



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:57 AM UTC

PDB ID : 4Y49 / pdb_00004y49
Title : Crystal structure of yeast N-terminal acetyltransferase (ppGpp) NatE in complex with a bisubstrate
Authors : Dong, J.; Wang, S.; York, J.D.
Deposited on : 2015-02-10
Resolution : 3.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

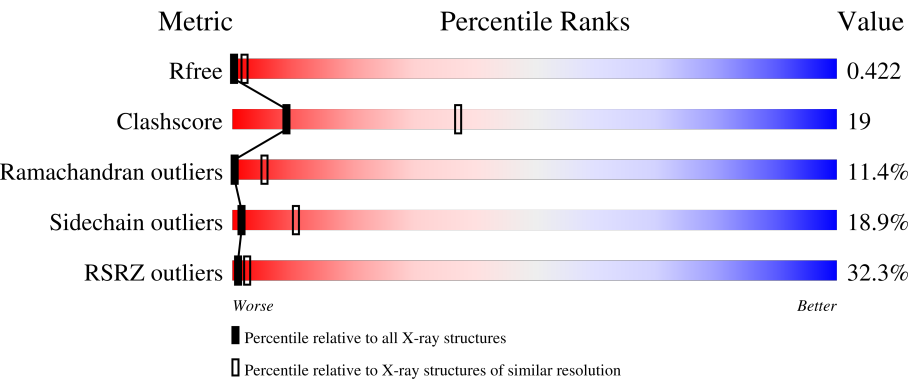
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.95 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	854	27% 56%26%6%10%
1	G	854	31% 58%24%7%10%
1	M	854	29% 58%24%7%10%
2	B	238	23% 37%24%8%31%
2	H	238	26% 43%20%5%31%

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Mol	Chain	Length	Quality of chain
2	N	238	
3	C	176	
3	I	176	
3	O	176	
4	E	8	
4	K	8	
4	Q	8	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20122 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 N-terminal acetyltransferase A complex subunit NAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	0	0	0
			4636	2891	860	877	8			
1	G	770	Total	C	N	O	S	0	0	0
			4656	2910	855	881	10			
1	M	769	Total	C	N	O	S	0	0	0
			4624	2889	848	877	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	TYR	GLU	conflict	UNP P12945
G	31	TYR	GLU	conflict	UNP P12945
M	31	TYR	GLU	conflict	UNP P12945

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1024	640	188	188	8			
2	H	164	Total	C	N	O	S	0	0	0
			1025	635	190	192	8			
2	N	164	Total	C	N	O	S	0	0	0
			1025	636	189	192	8			

- Molecule 3 is a protein called N-terminal acetyltransferase A complex subunit NAT5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	4	0	0
			888	555	168	163	2			
3	I	155	Total	C	N	O	S	3	0	0
			879	545	167	165	2			

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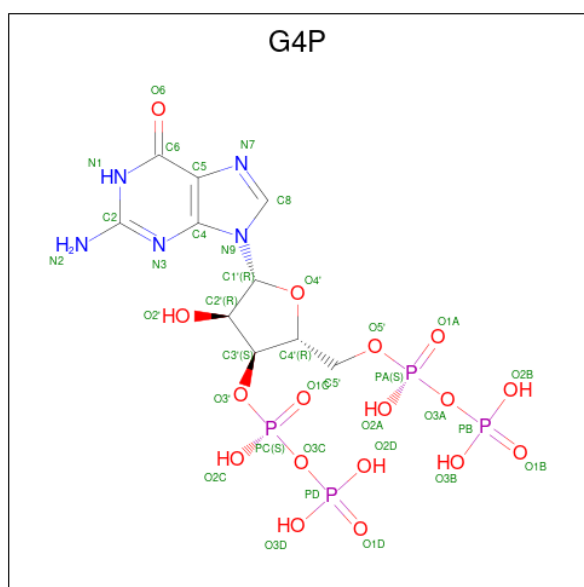
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	154	Total	C	N	O	S	1	1	0
			861	532	165	162	2			

- Molecule 4 is a protein called ALA-ALA-ALA-ALA-ALA-ALA.

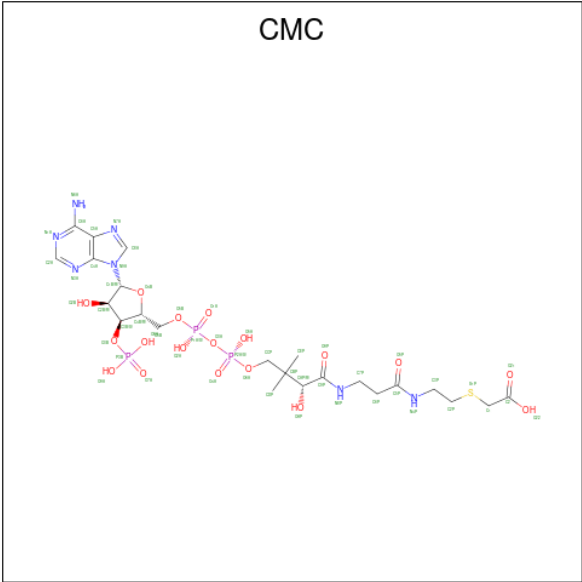
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O		0	0	0
			30	18	6	6				
4	K	6	Total	C	N	O		0	0	0
			30	18	6	6				
4	Q	6	Total	C	N	O		0	0	0
			30	18	6	6				

- Molecule 5 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



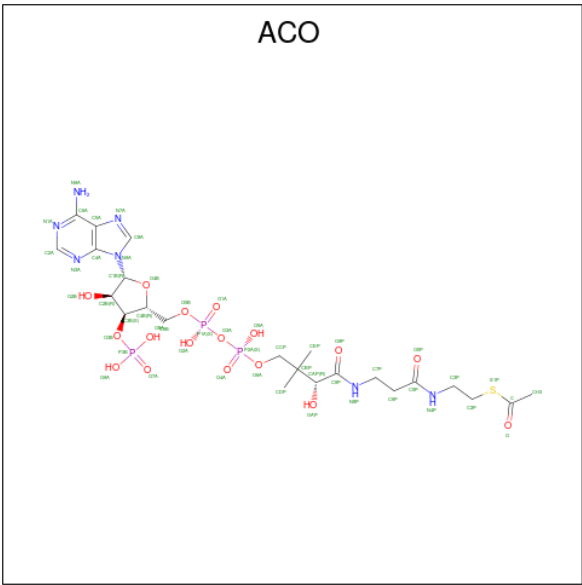
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	G	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
5	M	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 6 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		
6	H	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		
6	N	1	Total	C	N	O	P	S	51	0
			51	23	7	17	3	1		

- Molecule 7 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).

