



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:45 PM BST

PDB ID : 2OI6  
Title : E. coli GlmU- Complex with UDP-GlcNAc, CoA and GlcN-1-PO4  
Authors : Olsen, L.R.; Vetting, M.W.; Roderick, S.L.  
Deposited on : 2007-01-10  
Resolution : 2.20 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](mailto: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.

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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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

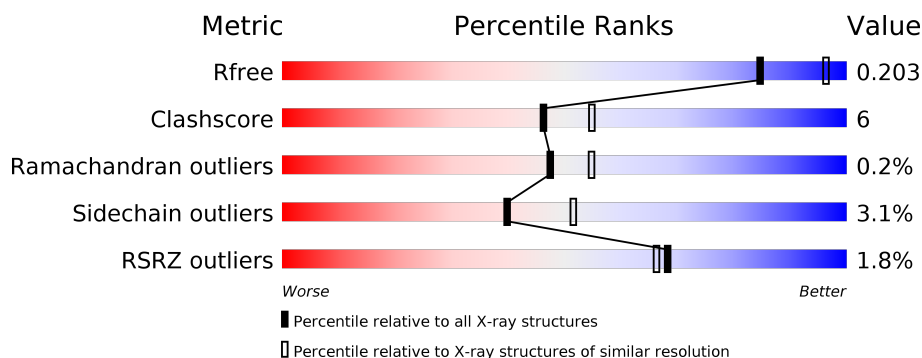
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	456	<div> <div> <div>0%</div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>
1	B	456	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>

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	MG	A	6004	-	-	-	X

## 2 Entry composition [i](#)

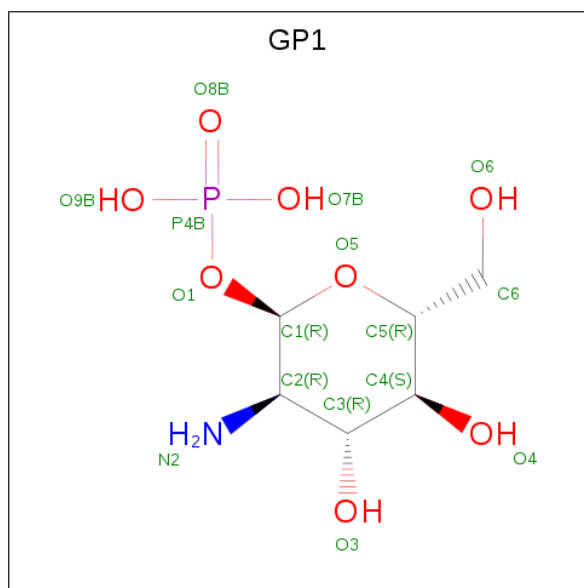
There are 8 unique types of molecules in this entry. The entry contains 7659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional protein glmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3387	2114	610	651	12			
1	B	452	Total	C	N	O	S	0	0	0
			3421	2133	618	658	12			

- Molecule 2 is 2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (three-letter code: GP1) (formula:  $C_6H_{14}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

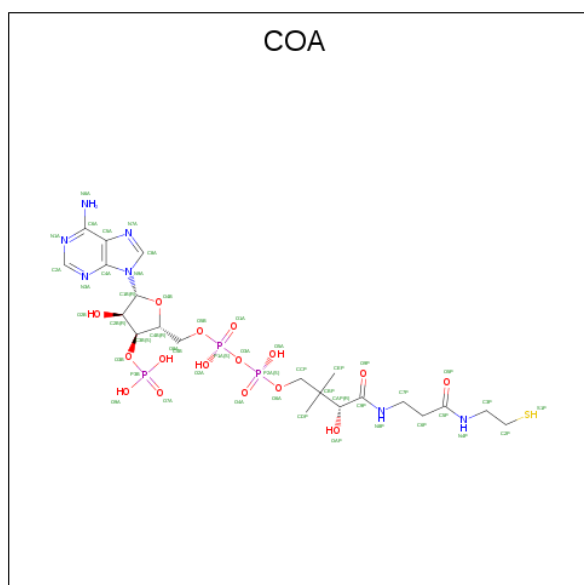
- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

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

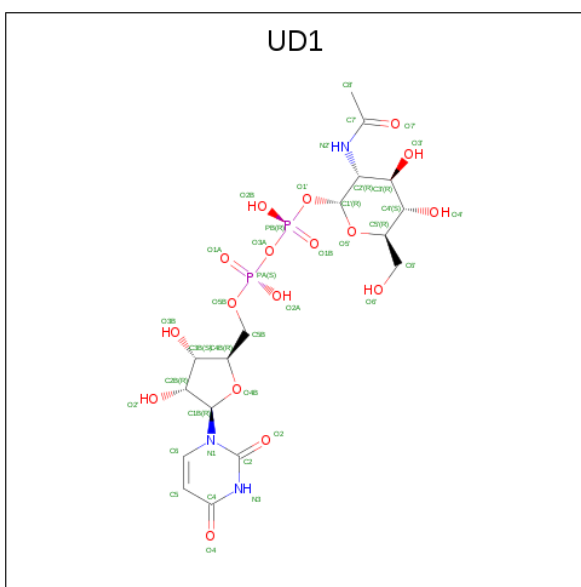
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



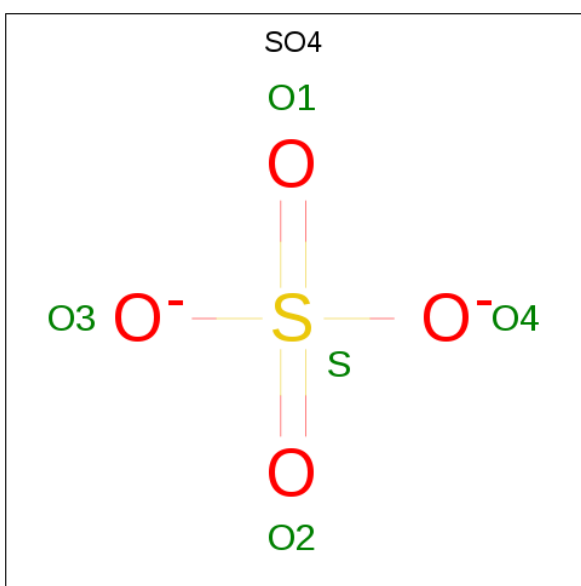
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total 39	C 17	N 3	O 17	P 2	0	0
6	B	1	Total 39	C 17	N 3	O 17	P 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

