



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 09:45 am BST

PDB ID : 4ACB / pdb_00004acb
Title : CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR
SELB FROM METHANOCOCCUS MARIPALUDIS IN COMPLEX WITH
THE GTP ANALOGUE GPPNHP
Authors : Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on : 2011-12-14
Resolution : 3.34 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	:	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

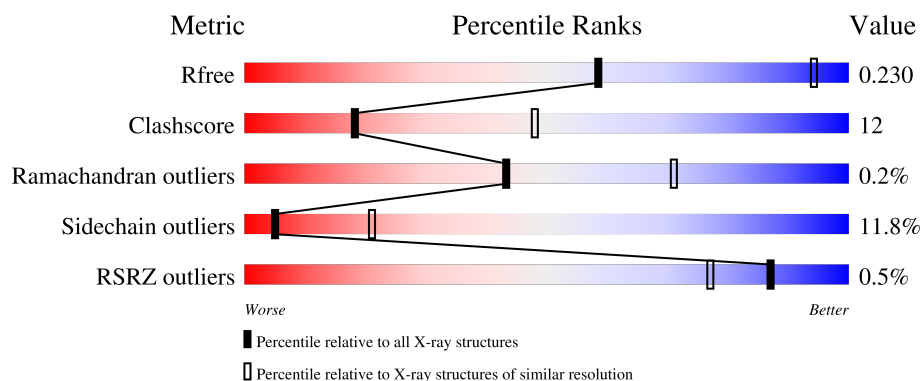
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	482	% 65% 24% • 6%
1	B	482	% 63% 28% • 5%
1	C	482	 64% 29% 5% •
1	D	482	% 64% 27% 5% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MMC	D	470	-	-	X	-
4	MMC	D	471	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14623 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 TRANSLATION ELONGATION FACTOR SELB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3498	2236	597	651	14			
1	B	456	Total	C	N	O	S	0	0	0
			3525	2253	603	655	14			
1	C	471	Total	C	N	O	S	0	0	0
			3643	2323	627	679	14			
1	D	467	Total	C	N	O	S	0	0	0
			3607	2301	618	675	13			

There are 56 discrepancies between the modelled and reference sequences:

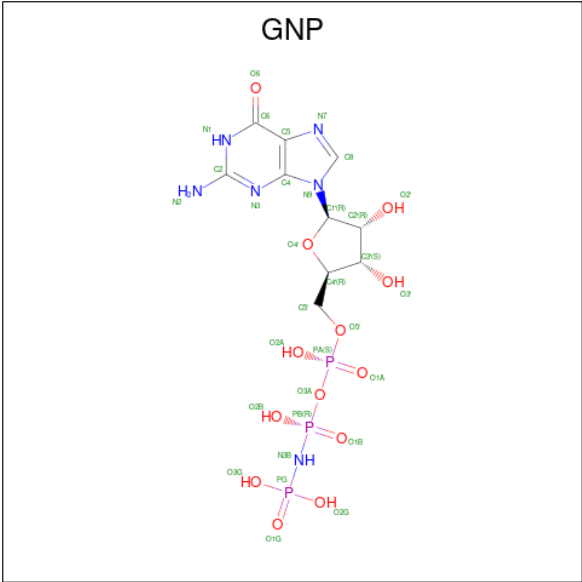
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8J307
A	-12	HIS	-	expression tag	UNP Q8J307
A	-11	HIS	-	expression tag	UNP Q8J307
A	-10	HIS	-	expression tag	UNP Q8J307
A	-9	HIS	-	expression tag	UNP Q8J307
A	-8	HIS	-	expression tag	UNP Q8J307
A	-7	HIS	-	expression tag	UNP Q8J307
A	-6	SER	-	expression tag	UNP Q8J307
A	-5	ILE	-	expression tag	UNP Q8J307
A	-4	GLU	-	expression tag	UNP Q8J307
A	-3	GLY	-	expression tag	UNP Q8J307
A	-2	ARG	-	expression tag	UNP Q8J307
A	-1	PRO	-	expression tag	UNP Q8J307
A	0	HIS	-	expression tag	UNP Q8J307
B	-13	MET	-	expression tag	UNP Q8J307
B	-12	HIS	-	expression tag	UNP Q8J307
B	-11	HIS	-	expression tag	UNP Q8J307
B	-10	HIS	-	expression tag	UNP Q8J307
B	-9	HIS	-	expression tag	UNP Q8J307
B	-8	HIS	-	expression tag	UNP Q8J307
B	-7	HIS	-	expression tag	UNP Q8J307

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP Q8J307
B	-5	ILE	-	expression tag	UNP Q8J307
B	-4	GLU	-	expression tag	UNP Q8J307
B	-3	GLY	-	expression tag	UNP Q8J307
B	-2	ARG	-	expression tag	UNP Q8J307
B	-1	PRO	-	expression tag	UNP Q8J307
B	0	HIS	-	expression tag	UNP Q8J307
C	-13	MET	-	expression tag	UNP Q8J307
C	-12	HIS	-	expression tag	UNP Q8J307
C	-11	HIS	-	expression tag	UNP Q8J307
C	-10	HIS	-	expression tag	UNP Q8J307
C	-9	HIS	-	expression tag	UNP Q8J307
C	-8	HIS	-	expression tag	UNP Q8J307
C	-7	HIS	-	expression tag	UNP Q8J307
C	-6	SER	-	expression tag	UNP Q8J307
C	-5	ILE	-	expression tag	UNP Q8J307
C	-4	GLU	-	expression tag	UNP Q8J307
C	-3	GLY	-	expression tag	UNP Q8J307
C	-2	ARG	-	expression tag	UNP Q8J307
C	-1	PRO	-	expression tag	UNP Q8J307
C	0	HIS	-	expression tag	UNP Q8J307
D	-13	MET	-	expression tag	UNP Q8J307
D	-12	HIS	-	expression tag	UNP Q8J307
D	-11	HIS	-	expression tag	UNP Q8J307
D	-10	HIS	-	expression tag	UNP Q8J307
D	-9	HIS	-	expression tag	UNP Q8J307
D	-8	HIS	-	expression tag	UNP Q8J307
D	-7	HIS	-	expression tag	UNP Q8J307
D	-6	SER	-	expression tag	UNP Q8J307
D	-5	ILE	-	expression tag	UNP Q8J307
D	-4	GLU	-	expression tag	UNP Q8J307
D	-3	GLY	-	expression tag	UNP Q8J307
D	-2	ARG	-	expression tag	UNP Q8J307
D	-1	PRO	-	expression tag	UNP Q8J307
D	0	HIS	-	expression tag	UNP Q8J307

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

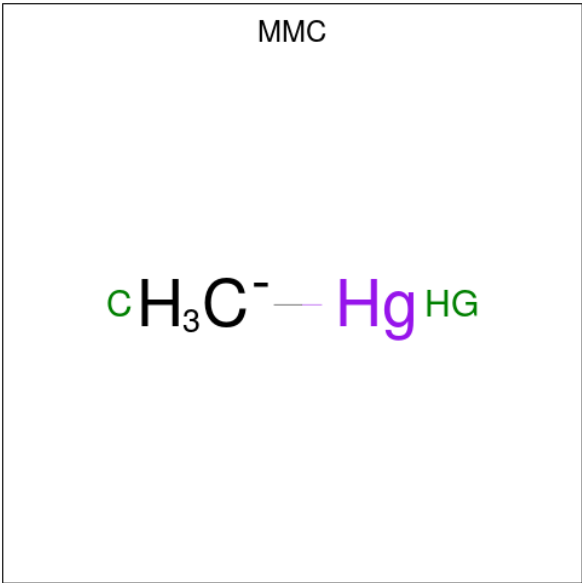


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

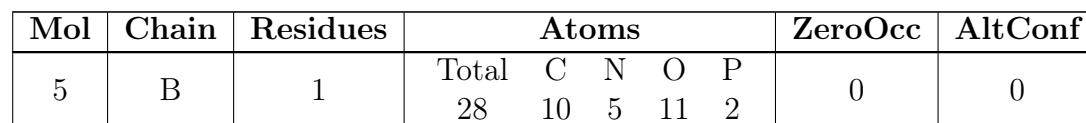
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is METHYL MERCURY ION (CCD ID: MMC) (formula: CH₃Hg).



