



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 09:18 PM EDT

PDB ID : 1I1D
Title : CRYSTAL STRUCTURE OF YEAST GNA1 BOUND TO COA AND GLNAC-6P
Authors : Peneff, C.; Mengin-Lecreulx, D.; Bourne, Y.
Deposited on : 2001-02-01
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.34
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) : 2.34

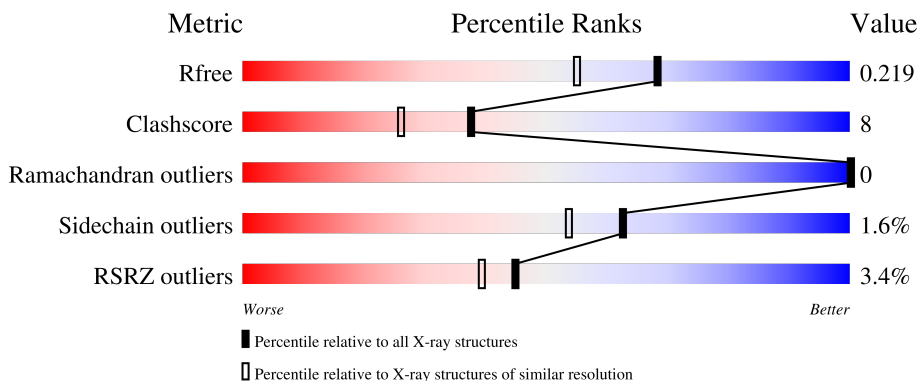
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	161	 2% 86% 10% ..
1	B	161	 3% 84% 11% ..
1	C	161	 4% 74% 21% ..
1	D	161	 4% 86% 13% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5713 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.

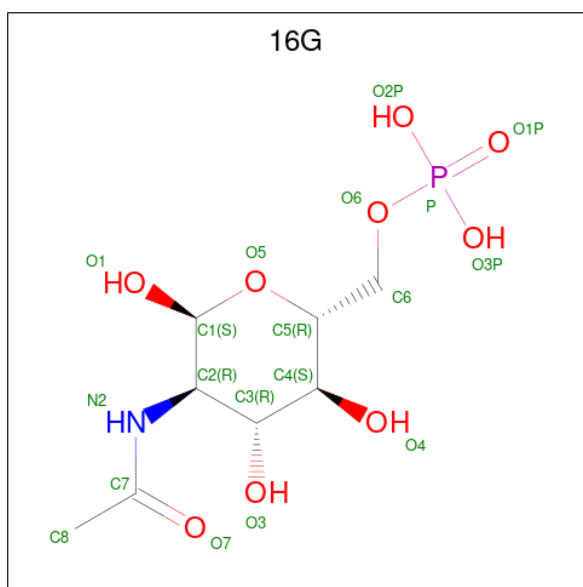
- Molecule 1 is a protein called GLUCOSAMINE-PHOSPHATE N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	Total 1257	C 804	N 206	O 237	S 10	0	4	0
1	B	154	Total 1240	C 792	N 204	O 234	S 10	0	4	0
1	C	155	Total 1236	C 789	N 202	O 234	S 11	0	1	0
1	D	161	Total 1283	C 814	N 210	O 248	S 11	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

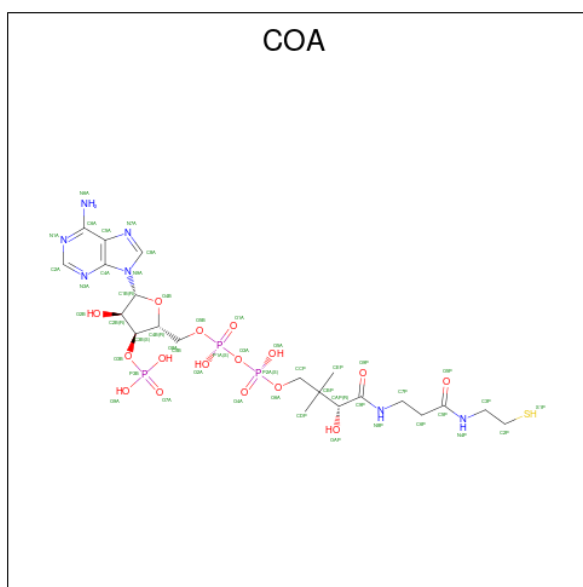
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP P43577
A	0	SER	-	cloning artifact	UNP P43577
A	39	CYS	SER	engineered mutation	UNP P43577
B	-1	GLY	-	cloning artifact	UNP P43577
B	0	SER	-	cloning artifact	UNP P43577
B	39	CYS	SER	engineered mutation	UNP P43577
C	-1	GLY	-	cloning artifact	UNP P43577
C	0	SER	-	cloning artifact	UNP P43577
C	39	CYS	SER	engineered mutation	UNP P43577
D	-1	GLY	-	cloning artifact	UNP P43577
D	0	SER	-	cloning artifact	UNP P43577
D	39	CYS	SER	engineered mutation	UNP P43577

- Molecule 2 is 2-acetamido-2-deoxy-6-O-phosphono-alpha-D-glucopyranose (three-letter code: 16G) (formula: C₈H₁₆NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
2	B	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
2	D	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



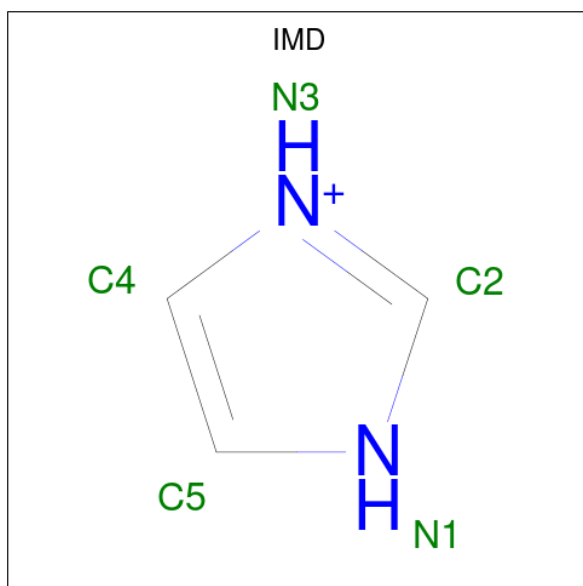
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	45	19	7	16	3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	5	3	2	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	170	Total	O	0	0
			170	170		
5	C	117	Total	O	0	0
			117	117		
5	D	103	Total	O	0	0
			103	103		

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.

