



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 10:31 AM EDT

PDB ID : 4X0O  
Title : Beta-ketoacyl-(acyl carrier protein) synthase III-2 (FabH2) from *Vibrio cholerae* soaked with Acetyl-CoA  
Authors : Hou, J.; Chruszcz, M.; Zheng, H.; Cooper, D.R.; Chordia, M.D.; Zimmerman, M.D.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2014-11-21  
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 : 2.27  
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) : 2.27

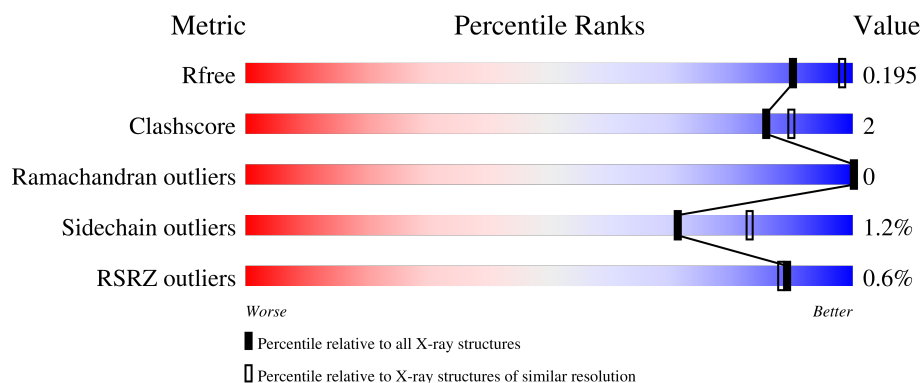
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

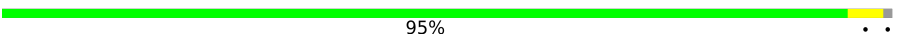
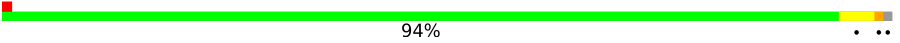
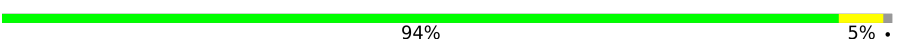
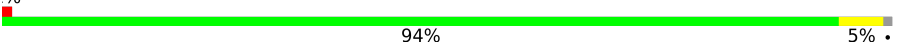
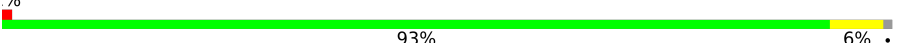
The reported resolution of this entry is 2.20 Å.

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 of 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	362	 95% . .
1	B	362	 94% . .
1	C	362	 94% 5% .
1	E	362	 94% 5% .
1	F	362	 93% 6% .

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Mol	Chain	Length	Quality of chain
1	G	362	<div><div>%</div><div><div></div><div>94%</div><div>5% •</div></div></div>
1	H	362	<div><div>%</div><div><div></div><div>94%</div><div>5% •</div></div></div>
2	D	362	<div><div>%</div><div><div></div><div>94%</div><div>• •</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22469 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.

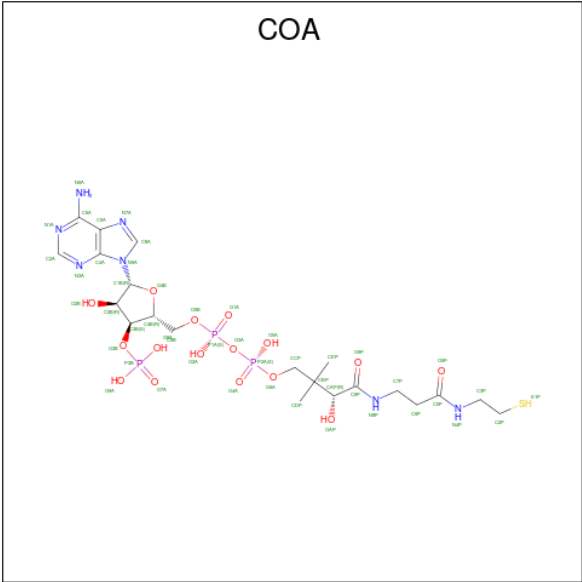
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2671	1682	468	508	13			
1	B	359	Total	C	N	O	S	0	0	0
			2669	1682	468	506	13			
1	C	359	Total	C	N	O	S	0	2	0
			2694	1694	474	513	13			
1	E	360	Total	C	N	O	S	0	1	0
			2679	1685	468	513	13			
1	F	359	Total	C	N	O	S	0	1	0
			2689	1691	472	513	13			
1	G	359	Total	C	N	O	S	0	1	0
			2701	1701	475	512	13			
1	H	358	Total	C	N	O	S	0	3	0
			2709	1704	480	512	13			

- Molecule 2 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	359	Total	C	N	O	S	0	3	0
			2712	1706	479	514	13			

- Molecule 3 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	
3	A	1	Total	C	N	O	P	0	0	
			27	10	5	10	2			
3	B	1	Total	C	N	O	P	0	0	
			21	9	5	6	1			
3	D	1	Total	C	N	O	P	0	0	
			21	9	5	6	1			
3	E	1	Total	C	N	O	P	0	0	
			27	10	5	10	2			
3	F	1	Total	C	N	O	P	0	0	
			31	10	5	13	3			
3	G	1	Total	C	N	O	P	0	0	
			31	10	5	13	3			
3	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