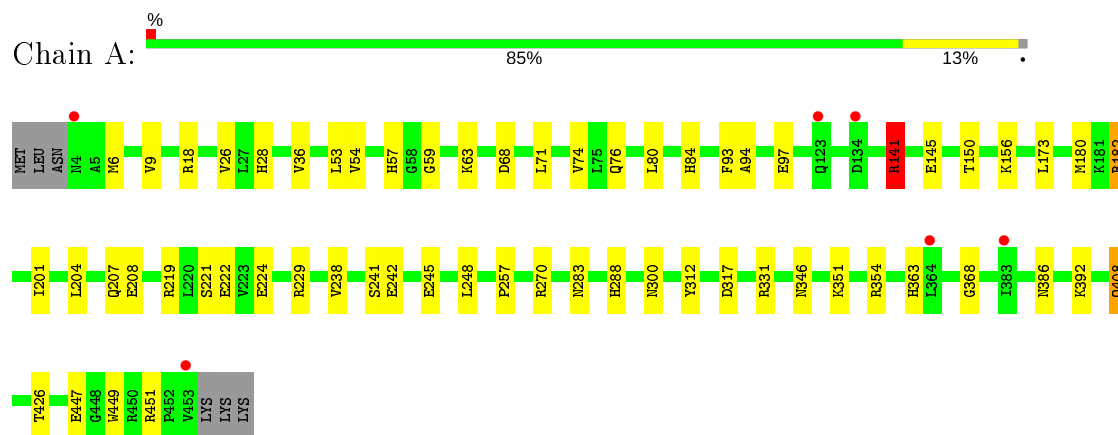
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	307	Total 307	O 307	0	0
8	B	328	Total 328	O 328	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: Bifunctional protein glmU





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.76 Å   102.76 Å   644.83 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	38.96 – 2.20 38.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.96-2.20) 98.1 (38.95-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.20 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.178   ,   0.208 0.174   ,   0.203	Depositor DCC
$R_{free}$ test set	3253 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, UD1, CO, COA, SO4, GP1

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	0.82	1/3435 (0.0%)	0.86	2/4658 (0.0%)
1	B	0.81	1/3469 (0.0%)	0.89	9/4700 (0.2%)
All	All	0.82	2/6904 (0.0%)	0.87	11/9358 (0.1%)

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	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	MET	SD-CE	-5.21	1.48	1.77
1	B	112	GLU	CB-CG	5.13	1.61	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	B	399	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	305	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	451	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	141	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	141	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	333	ARG	NE-CZ-NH2	-5.49	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	107	PRO	N-CA-C	5.11	125.39	112.10
1	B	182	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	255	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	TYR	Sidechain
1	B	312	TYR	Sidechain

## 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	3387	0	3400	38	0
1	B	3421	0	3447	50	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	48	0	32	0	0
5	B	48	0	32	0	0
6	A	39	0	25	0	0
6	B	39	0	25	2	0
7	B	5	0	0	0	0
8	A	307	0	0	3	0
8	B	328	0	0	8	0
All	All	7659	0	6961	88	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 6.

All (88) 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:B:270:ARG:H	1:B:288:HIS:HD2	1.16	0.92
1:A:270:ARG:H	1:A:288:HIS:HD2	1.18	0.88
1:A:141:ARG:HH11	1:A:141:ARG:HG3	1.38	0.85
1:B:453:VAL:HG22	1:B:454:LYS:H	1.43	0.83
1:A:76:GLN:HE21	1:A:84:HIS:HD2	1.26	0.83
1:A:221:SER:HA	1:A:224:GLU:HG3	1.64	0.80
1:B:270:ARG:H	1:B:288:HIS:CD2	2.03	0.74
1:B:115:GLN:HA	1:B:115:GLN:HE21	1.57	0.70
1:A:180:MET:HE1	1:A:201:ILE:HD13	1.74	0.69
1:A:248:LEU:HD11	1:A:257:PRO:HG3	1.75	0.69
1:A:270:ARG:H	1:A:288:HIS:CD2	2.08	0.67
1:A:238:VAL:O	1:A:242:GLU:HG3	1.95	0.66
1:B:19:MET:HG3	1:B:25:LYS:HG3	1.77	0.66
1:A:59:GLY:O	1:A:63:LYS:HD3	1.95	0.66
1:B:375:ASN:HB2	8:B:8419:HOH:O	1.96	0.66
1:A:76:GLN:HE21	1:A:84:HIS:CD2	2.11	0.65
1:A:141:ARG:NH1	1:A:141:ARG:HG3	2.12	0.64
1:B:28:HIS:HD2	8:B:8076:HOH:O	1.82	0.62
1:A:204:LEU:O	1:A:207:GLN:HG2	2.01	0.61
1:B:182:ARG:NH2	1:B:208:GLU:OE2	2.35	0.60
1:B:453:VAL:HG22	1:B:454:LYS:N	2.15	0.60
1:B:453:VAL:O	1:B:454:LYS:HG2	2.01	0.59
1:B:133:LEU:HD21	8:B:8404:HOH:O	2.01	0.58
1:B:386:ASN:O	1:B:392:LYS:HA	2.02	0.58
1:B:112:GLU:CD	1:B:112:GLU:H	2.06	0.58
1:B:26:VAL:HB	1:B:36:VAL:HB	1.86	0.57
1:B:255:ARG:HB2	1:B:275:ASP:HA	1.88	0.56
1:A:26:VAL:HB	1:A:36:VAL:HB	1.89	0.54
1:A:141:ARG:NH1	1:A:141:ARG:CG	2.69	0.53
1:B:94:ALA:HB3	1:B:97:GLU:HG2	1.90	0.53
1:A:141:ARG:HH11	1:A:141:ARG:CG	2.07	0.53
1:A:300:ASN:O	1:A:317:ASP:HA	2.11	0.51
1:B:6:MET:HE3	1:B:118:ARG:HD2	1.94	0.50
1:B:139:TYR:CD2	6:B:4001:UD1:H6'2	2.47	0.50
1:B:364:LEU:O	1:B:381:GLY:HA2	2.12	0.49
1:B:248:LEU:HD11	1:B:257:PRO:HG3	1.94	0.49
1:B:300:ASN:O	1:B:317:ASP:HA	2.11	0.49
1:B:16:GLY:HA3	1:B:25:LYS:HE2	1.95	0.49
1:B:229:ARG:HG2	8:B:8042:HOH:O	2.12	0.49
1:B:12:ALA:HB1	1:B:26:VAL:HG21	1.94	0.48
1:B:6:MET:HG2	1:B:118:ARG:CZ	2.43	0.48
1:A:204:LEU:O	1:A:207:GLN:CG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:HD2	8:A:8060:HOH:O	2.13	0.47
1:B:141:ARG:HG3	1:B:165:ILE:HB	1.96	0.47
1:A:351:LYS:O	1:A:368:GLY:HA2	2.15	0.47
1:A:68:ASP:HB2	1:A:71:LEU:HG	1.98	0.46
1:B:4:ASN:ND2	8:B:8278:HOH:O	2.48	0.46
1:A:207:GLN:HG3	1:A:208:GLU:N	2.30	0.46
1:B:182:ARG:HH22	1:B:208:GLU:CD	2.18	0.46
1:A:219:ARG:O	1:A:222:GLU:HB2	2.16	0.46
1:B:98:ASP:OD1	1:B:121:LYS:HE2	2.16	0.45
1:B:19:MET:CG	1:B:25:LYS:HG3	2.45	0.45
1:A:9:VAL:HG21	1:A:93:PHE:CZ	2.51	0.45
1:A:145:GLU:HB2	1:A:150:THR:HG21	1.99	0.45
1:B:115:GLN:HA	1:B:115:GLN:NE2	2.30	0.45
1:B:139:TYR:HD2	6:B:4001:UD1:H6'2	1.82	0.45
1:B:333:ARG:HB3	1:B:334:PRO:HD2	1.98	0.45
1:A:408:GLN:HE21	1:A:408:GLN:HB2	1.60	0.44
1:B:337:GLU:O	1:B:354:ARG:HA	2.18	0.44
1:A:28:HIS:HE1	1:A:229:ARG:NH2	2.16	0.44
1:A:156:LYS:HG2	8:A:8265:HOH:O	2.17	0.44
1:B:115:GLN:NE2	8:B:8468:HOH:O	2.48	0.44
1:B:372:ILE:HD12	1:B:397:ILE:HD12	2.00	0.43
1:A:54:VAL:HA	1:A:74:VAL:O	2.18	0.43
1:A:94:ALA:HB3	1:A:97:GLU:HG2	2.00	0.43
1:B:345:GLY:HA3	1:B:362:GLY:O	2.19	0.43
1:A:408:GLN:NE2	1:A:426:THR:OG1	2.48	0.43
1:B:6:MET:HE1	1:B:174:ILE:HD12	2.01	0.43
1:B:108:LEU:HB2	1:B:222:GLU:HA	2.01	0.42
1:A:386:ASN:O	1:A:392:LYS:HA	2.18	0.42
1:B:218:GLN:HB2	1:B:219:ARG:HD3	2.00	0.42
1:A:173:LEU:C	1:A:173:LEU:HD12	2.40	0.42
1:B:219:ARG:O	1:B:222:GLU:HG2	2.20	0.42
1:B:288:HIS:HE1	8:B:8424:HOH:O	2.01	0.42
1:A:204:LEU:O	1:A:208:GLU:HG3	2.19	0.42
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.86	0.42
1:A:283:ASN:O	1:A:300:ASN:HA	2.21	0.41
1:A:63:LYS:HE2	8:A:8415:HOH:O	2.20	0.41
1:B:309:ILE:HD12	1:B:326:ILE:HD11	2.01	0.41
1:B:82:THR:OG1	1:B:198:ILE:HG22	2.20	0.41
1:B:141:ARG:O	1:B:152:ILE:HA	2.21	0.41
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.85	0.41
1:B:54:VAL:HA	1:B:74:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:O	1:B:153:VAL:HG13	2.21	0.41
1:A:80:LEU:HB2	1:A:84:HIS:CG	2.55	0.41
1:B:156:LYS:HG2	8:B:8247:HOH:O	2.20	0.40
1:A:241:SER:O	1:A:245:GLU:HG3	2.21	0.40
1:B:15:LYS:HB2	1:B:57:HIS:CG	2.57	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	448/456 (98%)	439 (98%)	9 (2%)	0	100	100
1	B	450/456 (99%)	434 (96%)	14 (3%)	2 (0%)	34	37
All	All	898/912 (98%)	873 (97%)	23 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ASN
1	B	56	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	352/362 (97%)	341 (97%)	11 (3%)	40	51
1	B	358/362 (99%)	347 (97%)	11 (3%)	40	51
All	All	710/724 (98%)	688 (97%)	22 (3%)	40	51