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

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



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- Diagram illustrating the Lewis structure of the sulfate ion (SO_4^{2-}). The central sulfur atom (S) is bonded to four oxygen atoms (O). Two oxygen atoms are double-bonded to sulfur (top and bottom), and two are single-bonded (left and right). Each single-bonded oxygen has a negative charge (O^-). The sulfur atom has a formal charge of +6, indicated by a green 'S' with a '+' sign. The oxygen atoms are labeled O1, O2, O3, and O4 in green. The overall charge is -2, indicated by a green '2-'.

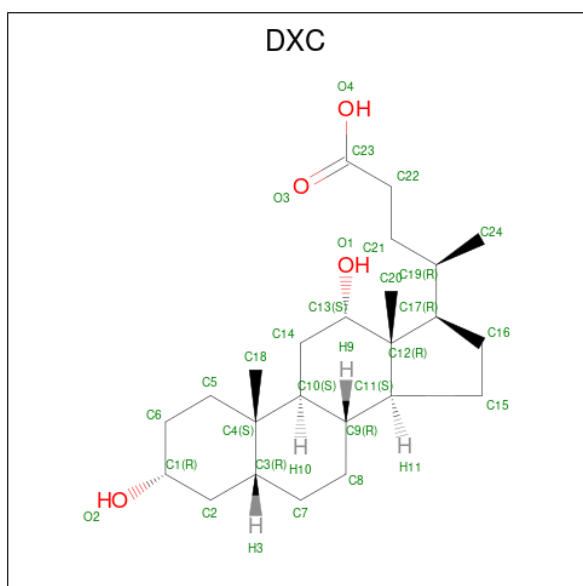
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	C	1	Total 5	O 4	S 1	0	0



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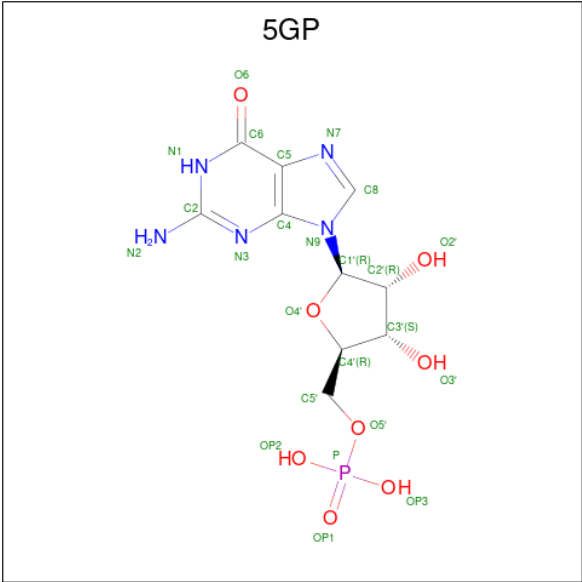
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (CCD ID: DXC) (formula: C₂₄H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			28	24	4		
7	C	1	Total	C	O	0	0
			28	24	4		
7	C	1	Total	C	O	0	0
			28	24	4		
7	C	1	Total	C	O	0	0
			28	24	4		
7	C	1	Total	C	O	0	0
			28	24	4		
7	C	1	Total	C	O	0	0
			28	24	4		

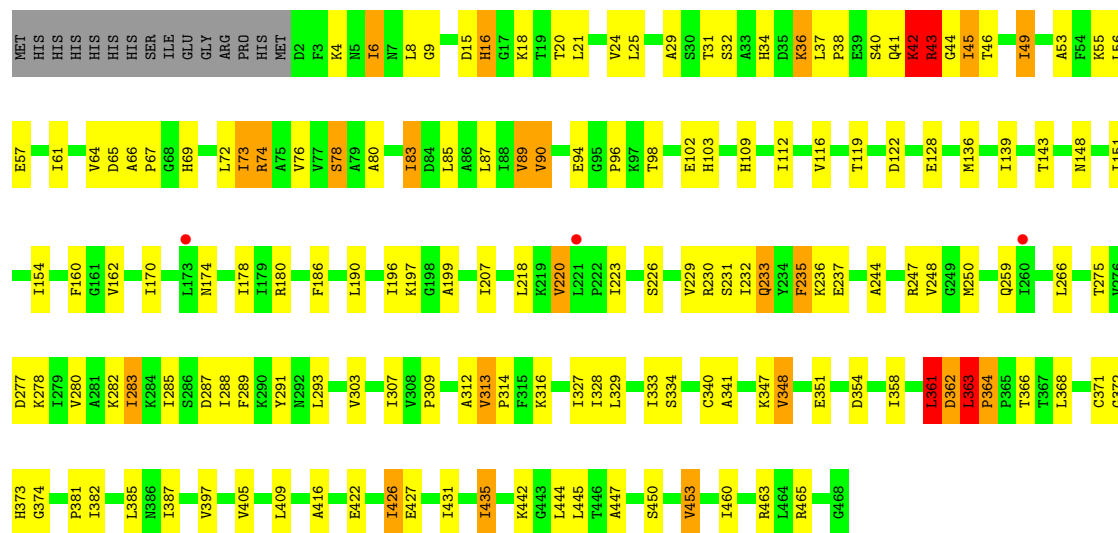
- Molecule 8 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O	0	0
			2 2		
9	B	4	Total O	0	0
			4 4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	146.63Å 146.63Å 297.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.34 19.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	82.8 (19.94-3.34) 88.0 (19.94-3.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.223 0.189 , 0.230	Depositor DCC
R_{free} test set	2214 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	110.2	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 174.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14623	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5GP, GDP, MMC, DXC, SO4, GNP

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	0.42	0/3543	0.89	3/4771 (0.1%)
1	B	0.48	0/3569	0.91	6/4804 (0.1%)
1	C	0.54	0/3692	0.96	9/4973 (0.2%)
1	D	0.39	0/3654	0.91	13/4922 (0.3%)
All	All	0.46	0/14458	0.92	31/19470 (0.2%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	363	LEU	CA-C-N	9.75	130.42	120.38
1	D	363	LEU	C-N-CA	9.75	130.42	120.38
1	D	364	PRO	N-CA-C	7.71	120.10	110.70
1	D	283	ILE	N-CA-C	7.26	118.35	107.75
1	B	308	VAL	N-CA-C	6.89	115.81	107.61

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	3498	0	3691	79	0
1	B	3525	0	3730	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3643	0	3842	84	0
1	D	3607	0	3803	110	0
2	A	32	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	2	0
4	D	8	0	0	5	0
5	B	28	0	12	2	0
6	B	10	0	0	2	0
6	C	20	0	0	2	0
7	B	28	0	39	4	0
7	C	168	0	234	15	0
8	B	24	0	12	2	0
9	A	2	0	0	0	0
9	B	4	0	0	0	0
All	All	14623	0	15376	363	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 12.

The worst 5 of 363 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:C:6:ILE:HD12	1:C:173:LEU:HD13	1.54	0.90
1:C:338:CYS:HB2	4:C:1484:MMC:C	2.05	0.86
1:D:43:ARG:HD3	1:D:45:ILE:HD11	1.57	0.85
1:D:283:ILE:HG13	1:D:340:CYS:HB2	1.61	0.82
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.61	0.80

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	448/482 (93%)	422 (94%)	26 (6%)	0	100	100
1	B	452/482 (94%)	433 (96%)	19 (4%)	0	100	100
1	C	469/482 (97%)	437 (93%)	30 (6%)	2 (0%)	30	59
1	D	465/482 (96%)	437 (94%)	27 (6%)	1 (0%)	43	71
All	All	1834/1928 (95%)	1729 (94%)	102 (6%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	C	57	GLU
1	C	47	ILE

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	390/416 (94%)	347 (89%)	43 (11%)	6	23
1	B	392/416 (94%)	353 (90%)	39 (10%)	7	28
1	C	406/416 (98%)	347 (86%)	59 (14%)	3	14
1	D	402/416 (97%)	355 (88%)	47 (12%)	5	21
All	All	1590/1664 (96%)	1402 (88%)	188 (12%)	5	21

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	293	LEU
1	D	20	THR
1	C	319	THR
1	C	368	LEU
1	D	43	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	233	GLN
1	D	373	HIS
1	C	181	ASN
1	C	233	GLN
1	D	58	ASN