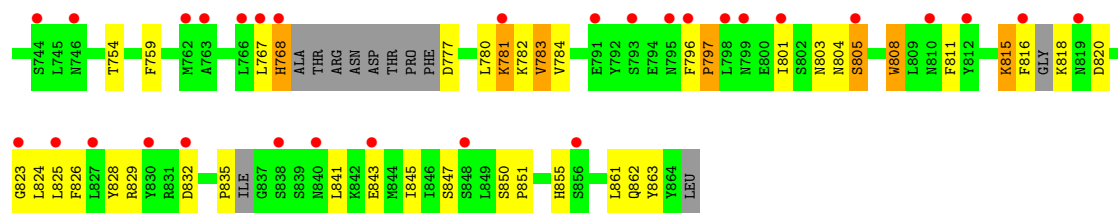


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

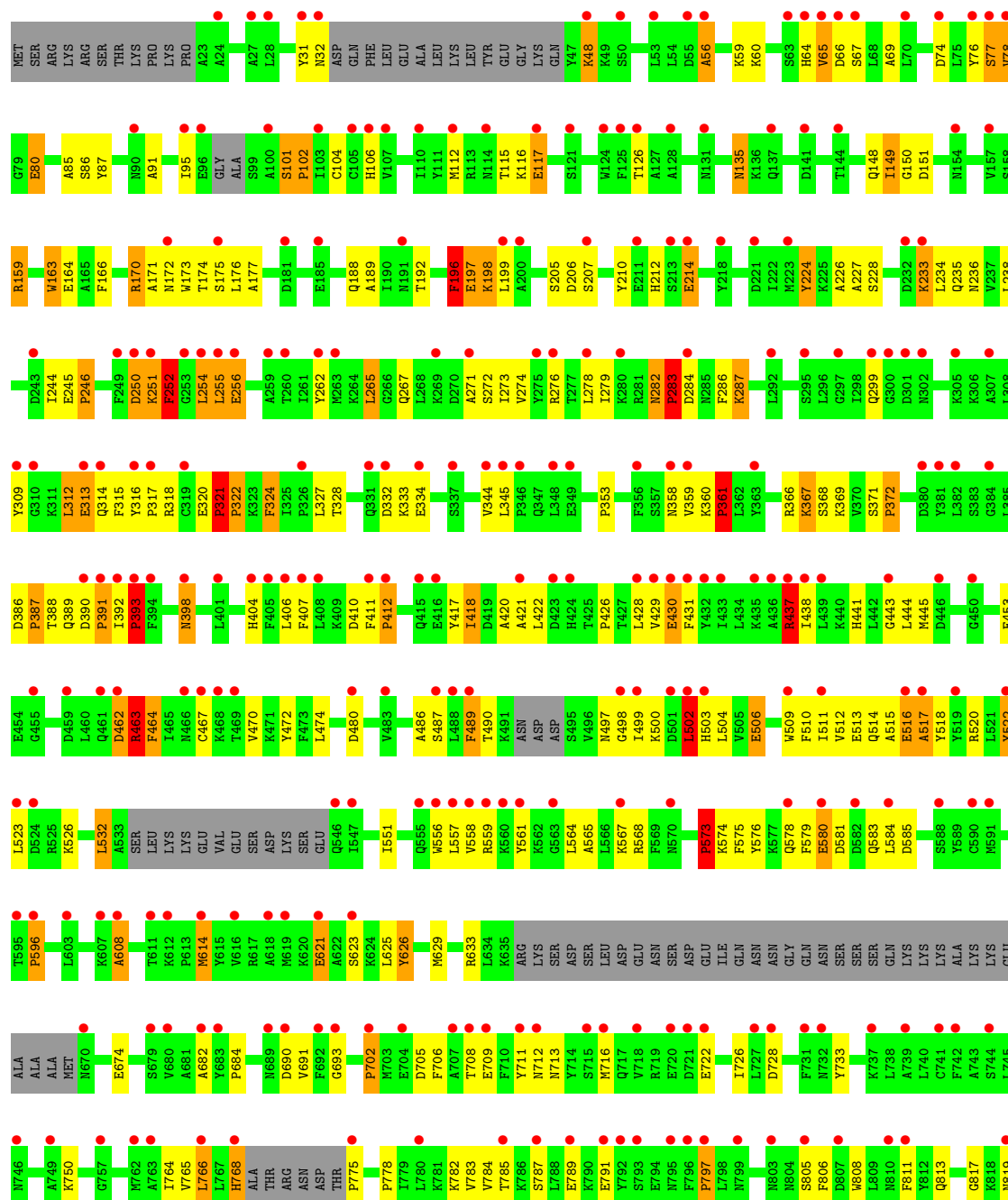
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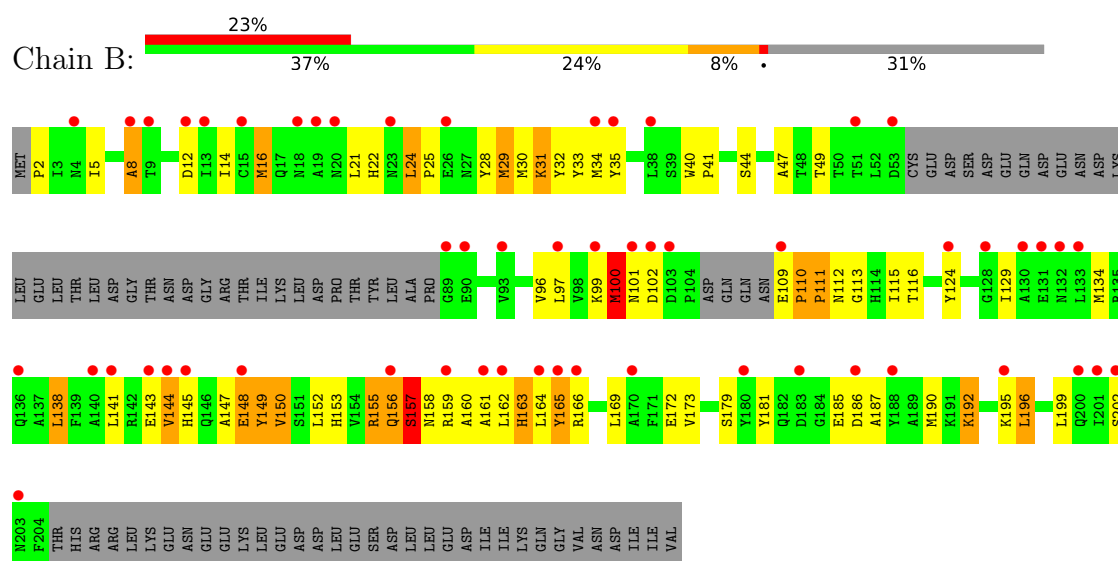
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
7	O	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		



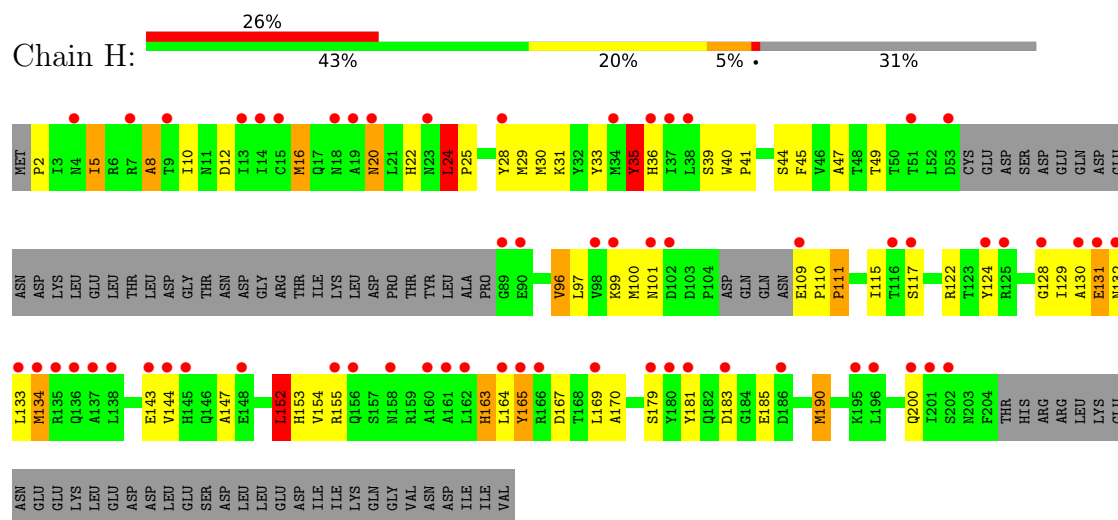
● Molecule 1: N-terminal acetyltransferase A complex subunit NAT1



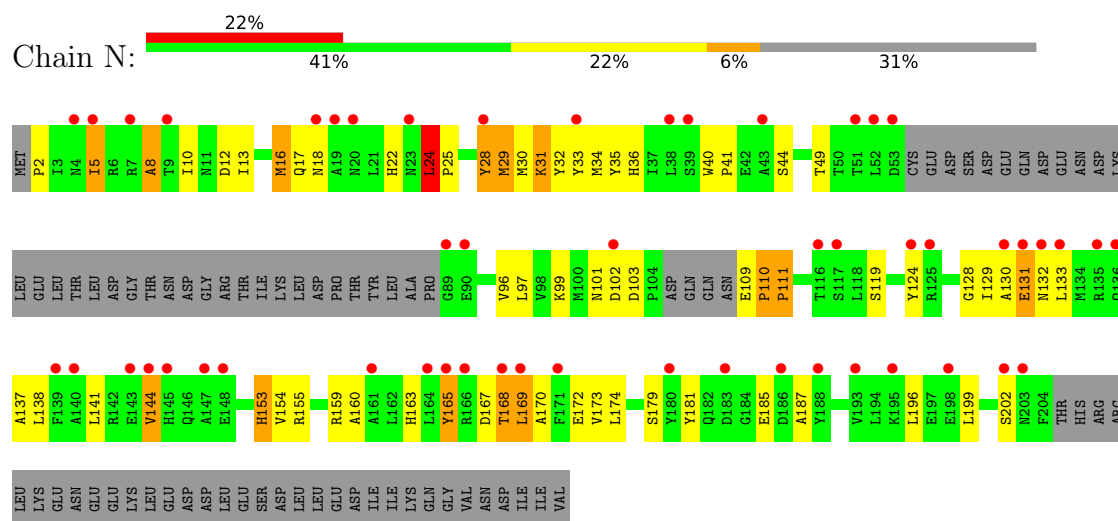




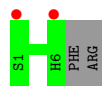
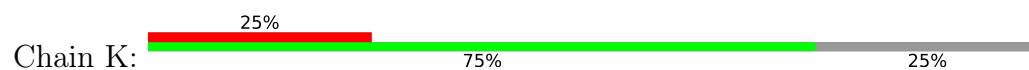
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1