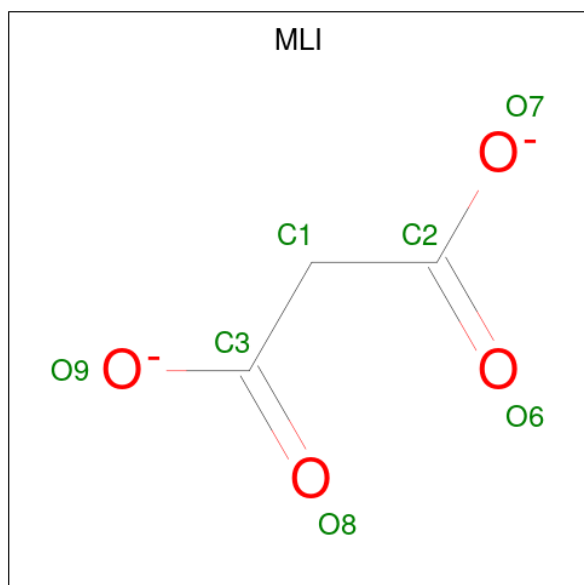
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Na	0	0
			1	1		
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	1
			81	81		
6	B	86	Total	O	0	1
			87	87		
6	C	101	Total	O	0	0
			101	101		
6	D	106	Total	O	0	0
			106	106		
6	E	75	Total	O	0	1
			76	76		
6	F	100	Total	O	0	0
			100	100		

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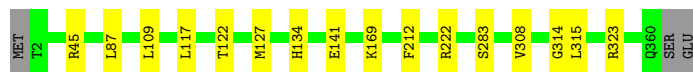
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	90	Total	O	0	0
			90	90		
6	H	84	Total	O	0	0
			84	84		

### 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: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2

Chain A:  95%



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2

Chain B:  94%



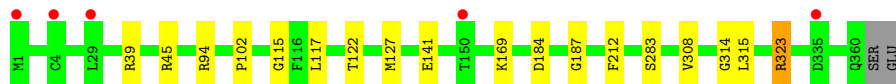
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2

Chain C:  94%



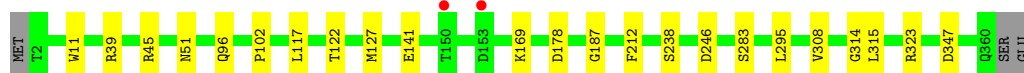
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2

Chain E:  94%



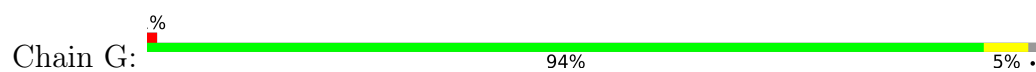
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2

