WORLD WIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 06:07 PM EDT

PDB ID	:	1CJU
Title	:	COMPLEX OF GS-ALPHA WITH THE CATALYTIC DOMAINS OF MAM-MALIAN ADENYLYL CYCLASE: COMPLEX WITH BETA-L-2',3'-DIDE OXYATP AND MG
Authors	:	Tesmer, J.J.G.; Sprang, S.R.
Deposited on	:	1999-04-16
Resolution	:	2.80 Å(reported)

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

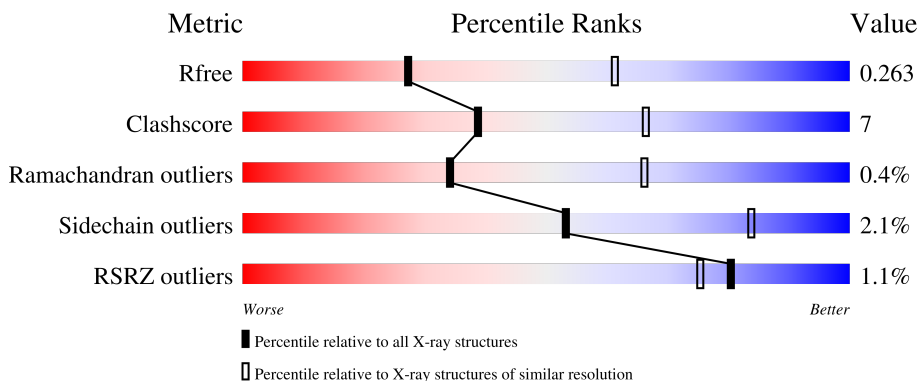|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		2.1%
RSRZ outliers		1.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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	217	% 69% 18% · 13%
2	B	212	2% 69% 19% 11%
3	C	402	69% 13% 18%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 5793 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 ADENYLATE CYCLASE, TYPE V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	MET	VAL	engineered mutation	UNP P30803

- Molecule 2 is a protein called ADENYLATE CYCLASE, TYPE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1471	939	242	280	10			

- Molecule 3 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN G(S).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	331	Total	C	N	O	S	0	0	0
			2710	1718	472	507	13			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FORSKOLIN (three-letter code: FOK) (formula: $C_{22}H_{34}O_7$).
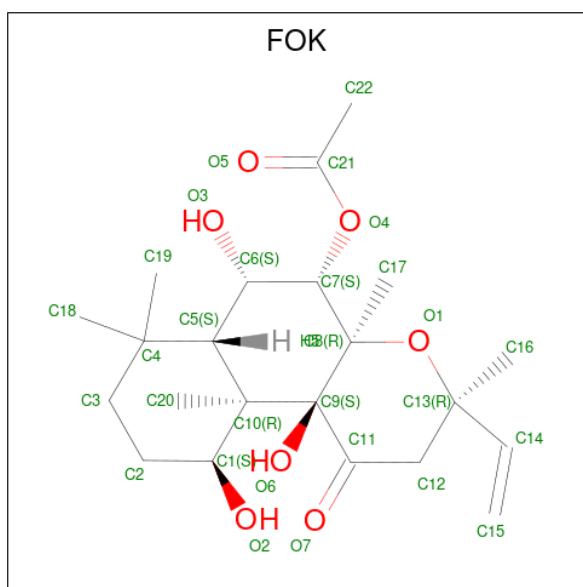
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 29	C 22	O 7	0	0

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: DAD) (formula: $C_{10}H_{16}N_5O_{11}P_3$).
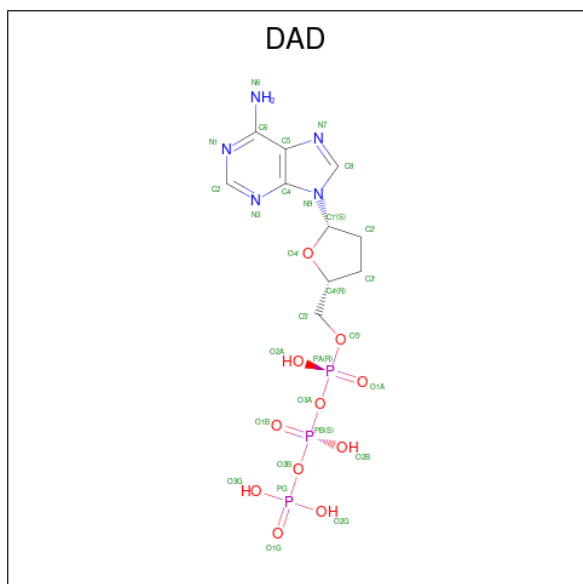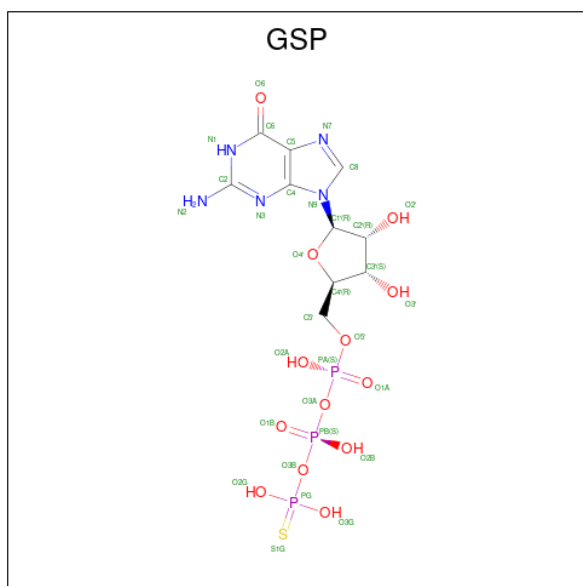