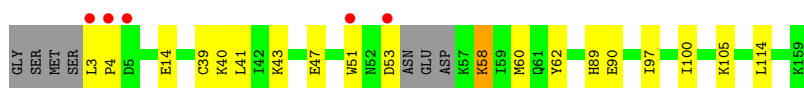
- Molecule 1: GLUCOSAMINE-PHOSPHATE N-ACETYLTRANSFERASE

Chain A: 




- Molecule 1: GLUCOSAMINE-PHOSPHATE N-ACETYLTRANSFERASE

Chain B: 




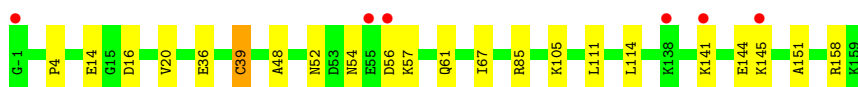
- Molecule 1: GLUCOSAMINE-PHOSPHATE N-ACETYLTRANSFERASE

Chain C: 



- Molecule 1: GLUCOSAMINE-PHOSPHATE N-ACETYLTRANSFERASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.01Å 51.62Å 91.66Å 90.00° 107.98° 90.00°	Depositor
Resolution (Å)	24.12 – 1.80 35.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.12-1.80) 97.0 (35.98-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.80	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.183 , 0.223 0.179 , 0.219	Depositor DCC
R_{free} test set	1123 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5713	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, 16G, COA

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	0/1298	0.88	1/1744 (0.1%)
1	B	0.82	0/1282	0.84	0/1724
1	C	0.80	1/1260 (0.1%)	0.84	0/1695
1	D	0.73	0/1313	0.83	2/1767 (0.1%)
All	All	0.80	1/5153 (0.0%)	0.85	3/6930 (0.0%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	GLU	CB-CG	5.63	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	158	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	85	ARG	NE-CZ-NH2	-5.43	117.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	62	TYR	Sidechain

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	1257	0	1279	19	0
1	B	1240	0	1249	20	0
1	C	1236	0	1253	32	0
1	D	1283	0	1291	15	0
2	A	19	0	14	0	0
2	B	19	0	14	0	0
2	D	19	0	14	1	0
3	A	48	0	31	0	0
3	B	45	0	26	0	0
4	A	5	0	5	0	0
5	A	152	0	0	3	1
5	B	170	0	0	6	0
5	C	117	0	0	5	1
5	D	103	0	0	3	0
All	All	5713	0	5176	80	1

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 8.

All (80) 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:A:61:GLN:NE2	1:D:61:GLN:OE1	1.95	0.98
1:B:3:LEU:HB3	1:B:4:PRO:HD2	1.52	0.90
1:C:19:GLN:HE22	1:C:74:THR:HA	1.38	0.88
1:A:66[B]:VAL:HG13	1:A:75:VAL:HG13	1.56	0.88
1:C:19:GLN:HE22	1:C:74:THR:CA	1.92	0.83
1:B:3:LEU:HB3	1:B:4:PRO:CD	2.09	0.82
1:D:105:LYS:HG2	5:D:940:HOH:O	1.84	0.77
1:C:28:THR:HG22	1:C:29:THR:H	1.49	0.76
1:A:66[B]:VAL:HG11	1:A:75:VAL:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:HE2	5:C:262:HOH:O	1.87	0.74
1:B:39[B]:CYS:SG	5:B:1037:HOH:O	2.46	0.73
1:D:61:GLN:NE2	5:D:963:HOH:O	2.22	0.72
1:C:14:GLU:OE1	1:C:39[A]:CYS:SG	2.46	0.72
1:A:66[B]:VAL:CG1	1:A:75:VAL:HG13	2.20	0.70
1:A:89:HIS:HE1	2:D:908:16G:O3P	1.74	0.70
1:A:14:GLU:OE2	1:A:39:CYS:HB2	1.92	0.70
1:C:19:GLN:NE2	1:C:75:VAL:H	1.92	0.67
1:C:19:GLN:NE2	1:C:74:THR:HA	2.11	0.65
1:A:43[B]:LYS:HG2	5:A:1052:HOH:O	1.98	0.62
1:A:9:ILE:HD13	1:A:118[A]:GLN:HG2	1.81	0.62
1:B:58:LYS:HE2	1:B:60[B]:MET:CE	2.31	0.60
1:D:54:ASN:ND2	1:D:57:LYS:HD2	2.17	0.60
1:B:51:TRP:CZ2	1:B:53:ASP:HA	2.37	0.59
1:B:105:LYS:NZ	5:B:979:HOH:O	2.35	0.59
1:C:72:THR:OG1	1:C:74:THR:HB	2.03	0.58
1:C:43:LYS:O	1:C:47:GLU:HG3	2.04	0.58
1:B:89[A]:HIS:CE1	1:C:28:THR:HG21	2.40	0.57
1:A:43[B]:LYS:HE3	5:A:1052:HOH:O	2.04	0.57
1:C:28:THR:HG22	1:C:29:THR:N	2.17	0.57
1:B:14:GLU:HG3	5:B:1044:HOH:O	2.05	0.56
1:D:141:LYS:O	1:D:145:LYS:HG2	2.07	0.55
1:D:141:LYS:HD3	1:D:144:GLU:OE2	2.06	0.55
1:B:53:ASP:HB2	5:B:1038:HOH:O	2.07	0.53
1:C:86:LYS:O	1:C:91:LEU:HA	2.10	0.52
1:B:14:GLU:OE2	1:B:39[B]:CYS:SG	2.48	0.51
1:A:9:ILE:HG12	1:A:65[A]:MET:CE	2.41	0.51
1:C:50:VAL:HG13	1:C:51:TRP:N	2.25	0.51
1:C:34:THR:HB	1:C:36:GLU:OE1	2.11	0.51
1:C:140:VAL:O	1:C:144:GLU:HG3	2.11	0.51
1:D:48:ALA:HB1	1:D:61:GLN:NE2	2.27	0.49
1:B:62:TYR:OH	5:B:1073:HOH:O	2.20	0.49
1:A:26:VAL:O	1:A:26:VAL:HG12	2.13	0.49
1:C:50:VAL:CG1	1:C:51:TRP:N	2.76	0.48
1:C:83:ILE:HG22	1:C:93:LEU:HD22	1.96	0.48
1:D:36:GLU:HG3	5:D:949:HOH:O	2.12	0.48
1:B:3:LEU:C	1:B:4:PRO:O	2.50	0.47
1:A:9:ILE:HG12	1:A:65[A]:MET:HE3	1.95	0.47
1:D:67:ILE:HG21	1:D:111:LEU:HD11	1.97	0.47
1:C:150:ASN:C	1:C:150:ASN:HD22	2.17	0.46
1:D:14:GLU:OE2	1:D:39[A]:CYS:SG	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:OE2	1:A:39:CYS:CB	2.63	0.46
1:C:85:ARG:HB2	5:C:253:HOH:O	2.16	0.46
1:C:25:LYS:NZ	5:C:261:HOH:O	2.49	0.46
1:C:58:LYS:HE2	1:C:60:MET:SD	2.56	0.45
1:B:90:GLU:HG3	1:C:30:VAL:O	2.16	0.45
1:C:36:GLU:H	1:C:36:GLU:CD	2.20	0.45
1:C:7:PHE:CE1	1:C:111:LEU:HD21	2.52	0.45
1:A:86:LYS:O	1:A:91:LEU:HA	2.18	0.44
1:D:16:ASP:HB3	1:D:20:VAL:HG23	2.00	0.43
1:D:54:ASN:HD21	1:D:57:LYS:HD2	1.84	0.43
1:C:19:GLN:HE22	1:C:75:VAL:N	2.17	0.43
1:D:4:PRO:HD2	1:D:114:LEU:HD21	2.01	0.43
1:C:19:GLN:NE2	1:C:75:VAL:N	2.63	0.42
1:B:41:LEU:HD13	1:C:85:ARG:HG2	2.02	0.42
1:A:1:MET:CE	5:A:1062:HOH:O	2.67	0.42
1:B:4:PRO:HD3	1:B:114:LEU:HD13	2.01	0.42
1:B:40:LYS:NZ	5:B:975:HOH:O	2.51	0.42
1:C:129:TYR:OH	5:C:262:HOH:O	2.20	0.42
1:A:105:LYS:HA	1:A:105:LYS:NZ	2.34	0.42
1:A:150:ASN:HD22	1:A:150:ASN:C	2.22	0.42
1:D:141:LYS:HD3	1:D:141:LYS:HA	1.65	0.42
1:A:66[B]:VAL:HG11	1:A:75:VAL:CG2	2.43	0.41
1:B:97:ILE:HG23	1:B:100:ILE:HD11	2.01	0.41
1:B:89[A]:HIS:NE2	1:C:28:THR:HG21	2.36	0.41
1:C:16:ASP:HB3	1:C:20:VAL:HG23	2.03	0.41
1:C:85:ARG:CB	5:C:253:HOH:O	2.69	0.41
1:B:43:LYS:O	1:B:47:GLU:HG3	2.21	0.40
1:C:150:ASN:HD22	1:C:151:ALA:N	2.19	0.40
1:A:156:GLN:HG2	1:D:151:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1013:HOH:O	5:C:205:HOH:O[2_656]	2.18	0.02