Chain F:  93%



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2





- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2



- Molecule 2: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.76Å 86.98Å 157.34Å 90.06° 89.96° 90.08°	Depositor
Resolution (Å)	26.70 – 2.20 26.68 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.9 (26.70-2.20) 95.9 (26.68-2.19)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.173 , 0.201 0.177 , 0.195	Depositor DCC
$R_{free}$ test set	8101 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.367 for h,-k,-l 0.367 for -h,k,-l 0.450 for -h,-k,l	Xtriage
Reported twinning fraction	0.394 for H, K, L 0.233 for -h,-k,l 0.224 for h,-k,-l 0.148 for -H, K, -L	Depositor
Outliers	0 of 161071 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2078e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, MLI, SCY, 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	0.46	0/2716	0.64	1/3700 (0.0%)
1	B	0.52	0/2711	0.66	1/3692 (0.0%)
1	C	0.46	0/2737	0.63	1/3727 (0.0%)
1	E	0.45	0/2721	0.65	2/3707 (0.1%)
1	F	0.51	0/2731	0.64	0/3717
1	G	0.45	0/2747	0.67	2/3736 (0.1%)
1	H	0.48	0/2751	0.64	0/3741
2	D	0.53	0/2774	0.70	4/3775 (0.1%)
All	All	0.48	0/21888	0.65	11/29795 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	39	ARG	NE-CZ-NH1	11.49	126.05	120.30
2	D	323	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	E	323	ARG	NE-CZ-NH2	8.37	124.48	120.30
2	D	117	LEU	CB-CG-CD2	7.41	123.60	111.00
1	G	39	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	C	323	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	323	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	39	ARG	NE-CZ-NH2	5.99	123.29	120.30
2	D	323	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	D	113	CYS	N-CA-CB	5.49	120.48	110.60
1	E	323	ARG	NE-CZ-NH1	-5.42	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2671	0	2591	9	0
1	B	2669	0	2593	12	0
1	C	2694	0	2602	8	0
1	E	2679	0	2592	12	0
1	F	2689	0	2617	19	0
1	G	2701	0	2645	14	0
1	H	2709	0	2644	14	0
2	D	2712	0	2653	9	0
3	A	27	0	11	0	0
3	B	21	0	8	0	0
3	D	21	0	8	0	0
3	E	27	0	11	1	0
3	F	31	0	11	0	0
3	G	31	0	11	0	0
3	H	48	0	32	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	G	7	0	2	0	0
6	A	81	0	0	2	0
6	B	87	0	0	4	0
6	C	101	0	0	2	0
6	D	106	0	0	3	0
6	E	76	0	0	4	0
6	F	100	0	0	6	0
6	G	90	0	0	4	0
6	H	84	0	0	4	0
All	All	22469	0	21031	92	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 2.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:GLN:OE1	2:D:237:ARG:NH2	2.06	0.88
1:H:180:GLN:OE1	1:H:237:ARG:NH2	2.07	0.86
1:G:180:GLN:OE1	1:G:237:ARG:NH2	2.07	0.85
1:A:87:LEU:O	6:A:501:HOH:O	1.95	0.83
1:H:311[A]:PHE:CE1	1:H:315:LEU:HD12	2.17	0.78
1:B:153:ASP:CB	6:B:581:HOH:O	2.34	0.75
1:H:184[A]:ASP:OD1	6:H:502:HOH:O	2.09	0.71
1:F:323:ARG:NH2	6:F:503:HOH:O	2.25	0.69
1:F:178[B]:ASP:OD2	1:F:238:SER:HB3	1.94	0.68
1:E:115:GLY:HA3	6:E:552:HOH:O	1.95	0.65
1:F:96:GLN:NE2	6:F:504:HOH:O	2.30	0.65
1:G:2:THR:N	6:G:503:HOH:O	2.30	0.64
1:F:102:PRO:O	6:F:501:HOH:O	2.15	0.64
1:G:131:HIS:CD2	1:G:131:HIS:O	2.51	0.62
2:D:323:ARG:HG2	6:D:592:HOH:O	2.00	0.62
1:E:187:GLY:O	1:E:315:LEU:CD2	2.49	0.61
1:B:187:GLY:O	1:B:315:LEU:CD2	2.49	0.61
1:F:187:GLY:O	1:F:315:LEU:CD2	2.49	0.61
1:H:187:GLY:O	1:H:315:LEU:CD2	2.49	0.61
1:G:131:HIS:O	1:G:131:HIS:HD2	1.86	0.58
1:C:35:TRP:CZ2	1:C:39:ARG:HD2	2.38	0.58
1:E:323:ARG:NH2	6:E:502:HOH:O	2.36	0.58
1:C:141:GLU:HG3	1:C:283:SER:HB3	1.86	0.57
1:B:141:GLU:HG3	1:B:283:SER:HB3	1.87	0.57
2:D:141:GLU:HG3	2:D:283:SER:HB3	1.87	0.57
1:F:51:ASN:HA	6:F:518:HOH:O	2.03	0.57
1:E:141:GLU:HG3	1:E:283:SER:HB3	1.88	0.55
1:H:141:GLU:HG3	1:H:283:SER:HB3	1.89	0.55
1:A:141:GLU:HG3	1:A:283:SER:HB3	1.89	0.55
1:F:141:GLU:HG3	1:F:283:SER:HB3	1.89	0.54
1:G:141:GLU:HG3	1:G:283:SER:HB3	1.90	0.54
1:H:311[A]:PHE:CZ	1:H:315:LEU:HD12	2.42	0.54
1:H:323:ARG:NH2	6:H:510:HOH:O	2.42	0.53
1:A:134:HIS:HD2	6:A:535:HOH:O	1.90	0.53
1:B:178:ASP:HB2	6:B:521:HOH:O	2.08	0.52
1:C:148:ASP:N	6:C:508:HOH:O	2.36	0.52
1:F:246:ASP:OD1	6:F:502:HOH:O	2.19	0.51
1:B:323:ARG:NH2	6:B:504:HOH:O	2.43	0.50
1:F:347:ASP:HB3	6:F:566:HOH:O	2.11	0.49
1:C:314:GLY:N	1:C:315:LEU:HA	2.28	0.49
2:D:314:GLY:N	2:D:315:LEU:HA	2.28	0.49
1:G:222:ARG:HD3	1:G:315:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:GLY:O	1:F:315:LEU:HD23	2.13	0.48
1:B:187:GLY:O	1:B:315:LEU:HD23	2.13	0.48
1:H:187:GLY:O	1:H:315:LEU:HD23	2.13	0.48
1:E:187:GLY:O	1:E:315:LEU:HD23	2.13	0.48
1:B:212:PHE:HB3	6:B:522:HOH:O	2.14	0.48
1:E:122:THR:HG23	1:G:122:THR:HG23	1.96	0.47
1:C:194:PRO:HD2	6:C:529:HOH:O	2.14	0.47
1:H:326:GLU:HG2	6:H:537:HOH:O	2.14	0.47
1:F:117:LEU:HD11	1:F:308:VAL:HG11	1.97	0.47
1:H:130:SER:OG	6:H:501:HOH:O	2.06	0.47
1:A:222:ARG:HD3	1:A:315:LEU:CD1	2.45	0.46
3:H:401:COA:O6A	3:H:401:COA:OAP	2.33	0.46
1:G:314:GLY:N	1:G:315:LEU:HA	2.31	0.46
1:A:314:GLY:N	1:A:315:LEU:HA	2.31	0.45
1:F:117:LEU:HA	1:F:117:LEU:HD13	1.70	0.45
1:E:314:GLY:N	1:E:315:LEU:HA	2.32	0.45
1:H:314:GLY:N	1:H:315:LEU:HA	2.32	0.44
2:D:184[A]:ASP:OD2	6:D:501:HOH:O	2.21	0.44
1:E:117:LEU:HD11	1:E:308:VAL:CG1	2.48	0.44
1:G:2:THR:HA	6:G:536:HOH:O	2.16	0.44
1:F:314:GLY:N	1:F:315:LEU:HA	2.33	0.44
1:C:127:MET:O	1:C:169:LYS:CE	2.66	0.44
1:A:127:MET:O	1:A:169:LYS:CE	2.66	0.44
1:E:184:ASP:HB2	6:E:547:HOH:O	2.17	0.44
2:D:127:MET:O	2:D:169:LYS:CE	2.67	0.43
1:A:122:THR:HG23	1:C:122:THR:HG23	2.01	0.43
1:G:311[B]:PHE:HZ	1:G:315:LEU:HD13	1.84	0.43
1:B:314:GLY:N	1:B:315:LEU:HA	2.33	0.43
1:E:127:MET:O	1:E:169:LYS:CE	2.67	0.43
1:A:117:LEU:HD11	1:A:308:VAL:CG1	2.48	0.43
1:F:117:LEU:HD11	1:F:308:VAL:CG1	2.49	0.43
1:F:117:LEU:HD21	1:F:308:VAL:CG1	2.48	0.43
1:G:127:MET:O	1:G:169:LYS:CE	2.67	0.43
1:B:127:MET:O	1:B:169:LYS:CE	2.67	0.43
1:H:117:LEU:HD11	1:H:308:VAL:CG1	2.48	0.43
1:F:127:MET:O	1:F:169:LYS:CE	2.68	0.42
1:H:127:MET:O	1:H:169:LYS:CE	2.67	0.42
3:E:400:COA:O2A	3:E:400:COA:H4B	2.19	0.42
1:G:47:ILE:O	6:G:501:HOH:O	2.21	0.42
1:B:117:LEU:HD11	1:B:308:VAL:CG1	2.49	0.42
2:D:115:GLY:HA3	6:D:562:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:HG23	2:D:122:THR:HG23	2.01	0.42
1:E:102:PRO:HA	6:E:515:HOH:O	2.20	0.42
1:F:117:LEU:HD22	1:F:117:LEU:N	2.35	0.42
1:F:122:THR:HG23	1:H:122:THR:HG23	2.02	0.41
1:B:109:LEU:HG	2:D:107:PHE:CD2	2.55	0.41
1:F:11:TRP:CD2	1:F:295:LEU:HD13	2.55	0.41
1:G:351:LYS:NZ	6:G:514:HOH:O	2.46	0.41
1:A:109:LEU:HG	1:C:107:PHE:CD2	2.56	0.41
1:E:94:ARG:HB2	1:G:188:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	B	356/362 (98%)	343 (96%)	13 (4%)	0	100	100
1	C	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
1	E	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
1	F	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	G	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	H	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
2	D	360/362 (99%)	347 (96%)	13 (4%)	0	100	100
All	All	2861/2896 (99%)	2760 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	268/284 (94%)	266 (99%)	2 (1%)	84	91
1	B	267/284 (94%)	264 (99%)	3 (1%)	73	85
1	C	270/284 (95%)	265 (98%)	5 (2%)	57	71
1	E	269/284 (95%)	266 (99%)	3 (1%)	73	85
1	F	272/284 (96%)	269 (99%)	3 (1%)	73	85
1	G	275/284 (97%)	271 (98%)	4 (2%)	65	78
1	H	274/284 (96%)	272 (99%)	2 (1%)	84	91
2	D	277/285 (97%)	273 (99%)	4 (1%)	67	80
All	All	2172/2273 (96%)	2146 (99%)	26 (1%)	71	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	212	PHE
1	B	39	ARG
1	B	45	ARG
1	B	212	PHE
1	C	45	ARG
1	C	117	LEU
1	C	153[A]	ASP
1	C	153[B]	ASP
1	C	212	PHE
2	D	39	ARG
2	D	45	ARG
2	D	117	LEU
2	D	212	PHE
1	E	39	ARG
1	E	45	ARG
1	E	212	PHE
1	F	39	ARG
1	F	45	ARG