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 29	C 10	N 5	O 11	P 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Cl 1	0	0

- Molecule 8 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

GSP

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	C	1	32	10	5	13	3	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total 7	O 7	0	0
9	B	13	Total 13	O 13	0	0
9	C	22	Total 22	O 22	0	0

3 Residue-property plots ⓘ

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.
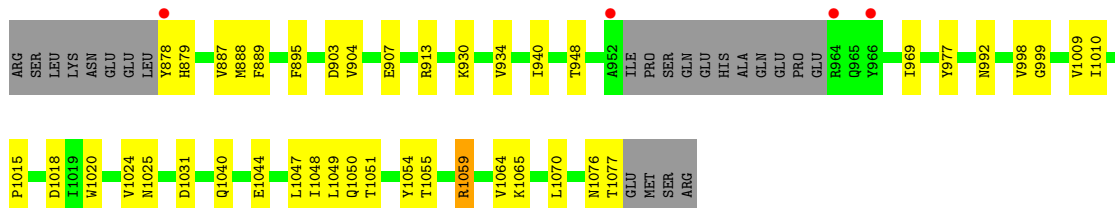
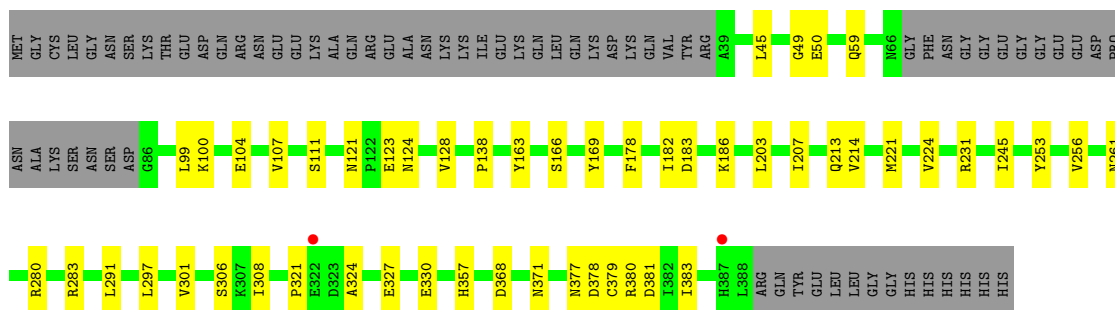• Molecule 1: ADENYLATE CYCLASE, TYPE V

Chain A:
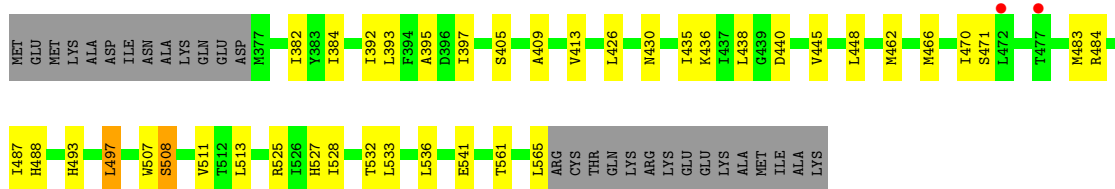
• Molecule 2: ADENYLATE CYCLASE, TYPE II

Chain B:

• Molecule 3: GUANINE NUCLEOTIDE-BINDING PROTEIN G(S)

Chain C:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.30Å 134.20Å 71.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 37.83 – 2.81	Depositor EDS
% Data completeness (in resolution range)	77.7 (15.00-2.80) 77.7 (37.83-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.81Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.222 , 0.284 0.210 , 0.263	Depositor DCC
R_{free} test set	2191 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	1.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5793	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOK, DAD, GSP, CL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/1504	0.59	0/2027
2	B	0.44	0/1497	0.62	0/2021
3	C	0.41	0/2767	0.60	0/3744
All	All	0.41	0/5768	0.60	0/7792

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 ⓘ

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	1476	0	1450	25	0
2	B	1471	0	1468	31	0
3	C	2710	0	2657	28	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	29	0	34	6	0
6	A	29	0	12	2	0
7	C	1	0	0	0	0
8	C	32	0	12	1	0
9	A	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	13	0	0	0	0
9	C	22	0	0	1	0
All	All	5793	0	5633	85	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 7.

