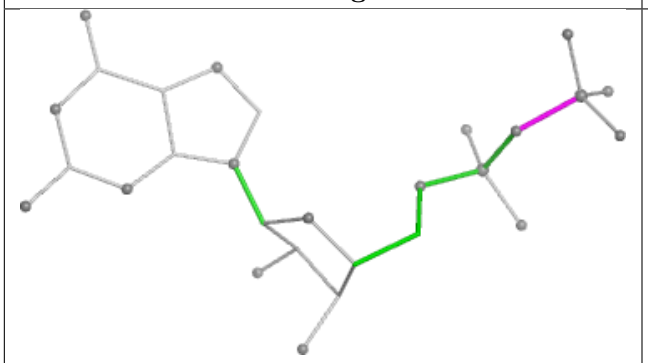
Ligand GDP D 1001



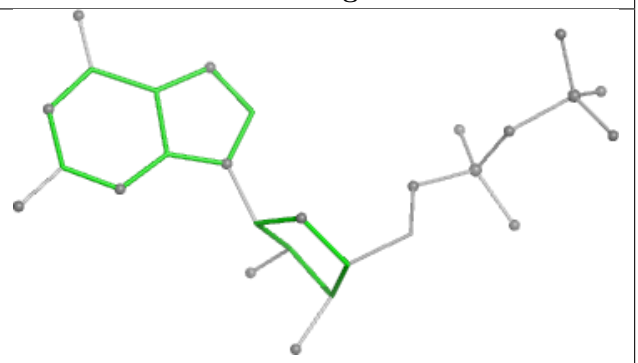
Bond lengths



Bond angles

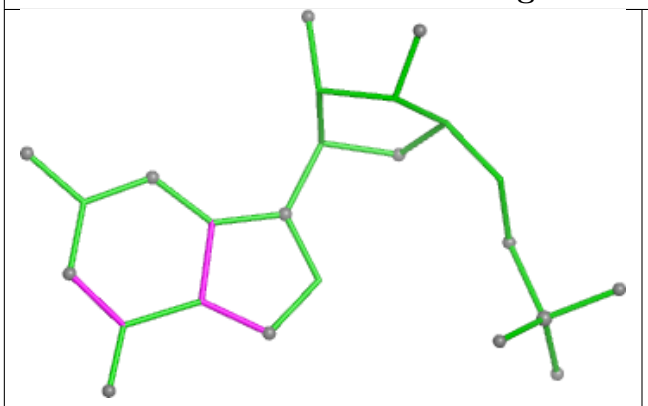


Torsions

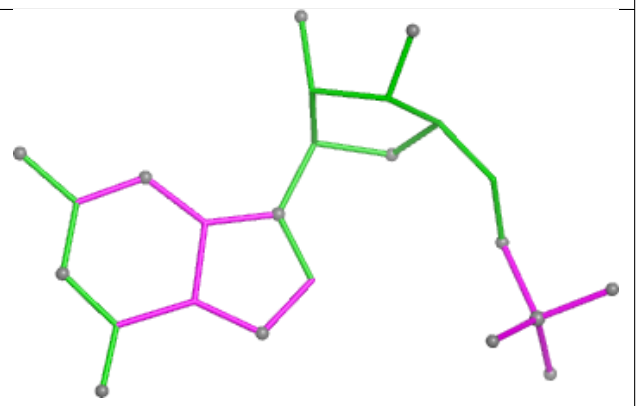


Rings

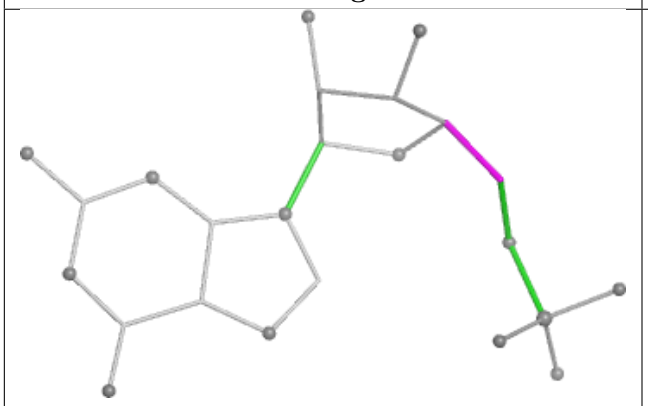
Ligand 5GP D 3001



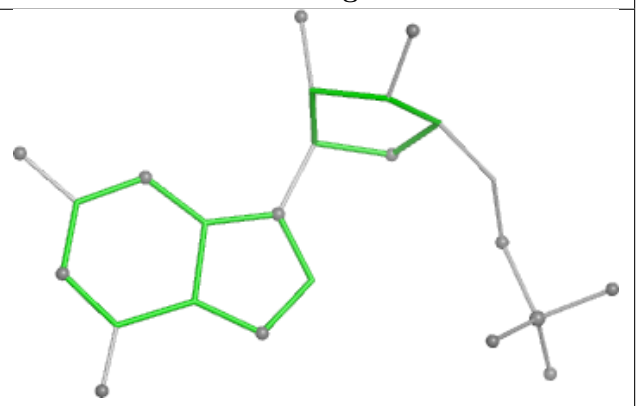
Bond lengths



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 (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	290/294 (98%)	-1.67	0	100	100	13, 28, 56, 68	12 (4%)
1	B	290/294 (98%)	-1.66	0	100	100	15, 29, 75, 85	10 (3%)
1	C	290/294 (98%)	-1.67	0	100	100	8, 31, 57, 65	12 (4%)
2	D	281/284 (98%)	-1.65	0	100	100	10, 28, 65, 71	8 (2%)
2	E	279/284 (98%)	-1.65	0	100	100	13, 29, 69, 75	9 (3%)
2	F	260/284 (91%)	-1.64	0	100	100	18, 32, 70, 77	4 (1%)
All	All	1690/1734 (97%)	-1.66	0	100	100	8, 30, 67, 85	55 (3%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	5GP	D	3001	24/24	0.99	0.02	39,41,49,49	0

Continued on next page...