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Mol	Chain	Res	Type
1	F	212	PHE
1	G	39	ARG
1	G	45	ARG
1	G	117	LEU
1	G	212	PHE
1	H	45	ARG
1	H	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	134	HIS
1	B	37	GLN
1	B	180	GLN
1	B	186	GLN
1	C	37	GLN
2	D	37	GLN
1	E	37	GLN
1	F	3	GLN
1	F	37	GLN
1	G	37	GLN
1	G	131	HIS
1	H	3	GLN
1	H	37	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
1	SCY	C	113	1	7,8,9	0.75	0	3,9,11	0.60	0
1	SCY	A	113	1	7,8,9	0.89	0	3,9,11	0.58	0
1	SCY	B	113	1	7,8,9	0.90	0	3,9,11	0.53	0
1	SCY	H	113	1	7,8,9	0.88	0	3,9,11	0.60	0
1	SCY	E	113	1	7,8,9	0.78	0	3,9,11	0.57	0
1	SCY	F	113	1	7,8,9	0.95	0	3,9,11	0.53	0
1	SCY	G	113	1	7,8,9	0.86	0	3,9,11	0.59	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
1	SCY	C	113	1	-	0/5/7/9	-
1	SCY	A	113	1	-	0/5/7/9	-
1	SCY	B	113	1	-	0/5/7/9	-
1	SCY	H	113	1	-	0/5/7/9	-
1	SCY	E	113	1	-	0/5/7/9	-
1	SCY	F	113	1	-	0/5/7/9	-
1	SCY	G	113	1	-	0/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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
3	COA	B	400	-	20,23,50	1.11	2 (10%)	20,35,75	1.60	4 (20%)
3	COA	D	400	-	20,23,50	1.13	1 (5%)	20,35,75	1.70	4 (20%)
3	COA	E	400	-	26,29,50	1.29	3 (11%)	31,45,75	1.48	6 (19%)
3	COA	A	400	-	26,29,50	1.08	1 (3%)	31,45,75	1.27	4 (12%)
5	MLI	G	403	-	0,6,6	-	-	0,7,7	-	-
3	COA	G	401	-	28,33,50	1.33	4 (14%)	35,52,75	1.35	5 (14%)
3	COA	F	401	-	28,33,50	1.29	4 (14%)	35,52,75	1.38	6 (17%)
3	COA	H	401	-	41,50,50	0.87	2 (4%)	52,75,75	1.46	9 (17%)