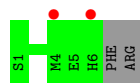
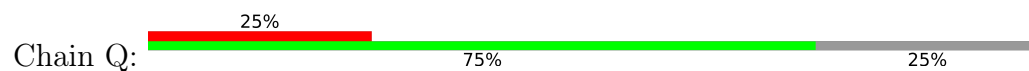
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ARD1



- Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA



- Molecule 4: ALA-ALA-ALA-ALA-ALA-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.72Å 146.49Å 254.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.95 49.63 – 3.95	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.63-3.95) 96.5 (49.63-3.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.355 , 0.421 0.366 , 0.422	Depositor DCC
R_{free} test set	1815 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20122	wwPDB-VP
Average B, all atoms (Å ²)	85.0	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 92.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9860e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, CMC, ACO

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	1.37	26/4701 (0.6%)	1.24	34/6458 (0.5%)
1	G	1.31	18/4725 (0.4%)	1.29	38/6500 (0.6%)
1	M	1.19	15/4689 (0.3%)	1.25	32/6453 (0.5%)
2	B	1.44	16/1040 (1.5%)	1.33	10/1424 (0.7%)
2	H	1.26	5/1041 (0.5%)	1.26	7/1424 (0.5%)
2	N	1.14	5/1040 (0.5%)	1.23	10/1423 (0.7%)
3	C	2.02	4/900 (0.4%)	1.46	12/1243 (1.0%)
3	I	1.85	9/889 (1.0%)	1.45	13/1224 (1.1%)
3	O	1.05	0/870	1.24	10/1197 (0.8%)
4	E	1.48	0/29	1.65	0/39
4	K	1.59	0/29	1.51	0/39
4	Q	1.49	0/29	1.20	0/39
All	All	1.35	98/19982 (0.5%)	1.28	166/27463 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	M	0	2
3	C	0	1
3	I	0	1
All	All	0	6

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	35	PHE	C-N	-33.66	0.90	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	36	PHE	C-O	33.03	1.63	1.24
1	G	768	HIS	C-O	32.03	1.87	1.23
3	I	36	PHE	N-CA	31.89	1.87	1.46
1	A	768	HIS	C-O	25.36	1.74	1.23

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	35	PHE	O-C-N	-21.17	96.58	122.20
3	I	36	PHE	N-CA-CB	14.02	134.18	110.49
3	C	36	PHE	O-C-N	-13.73	107.57	122.12
1	G	851	PRO	N-CA-CB	12.68	111.35	102.35
1	A	851	PRO	N-CA-CB	12.36	110.90	102.25

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	781	LYS	Peptide
3	C	36	PHE	Mainchain
1	G	806	PHE	Peptide
3	I	16	LEU	Mainchain
1	M	171	ALA	Peptide

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	4636	0	2969	146	0
1	G	4656	0	2966	140	0
1	M	4624	0	2960	154	0
2	B	1024	0	710	42	0
2	H	1025	0	695	28	0
2	N	1025	0	699	28	0
3	C	888	0	539	29	0
3	I	879	0	527	32	0
3	O	861	0	511	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	30	0	14	0	0
4	K	30	0	14	0	0
4	Q	30	0	14	0	0
5	A	36	0	11	1	0
5	G	36	0	11	3	0
5	M	36	0	11	0	0
6	B	51	0	31	0	0
6	H	51	0	31	0	0
6	N	51	0	31	0	0
7	C	51	0	34	10	0
7	I	51	0	34	9	0
7	O	51	0	34	5	0
All	All	20122	0	12846	606	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 19.

The worst 5 of 606 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:G:614:MET:CB	1:G:614:MET:CG	1.77	1.62
1:M:185:GLU:CD	1:M:185:GLU:CG	1.84	1.49
1:M:215:CYS:CB	1:M:215:CYS:SG	2.08	1.42
1:A:467:CYS:SG	1:A:467:CYS:CB	2.09	1.41
2:B:29:MET:CG	2:B:29:MET:SD	2.15	1.33

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	751/854 (88%)	487 (65%)	185 (25%)	79 (10%)	0	7
1	G	754/854 (88%)	494 (66%)	179 (24%)	81 (11%)	0	6
1	M	753/854 (88%)	504 (67%)	173 (23%)	76 (10%)	0	8
2	B	158/238 (66%)	94 (60%)	39 (25%)	25 (16%)	0	3
2	H	158/238 (66%)	91 (58%)	49 (31%)	18 (11%)	0	5
2	N	158/238 (66%)	93 (59%)	42 (27%)	23 (15%)	0	3
3	C	150/176 (85%)	94 (63%)	35 (23%)	21 (14%)	0	3
3	I	149/176 (85%)	89 (60%)	37 (25%)	23 (15%)	0	3
3	O	147/176 (84%)	90 (61%)	41 (28%)	16 (11%)	0	6
4	E	4/8 (50%)	4 (100%)	0	0	100	100
4	K	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
4	Q	4/8 (50%)	4 (100%)	0	0	100	100
All	All	3190/3828 (83%)	2047 (64%)	781 (24%)	362 (11%)	0	5

5 of 362 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	101	SER
1	A	116	LYS
1	A	135	ASN
1	A	163	TRP

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	186/759 (24%)	150 (81%)	36 (19%)	1	9
1	G	189/759 (25%)	144 (76%)	45 (24%)	1	5
1	M	188/759 (25%)	155 (82%)	33 (18%)	2	12
2	B	51/216 (24%)	45 (88%)	6 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	51/216 (24%)	40 (78%)	11 (22%)	1	6
2	N	51/216 (24%)	43 (84%)	8 (16%)	2	15
3	C	29/153 (19%)	22 (76%)	7 (24%)	1	5
3	I	28/153 (18%)	25 (89%)	3 (11%)	6	24
3	O	25/153 (16%)	23 (92%)	2 (8%)	11	35
All	All	798/3384 (24%)	647 (81%)	151 (19%)	1	10

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	224	TYR
2	N	24	LEU
1	M	291	LEU
1	M	522	TYR
3	O	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	114	HIS
1	M	135	ASN
1	M	347	GLN
1	M	236	ASN
1	G	282	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 oligosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	G4P	A	901	-	36,38,38	1.58	5 (13%)	56,61,61	1.70	12 (21%)
6	CMC	H	301	-	51,53,54	1.12	5 (9%)	72,78,80	1.69	13 (18%)
6	CMC	N	301	-	51,53,54	1.13	5 (9%)	72,78,80	1.71	15 (20%)
7	ACO	O	201	-	51,53,53	1.37	6 (11%)	73,79,79	1.79	11 (15%)
5	G4P	G	901	-	36,38,38	3.96	8 (22%)	56,61,61	2.17	17 (30%)
7	ACO	C	201	-	51,53,53	1.27	4 (7%)	73,79,79	2.14	18 (24%)
5	G4P	M	901	-	36,38,38	1.47	4 (11%)	56,61,61	1.82	9 (16%)
7	ACO	I	201	-	51,53,53	1.59	8 (15%)	73,79,79	2.22	25 (34%)
6	CMC	B	301	-	51,53,54	1.13	6 (11%)	72,78,80	1.69	14 (19%)

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
5	G4P	A	901	-	-	7/27/43/43	0/3/3/3
6	CMC	H	301	-	-	2/50/67/68	0/3/3/3
6	CMC	N	301	-	-	3/50/67/68	0/3/3/3
7	ACO	O	201	-	-	18/51/67/67	0/3/3/3
5	G4P	G	901	-	-	4/27/43/43	0/3/3/3
7	ACO	C	201	-	-	22/51/67/67	0/3/3/3
5	G4P	M	901	-	-	8/27/43/43	0/3/3/3
7	ACO	I	201	-	-	24/51/67/67	0/3/3/3
6	CMC	B	301	-	-	3/50/67/68	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	901	G4P	PC-O3C	20.03	1.81	1.59
5	G	901	G4P	PA-O3A	7.30	1.67	1.59
7	I	201	ACO	C5A-C4A	6.12	1.50	1.39
5	G	901	G4P	PD-O1D	5.17	1.66	1.50
5	A	901	G4P	PC-O3C	5.03	1.64	1.59