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	53	LEU
1	A	57	HIS
1	A	141	ARG
1	A	182	ARG
1	A	331	ARG
1	A	346	ASN
1	A	363	HIS
1	A	408	GLN
1	A	447	GLU
1	A	449	TRP
1	B	112	GLU
1	B	115	GLN
1	B	123	GLN
1	B	160	ASP
1	B	207	GLN
1	B	219	ARG
1	B	235	LEU
1	B	255	ARG
1	B	331	ARG
1	B	346	ASN
1	B	363	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	84	HIS
1	A	88	GLN
1	A	123	GLN
1	A	207	GLN
1	A	288	HIS
1	A	363	HIS
1	A	408	GLN

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Mol	Chain	Res	Type
1	B	28	HIS
1	B	38	HIS
1	B	64	GLN
1	B	70	ASN
1	B	72	ASN
1	B	115	GLN
1	B	123	GLN
1	B	193	GLN
1	B	218	GLN
1	B	243	GLN
1	B	288	HIS
1	B	363	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GP1	B	5001	-	15,16,16	3.28	10 (66%)	23,24,24	0.92	1 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	UD1	B	4001	4	34,41,41	2.28	6 (17%)	45,62,62	1.03	5 (11%)
6	UD1	A	4000	-	34,41,41	2.24	3 (8%)	45,62,62	0.94	3 (6%)
5	COA	A	2000	-	41,50,50	1.69	8 (19%)	52,75,75	1.36	5 (9%)
2	GP1	A	5000	-	15,16,16	2.59	8 (53%)	23,24,24	1.11	3 (13%)
5	COA	B	2001	-	41,50,50	1.57	6 (14%)	52,75,75	1.21	5 (9%)
7	SO4	B	7000	-	4,4,4	0.37	0	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GP1	B	5001	-	-	2/6/27/27	0/1/1/1
6	UD1	B	4001	4	-	3/24/63/63	0/3/3/3
6	UD1	A	4000	-	-	0/24/63/63	0/3/3/3
5	COA	A	2000	-	-	2/44/64/64	0/3/3/3
2	GP1	A	5000	-	-	4/6/27/27	0/1/1/1
5	COA	B	2001	-	-	1/44/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4000	UD1	C6-N1	11.21	1.49	1.35
6	B	4001	UD1	C6-N1	10.85	1.49	1.35
2	B	5001	GP1	P4B-O1	-6.70	1.46	1.59
5	B	2001	COA	C4A-N3A	5.27	1.42	1.35
5	A	2000	COA	C6P-C5P	5.21	1.61	1.51
2	B	5001	GP1	C3-C2	5.15	1.60	1.53
2	A	5000	GP1	P4B-O1	-4.60	1.50	1.59
2	B	5001	GP1	C1-C2	4.27	1.60	1.52
2	A	5000	GP1	C1-C2	4.12	1.60	1.52
5	A	2000	COA	C3P-N4P	3.92	1.55	1.46
2	B	5001	GP1	O5-C1	3.76	1.51	1.41
5	A	2000	COA	C4A-N3A	3.74	1.40	1.35
2	A	5000	GP1	C4-C5	3.60	1.60	1.53
2	A	5000	GP1	O5-C1	3.54	1.50	1.41
2	B	5001	GP1	C4-C5	3.51	1.60	1.53
5	B	2001	COA	C6P-C5P	3.49	1.58	1.51
2	B	5001	GP1	O5-C5	3.43	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	GP1	C4-C3	3.24	1.60	1.52
6	B	4001	UD1	C4-N3	3.06	1.38	1.33
5	B	2001	COA	P3B-O3B	2.94	1.64	1.59
2	A	5000	GP1	C3-C2	2.91	1.57	1.53