All (85) 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:B:1040:GLN:HE22	2:B:1059:ARG:HH11	1.15	0.89
2:B:1040:GLN:HE22	2:B:1059:ARG:NH1	1.73	0.86
1:A:382:ILE:HD11	1:A:384:ILE:HD12	1.58	0.84
5:A:101:FOK:H173	5:A:101:FOK:H201	1.61	0.81
1:A:462:MET:HG3	1:A:466:MET:HE3	1.59	0.81
1:A:525:ARG:HH22	1:A:565:LEU:HD23	1.48	0.78
1:A:487:ILE:HB	1:A:528:ILE:HG22	1.75	0.69
2:B:904:VAL:HG11	3:C:207:ILE:HG21	1.79	0.65
3:C:124:ASN:O	3:C:128:VAL:HG23	1.98	0.64
6:A:102:DAD:H8	2:B:1025:ASN:ND2	2.13	0.64
3:C:121:ASN:HB3	3:C:123:GLU:OE1	2.01	0.61
3:C:256:VAL:HG11	3:C:261:ASN:C	2.22	0.60
5:A:101:FOK:H202	5:A:101:FOK:H193	1.83	0.59
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.84	0.59
1:A:488:HIS:CE1	1:A:513:LEU:HD23	2.39	0.58
3:C:321:PRO:HG2	3:C:324:ALA:HB2	1.86	0.57
1:A:426:LEU:HB2	1:A:462:MET:HE1	1.87	0.56
3:C:100:LYS:O	3:C:104:GLU:HG2	2.06	0.55
3:C:203:LEU:HD12	8:C:405:GSP:S1G	2.46	0.54
2:B:1040:GLN:NE2	2:B:1059:ARG:HH11	1.96	0.53
2:B:969:ILE:HD12	2:B:1048:ILE:HG21	1.89	0.53
2:B:1009:VAL:HG12	2:B:1010:ILE:N	2.24	0.52
1:A:507:TRP:O	1:A:508:SER:HB3	2.10	0.51
1:A:430:ASN:HD22	1:A:462:MET:HA	1.75	0.51
1:A:527:HIS:NE2	1:A:561:THR:HB	2.26	0.51
5:A:101:FOK:H152	2:B:895:PHE:CE2	2.45	0.51
1:A:397:ILE:CG1	1:A:440:ASP:HB2	2.40	0.51
1:A:497:LEU:HD22	1:A:507:TRP:CZ2	2.46	0.51
2:B:878:TYR:HD1	2:B:879:HIS:H	1.58	0.51
2:B:1044:GLU:CD	2:B:1044:GLU:H	2.15	0.51
3:C:183:ASP:HA	3:C:186:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:101:FOK:H163	5:A:101:FOK:H171	1.92	0.50
3:C:99:LEU:HD21	3:C:182:ILE:HG12	1.93	0.50
3:C:291:LEU:HD13	9:C:417:HOH:O	2.11	0.50
3:C:166:SER:HA	3:C:169:TYR:CE2	2.48	0.49
2:B:1009:VAL:HG12	2:B:1010:ILE:H	1.76	0.49
3:C:45:LEU:HD23	3:C:245:ILE:CG2	2.43	0.49
1:A:438:LEU:HD13	2:B:940:ILE:HG23	1.94	0.48
1:A:533:LEU:HD12	1:A:536:LEU:HD12	1.95	0.48
3:C:99:LEU:HD13	3:C:178:PHE:HB3	1.96	0.48
5:A:101:FOK:H152	2:B:895:PHE:HE2	1.78	0.48
1:A:430:ASN:ND2	1:A:462:MET:HA	2.29	0.48
3:C:49:GLY:O	3:C:50:GLU:HB2	2.15	0.47
2:B:878:TYR:CD1	2:B:879:HIS:N	2.83	0.47
2:B:977:TYR:OH	2:B:1077:THR:HA	2.14	0.47
3:C:368:ASP:HB3	3:C:371:ASN:HB3	1.97	0.47
2:B:904:VAL:HG11	3:C:207:ILE:CG2	2.43	0.47
2:B:1018:ASP:HB3	2:B:1020:TRP:CH2	2.49	0.46
6:A:102:DAD:O1G	2:B:1065:LYS:NZ	2.46	0.46
2:B:1049:LEU:O	2:B:1054:TYR:HB2	2.16	0.46
1:A:470:ILE:HD13	1:A:483:MET:HB2	1.97	0.45
2:B:934:VAL:HA	2:B:948:THR:HG22	1.97	0.45