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	201	ACO	C5A-C4A-N3A	-7.12	116.91	126.72
7	C	201	ACO	C5A-C4A-N3A	-6.89	117.23	126.72
7	C	201	ACO	O3A-P2A-O4A	-6.21	92.04	110.70
5	M	901	G4P	C5-C4-N3	-5.88	119.03	128.39
7	I	201	ACO	CAP-C9P-N8P	5.74	127.39	116.48

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	G4P	O4'-C4'-C5'-O5'
5	A	901	G4P	C3'-C4'-C5'-O5'
5	G	901	G4P	C4'-C3'-O3'-PC
5	G	901	G4P	O4'-C1'-N9-C8
5	G	901	G4P	O4'-C1'-N9-C4

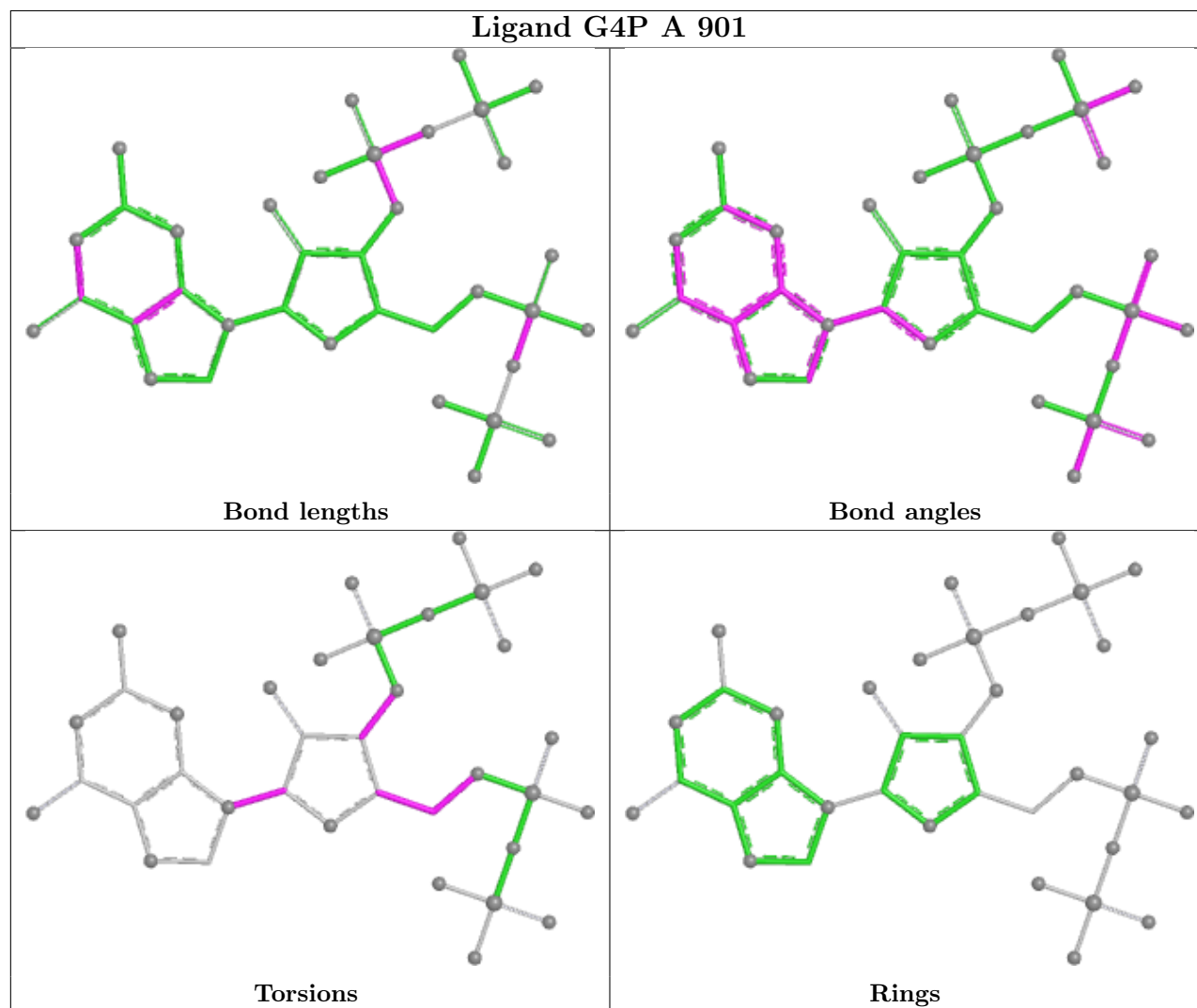
There are no ring outliers.

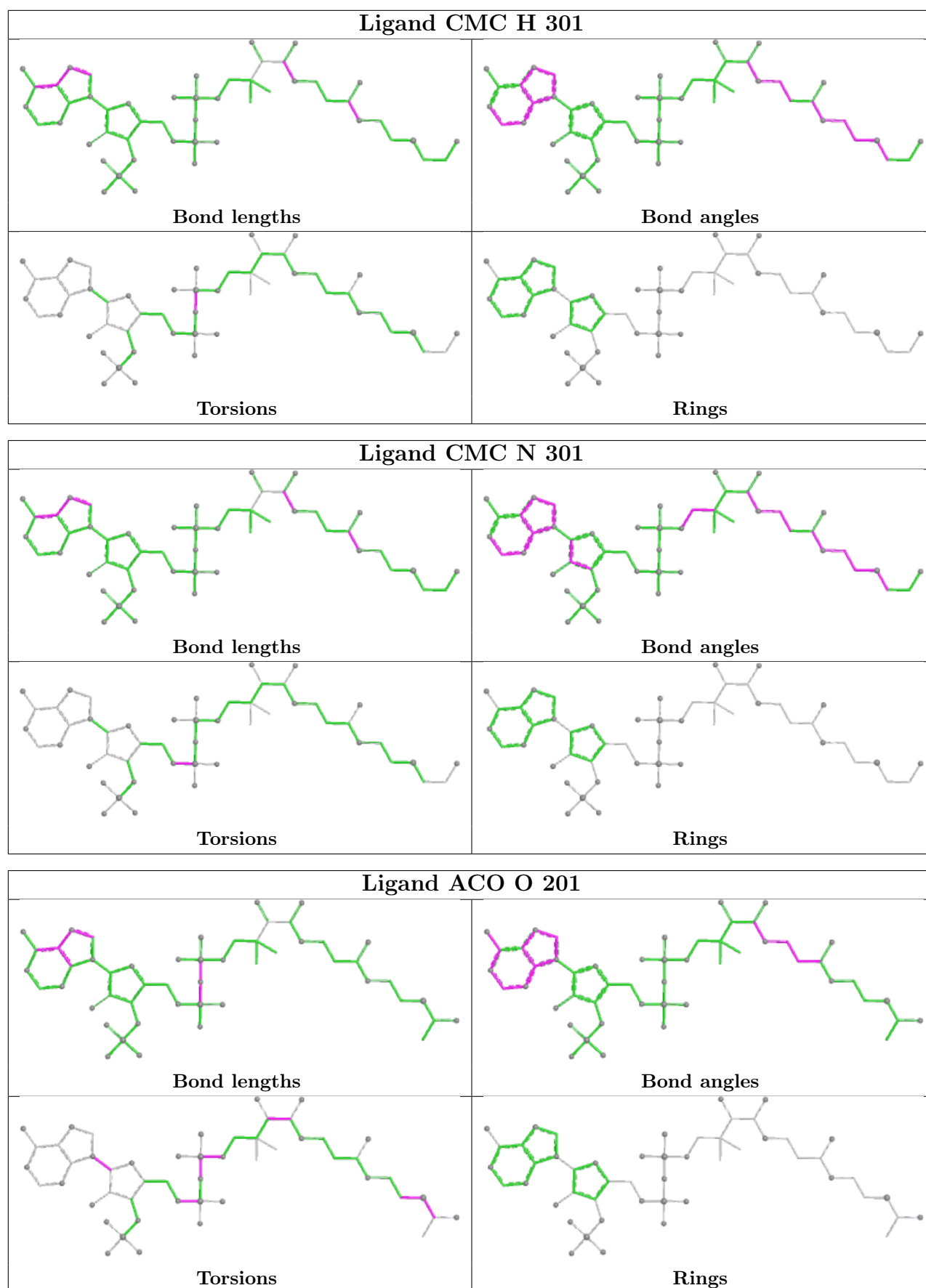
5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	G4P	1	0
7	O	201	ACO	5	0
5	G	901	G4P	3	0
7	C	201	ACO	10	0
7	I	201	ACO	9	0