5	B	2001	COA	C3P-N4P	2.85	1.52	1.46
5	A	2000	COA	C2A-N1A	2.85	1.39	1.33
5	A	2000	COA	O2B-C2B	2.72	1.49	1.43
5	A	2000	COA	P3B-O3B	2.71	1.64	1.59
6	A	4000	UD1	C4'-C5'	2.65	1.58	1.53
5	B	2001	COA	C2A-N1A	2.62	1.38	1.33
6	B	4001	UD1	C1'-C2'	2.62	1.57	1.53
5	A	2000	COA	C2P-S1P	2.61	1.90	1.80
5	A	2000	COA	C5P-N4P	2.51	1.39	1.33
6	B	4001	UD1	PA-O2A	-2.47	1.43	1.55
5	B	2001	COA	O2B-C2B	2.46	1.48	1.43
6	B	4001	UD1	C2'-N2'	2.43	1.49	1.45
2	A	5000	GP1	P4B-O9B	-2.32	1.45	1.54
2	B	5001	GP1	O4-C4	2.30	1.48	1.43
2	A	5000	GP1	C4-C3	2.21	1.58	1.52
6	B	4001	UD1	O5'-C5'	2.20	1.49	1.44
2	B	5001	GP1	P4B-O8B	-2.13	1.43	1.50
6	A	4000	UD1	O4B-C1B	-2.11	1.38	1.41
2	A	5000	GP1	O5-C5	2.10	1.49	1.44
2	B	5001	GP1	O3-C3	2.08	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2001	COA	C1B-N9A-C4A	-5.57	116.85	126.64
5	A	2000	COA	C1B-N9A-C4A	-5.43	117.10	126.64
5	A	2000	COA	C3P-N4P-C5P	3.97	130.22	122.84
2	A	5000	GP1	O5-C1-O1	-2.73	107.80	111.36
2	B	5001	GP1	C4-C3-C2	-2.61	106.58	111.07
6	B	4001	UD1	C3B-C2B-C1B	2.58	104.86	100.98
6	A	4000	UD1	O3A-PB-O1'	2.54	107.60	102.48
6	B	4001	UD1	O3A-PB-O1'	2.53	107.59	102.48
2	A	5000	GP1	O1-C1-C2	2.51	112.94	108.40
5	B	2001	COA	CDP-CBP-CCP	2.47	112.26	108.23
5	A	2000	COA	C6P-C5P-N4P	-2.30	112.56	116.42
6	A	4000	UD1	O5'-C1'-O1'	-2.28	108.38	111.36
6	B	4001	UD1	C5-C4-N3	-2.17	118.54	123.31
6	A	4000	UD1	C5-C4-N3	-2.14	118.60	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2000	COA	CEP-CBP-CAP	2.13	112.52	108.82
5	B	2001	COA	CEP-CBP-CAP	2.08	112.43	108.82
6	B	4001	UD1	O5'-C5'-C6'	2.05	111.54	106.44
6	B	4001	UD1	C6'-C5'-C4'	-2.05	108.20	113.00
5	B	2001	COA	O5A-P2A-O6A	2.04	117.22	107.75
2	A	5000	GP1	C4-C3-C2	-2.03	107.58	111.07
5	A	2000	COA	C5A-C6A-N6A	2.01	123.41	120.35
5	B	2001	COA	C6P-C7P-N8P	2.00	115.93	111.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2000	COA	S1P-C2P-C3P-N4P
6	B	4001	UD1	O4B-C1B-N1-C6
2	A	5000	GP1	O5-C5-C6-O6
2	B	5001	GP1	O5-C5-C6-O6
6	B	4001	UD1	C1'-O1'-PB-O3A
2	A	5000	GP1	C4-C5-C6-O6
2	B	5001	GP1	O5-C1-O1-P4B
5	B	2001	COA	P2A-O3A-P1A-O1A
6	B	4001	UD1	O5'-C5'-C6'-O6'
5	A	2000	COA	P2A-O3A-P1A-O1A
2	A	5000	GP1	C1-O1-P4B-O7B
2	A	5000	GP1	C1-O1-P4B-O8B

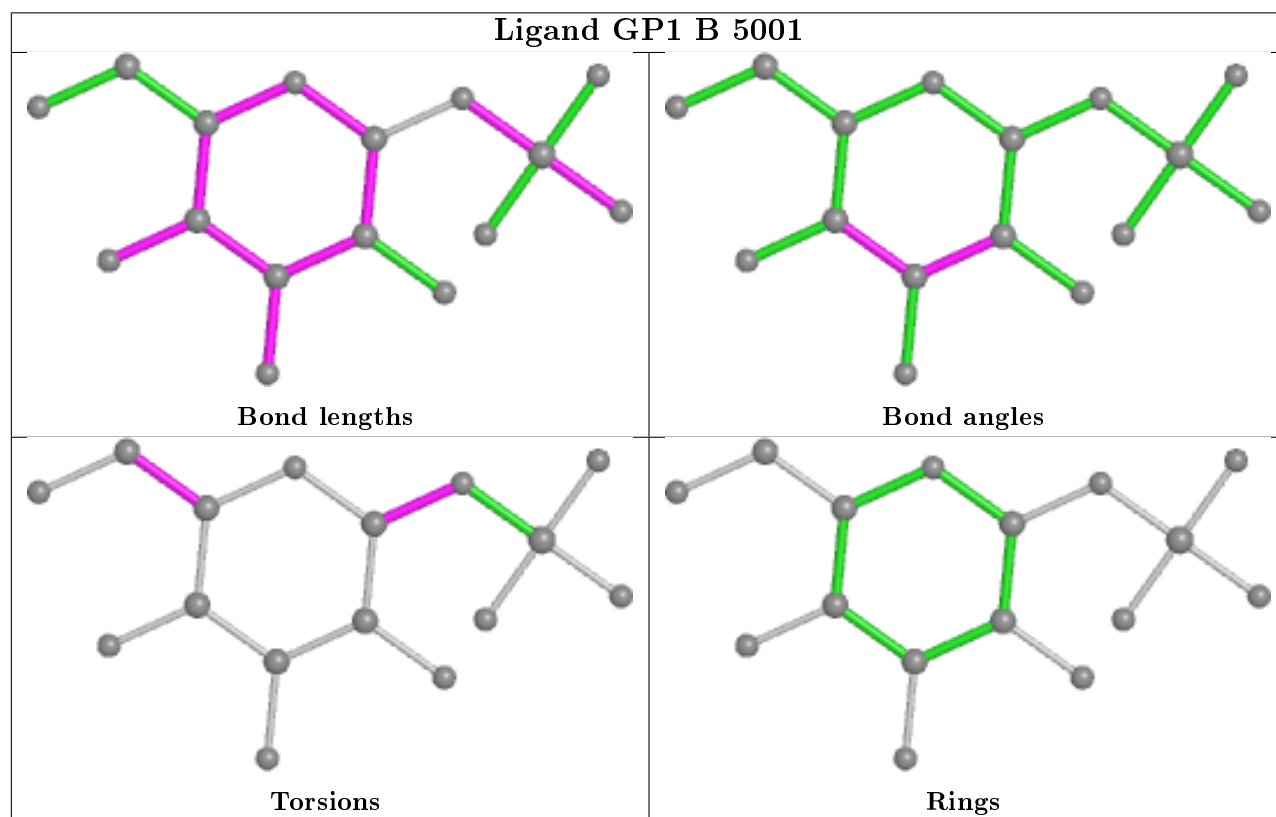
There are no ring outliers.