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 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\# Z > 2$
8	5GP	B	1474	-	26,26,26	0.97	1 (3%)	40,40,40	1.73	10 (25%)
4	MMC	A	1472	1	0,1,1	-	-	-		
5	GDP	B	1469	3	28,30,30	1.12	2 (7%)	44,47,47	1.80	7 (15%)
2	GNP	A	1469	3	33,34,34	1.41	4 (12%)	46,54,54	1.12	4 (8%)
6	SO4	C	1471	-	4,4,4	0.27	0	6,6,6	0.72	0
4	MMC	D	471	1	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DXC	C	1478	-	31,31,31	1.34	5 (16%)	49,49,49	1.85	16 (32%)
6	SO4	B	1472	-	4,4,4	0.14	0	6,6,6	0.15	0
7	DXC	C	1477	-	31,31,31	1.59	6 (19%)	49,49,49	1.86	13 (26%)
4	MMC	C	1484	1	0,1,1	-	-	-	-	-
4	MMC	A	1471	1	0,1,1	-	-	-	-	-
7	DXC	C	1476	-	31,31,31	1.48	5 (16%)	49,49,49	1.79	13 (26%)
4	MMC	D	472	1	0,1,1	-	-	-	-	-
4	MMC	D	470	1	0,1,1	-	-	-	-	-
4	MMC	C	1482	1	0,1,1	-	-	-	-	-
6	SO4	C	1472	-	4,4,4	0.25	0	6,6,6	0.20	0
7	DXC	C	1475	-	31,31,31	1.58	5 (16%)	49,49,49	2.22	18 (36%)
4	MMC	C	1485	1	0,1,1	-	-	-	-	-
4	MMC	B	1476	1	0,1,1	-	-	-	-	-
4	MMC	A	1473	1	0,1,1	-	-	-	-	-
4	MMC	A	1474	1	0,1,1	-	-	-	-	-
4	MMC	B	1475	1	0,1,1	-	-	-	-	-
6	SO4	C	1481	-	4,4,4	0.17	0	6,6,6	0.12	0
7	DXC	C	1479	-	31,31,31	1.53	8 (25%)	49,49,49	2.15	17 (34%)
4	MMC	C	1483	1	0,1,1	-	-	-	-	-
7	DXC	C	1480	-	31,31,31	1.61	7 (22%)	49,49,49	2.06	16 (32%)
4	MMC	B	1478	1	0,1,1	-	-	-	-	-
4	MMC	B	1477	1	0,1,1	-	-	-	-	-
6	SO4	C	1473	-	4,4,4	0.15	0	6,6,6	0.11	0
6	SO4	B	1471	-	4,4,4	0.15	0	6,6,6	0.08	0
7	DXC	B	1473	-	31,31,31	1.33	3 (9%)	49,49,49	2.07	15 (30%)