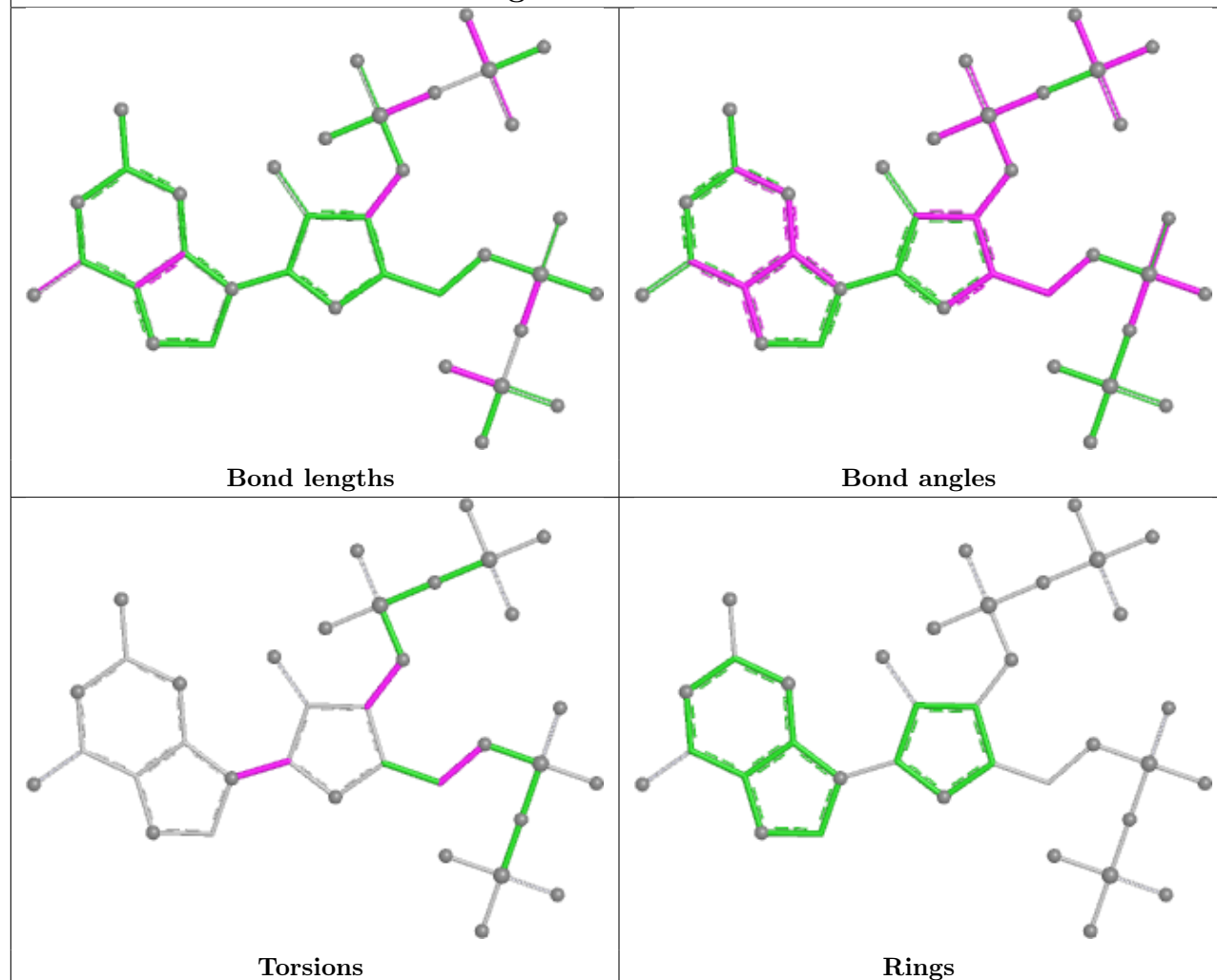
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