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	400	-	-	0/5/22/64	0/3/3/3
3	COA	D	400	-	-	3/5/22/64	0/3/3/3
3	COA	E	400	-	-	5/11/31/64	0/3/3/3
3	COA	A	400	-	-	5/11/31/64	0/3/3/3
5	MLI	G	403	-	-	0/0/4/4	-
3	COA	G	401	-	-	6/17/37/64	0/3/3/3
3	COA	F	401	-	-	5/17/37/64	0/3/3/3
3	COA	H	401	-	-	17/44/64/64	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	COA	P2A-O4A	3.85	1.63	1.50
3	F	401	COA	P2A-O4A	3.53	1.61	1.50
3	E	400	COA	P1A-O1A	3.48	1.61	1.50
3	G	401	COA	C5A-C4A	2.79	1.48	1.40
3	G	401	COA	O4B-C1B	2.70	1.44	1.41
3	F	401	COA	C5A-C4A	2.67	1.48	1.40
3	E	400	COA	O4B-C1B	2.66	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	COA	C5A-C4A	2.57	1.47	1.40
3	F	401	COA	O4B-C1B	2.56	1.44	1.41
3	A	400	COA	C5A-C4A	2.55	1.47	1.40
3	H	401	COA	C5A-C4A	2.51	1.47	1.40
3	E	400	COA	C5A-C4A	2.51	1.47	1.40
3	F	401	COA	C2A-N3A	2.44	1.36	1.32
3	G	401	COA	C2A-N3A	2.20	1.35	1.32
3	D	400	COA	C5A-C4A	2.10	1.46	1.40
3	H	401	COA	O4B-C1B	2.09	1.44	1.41
3	B	400	COA	C2A-N3A	2.04	1.35	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	COA	N3A-C2A-N1A	-4.17	122.16	128.68
3	H	401	COA	C6P-C7P-N8P	-4.17	103.48	111.90
3	F	401	COA	N3A-C2A-N1A	-3.85	122.67	128.68
3	E	400	COA	N3A-C2A-N1A	-3.84	122.68	128.68
3	G	401	COA	N3A-C2A-N1A	-3.71	122.89	128.68
3	H	401	COA	N3A-C2A-N1A	-3.70	122.89	128.68
3	B	400	COA	N3A-C2A-N1A	-3.50	123.21	128.68
3	A	400	COA	N3A-C2A-N1A	-3.43	123.32	128.68
3	F	401	COA	O6A-P2A-O5A	3.27	120.13	107.64
3	H	401	COA	CDP-CBP-CAP	3.20	114.38	108.82
3	G	401	COA	O6A-P2A-O5A	3.19	119.83	107.64
3	A	400	COA	C3B-C2B-C1B	3.09	106.74	99.89
3	H	401	COA	O4B-C1B-C2B	-3.04	102.48	106.93
3	G	401	COA	P1A-O3A-P2A	-2.83	123.12	132.83
3	E	400	COA	O3A-P1A-O2A	2.81	118.39	107.64
3	D	400	COA	C4A-C5A-N7A	-2.81	106.47	109.40
3	H	401	COA	C4A-C5A-N7A	-2.66	106.63	109.40
3	H	401	COA	O5P-C5P-C6P	-2.59	117.29	122.02
3	A	400	COA	O2A-P1A-O1A	2.51	120.50	110.68
3	B	400	COA	C4A-C5A-N7A	-2.50	106.79	109.40
3	A	400	COA	C4A-C5A-N7A	-2.48	106.81	109.40
3	E	400	COA	P1A-O5B-C5B	2.47	125.09	118.30
3	B	400	COA	C4B-C3B-C2B	2.44	106.55	102.28
3	B	400	COA	C3B-C2B-C1B	2.38	105.20	99.92
3	F	401	COA	C3B-C2B-C1B	2.32	105.02	99.89
3	G	401	COA	C4A-C5A-N7A	-2.31	106.99	109.40
3	D	400	COA	C2A-N1A-C6A	2.30	122.69	118.75
3	H	401	COA	P2A-O3A-P1A	-2.27	125.02	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	COA	C2A-N1A-C6A	2.27	122.63	118.75
3	F	401	COA	C2A-N1A-C6A	2.26	122.61	118.75
3	E	400	COA	C4A-C5A-N7A	-2.23	107.07	109.40
3	E	400	COA	C3B-C2B-C1B	2.15	104.64	99.89
3	D	400	COA	C4B-C3B-C2B	2.13	106.00	102.28
3	H	401	COA	C2A-N1A-C6A	2.11	122.36	118.75
3	F	401	COA	P1A-O3A-P2A	-2.10	125.61	132.83
3	H	401	COA	O9A-P3B-O8A	2.08	115.59	107.64
3	E	400	COA	C2A-N1A-C6A	2.02	122.20	118.75
3	F	401	COA	C4A-C5A-N7A	-2.01	107.30	109.40

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	COA	C3B-C4B-C5B-O5B
3	E	400	COA	C4B-C5B-O5B-P1A
3	E	400	COA	C5B-O5B-P1A-O2A
3	E	400	COA	C5B-O5B-P1A-O3A
3	H	401	COA	C3B-C4B-C5B-O5B
3	H	401	COA	O4B-C4B-C5B-O5B
3	H	401	COA	C5B-O5B-P1A-O2A
3	H	401	COA	C5B-O5B-P1A-O3A
3	H	401	COA	OAP-CAP-CBP-CCP
3	H	401	COA	C9P-CAP-CBP-CCP
3	H	401	COA	OAP-CAP-CBP-CDP
3	H	401	COA	C9P-CAP-CBP-CDP
3	H	401	COA	OAP-CAP-CBP-CEP
3	H	401	COA	C9P-CAP-CBP-CEP
3	H	401	COA	C5P-C6P-C7P-N8P
3	G	401	COA	C3B-C4B-C5B-O5B
3	G	401	COA	O4B-C4B-C5B-O5B
3	A	400	COA	C4B-C3B-O3B-P3B
3	A	400	COA	C2B-C3B-O3B-P3B
3	A	400	COA	O4B-C4B-C5B-O5B
3	E	400	COA	C5B-O5B-P1A-O1A
3	F	401	COA	P2A-O3A-P1A-O5B
3	G	401	COA	P2A-O3A-P1A-O5B
3	G	401	COA	C3B-O3B-P3B-O7A
3	H	401	COA	C3B-O3B-P3B-O9A
3	H	401	COA	P2A-O3A-P1A-O1A
3	A	400	COA	C4B-C5B-O5B-P1A