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	156/161 (97%)	154 (99%)	2 (1%)	0	100	100
1	B	154/161 (96%)	152 (99%)	2 (1%)	0	100	100
1	C	152/161 (94%)	150 (99%)	2 (1%)	0	100	100
1	D	161/161 (100%)	159 (99%)	2 (1%)	0	100	100
All	All	623/644 (97%)	615 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	142/142 (100%)	140 (99%)	2 (1%)	67	59
1	B	140/142 (99%)	139 (99%)	1 (1%)	84	81
1	C	138/142 (97%)	135 (98%)	3 (2%)	52	39
1	D	144/142 (101%)	140 (97%)	4 (3%)	43	30
All	All	564/568 (99%)	554 (98%)	10 (2%)	62	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	150	ASN

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Mol	Chain	Res	Type
1	B	58	LYS
1	C	18	GLU
1	C	50	VAL
1	C	150	ASN
1	D	39[A]	CYS
1	D	39[B]	CYS
1	D	52	ASN
1	D	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	63	ASN
1	A	89	HIS
1	A	107	GLN
1	A	150	ASN
1	B	61	GLN
1	B	107	GLN
1	B	109	GLN
1	C	19	GLN
1	C	61	GLN
1	C	63	ASN
1	C	107	GLN
1	C	150	ASN
1	D	52	ASN
1	D	63	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 monosaccharides in this entry.