3:C:163:TYR:O	3:C:166:SER:HB3	2.16	0.45
2:B:1055:THR:HG22	2:B:1076:ASN:HD22	1.81	0.45
1:A:541:GLU:HB3	1:A:565:LEU:HD12	1.99	0.44
2:B:1009:VAL:HG11	2:B:1015:PRO:HA	1.99	0.44
3:C:253:TYR:CZ	3:C:308:ILE:HG12	2.52	0.44
2:B:888:MET:HG2	2:B:889:PHE:N	2.32	0.44
2:B:913:ARG:HH11	2:B:913:ARG:HG3	1.83	0.44
3:C:280:ARG:HA	3:C:283:ARG:HE	1.83	0.44
5:A:101:FOK:H201	5:A:101:FOK:C17	2.40	0.43
3:C:214:VAL:HG11	3:C:380:ARG:HD3	2.00	0.43
3:C:107:VAL:CG1	3:C:128:VAL:HG13	2.47	0.43
2:B:1050:GLN:HA	2:B:1054:TYR:O	2.19	0.43
1:A:435:ILE:HG22	1:A:436:LYS:HG3	1.99	0.43
2:B:887:VAL:HG21	2:B:1024:VAL:HG22	2.00	0.43
1:A:508:SER:OG	1:A:511:VAL:HG23	2.18	0.43
3:C:377:ASN:HD22	3:C:377:ASN:HA	1.65	0.43
1:A:532:THR:O	1:A:536:LEU:HG	2.18	0.42
3:C:378:ASP:O	3:C:381:ASP:HB3	2.19	0.42
3:C:59:GLN:HA	3:C:59:GLN:OE1	2.19	0.42
3:C:327:GLU:HB2	3:C:330:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:379:CYS:O	3:C:383:ILE:HG13	2.19	0.42
2:B:998:VAL:HG12	2:B:999:GLY:N	2.35	0.42
2:B:930:LYS:HB3	2:B:930:LYS:HE2	1.91	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.20	0.41
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.82	0.41
1:A:392:ILE:HG23	1:A:445:VAL:HG12	2.02	0.41
2:B:1047:LEU:O	2:B:1051:THR:HG23	2.21	0.41
2:B:1064:VAL:HG21	2:B:1070:LEU:HD12	2.03	0.41
1:A:466:MET:O	1:A:470:ILE:HG13	2.20	0.41
1:A:393:LEU:C	1:A:393:LEU:HD23	2.42	0.41
1:A:395:ALA:HA	1:A:484:ARG:O	2.21	0.41
9:A:21:HOH:O	2:B:907:GLU:HB3	2.21	0.40
3:C:297:LEU:O	3:C:301:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/217 (86%)	181 (97%)	5 (3%)	1 (0%)	29	61
2	B	185/212 (87%)	178 (96%)	7 (4%)	0	100	100
3	C	327/402 (81%)	309 (94%)	16 (5%)	2 (1%)	25	56
All	All	699/831 (84%)	668 (96%)	28 (4%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	SER
3	C	138	PRO
3	C	231	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/182 (87%)	154 (98%)	4 (2%)	47	80
2	B	162/184 (88%)	158 (98%)	4 (2%)	47	80
3	C	298/357 (84%)	293 (98%)	5 (2%)	60	87
All	All	618/723 (86%)	605 (98%)	13 (2%)	53	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	SER
1	A	471	SER
1	A	493	HIS
1	A	497	LEU
2	B	903	ASP
2	B	992	ASN
2	B	1031	ASP
2	B	1059	ARG
3	C	111	SER
3	C	213	GLN
3	C	221	MET
3	C	306	SER
3	C	357	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	430	ASN
1	A	537	ASN
2	B	1025	ASN
2	B	1040	GLN
2	B	1050	GLN
2	B	1076	ASN
3	C	93	GLN