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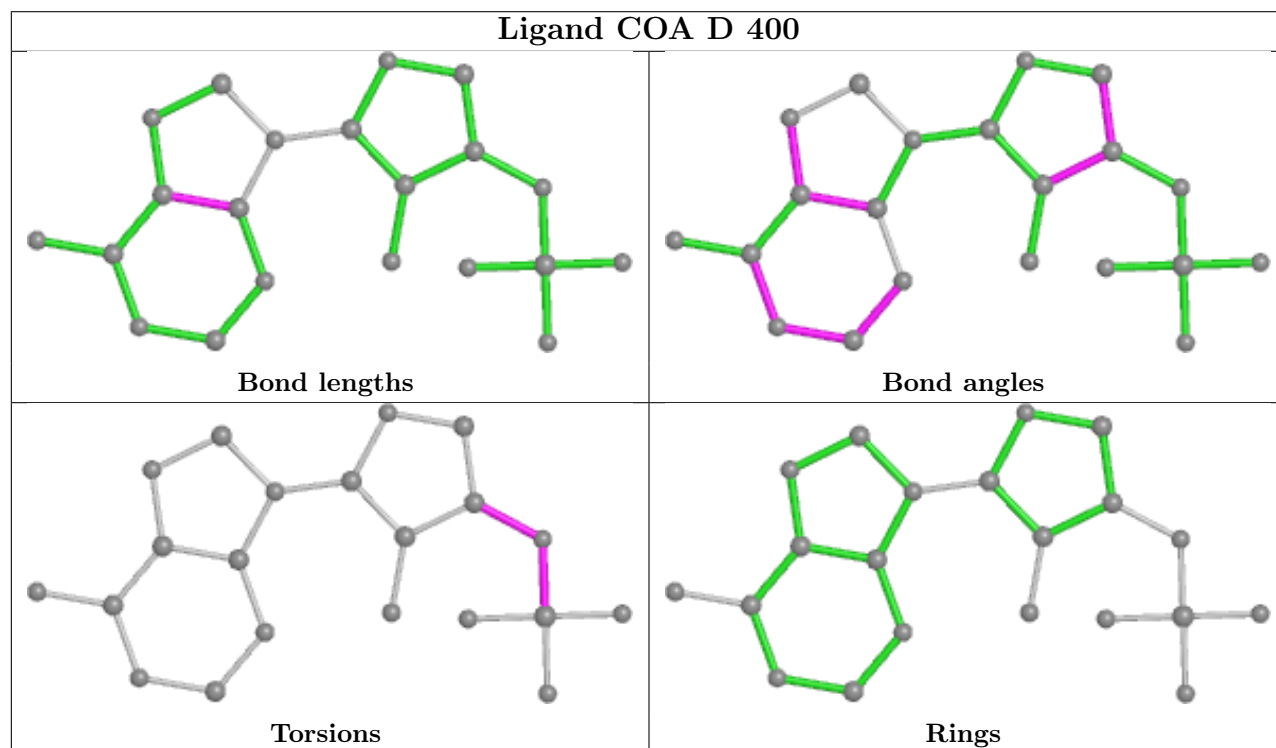
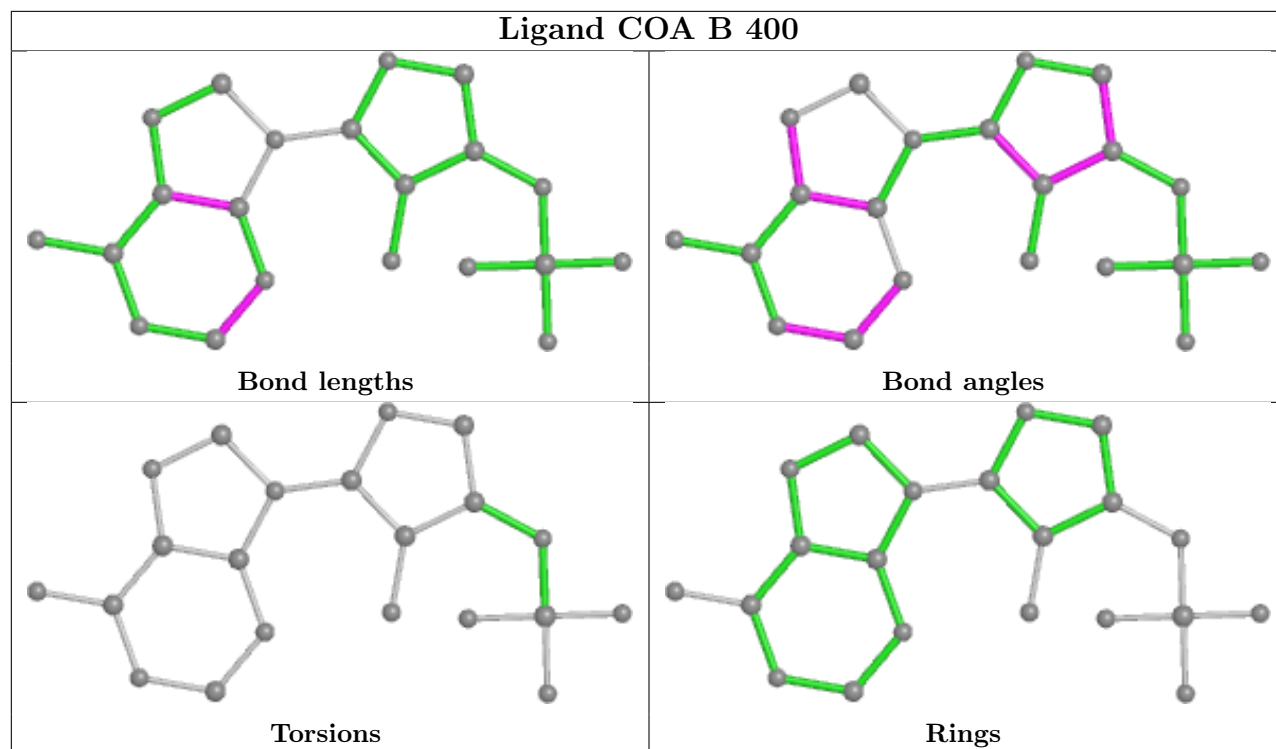
Mol	Chain	Res	Type	Atoms
3	D	400	COA	C4B-C3B-O3B-P3B
3	F	401	COA	C2B-C3B-O3B-P3B
3	F	401	COA	P1A-O3A-P2A-O4A
3	G	401	COA	C4B-C5B-O5B-P1A
3	E	400	COA	O4B-C4B-C5B-O5B
3	D	400	COA	C3B-O3B-P3B-O7A
3	F	401	COA	C3B-O3B-P3B-O7A
3	F	401	COA	P1A-O3A-P2A-O5A
3	H	401	COA	O5P-C5P-C6P-C7P
3	D	400	COA	C3B-O3B-P3B-O8A
3	G	401	COA	C3B-O3B-P3B-O9A
3	H	401	COA	N4P-C5P-C6P-C7P
3	H	401	COA	P2A-O3A-P1A-O2A
3	H	401	COA	CBP-CCP-O6A-P2A