5.6 Ligand geometry

6 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
3	COA	B	901	-	39,47,50	1.17	3 (7%)	49,72,75	1.03	3 (6%)
3	COA	A	900	-	41,50,50	1.39	5 (12%)	52,75,75	2.40	8 (15%)
2	16G	A	905	-	19,19,19	1.44	3 (15%)	28,28,28	1.44	3 (10%)
4	IMD	A	910	-	3,5,5	0.79	0	4,5,5	1.71	1 (25%)
2	16G	B	906	-	19,19,19	1.59	3 (15%)	28,28,28	1.21	3 (10%)
2	16G	D	908	-	19,19,19	1.82	4 (21%)	28,28,28	1.56	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	901	-	-	6/40/60/64	0/3/3/3
3	COA	A	900	-	-	7/44/64/64	0/3/3/3
2	16G	A	905	-	-	1/10/30/30	0/1/1/1
4	IMD	A	910	-	-	-	0/1/1/1
2	16G	B	906	-	-	1/10/30/30	0/1/1/1
2	16G	D	908	-	-	1/10/30/30	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	908	16G	C4-C5	-5.22	1.42	1.53
2	B	906	16G	C4-C5	-4.25	1.44	1.53
3	A	900	COA	C2A-N3A	4.12	1.38	1.32
2	A	905	16G	C4-C5	-3.85	1.44	1.53
3	A	900	COA	C2B-C1B	2.86	1.58	1.53
3	A	900	COA	P3B-O9A	-2.82	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	COA	C8A-N7A	-2.78	1.29	1.34
3	A	900	COA	O4B-C1B	2.47	1.44	1.41
3	B	901	COA	C4A-N3A	2.45	1.39	1.35
2	D	908	16G	C2-N2	-2.36	1.42	1.45
2	B	906	16G	O7-C7	-2.31	1.18	1.23
3	A	900	COA	C4A-N3A	2.11	1.38	1.35
2	A	905	16G	P-O2P	-2.10	1.46	1.54
3	B	901	COA	P3B-O3B	2.09	1.63	1.59
2	D	908	16G	P-O2P	-2.04	1.47	1.54
2	D	908	16G	O1-C1	2.03	1.46	1.39
2	A	905	16G	C8-C7	-2.02	1.46	1.50
2	B	906	16G	C8-C7	-2.01	1.46	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	COA	C3P-N4P-C5P	14.16	149.13	122.84
3	A	900	COA	C2P-C3P-N4P	-4.87	101.18	112.31
2	D	908	16G	C1-O5-C5	3.85	120.93	113.66
3	A	900	COA	O4B-C1B-C2B	-3.59	101.69	106.93
2	A	905	16G	C1-O5-C5	3.36	120.01	113.66
3	A	900	COA	CDP-CBP-CAP	3.28	114.50	108.82
2	A	905	16G	C2-N2-C7	-3.26	115.24	123.18
3	B	901	COA	O4B-C1B-C2B	-3.21	102.24	106.93
2	A	905	16G	C6-C5-C4	3.20	118.77	112.09
2	B	906	16G	C1-O5-C5	2.96	119.24	113.66
2	D	908	16G	O2P-P-O6	-2.86	99.13	106.73
2	D	908	16G	C2-N2-C7	-2.72	116.57	123.18
3	B	901	COA	O9A-P3B-O8A	2.60	117.56	107.64
2	D	908	16G	O2P-P-O1P	2.52	120.55	110.68
3	A	900	COA	O9A-P3B-O8A	2.47	117.09	107.64
3	A	900	COA	C7P-C6P-C5P	-2.47	108.24	112.36
4	A	910	IMD	C4-N3-C2	-2.44	98.51	105.91
2	B	906	16G	C6-C5-C4	2.36	117.03	112.09
3	B	901	COA	C4A-C5A-N7A	2.33	111.83	109.40
2	D	908	16G	O3P-P-O6	2.23	112.68	106.73
2	D	908	16G	C6-C5-C4	2.23	116.75	112.09
3	A	900	COA	C5A-C6A-N6A	2.21	123.70	120.35
2	D	908	16G	O5-C1-C2	-2.13	107.38	109.52
3	A	900	COA	O6A-CCP-CBP	-2.13	107.13	110.55
2	B	906	16G	C4-C3-C2	-2.01	107.40	110.34

There are no chirality outliers.

All (16) torsion outliers are listed below:

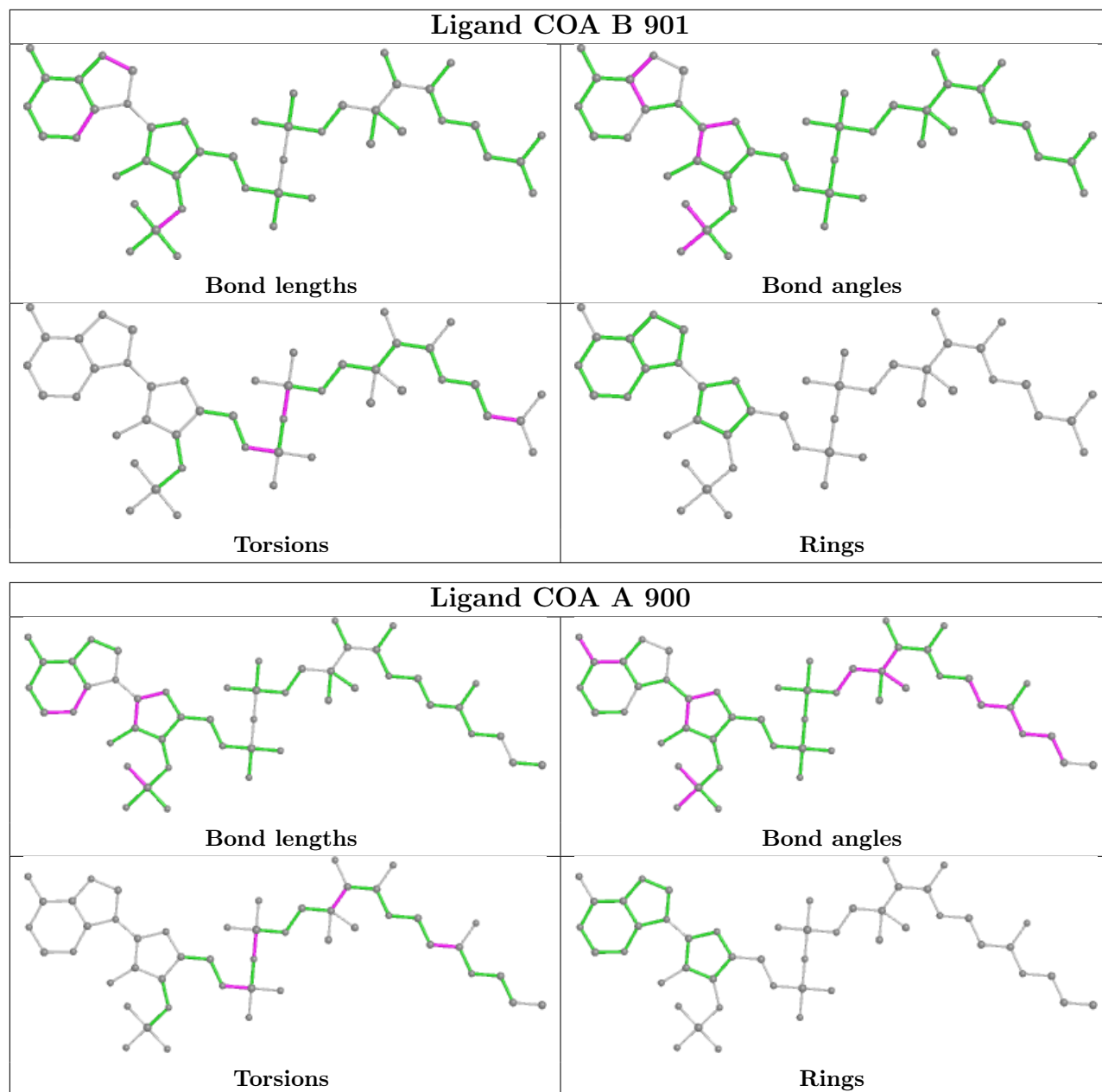
Mol	Chain	Res	Type	Atoms
2	A	905	16G	C4-C5-C6-O6
2	B	906	16G	C4-C5-C6-O6
2	D	908	16G	C4-C5-C6-O6
3	A	900	COA	C5B-O5B-P1A-O1A
3	A	900	COA	C5B-O5B-P1A-O2A
3	B	901	COA	C5B-O5B-P1A-O1A
3	B	901	COA	C5B-O5B-P1A-O2A
3	A	900	COA	O5P-C5P-C6P-C7P
3	B	901	COA	P1A-O3A-P2A-O5A
3	A	900	COA	P1A-O3A-P2A-O5A
3	A	900	COA	N4P-C5P-C6P-C7P
3	B	901	COA	O5P-C5P-C6P-C7P
3	B	901	COA	N4P-C5P-C6P-C7P
3	A	900	COA	C5B-O5B-P1A-O3A
3	A	900	COA	OAP-CAP-CBP-CEP
3	B	901	COA	C5B-O5B-P1A-O3A