4	MMC	D	469	1	0,1,1	-	-	-	-	-

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
8	5GP	B	1474	-	-	2/10/26/26	0/3/3/3
5	GDP	B	1469	3	-	7/16/32/32	0/3/3/3
7	DXC	C	1476	-	-	4/9/71/71	0/4/4/4
2	GNP	A	1469	3	-	5/18/38/38	0/3/3/3
7	DXC	C	1478	-	-	4/9/71/71	0/4/4/4
7	DXC	C	1480	-	-	4/9/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DXC	C	1475	-	-	6/9/71/71	0/4/4/4
7	DXC	C	1479	-	-	7/9/71/71	0/4/4/4
7	DXC	B	1473	-	-	2/9/71/71	0/4/4/4
7	DXC	C	1477	-	-	6/9/71/71	0/4/4/4

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	PB-O3A	-4.75	1.53	1.59
7	C	1475	DXC	C12-C13	-4.61	1.47	1.54
7	C	1477	DXC	C18-C4	-3.87	1.47	1.54
7	C	1477	DXC	C12-C13	-3.85	1.48	1.54
7	C	1480	DXC	C18-C4	-3.80	1.47	1.54

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1469	GDP	C5-C4-N3	-6.03	118.67	128.46
7	C	1478	DXC	C10-C14-C13	-5.61	106.89	114.30
8	B	1474	5GP	C5-C4-N3	-5.41	119.69	128.46
7	C	1475	DXC	C15-C11-C12	-5.37	98.29	103.55
7	C	1479	DXC	C18-C4-C3	-5.14	101.64	110.36

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1469	GNP	PB-N3B-PG-O1G
2	A	1469	GNP	PG-N3B-PB-O1B
2	A	1469	GNP	PG-N3B-PB-O3A
2	A	1469	GNP	PA-O3A-PB-O1B
2	A	1469	GNP	PA-O3A-PB-O2B

There are no ring outliers.

19 monomers are involved in 36 short contacts:

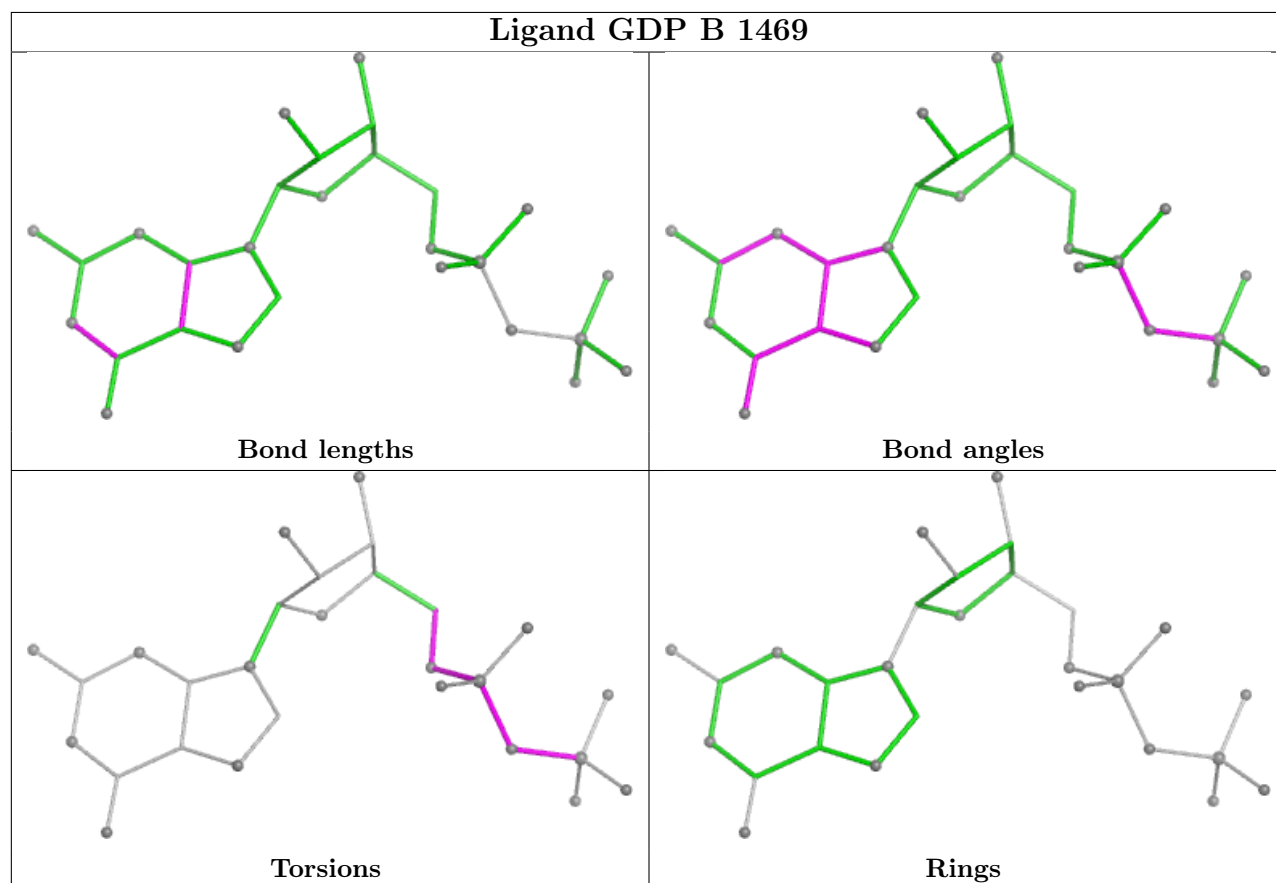
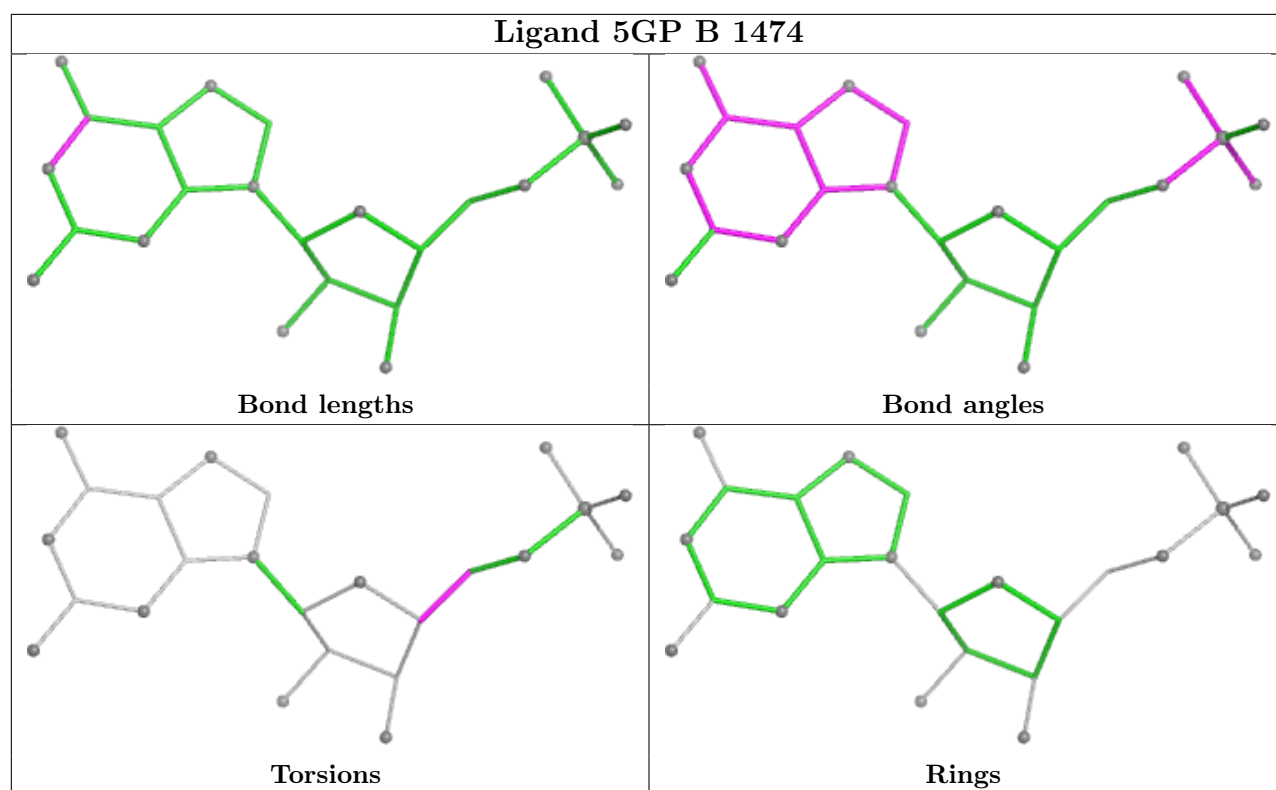
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1474	5GP	2	0
5	B	1469	GDP	2	0
2	A	1469	GNP	2	0