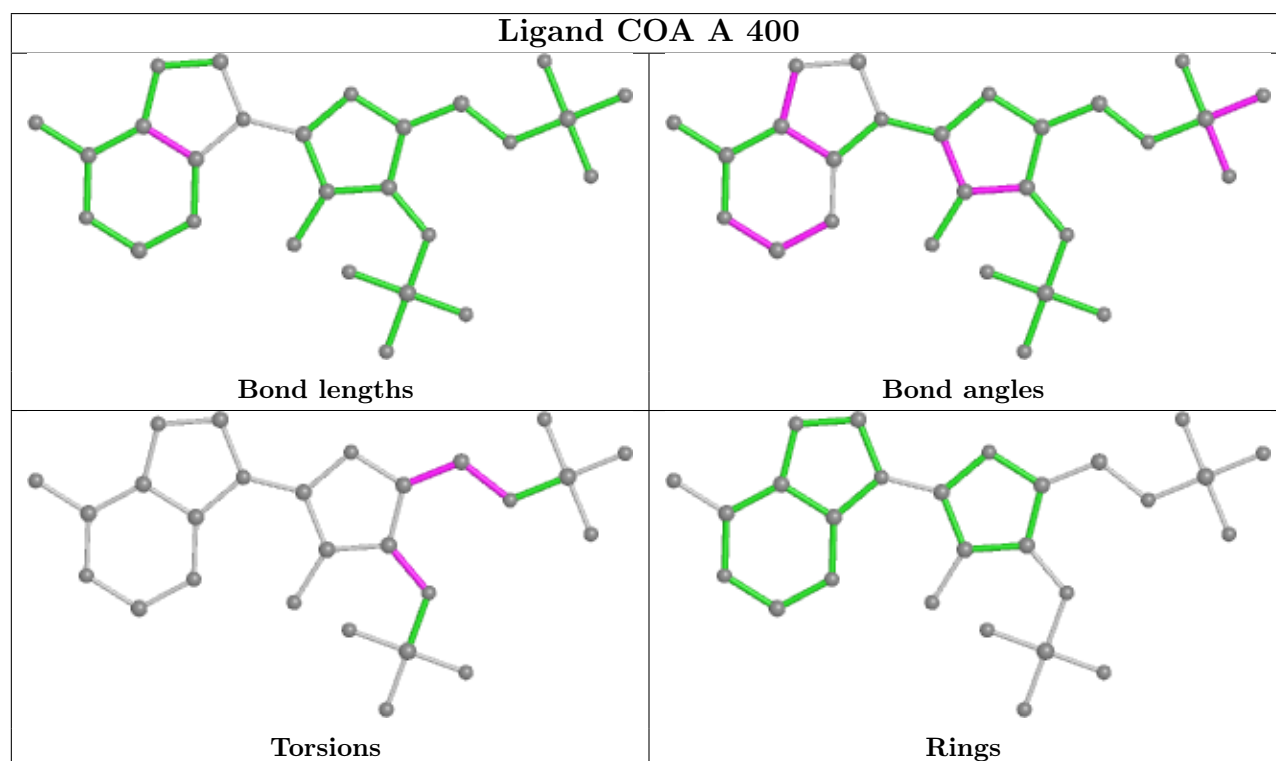
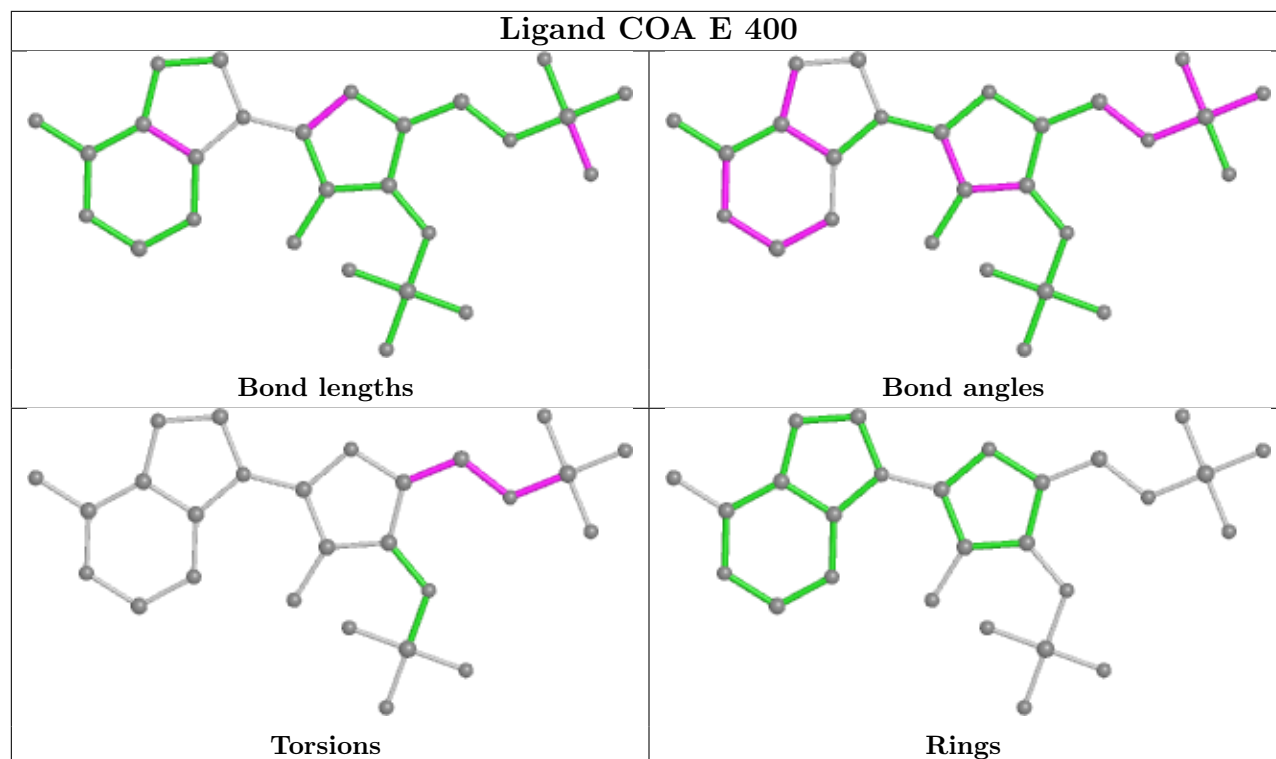
There are no ring outliers.