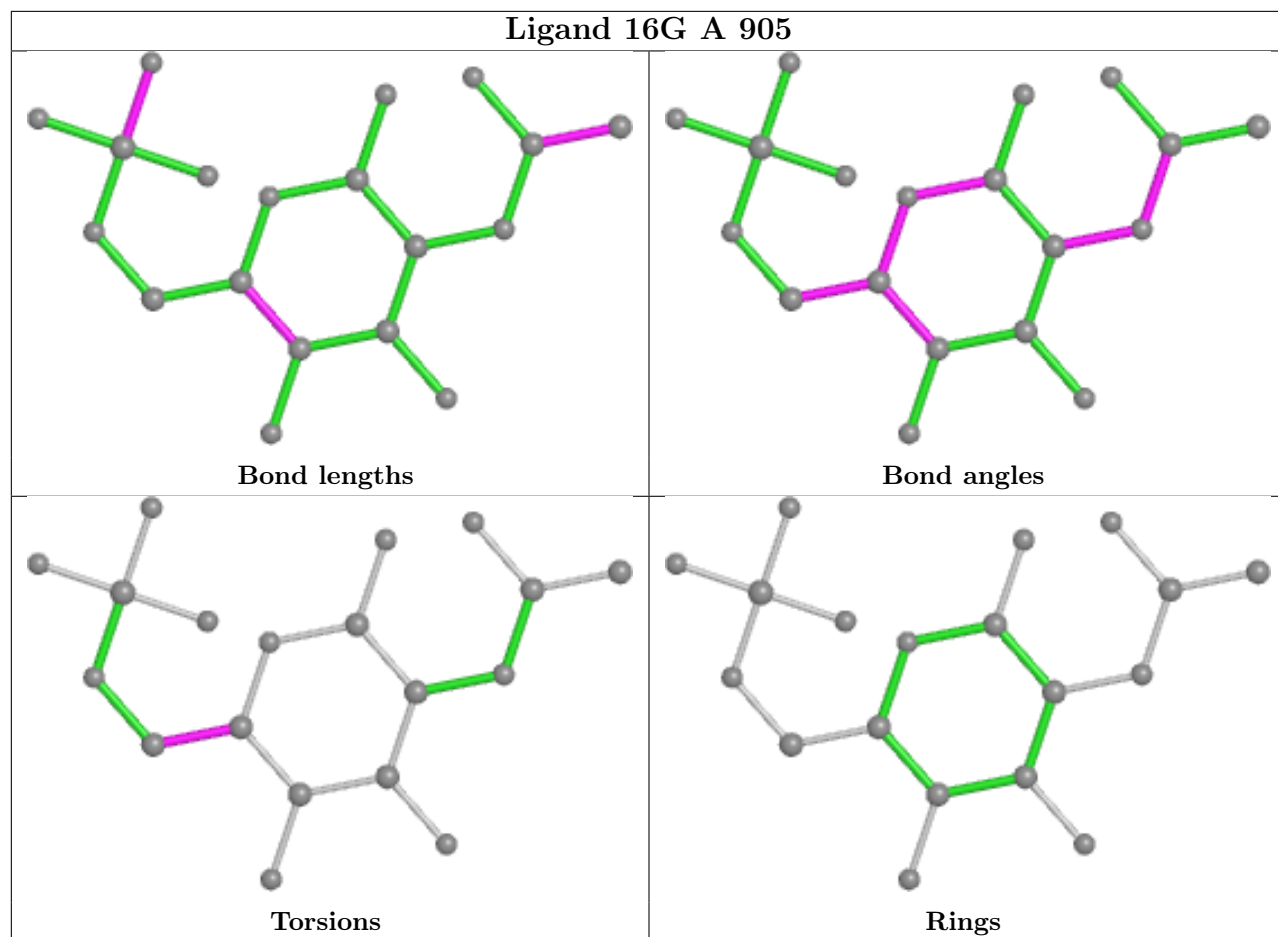
There are no ring outliers.