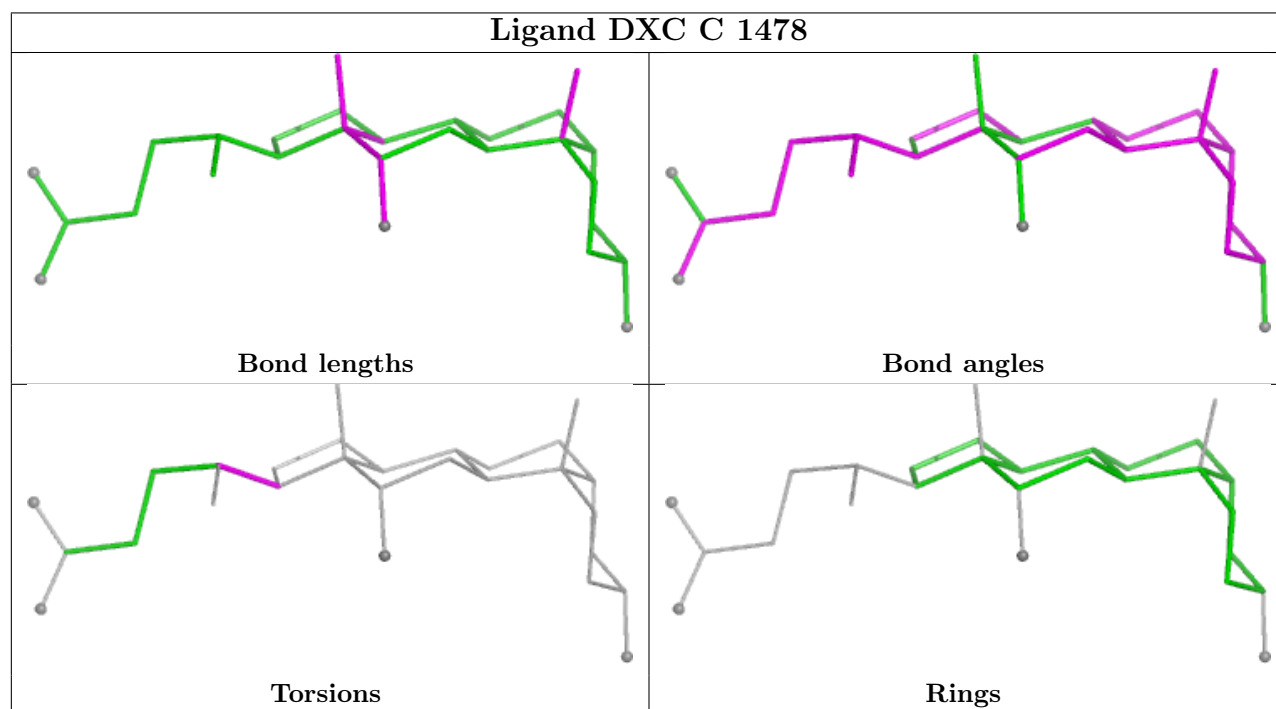
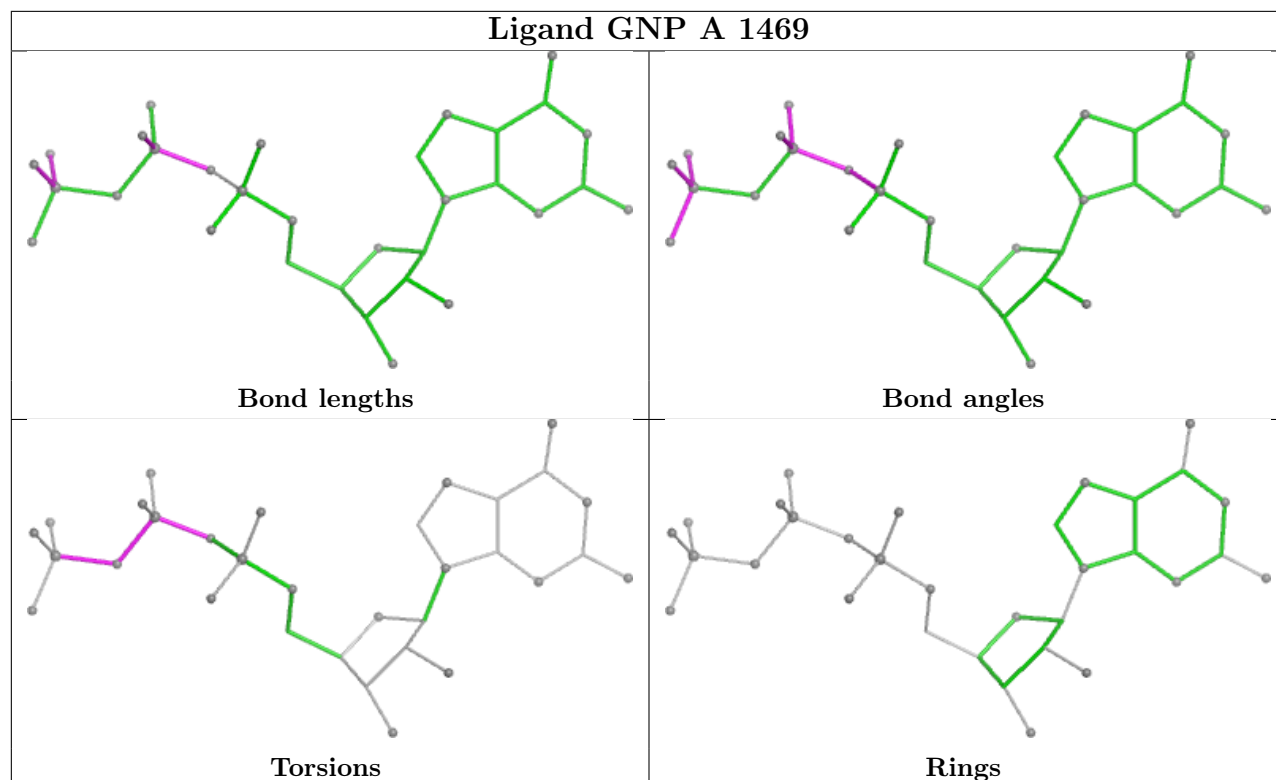
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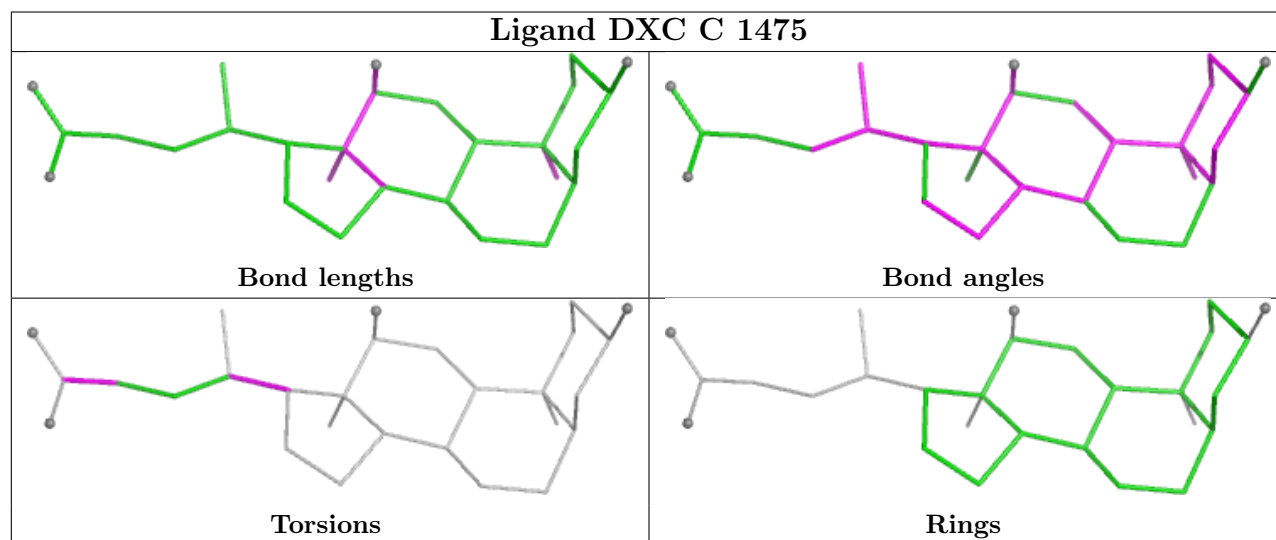
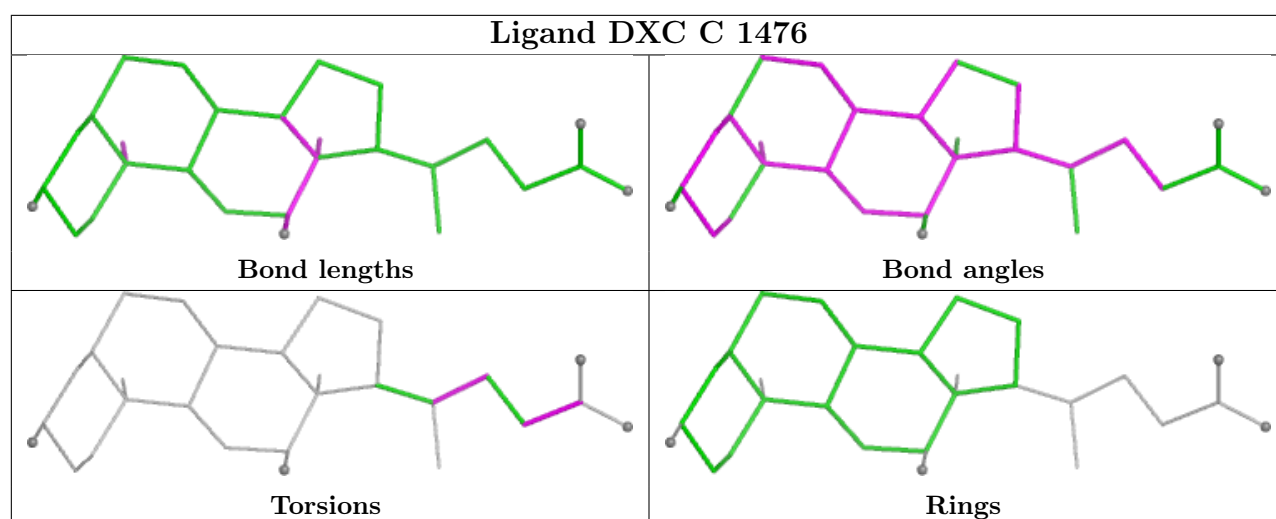
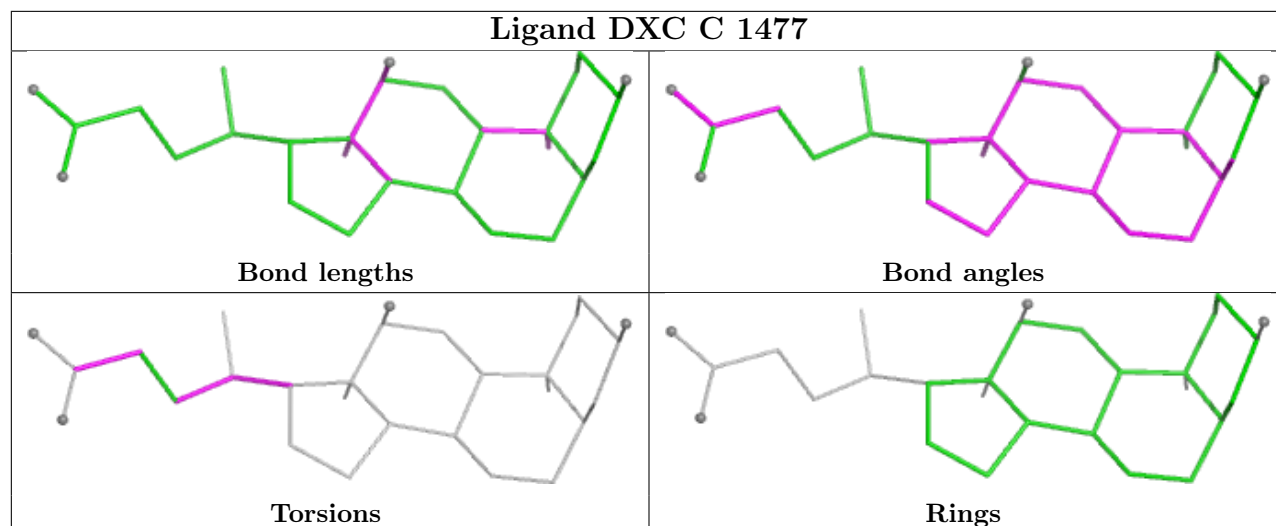
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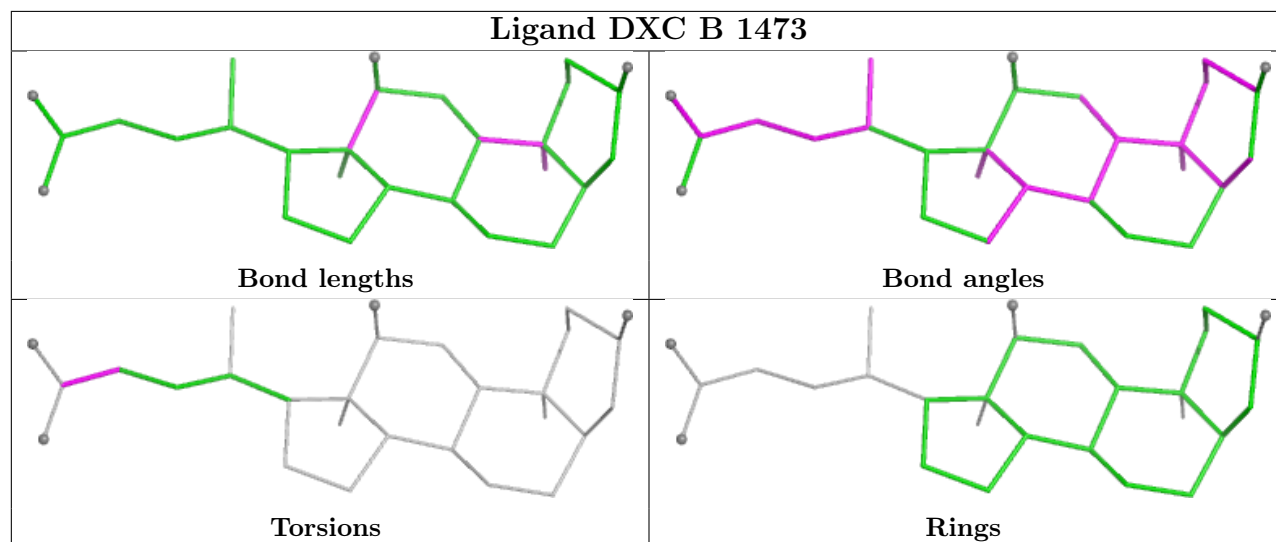
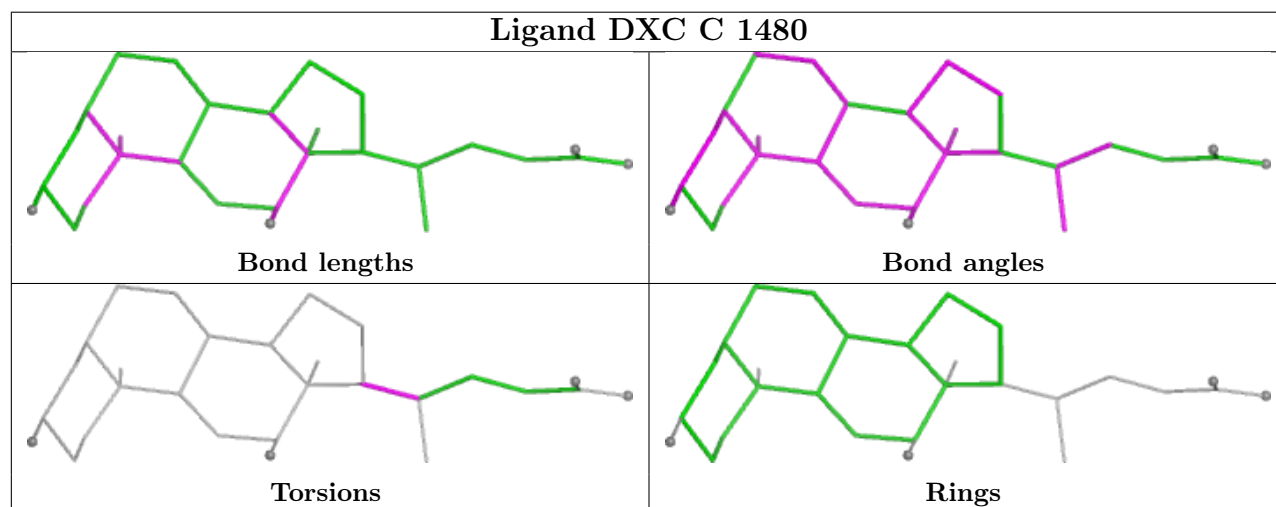