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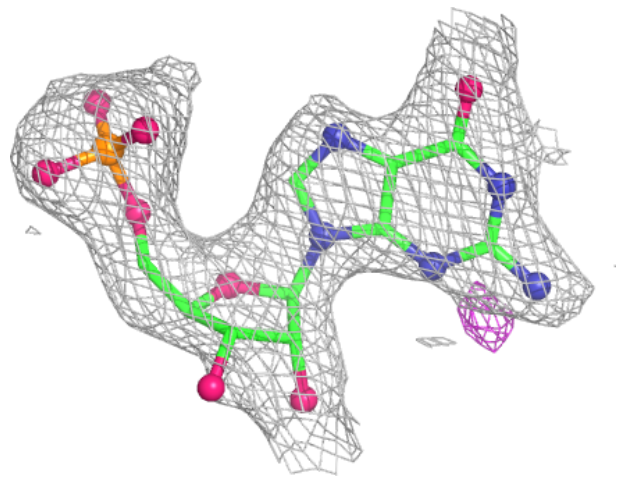
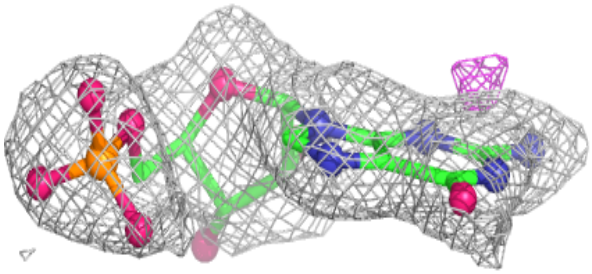
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	5GP	E	3001	24/24	0.99	0.02	33,36,48,48	0
6	5GP	F	3001	24/24	0.99	0.02	33,36,51,52	0
3	GDP	D	1001	28/28	1.00	0.01	9,16,17,18	0
3	GDP	E	1001	28/28	1.00	0.02	10,18,19,19	0
3	GDP	F	1001	28/28	1.00	0.01	12,17,18,19	0
4	MG	A	1002	1/1	1.00	0.01	12,12,12,12	0
4	MG	B	1002	1/1	1.00	0.02	17,17,17,17	0
4	MG	C	1002	1/1	1.00	0.01	18,18,18,18	0
4	MG	D	1002	1/1	1.00	0.01	13,13,13,13	0
4	MG	E	1002	1/1	1.00	0.01	15,15,15,15	0
4	MG	F	1002	1/1	1.00	0.01	15,15,15,15	0
5	ALF	A	1007	5/5	1.00	0.01	13,16,17,18	0
5	ALF	B	1007	5/5	1.00	0.01	18,19,19,20	0
5	ALF	C	1007	5/5	1.00	0.02	18,18,20,22	0
5	ALF	D	1007	5/5	1.00	0.01	12,12,14,16	0
5	ALF	E	1007	5/5	1.00	0.02	11,14,15,16	0
5	ALF	F	1007	5/5	1.00	0.01	15,15,16,16	0
3	GDP	A	1001	28/28	1.00	0.01	8,10,11,12	0
3	GDP	B	1001	28/28	1.00	0.01	13,16,17,17	0
3	GDP	C	1001	28/28	1.00	0.01	10,14,16,18	0