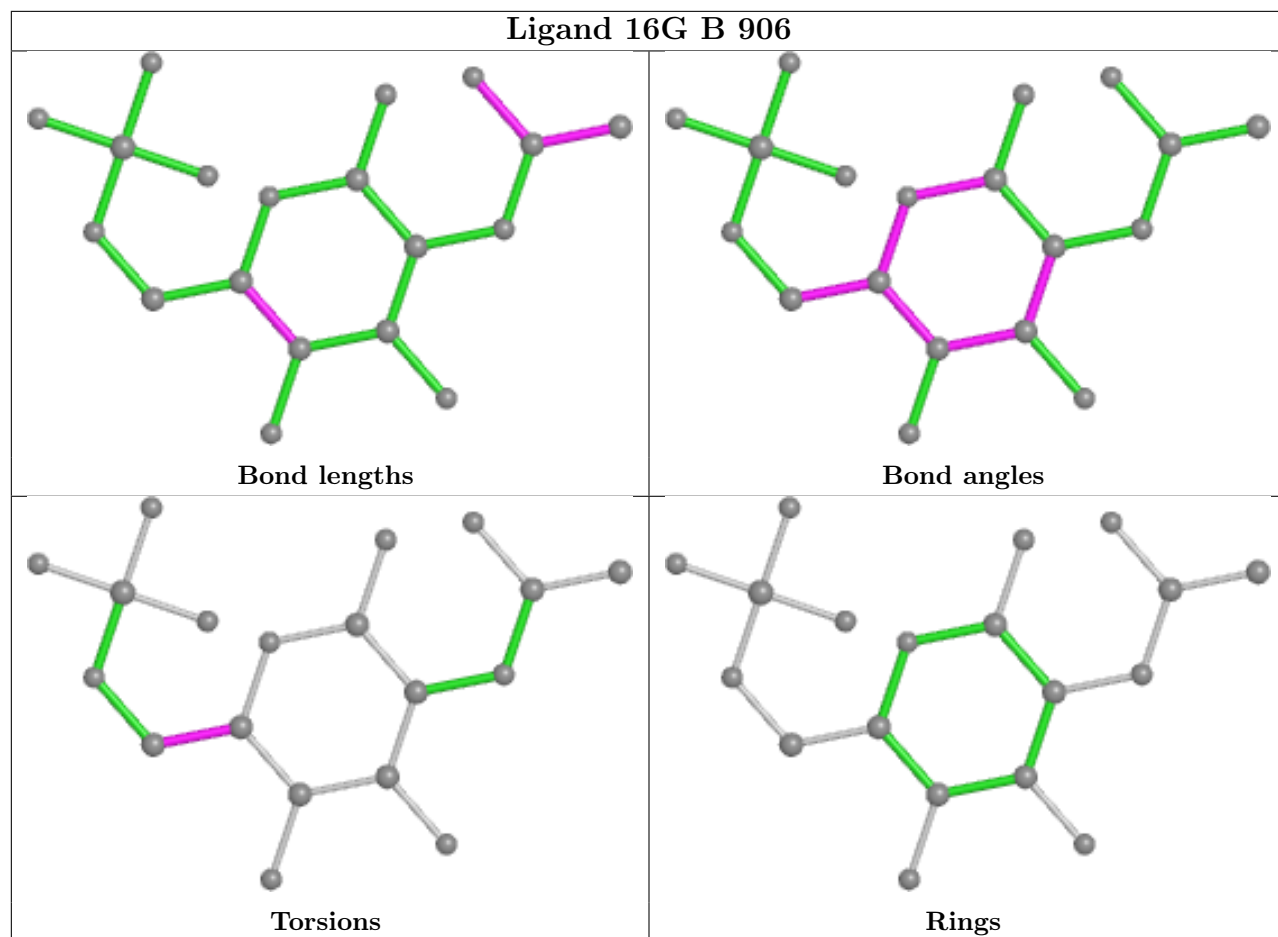
1 monomer is involved in 1 short contact:

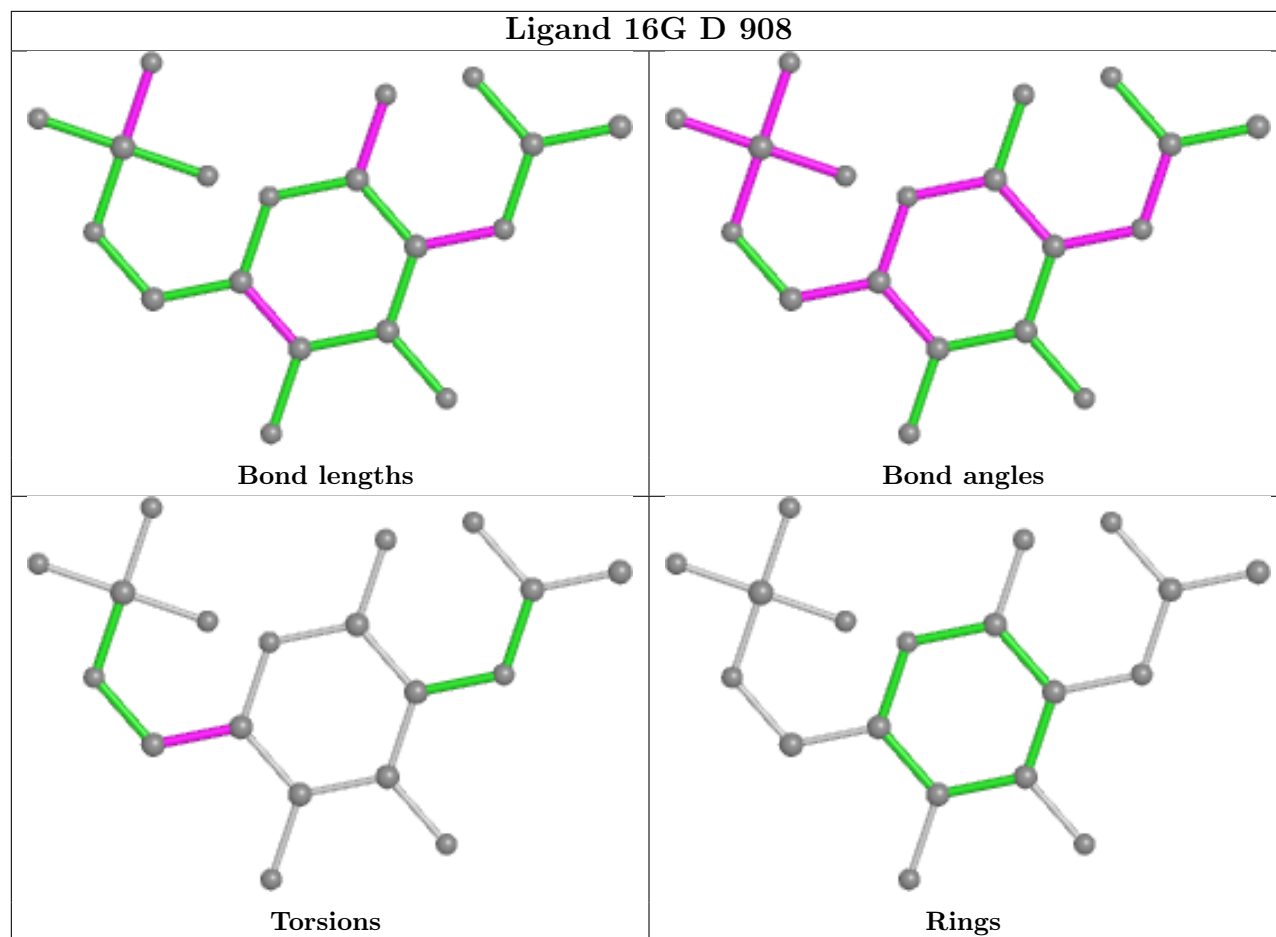
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	908	16G	1	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/161 (96%)	-0.21	3 (1%) 66 63	12, 20, 36, 60	0
1	B	154/161 (95%)	-0.36	5 (3%) 47 41	13, 20, 41, 59	0
1	C	155/161 (96%)	-0.25	7 (4%) 33 27	15, 26, 46, 63	0
1	D	161/161 (100%)	-0.15	6 (3%) 41 36	15, 26, 45, 65	0
All	All	626/644 (97%)	-0.24	21 (3%) 45 39	12, 23, 45, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	TRP	6.6
1	B	53	ASP	5.4
1	D	56	ASP	4.4
1	C	58	LYS	3.9
1	B	5	ASP	3.7
1	D	-1	GLY	3.5
1	C	50	VAL	3.4
1	A	53	ASP	3.2
1	C	32	THR	3.2
1	A	1	MET	3.1
1	D	145	LYS	2.9
1	C	0	SER	2.9
1	A	57	LYS	2.9
1	D	138	LYS	2.7
1	D	141	LYS	2.7
1	C	14	GLU	2.6
1	B	4	PRO	2.6
1	B	3	LEU	2.2
1	D	55	GLU	2.2
1	B	51	TRP	2.1
1	C	35	PRO	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