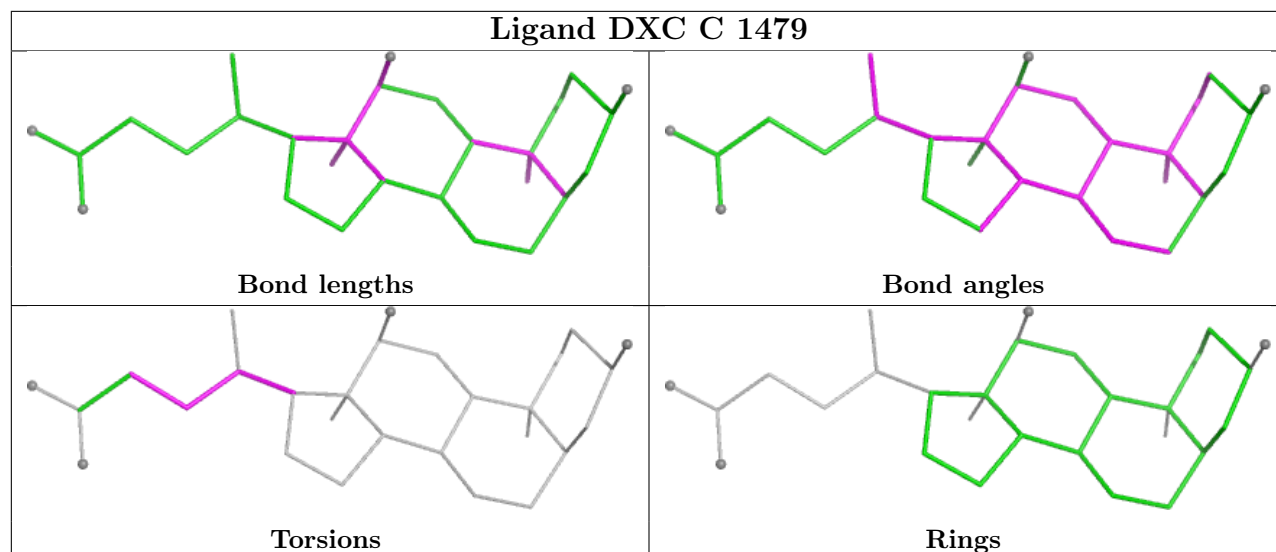
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1471	SO4	1	0
4	D	471	MMC	2	0
7	C	1478	DXC	2	0
6	B	1472	SO4	1	0
7	C	1477	DXC	3	0
4	C	1484	MMC	1	0
7	C	1476	DXC	2	0
4	D	472	MMC	1	0
4	D	470	MMC	2	0
7	C	1475	DXC	5	0
4	C	1485	MMC	1	0
7	C	1479	DXC	1	0
7	C	1480	DXC	2	0
6	C	1473	SO4	1	0
6	B	1471	SO4	1	0
7	B	1473	DXC	4	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.