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Mol	Chain	Res	Type
3	C	97	ASN
3	C	149	HIS
3	C	227	GLN
3	C	371	ASN
3	C	377	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	#$|Z| > 2$
6	DAD	A	102	4	25,31,31	0.83	0	26,48,48	1.85	4 (15%)
5	FOK	A	101	-	28,31,31	0.94	0	35,54,54	0.86	1 (2%)
8	GSP	C	405	4	26,34,34	1.16	2 (7%)	28,54,54	2.31	6 (21%)

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
6	DAD	A	102	4	-	5/18/31/31	0/3/3/3
5	FOK	A	101	-	-	5/7/80/80	0/3/3/3
8	GSP	C	405	4	-	1/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	405	GSP	C6-N1	3.52	1.39	1.33
8	C	405	GSP	C8-N7	-2.15	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	405	GSP	C5-C6-N1	-8.46	111.86	123.43
6	A	102	DAD	C2'-C1'-N9	6.90	125.47	112.48
8	C	405	GSP	C6-N1-C2	5.70	124.98	115.93
6	A	102	DAD	O4'-C1'-C2'	3.75	110.73	106.67
8	C	405	GSP	C2-N3-C4	-3.25	111.64	115.36
8	C	405	GSP	N3-C2-N1	-2.52	123.86	127.22
8	C	405	GSP	C6-C5-C4	-2.39	118.51	120.80
5	A	101	FOK	C20-C10-C1	-2.35	104.20	107.68
6	A	102	DAD	O2G-PG-O1G	2.28	119.61	110.68
8	C	405	GSP	PA-O3A-PB	-2.20	125.28	132.83
6	A	102	DAD	C5-C6-N6	2.04	123.46	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	101	FOK	O1-C13-C14-C15
5	A	101	FOK	C16-C13-C14-C15
6	A	102	DAD	PB-O3B-PG-O3G
6	A	102	DAD	C5'-O5'-PA-O3A
5	A	101	FOK	C22-C21-O4-C7
5	A	101	FOK	O5-C21-O4-C7
6	A	102	DAD	C4'-C5'-O5'-PA
6	A	102	DAD	C5'-O5'-PA-O1A
5	A	101	FOK	C12-C13-C14-C15
6	A	102	DAD	PB-O3B-PG-O1G
8	C	405	GSP	PA-O3A-PB-O2B

There are no ring outliers.

3 monomers are involved in 9 short contacts:

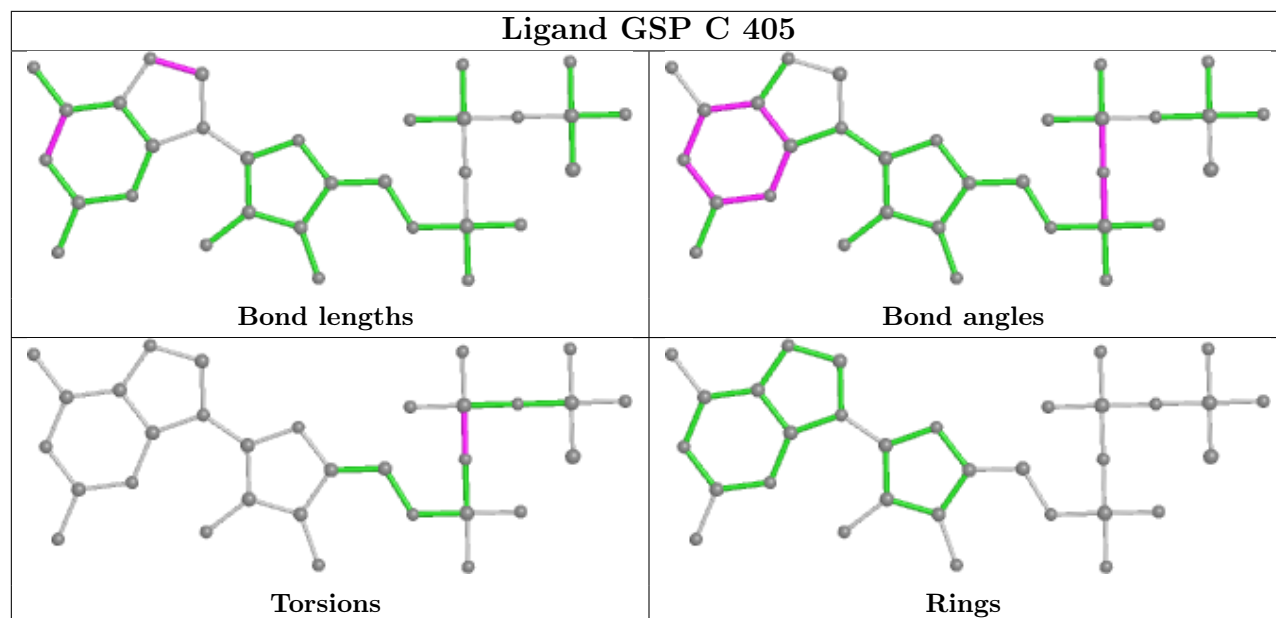| Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	102	DAD	2	0
5	A	101	FOK	6	0
8	C	405	GSP	1	0