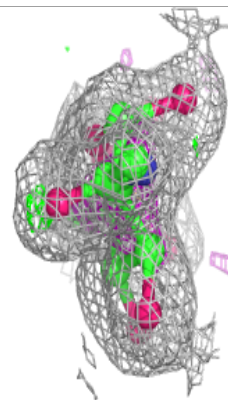
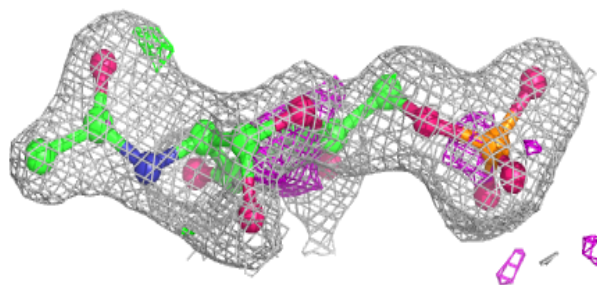
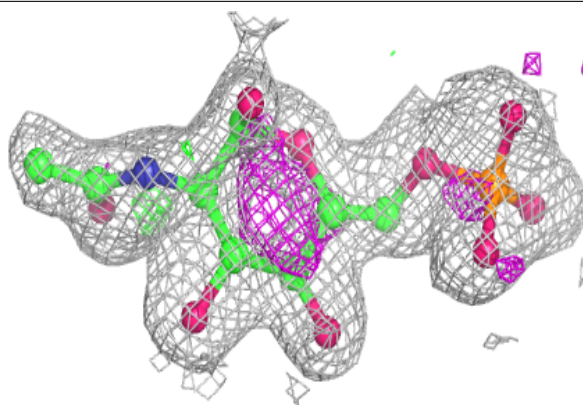
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	16G	D	908	19/19	0.88	0.13	25,34,38,40	0
2	16G	B	906	19/19	0.91	0.14	27,32,35,35	0
4	IMD	A	910	5/5	0.94	0.12	19,20,20,21	0
3	COA	A	900	48/48	0.97	0.10	14,19,38,52	0
2	16G	A	905	19/19	0.97	0.07	17,22,27,27	0
3	COA	B	901	45/48	0.98	0.08	14,18,32,35	0

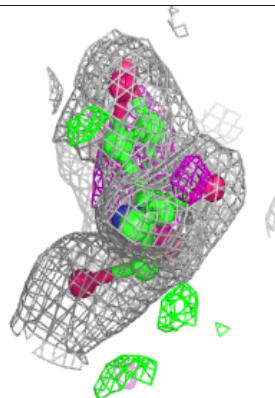
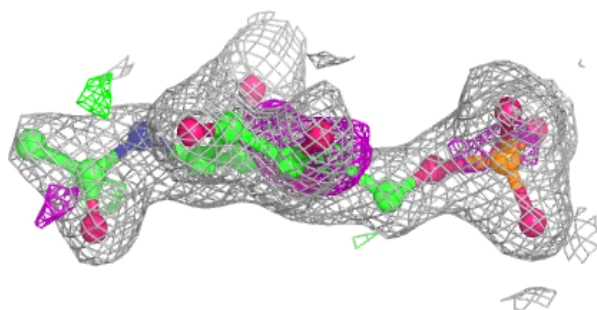
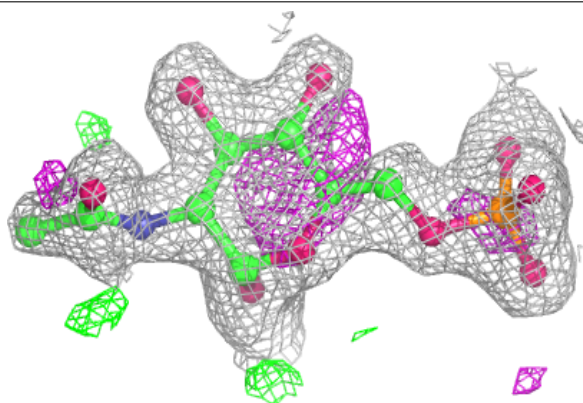
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 16G D 908:

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

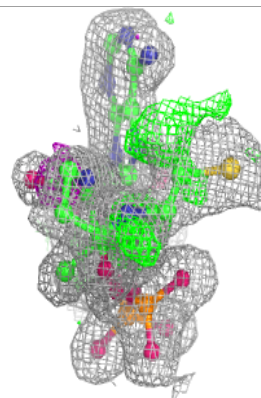
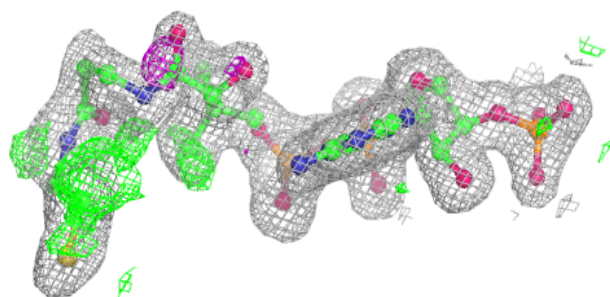
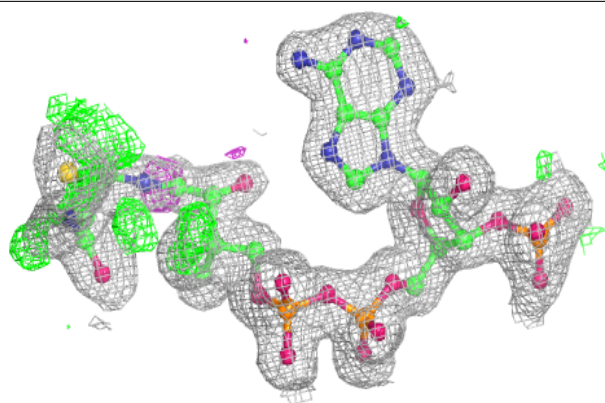
**Electron density around 16G B 906:**

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

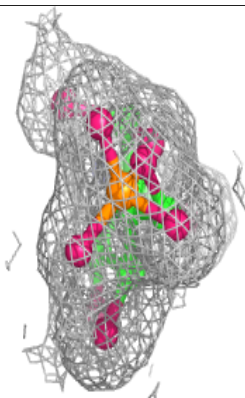
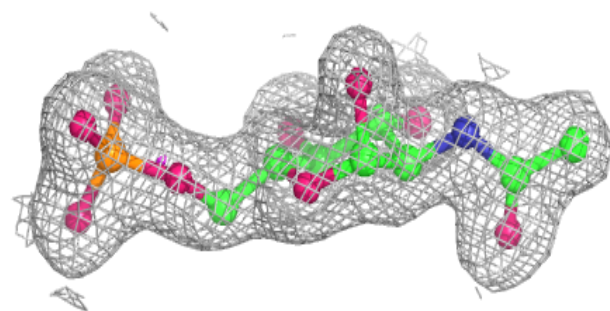
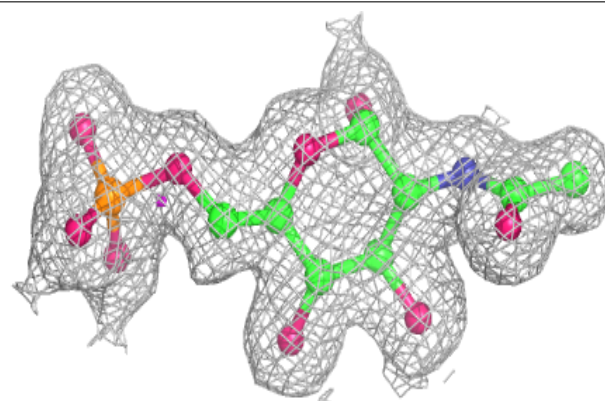


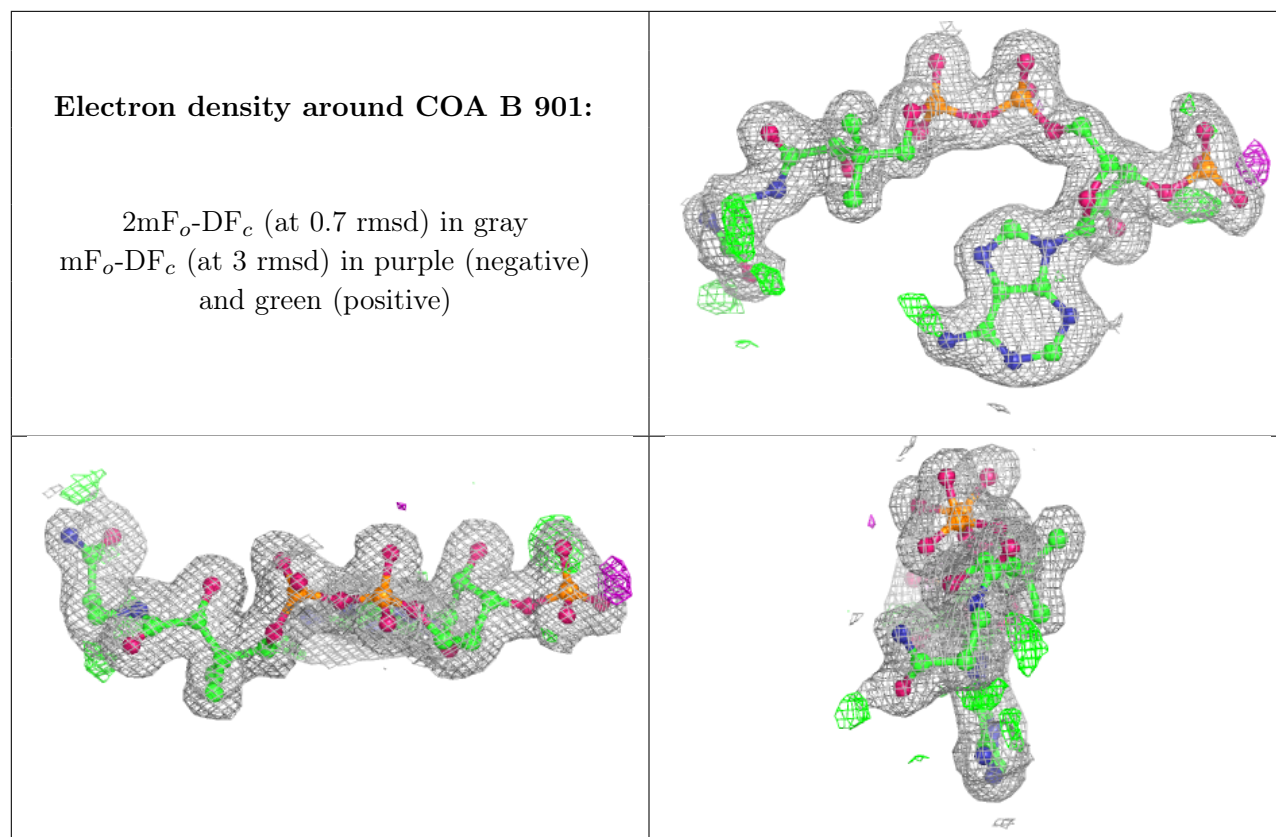
Electron density around COA A 900:

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

**Electron density around 16G A 905:**

$2mF_o-DF_c$ (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.