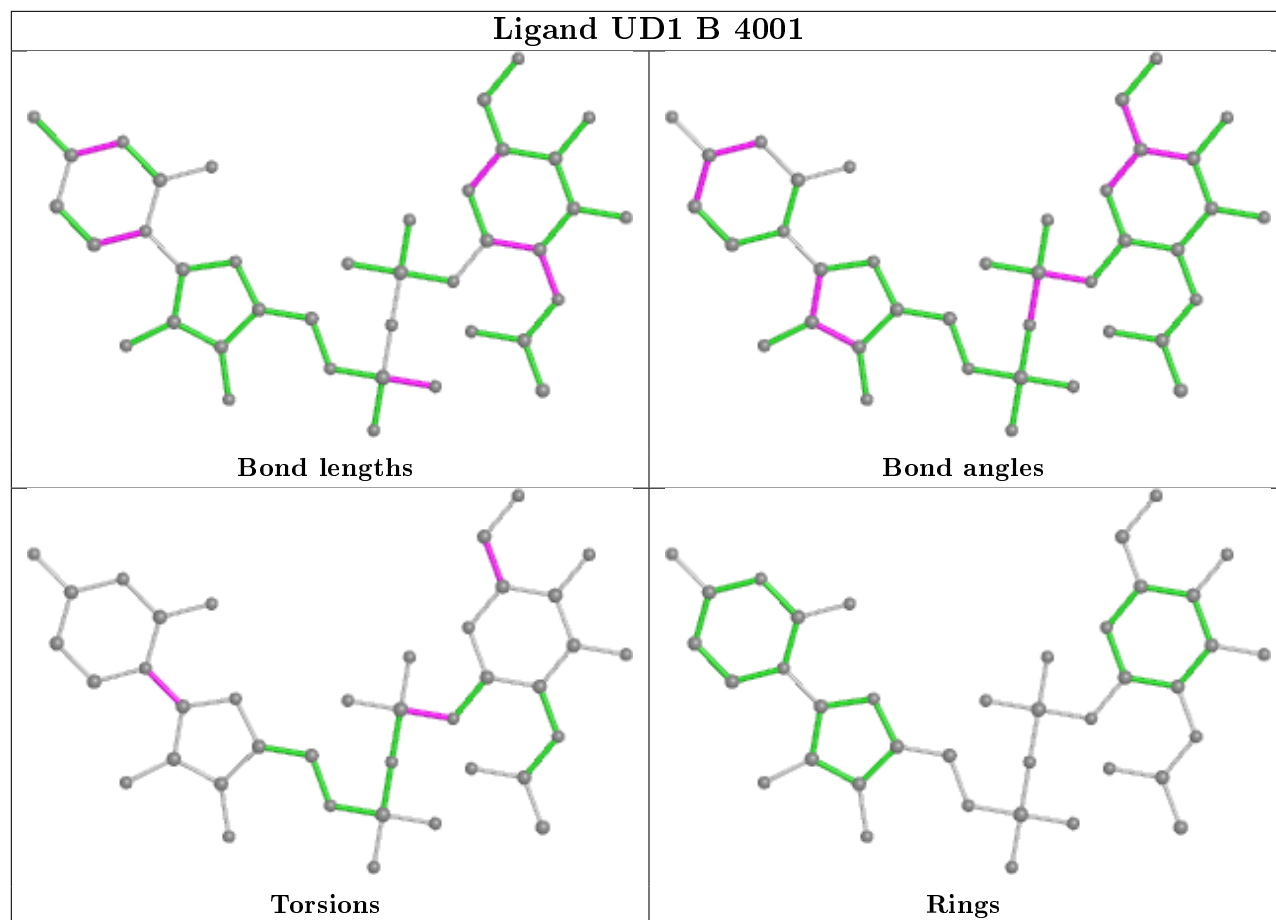
1 monomer is involved in 2 short contacts:

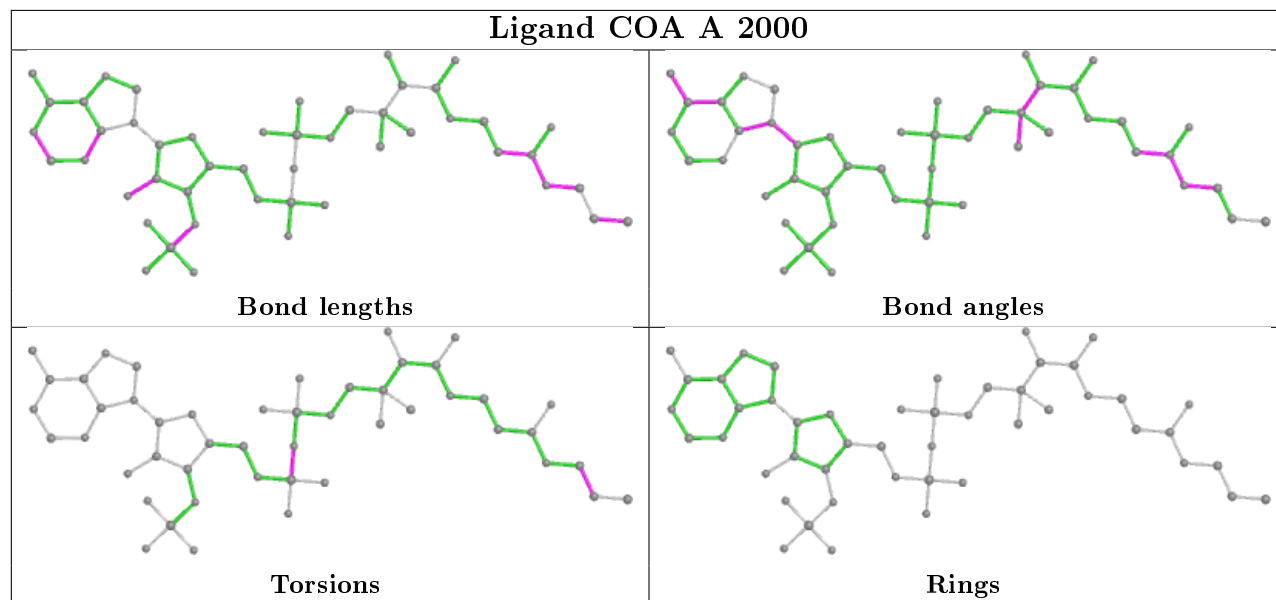
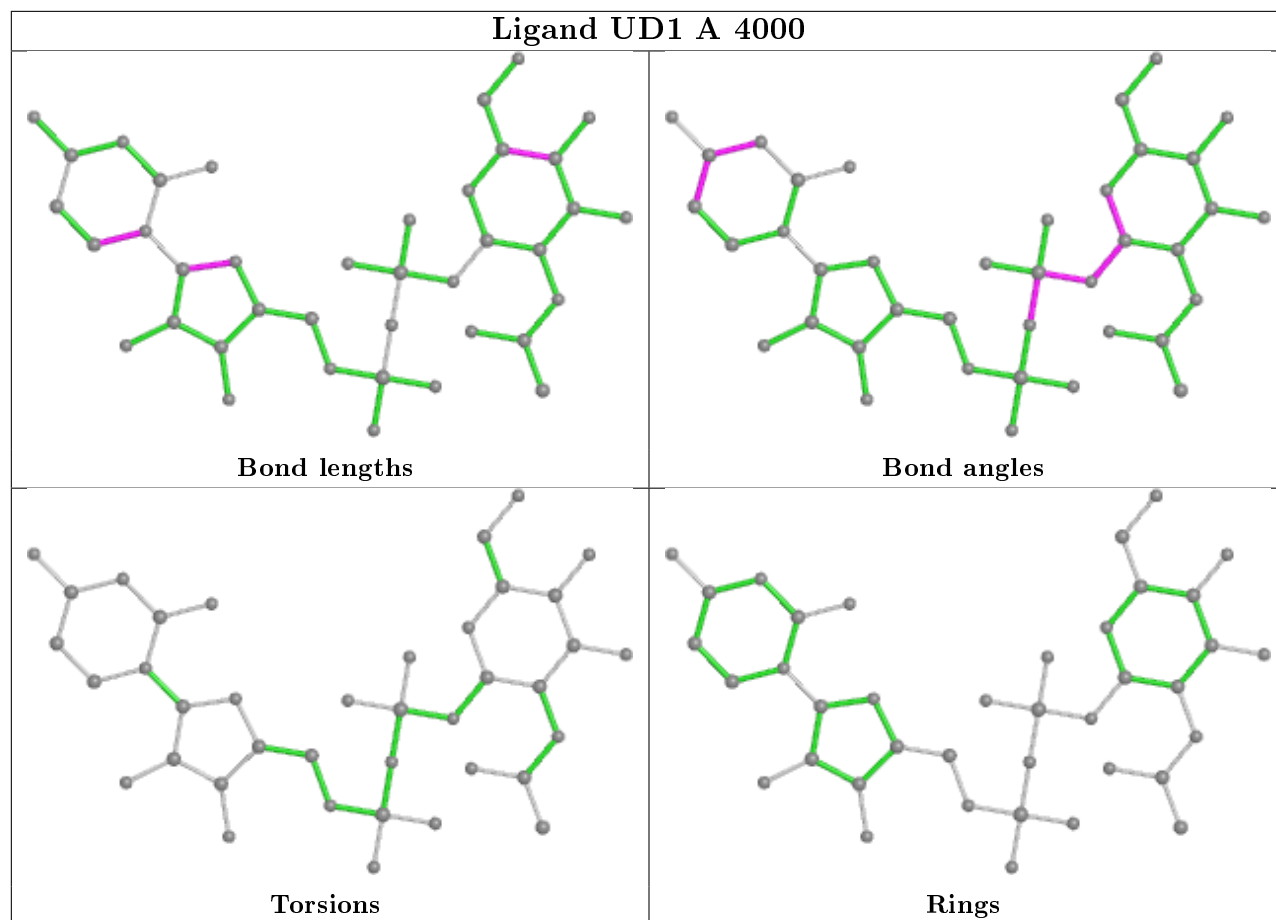
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4001	UD1	2	0

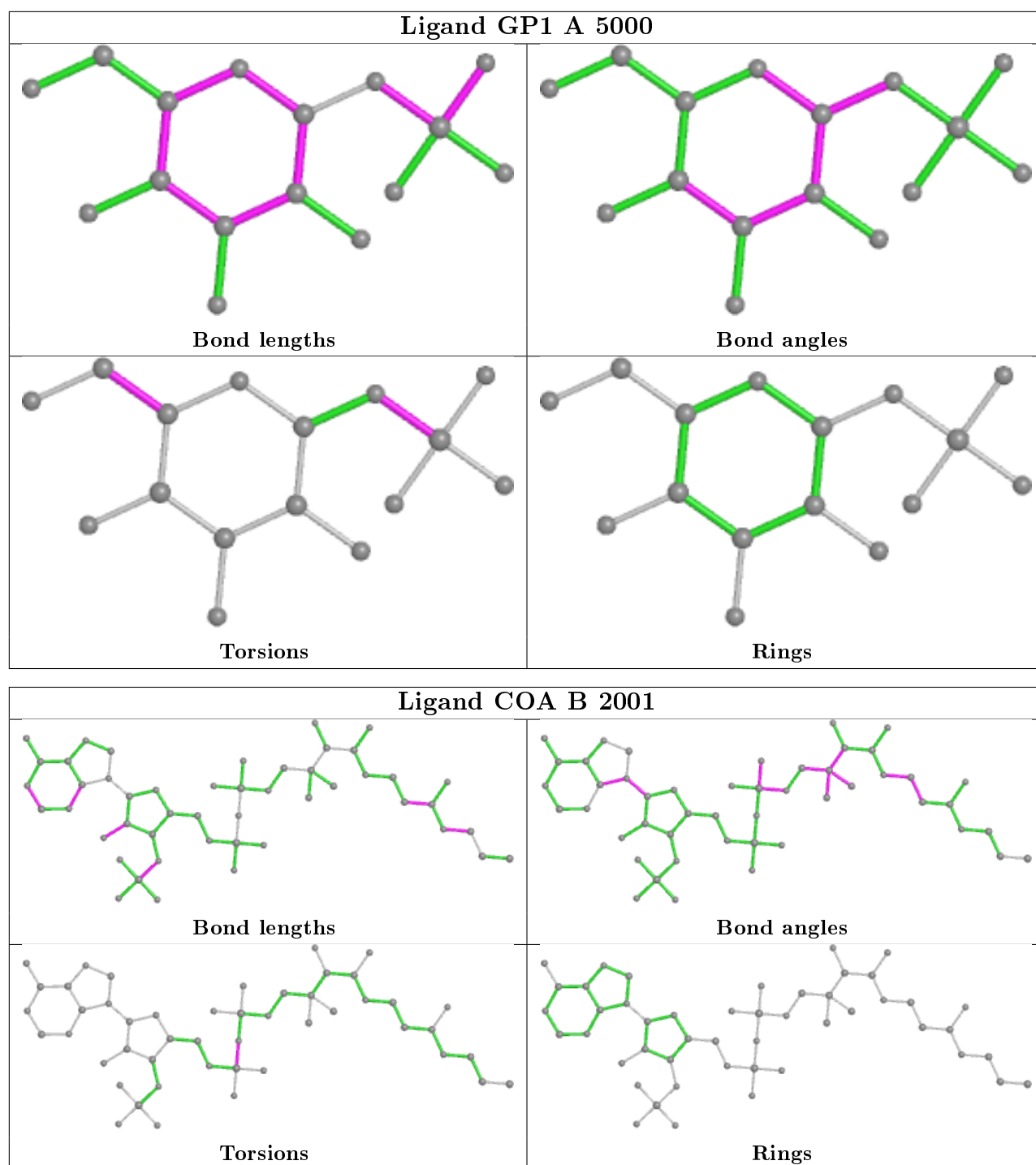
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/456 (98%)	-0.57	6 (1%) 77 75	10, 20, 37, 50	0
1	B	452/456 (99%)	-0.52	10 (2%) 62 59	11, 20, 38, 64	0
All	All	902/912 (98%)	-0.55	16 (1%) 68 66	10, 20, 38, 64	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	ASP	6.3
1	B	4	ASN	5.1
1	B	453	VAL	4.5
1	B	3	ASN	3.6
1	B	146	ASN	3.6
1	A	453	VAL	3.6
1	B	70	ASN	3.5
1	A	123	GLN	2.5
1	A	4	ASN	2.5
1	B	145	GLU	2.4
1	A	364	LEU	2.4
1	B	64	GLN	2.4
1	A	383	ILE	2.2
1	B	96	ASP	2.2
1	A	134	ASP	2.0
1	B	454	LYS	2.0