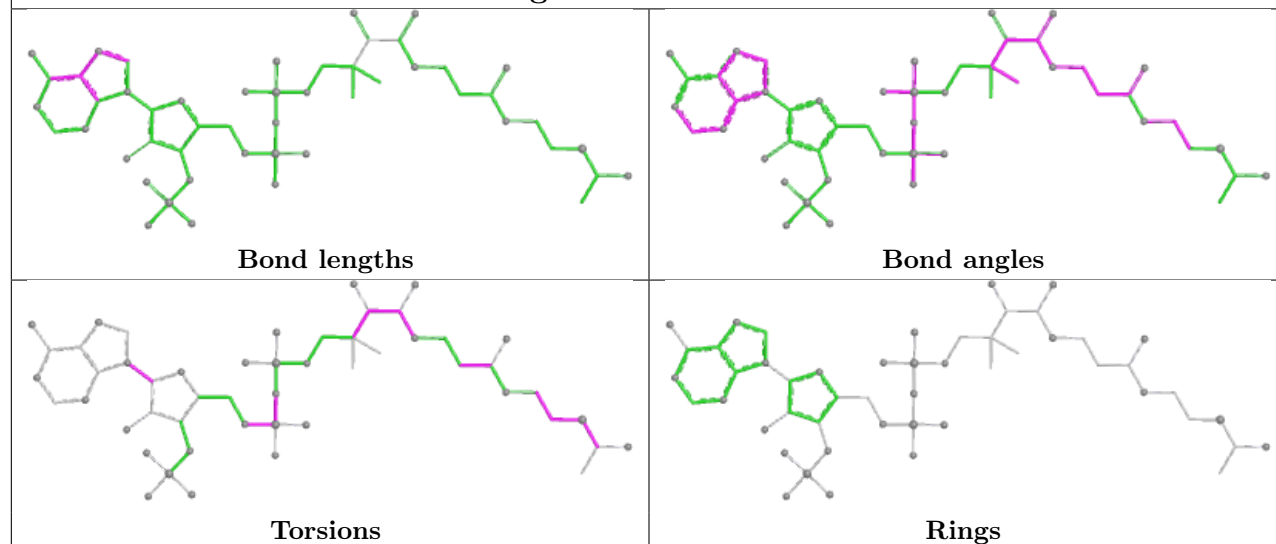


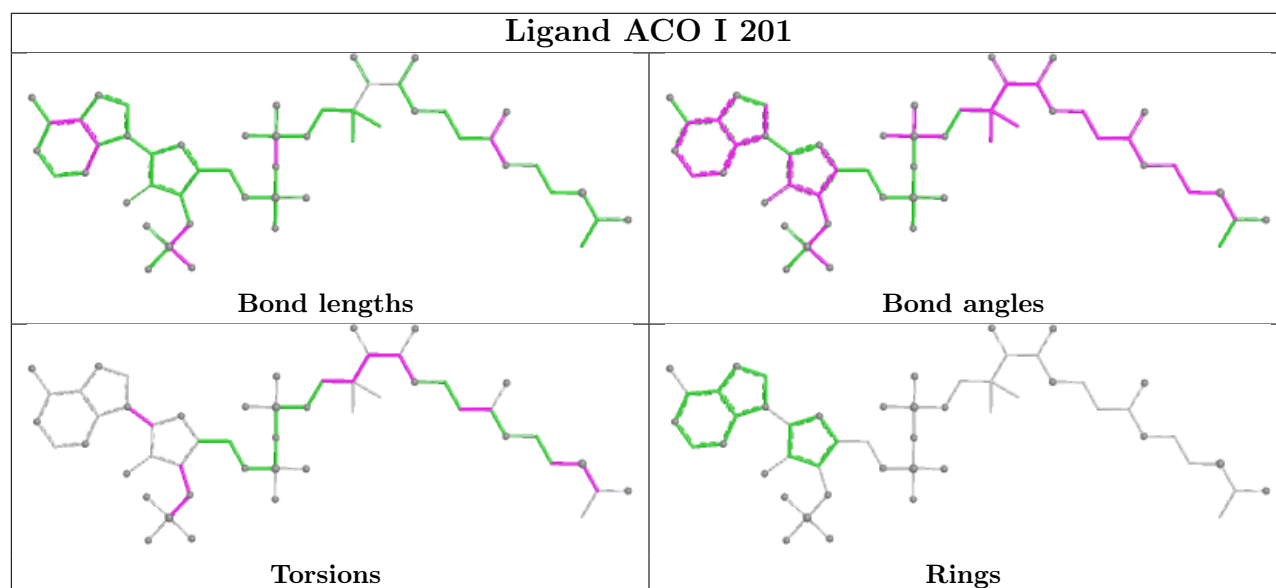
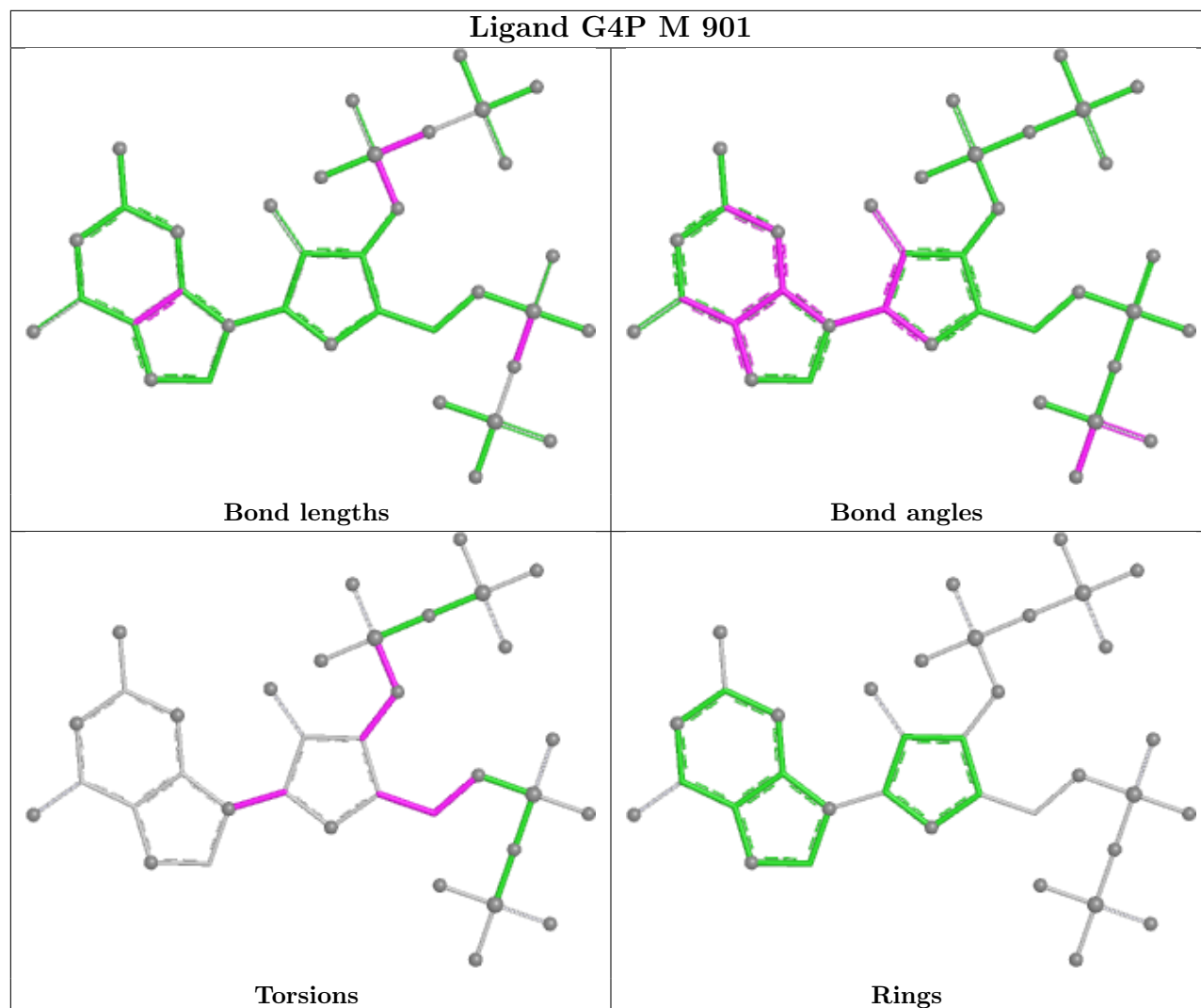


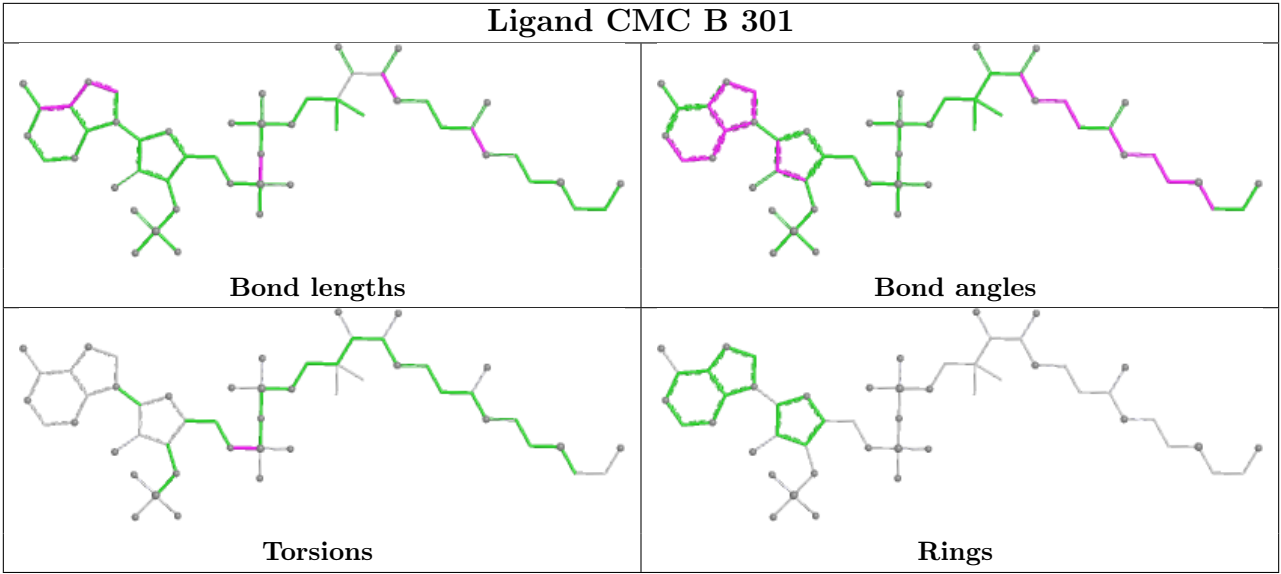
Ligand G4P G 901



Ligand ACO C 201







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	35:PHE	C	36:PHE	N	0.90

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	769/854 (90%)	1.67	234 (30%) 1 3	83, 86, 91, 94	0
1	G	770/854 (90%)	1.72	268 (34%) 1 2	73, 85, 88, 88	0
1	M	769/854 (90%)	1.68	244 (31%) 1 2	84, 86, 90, 92	0
2	B	164/238 (68%)	1.90	55 (33%) 1 2	48, 84, 86, 88	0
2	H	164/238 (68%)	1.78	62 (37%) 1 2	84, 85, 86, 87	0
2	N	164/238 (68%)	1.78	52 (31%) 1 2	54, 86, 87, 88	0
3	C	156/176 (88%)	1.60	43 (27%) 1 3	62, 86, 88, 88	2 (1%)
3	I	155/176 (88%)	1.74	55 (35%) 1 2	68, 87, 89, 90	2 (1%)
3	O	154/176 (87%)	1.60	42 (27%) 1 3	64, 90, 93, 93	2 (1%)
4	E	6/8 (75%)	1.85	2 (33%) 1 2	83, 83, 84, 84	0
4	K	6/8 (75%)	1.87	2 (33%) 1 2	84, 84, 85, 85	0
4	Q	6/8 (75%)	1.62	2 (33%) 1 2	85, 85, 85, 85	0
All	All	3283/3828 (85%)	1.70	1061 (32%) 1 2	48, 86, 90, 94	6 (0%)

The worst 5 of 1061 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	GLU	12.2
2	B	166	ARG	9.7
2	B	148	GLU	9.5
1	G	332	ASP	8.2
1	A	676	GLU	8.2

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](#)