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	452/482 (93%)	-0.47	3 (0%) 84 71	107, 205, 299, 372	0
1	B	456/482 (94%)	-0.48	3 (0%) 84 71	80, 153, 347, 414	0
1	C	471/482 (97%)	-0.53	1 (0%) 91 87	74, 123, 227, 308	0
1	D	467/482 (96%)	-0.23	3 (0%) 85 74	140, 274, 369, 416	0
All	All	1846/1928 (95%)	-0.43	10 (0%) 87 77	74, 188, 338, 416	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ILE	2.8
1	A	291	TYR	2.7
1	A	333	ILE	2.6
1	D	260	ILE	2.3
1	B	226	SER	2.3

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](#)

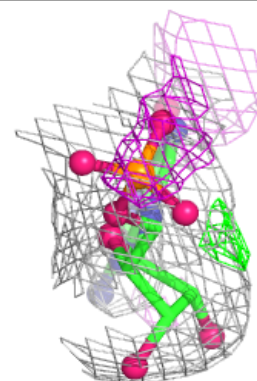
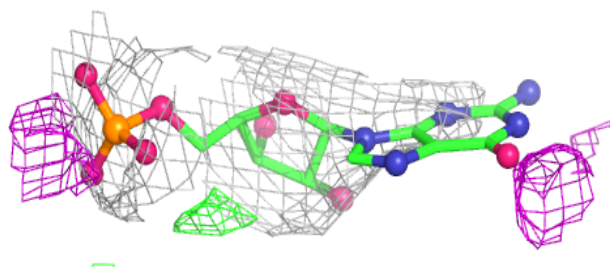
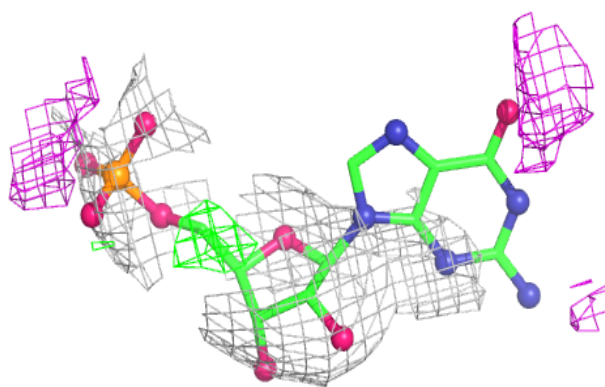
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
4	MMC	A	1472	2/2	0.69	0.28	190,190,190,307	2
6	SO4	C	1481	5/5	0.77	0.08	172,210,221,235	5
3	MG	B	1470	1/1	0.81	0.14	342,342,342,342	0
6	SO4	B	1471	5/5	0.82	0.13	205,213,271,283	0
8	5GP	B	1474	24/24	0.82	0.16	242,294,308,311	0
5	GDP	B	1469	28/28	0.85	0.09	126,197,212,235	0
4	MMC	B	1478	2/2	0.87	0.16	174,174,174,251	2
6	SO4	C	1473	5/5	0.88	0.04	164,166,220,230	5
4	MMC	D	470	2/2	0.89	0.15	180,180,180,242	2
6	SO4	C	1472	5/5	0.92	0.13	133,154,189,210	0
4	MMC	B	1476	2/2	0.93	0.14	181,181,181,232	2
6	SO4	B	1472	5/5	0.93	0.07	139,226,336,344	0
4	MMC	A	1474	2/2	0.94	0.11	168,168,168,215	2
6	SO4	C	1471	5/5	0.94	0.07	101,149,159,220	0
7	DXC	B	1473	28/28	0.94	0.10	68,97,134,143	0
2	GNP	A	1469	32/32	0.94	0.06	120,165,202,249	0
7	DXC	C	1476	28/28	0.96	0.10	159,168,217,253	0
7	DXC	C	1477	28/28	0.96	0.07	91,111,162,182	0
7	DXC	C	1480	28/28	0.96	0.07	63,85,106,127	0
4	MMC	D	469	2/2	0.96	0.07	248,248,248,255	2
7	DXC	C	1475	28/28	0.97	0.07	61,95,139,146	0
3	MG	A	1470	1/1	0.97	0.05	244,244,244,244	0
4	MMC	C	1483	2/2	0.97	0.07	150,150,150,174	2
7	DXC	C	1478	28/28	0.97	0.07	93,118,158,196	0
7	DXC	C	1479	28/28	0.97	0.08	82,104,174,196	28
4	MMC	D	471	2/2	0.97	0.13	296,296,296,317	2
4	MMC	D	472	2/2	0.97	0.16	154,154,154,216	2
4	MMC	B	1477	2/2	0.98	0.13	207,207,207,264	0
4	MMC	C	1485	2/2	0.98	0.15	78,78,78,123	2
4	MMC	A	1473	2/2	0.98	0.08	171,171,171,213	2
4	MMC	A	1471	2/2	0.99	0.10	215,215,215,235	2
4	MMC	C	1484	2/2	0.99	0.15	69,69,69,124	2
4	MMC	B	1475	2/2	1.00	0.07	73,73,73,112	2
4	MMC	C	1482	2/2	1.00	0.04	122,122,122,210	0

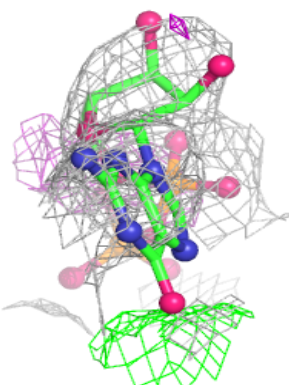
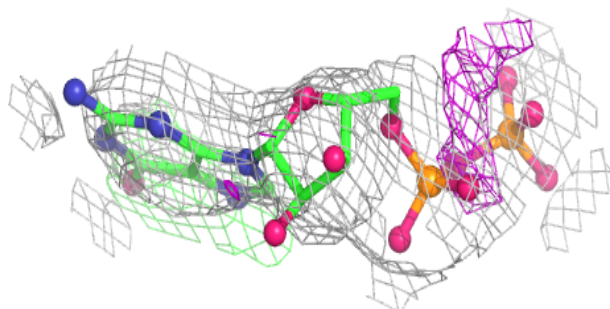
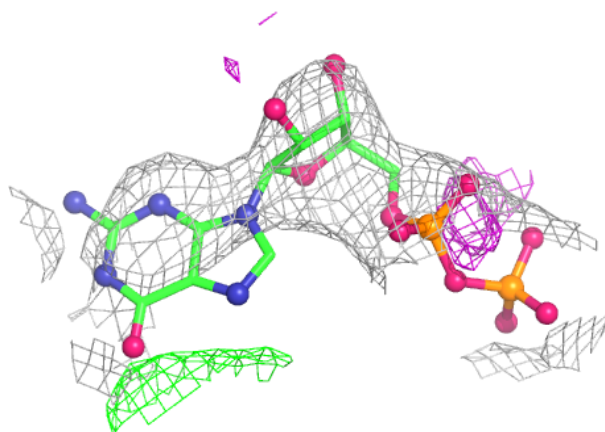
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP B 1474:

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

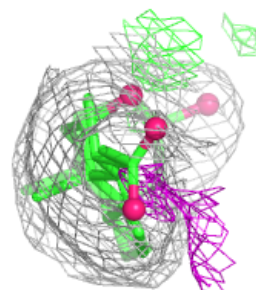
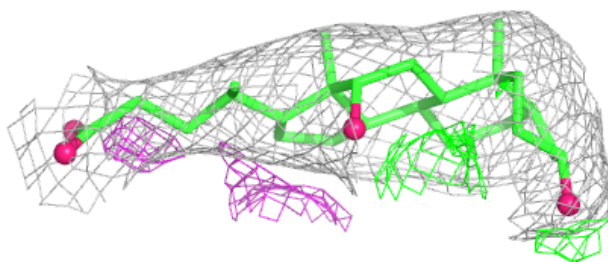
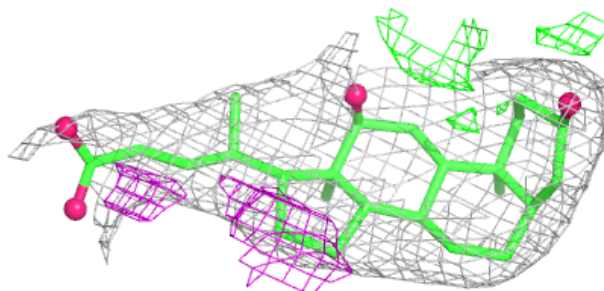
**Electron density around GDP B 1469:**

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and green (positive)

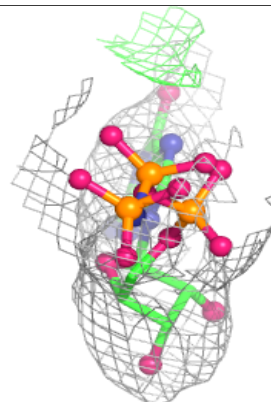
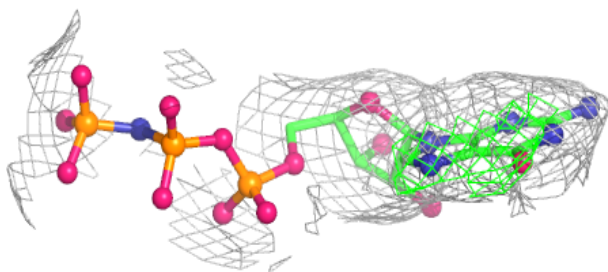
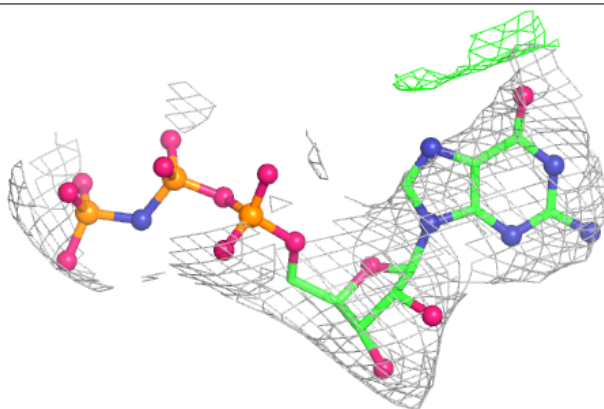