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 DAD A 102

Bond lengths

Bond angles

Torsions

Rings

Ligand FOK A 101

Bond lengths

Bond angles

Torsions

Rings

Ligand GSP C 405

Bond lengths

Bond angles

Torsions

Rings
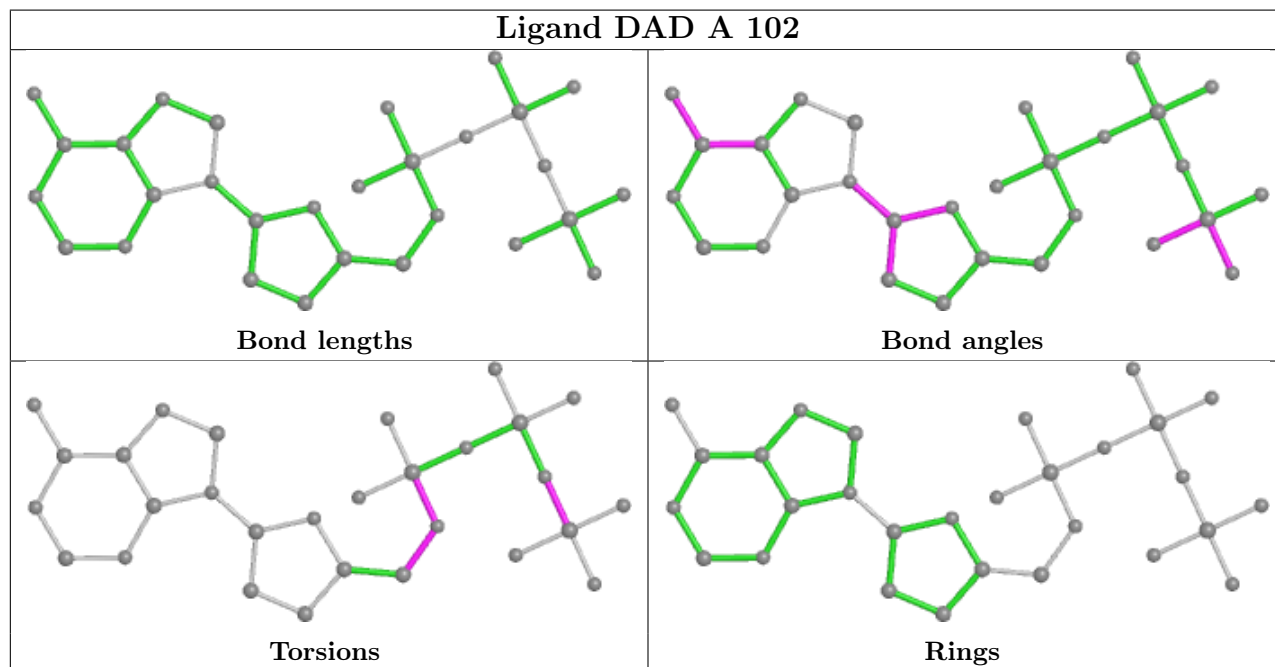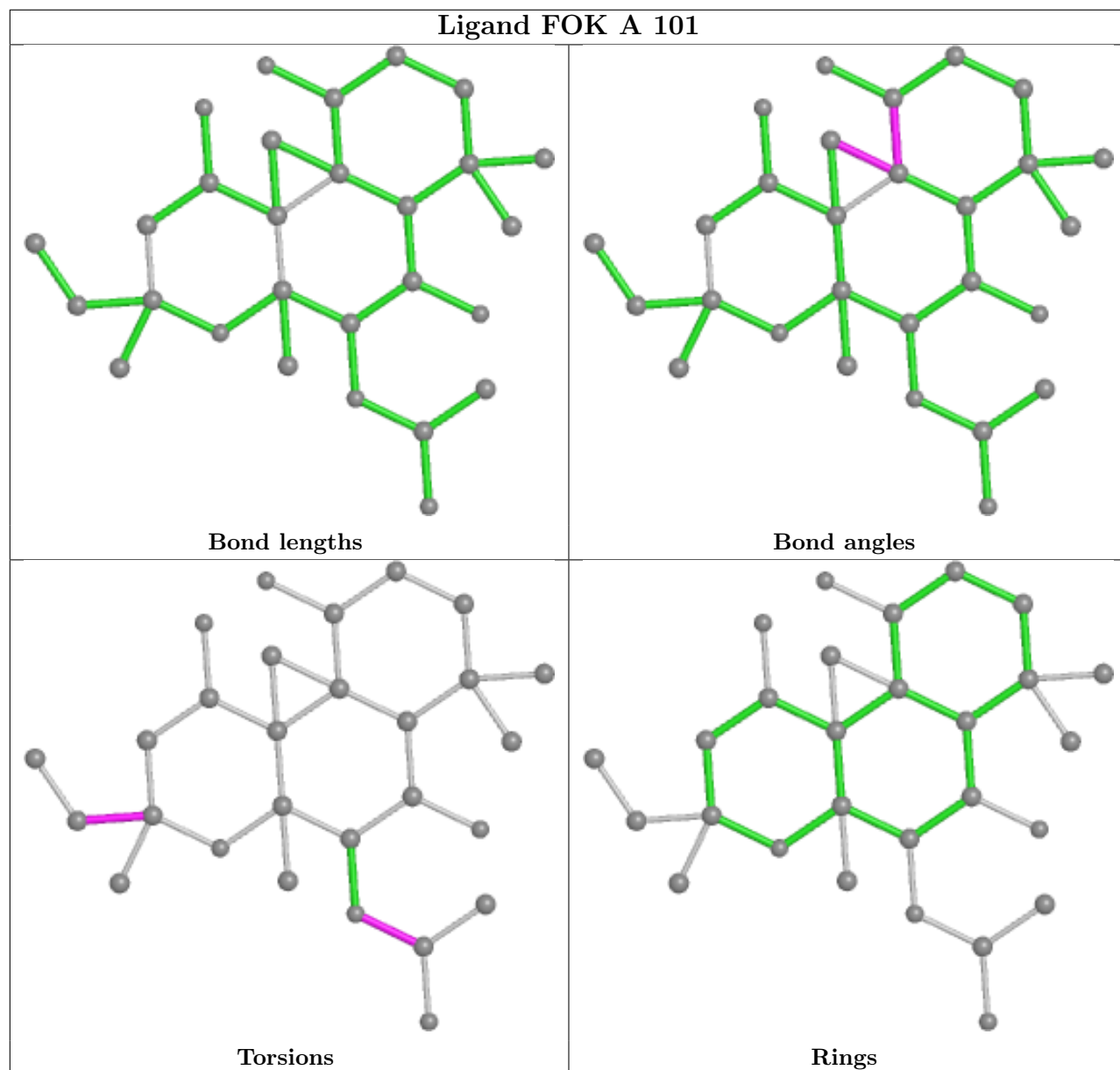
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	189/217 (87%)	-0.11	2 (1%)	80	75	25, 54, 71, 88	0
2	B	189/212 (89%)	-0.25	4 (2%)	63	54	16, 34, 62, 93	0
3	C	331/402 (82%)	-0.30	2 (0%)	89	86	20, 39, 66, 96	0