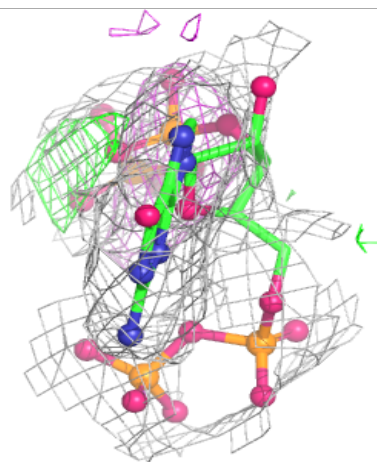
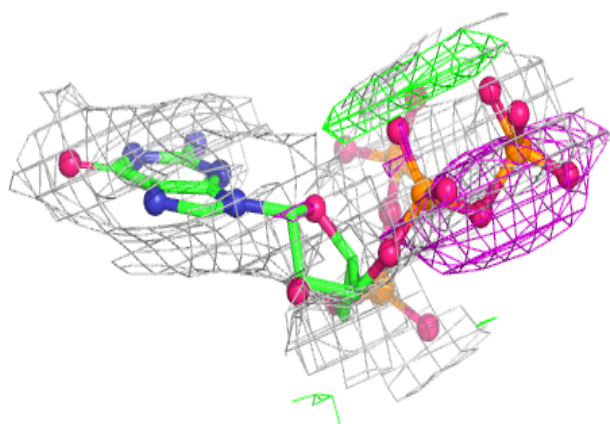
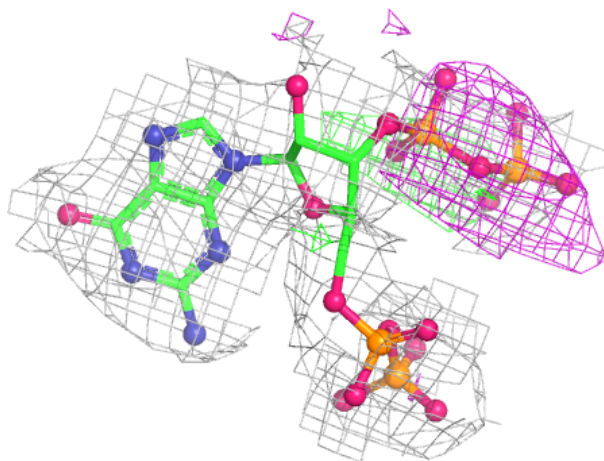
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	G4P	G	901	36/36	0.64	0.24	83,83,84,84	0
7	ACO	C	201	51/51	0.78	0.23	86,87,88,89	0
5	G4P	A	901	36/36	0.80	0.19	85,86,87,87	0
6	CMC	B	301	51/52	-	-	20,20,20,20	51
6	CMC	H	301	51/52	-	-	20,20,20,20	51
6	CMC	N	301	51/52	-	-	20,20,20,20	51
7	ACO	I	201	51/51	0.80	0.23	85,86,87,87	0
5	G4P	M	901	36/36	0.81	0.20	85,86,86,86	0
7	ACO	O	201	51/51	0.81	0.23	89,90,92,92	0

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

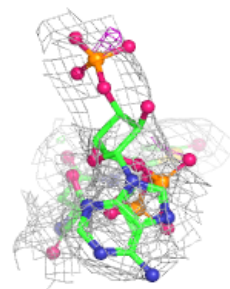
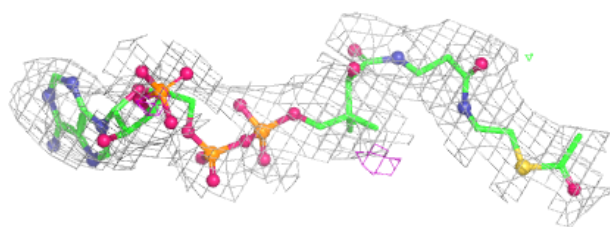
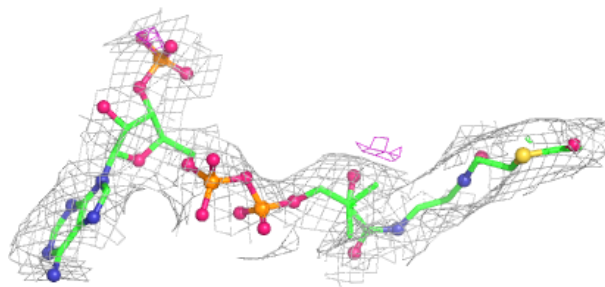
Electron density around G4P G 901:

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

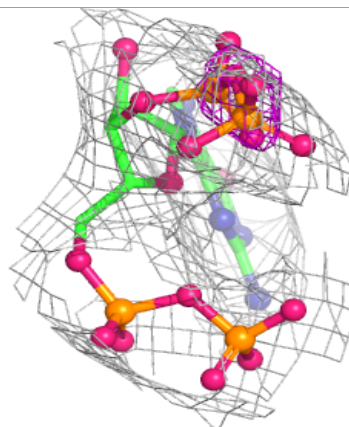
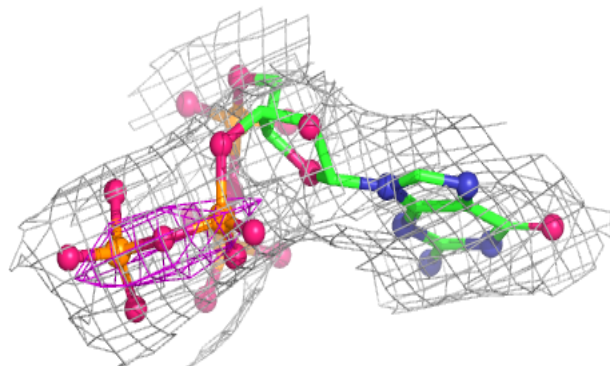
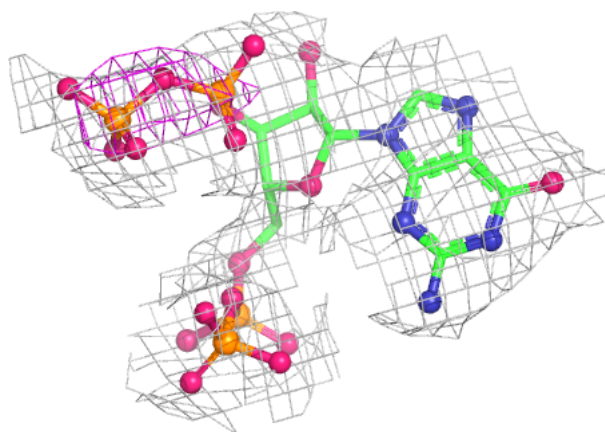


Electron density around ACO C 201:

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

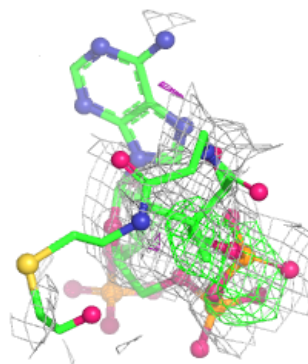
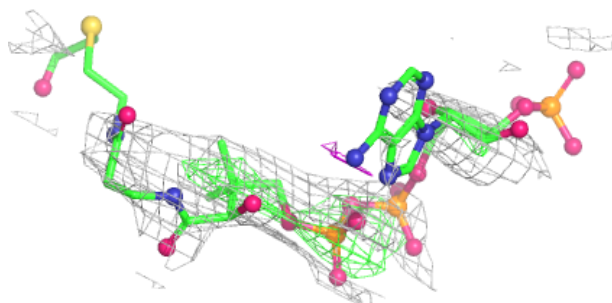
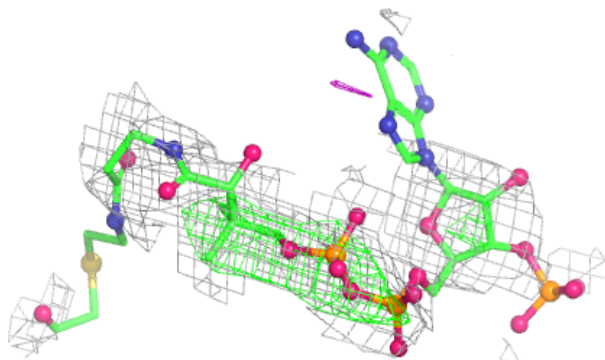
**Electron density around G4P A 901:**