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

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



## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

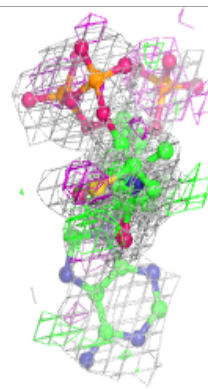
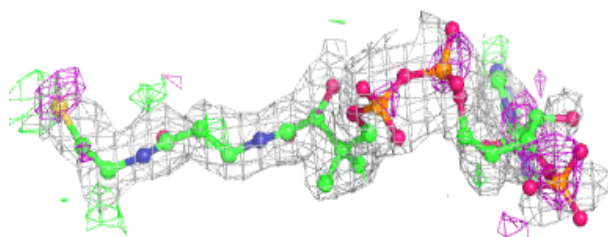
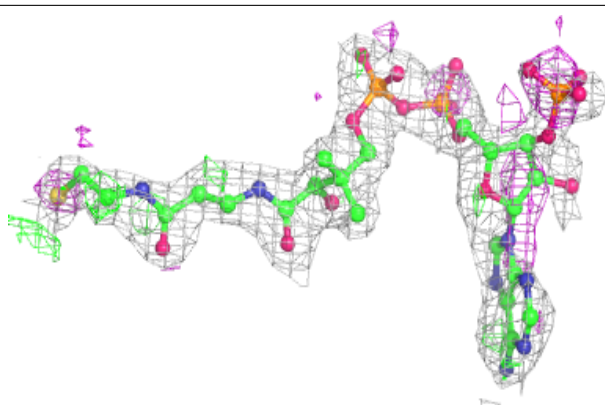
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	A	6004	1/1	0.17	0.60	43,43,43,43	1
4	MG	B	6001	1/1	0.47	0.21	20,20,20,20	1
5	COA	A	2000	48/48	0.76	0.23	20,62,80,82	0
5	COA	B	2001	48/48	0.79	0.23	21,63,80,81	0
2	GP1	A	5000	16/16	0.94	0.19	36,50,53,53	0
2	GP1	B	5001	16/16	0.95	0.19	31,46,48,49	0
6	UD1	A	4000	39/39	0.97	0.08	16,21,29,30	0
7	SO4	B	7000	5/5	0.98	0.07	26,30,31,33	0
6	UD1	B	4001	39/39	0.99	0.10	13,16,18,20	0
3	CO	A	6003	1/1	0.99	0.09	40,40,40,40	1
4	MG	B	6000	1/1	0.99	0.03	17,17,17,17	0
3	CO	B	6002	1/1	1.00	0.09	43,43,43,43	1

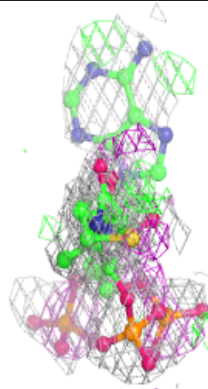
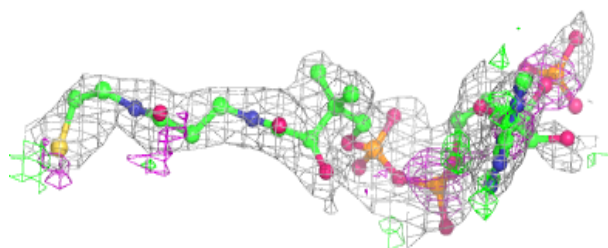
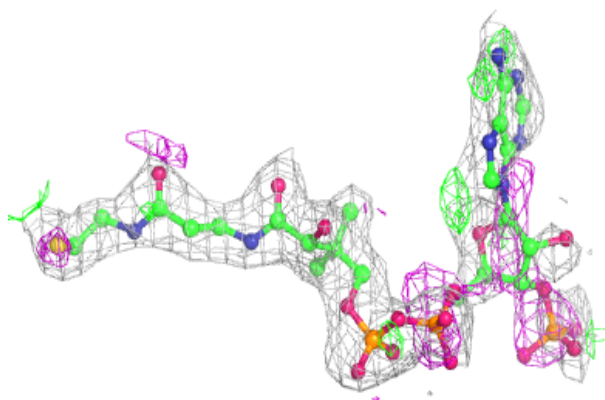
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around COA A 2000:**