Electron density around DXC B 1473:

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and green (positive)

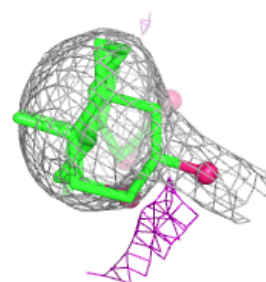
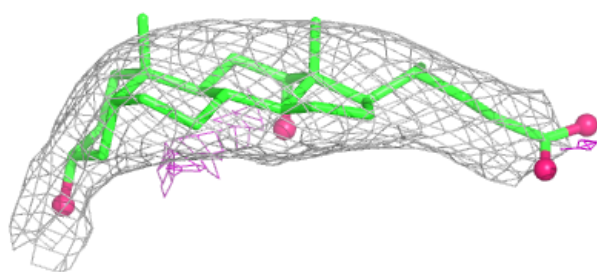
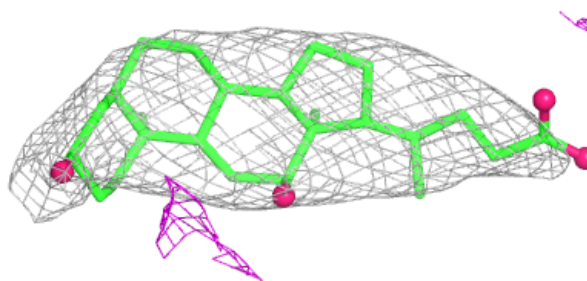
**Electron density around GNP A 1469:**

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and green (positive)

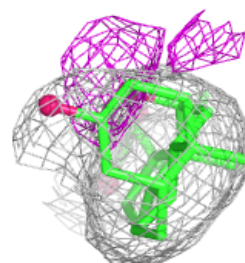
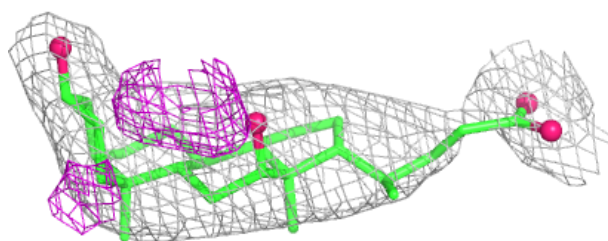
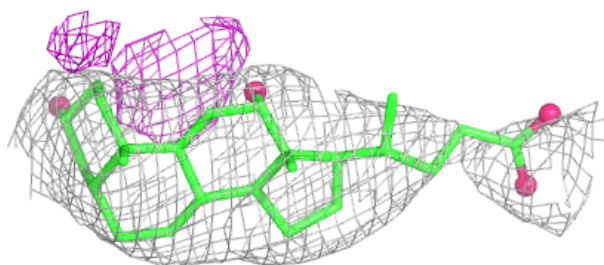


Electron density around DXC C 1476:

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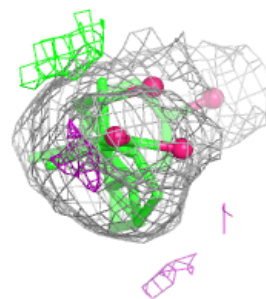
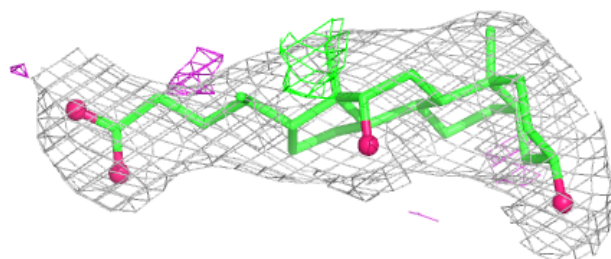
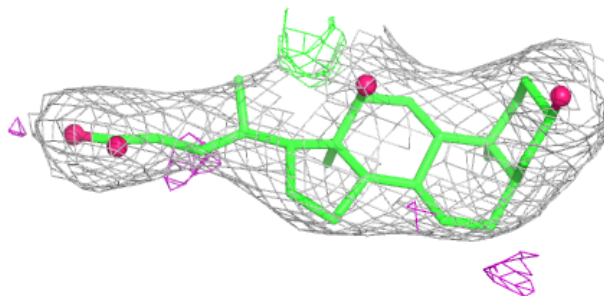
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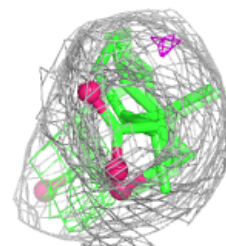
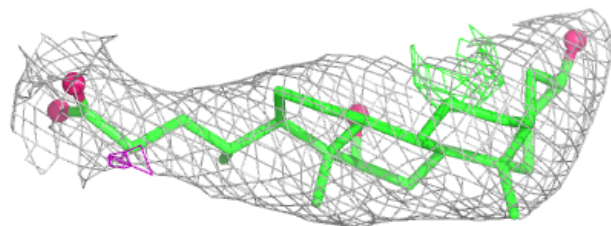
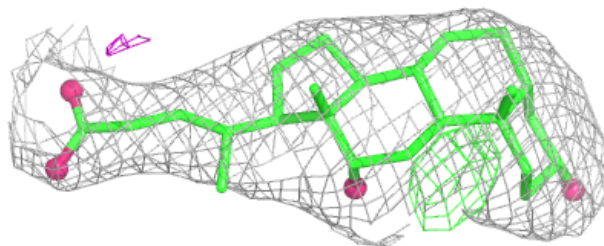


Electron density around DXC C 1480:

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

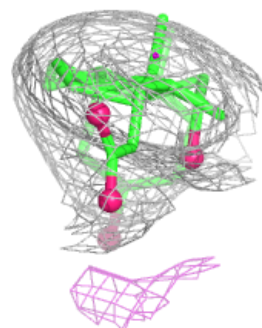
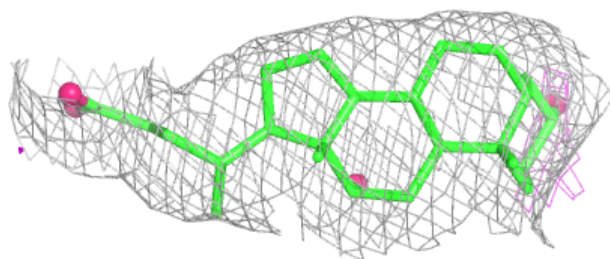
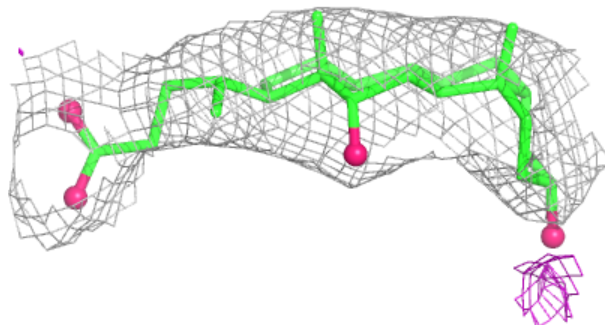
**Electron density around DXC C 1475:**

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

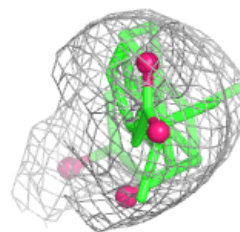
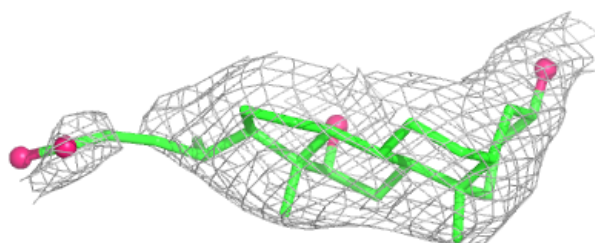
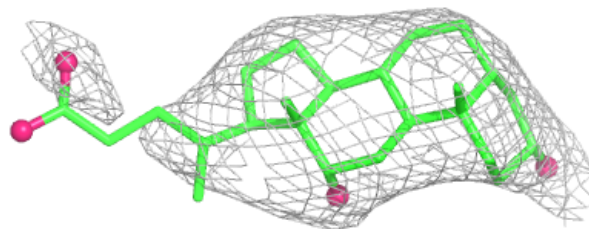


Electron density around DXC C 1478:

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

**Electron density around DXC C 1479:**

$2mF_o-DF_c$ (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.