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

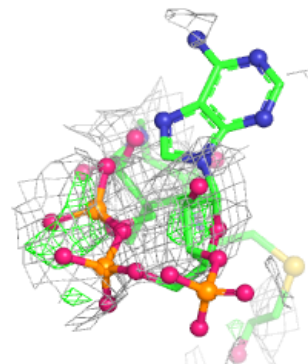
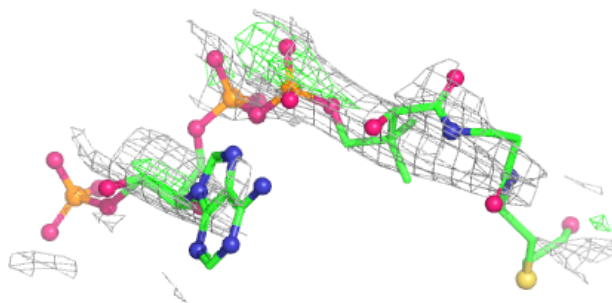
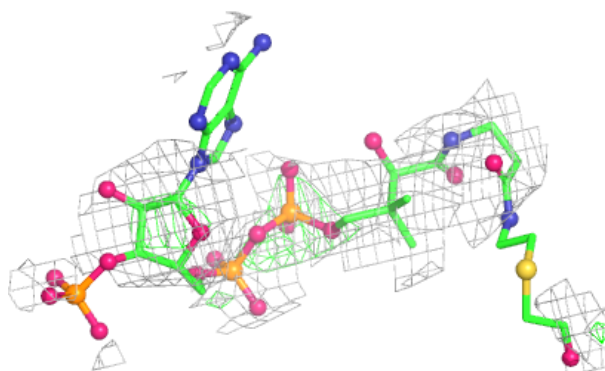


Electron density around CMC B 301:

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

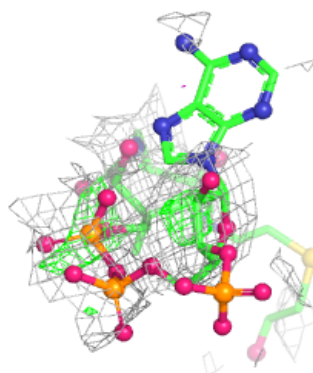
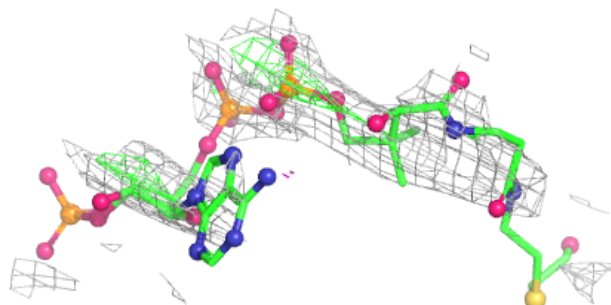
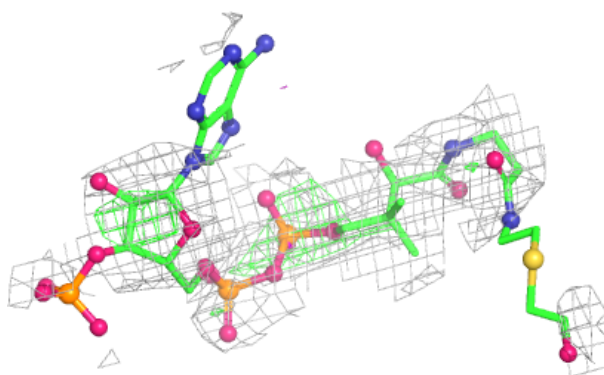
**Electron density around CMC H 301:**

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

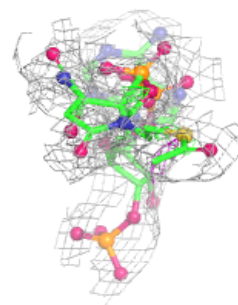
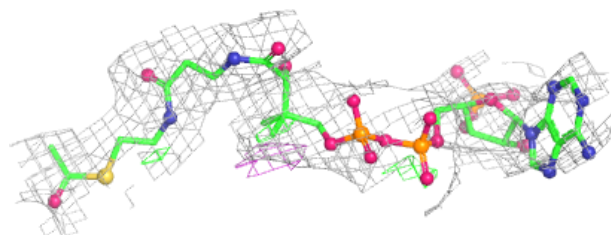
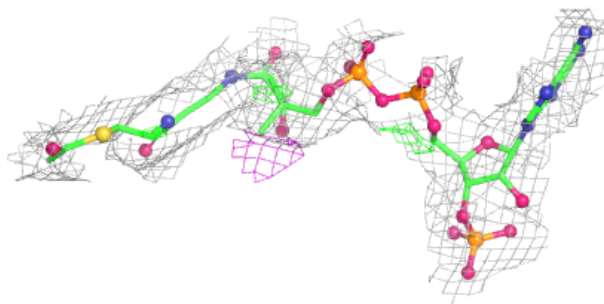


Electron density around CMC N 301:

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

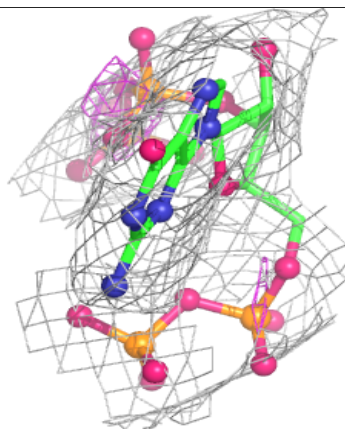
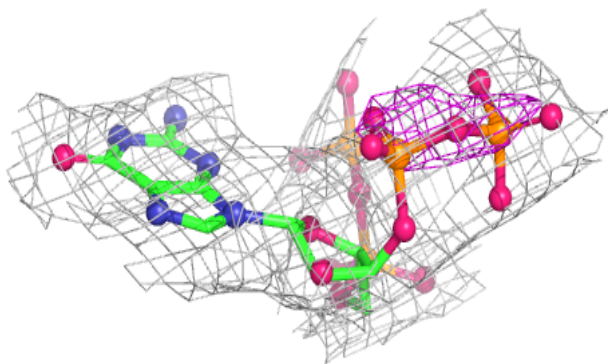
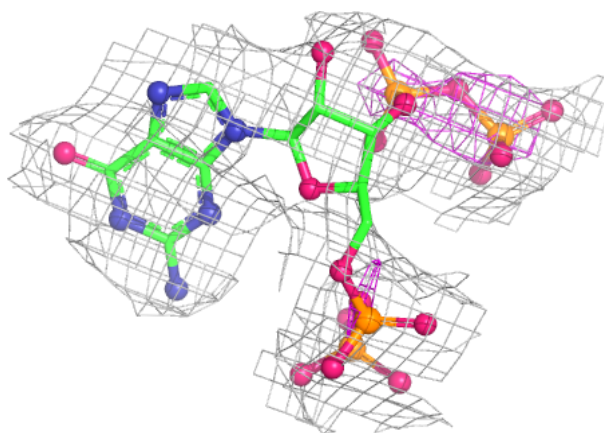
**Electron density around ACO I 201:**

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

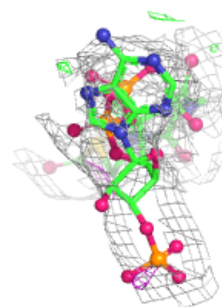
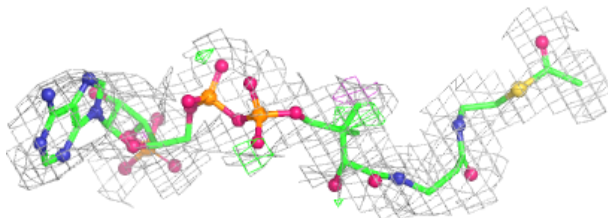
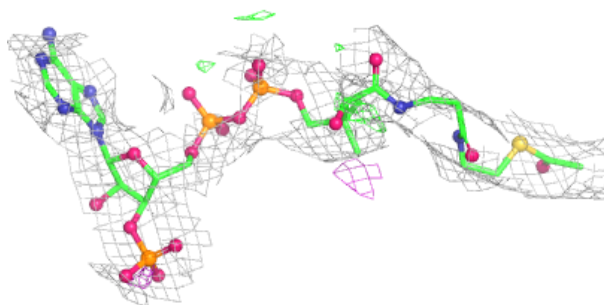


Electron density around G4P M 901:

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

**Electron density around ACO O 201:**

$2mF_o-DF_c$ (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.