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

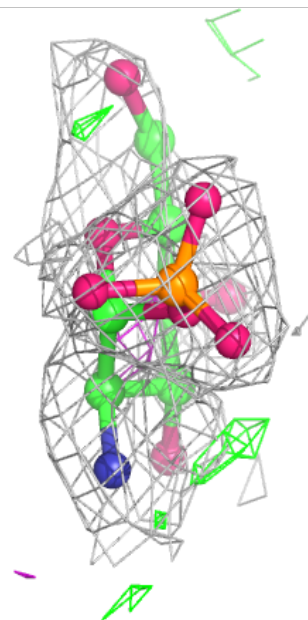
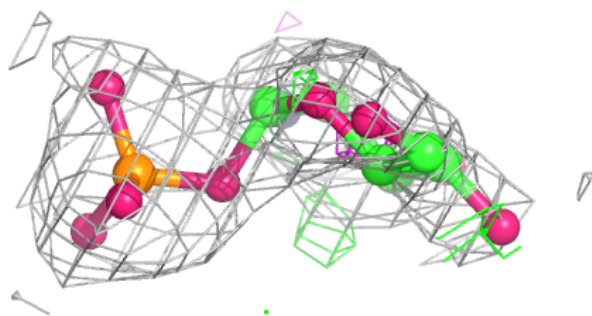
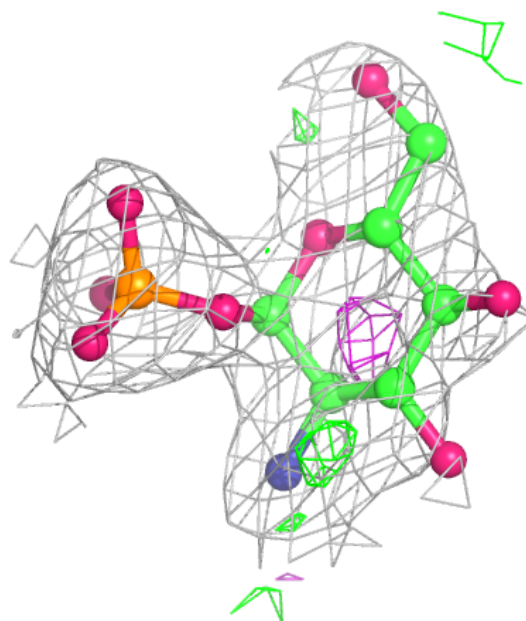
**Electron density around COA B 2001:**

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



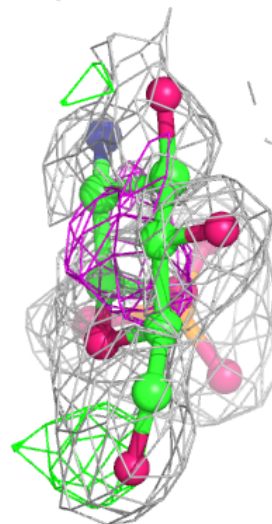
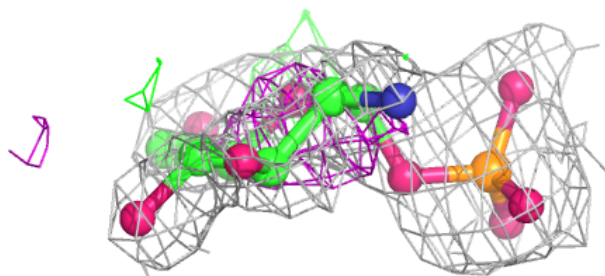
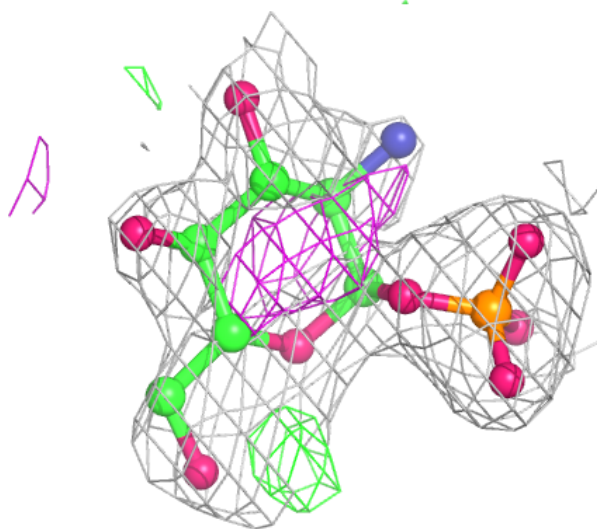
**Electron density around GP1 A 5000:**

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



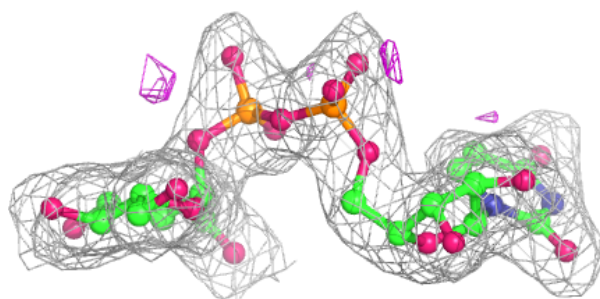
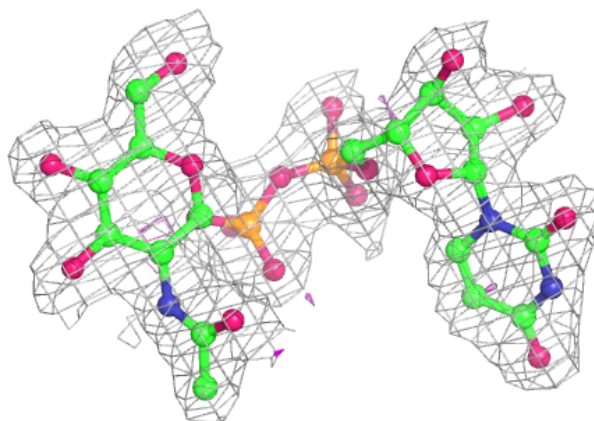
**Electron density around GP1 B 5001:**

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

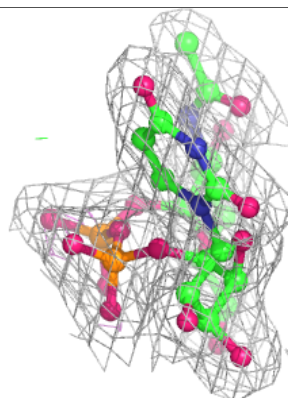
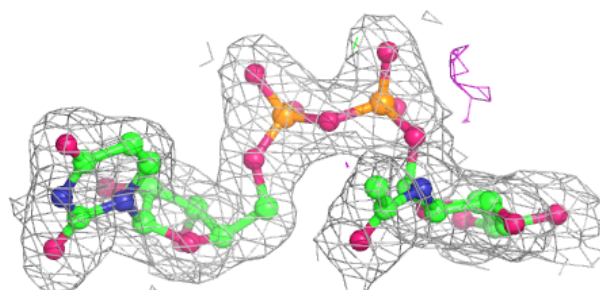
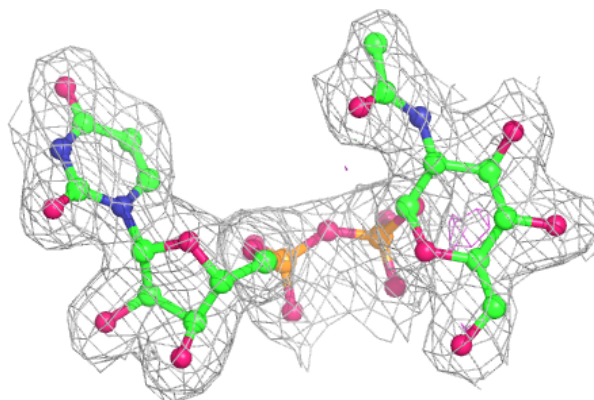


**Electron density around UD1 A 4000:**

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

**Electron density around UD1 B 4001:**

$2mF_o-DF_c$  (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.