All	All	709/831 (85%)	-0.24	8 (1%)	80	75	16, 41, 69, 96	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	964	ARG	3.6
2	B	952	ALA	3.5
3	C	322	GLU	2.7
1	A	472	LEU	2.7
3	C	387	HIS	2.7
2	B	878	TYR	2.4
2	B	966	TYR	2.3
1	A	477	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
4	MG	A	581	1/1	0.93	0.26	53,53,53,53	0
4	MG	A	582	1/1	0.97	0.15	19,19,19,19	0
5	FOK	A	101	29/29	0.97	0.17	20,24,27,29	0
7	CL	C	404	1/1	0.97	0.18	35,35,35,35	0
6	DAD	A	102	29/29	0.98	0.17	36,40,46,46	0
8	GSP	C	405	32/32	0.98	0.14	16,21,29,31	0
4	MG	C	403	1/1	0.99	0.07	2,2,2,2	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.
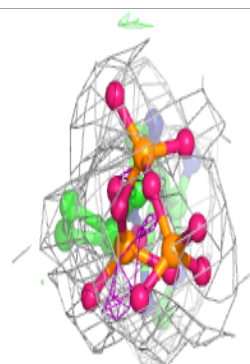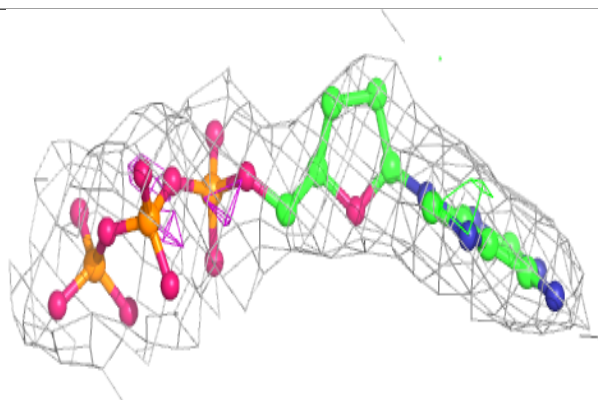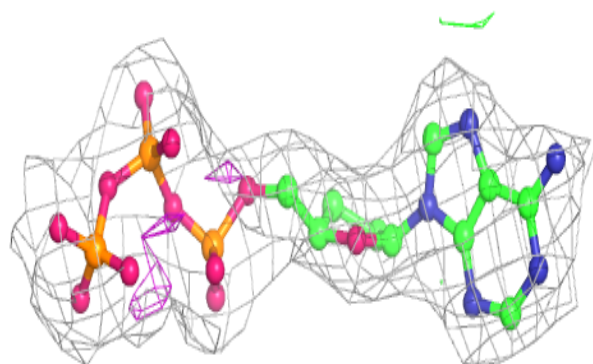
Electron density around FOK A 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
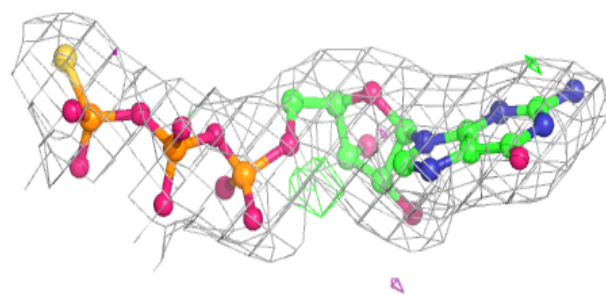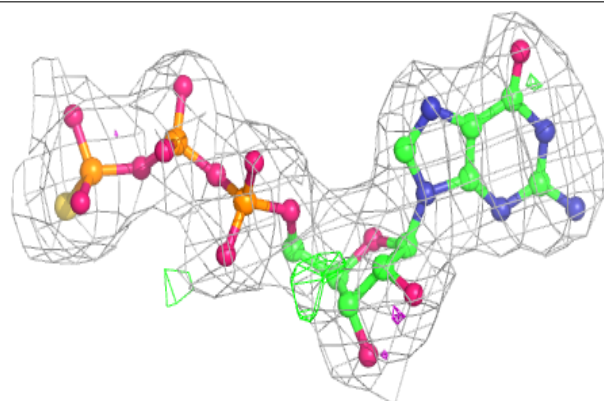and green (positive)
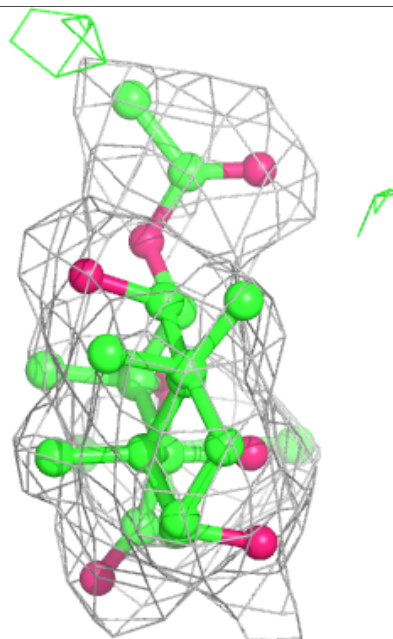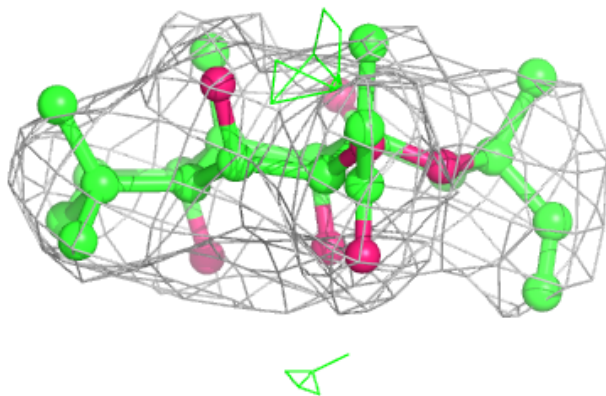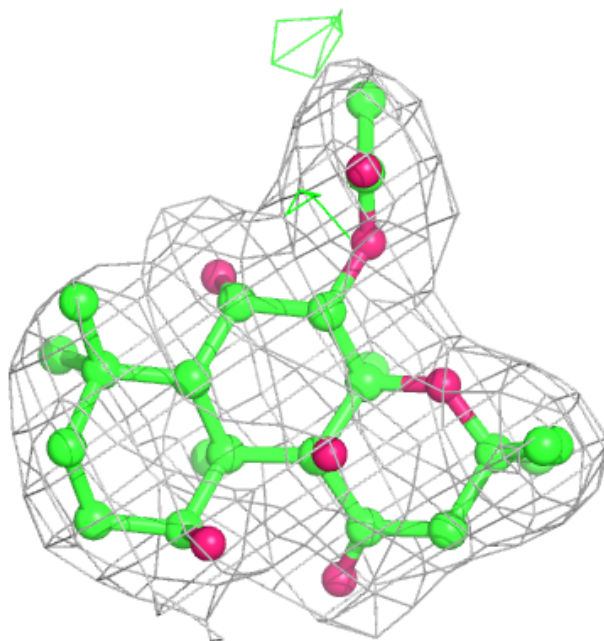
Electron density around DAD A 102:

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

Electron density around GSP C 405:

$2mF_o$-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.