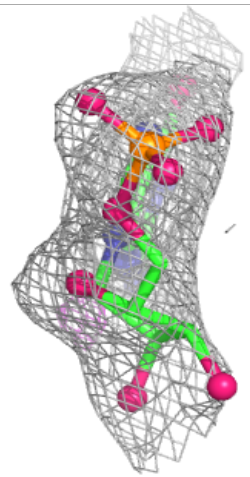
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP D 3001:

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

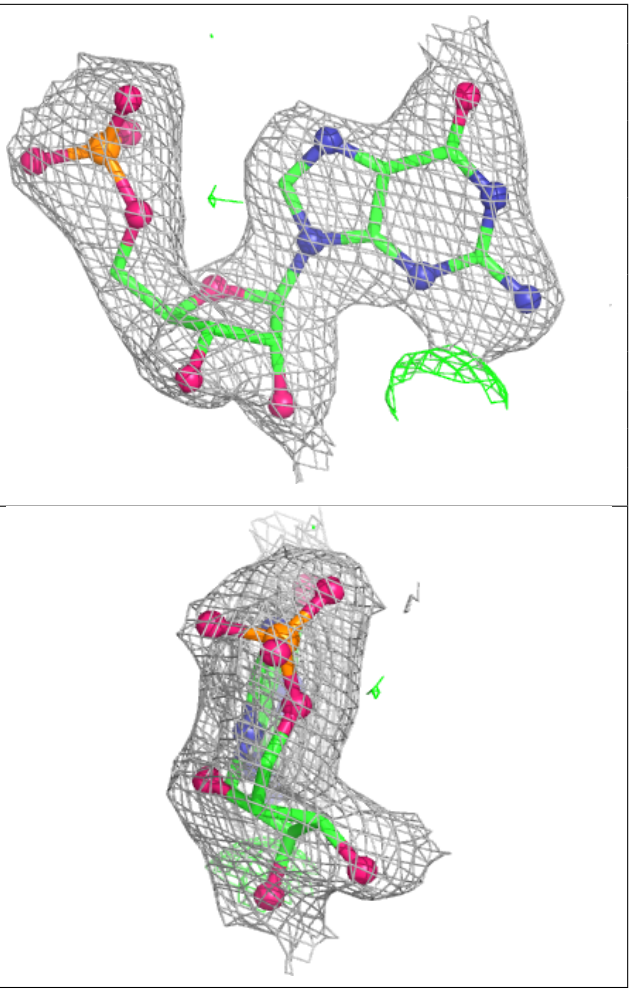






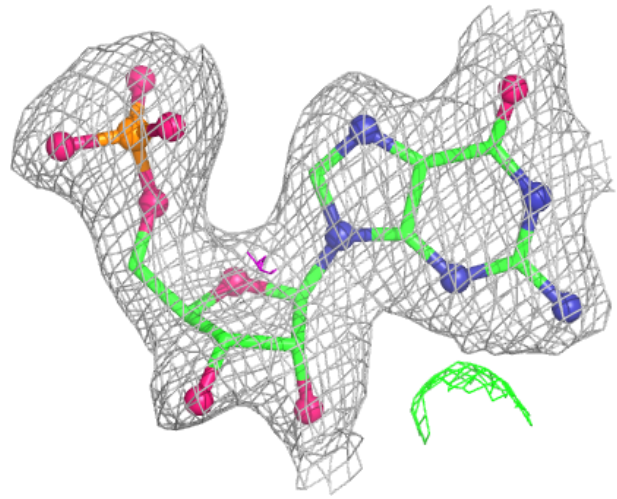
Electron density around 5GP E 3001:

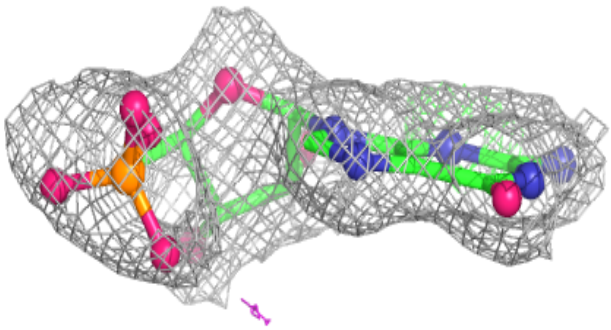
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

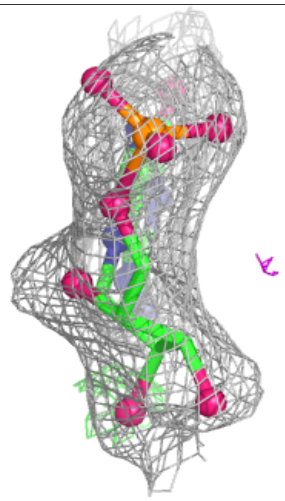


Electron density around 5GP F 3001:

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

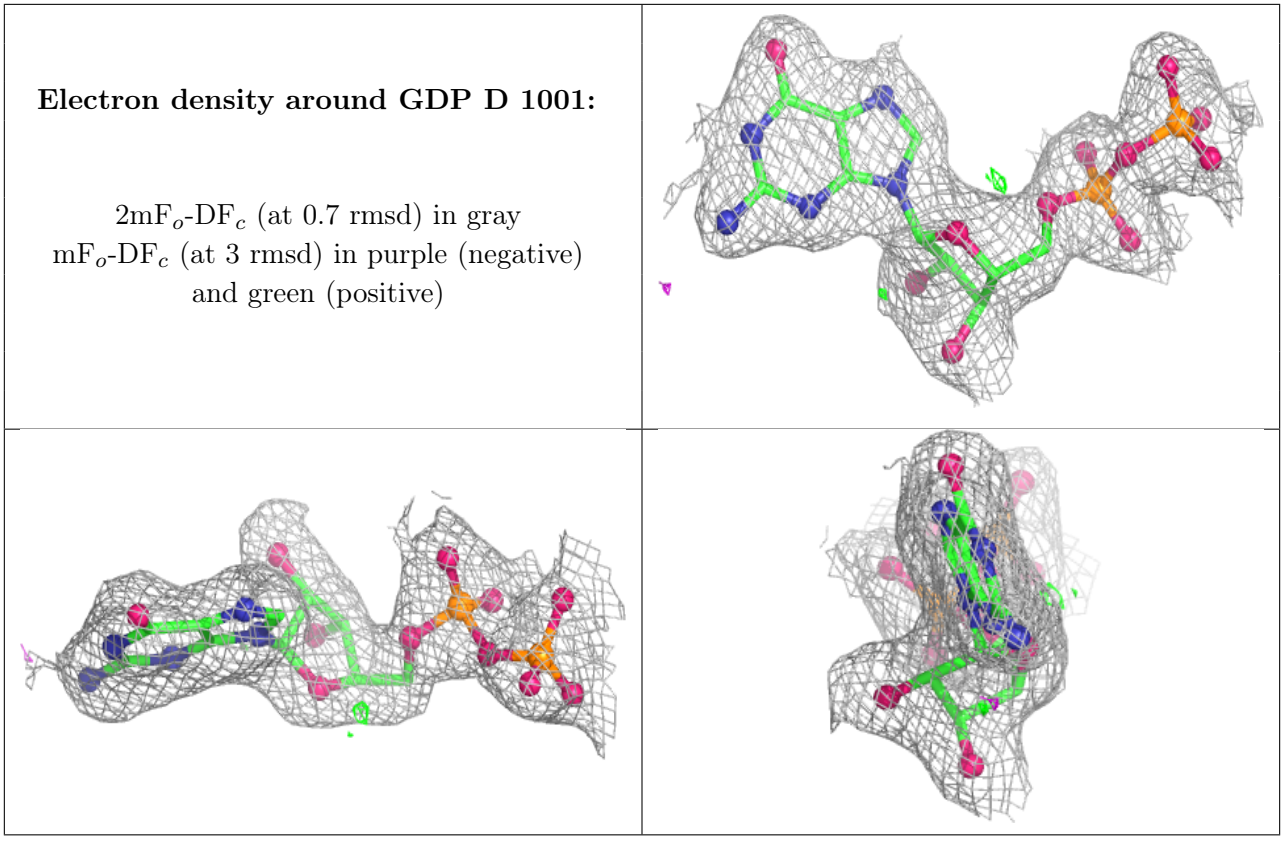






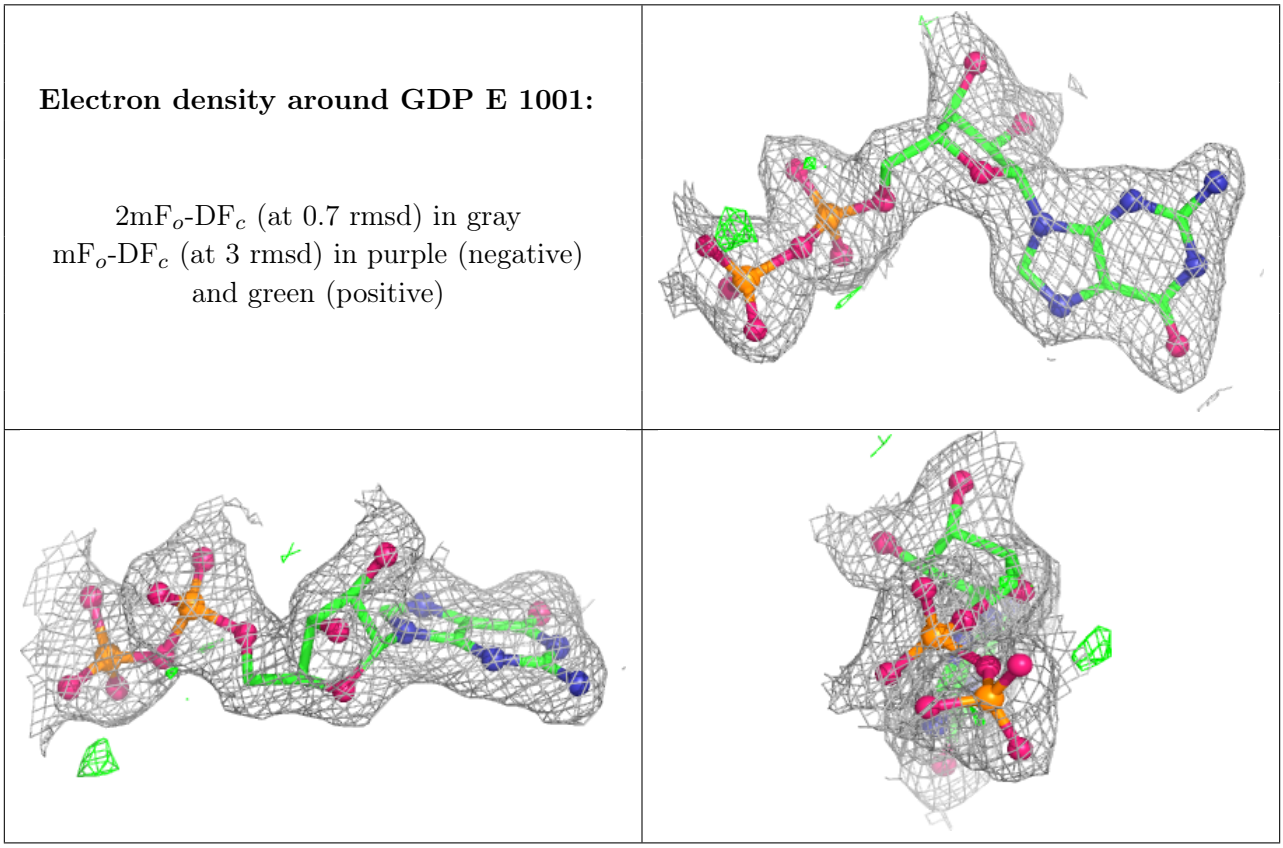
Electron density around GDP D 1001:

$2mF_o$-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 E 1001:

$2mF_o$-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 F 1001:

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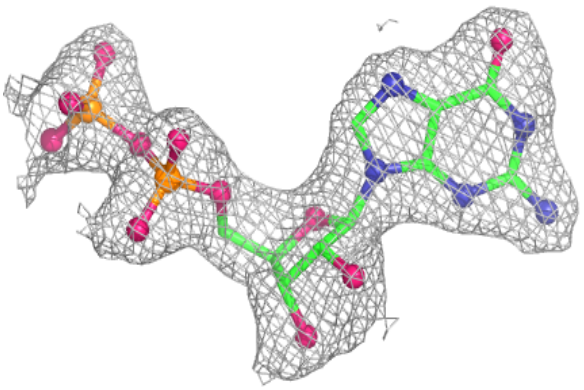
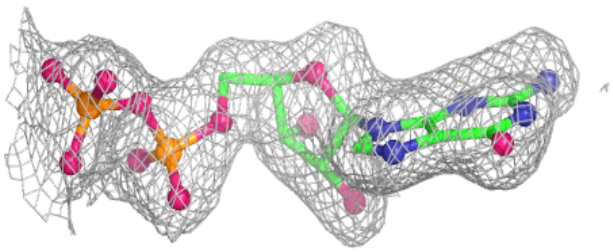
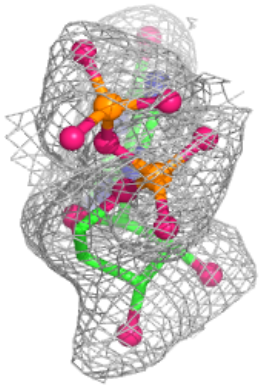
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

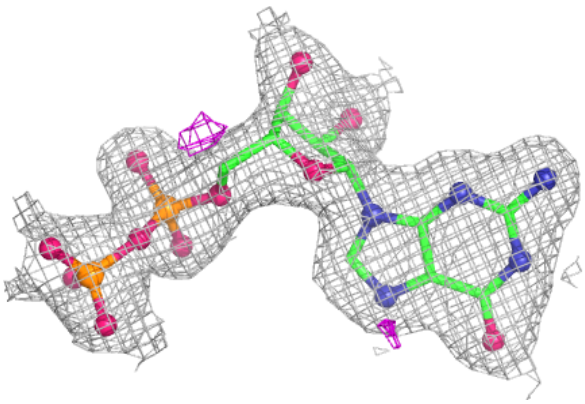


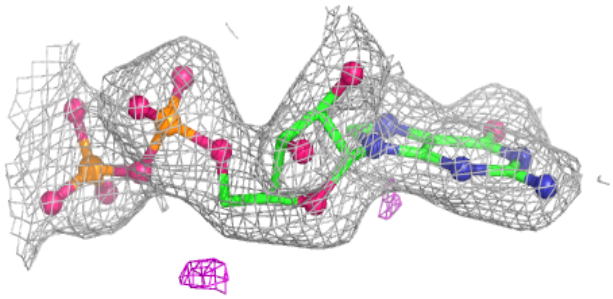


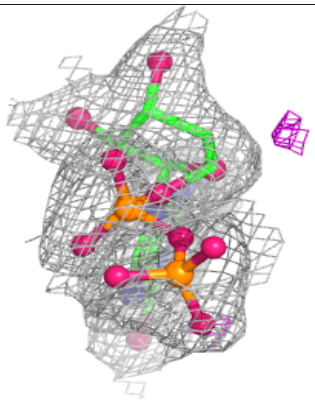


Electron density around GDP A 1001:

$2mF_o$-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 1001:

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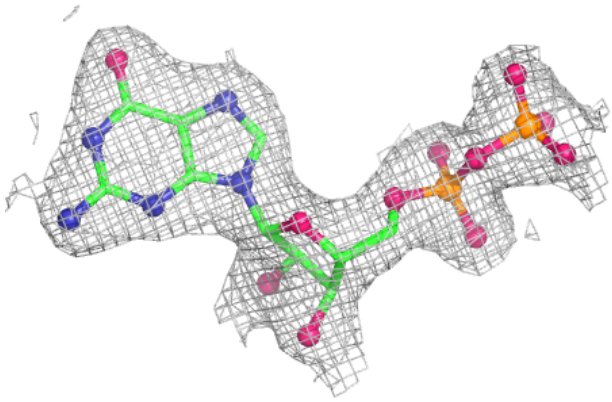
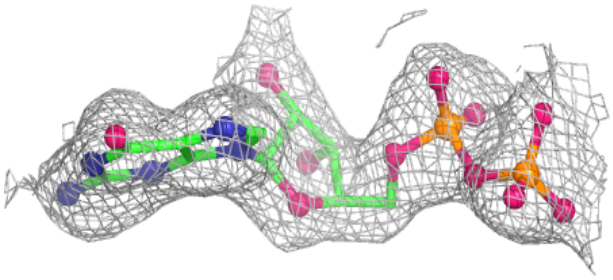
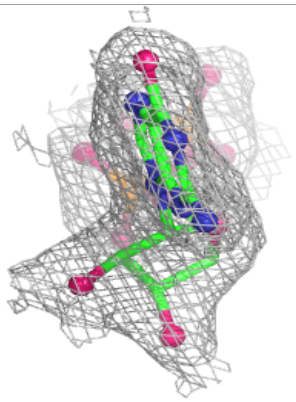
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

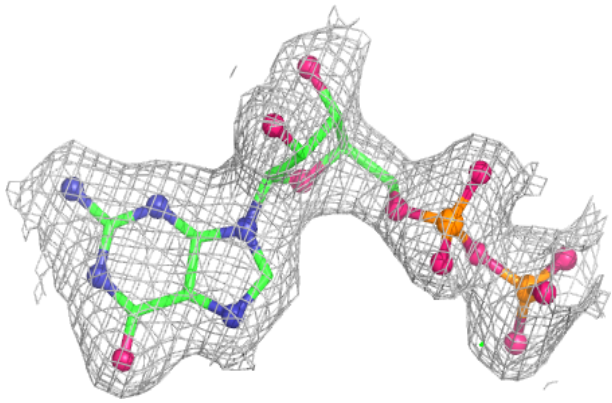


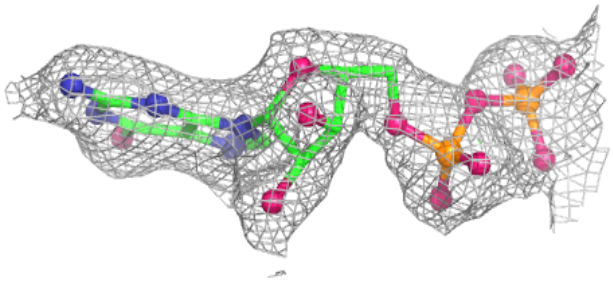


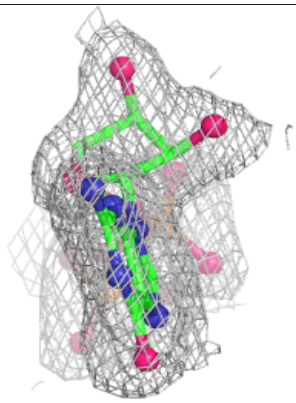


Electron density around GDP C 1001:

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







6.5 Other polymers (i)

There are no such residues in this entry.