2 monomers are involved in 2 short contacts:

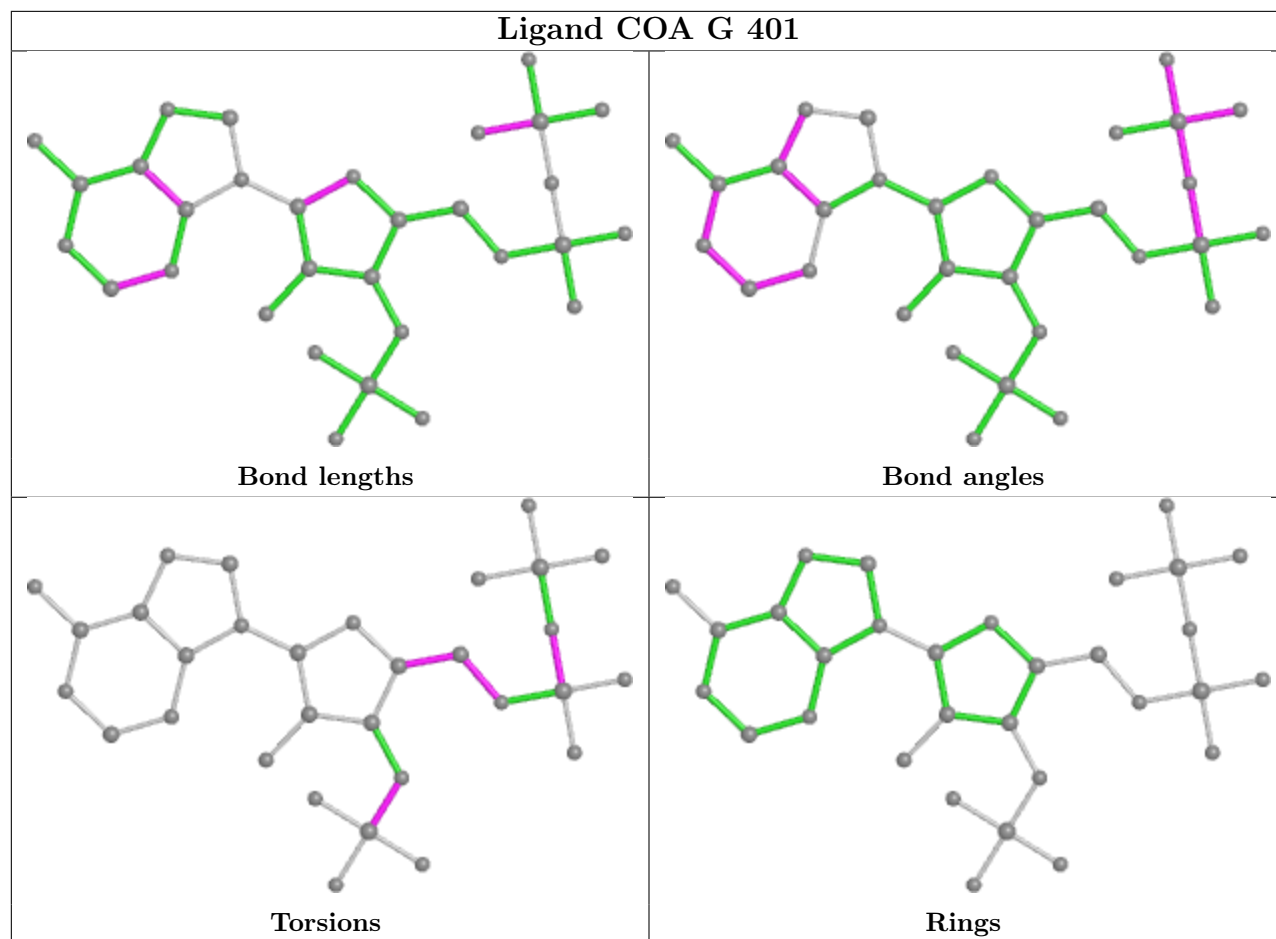
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	400	COA	1	0
3	H	401	COA	1	0

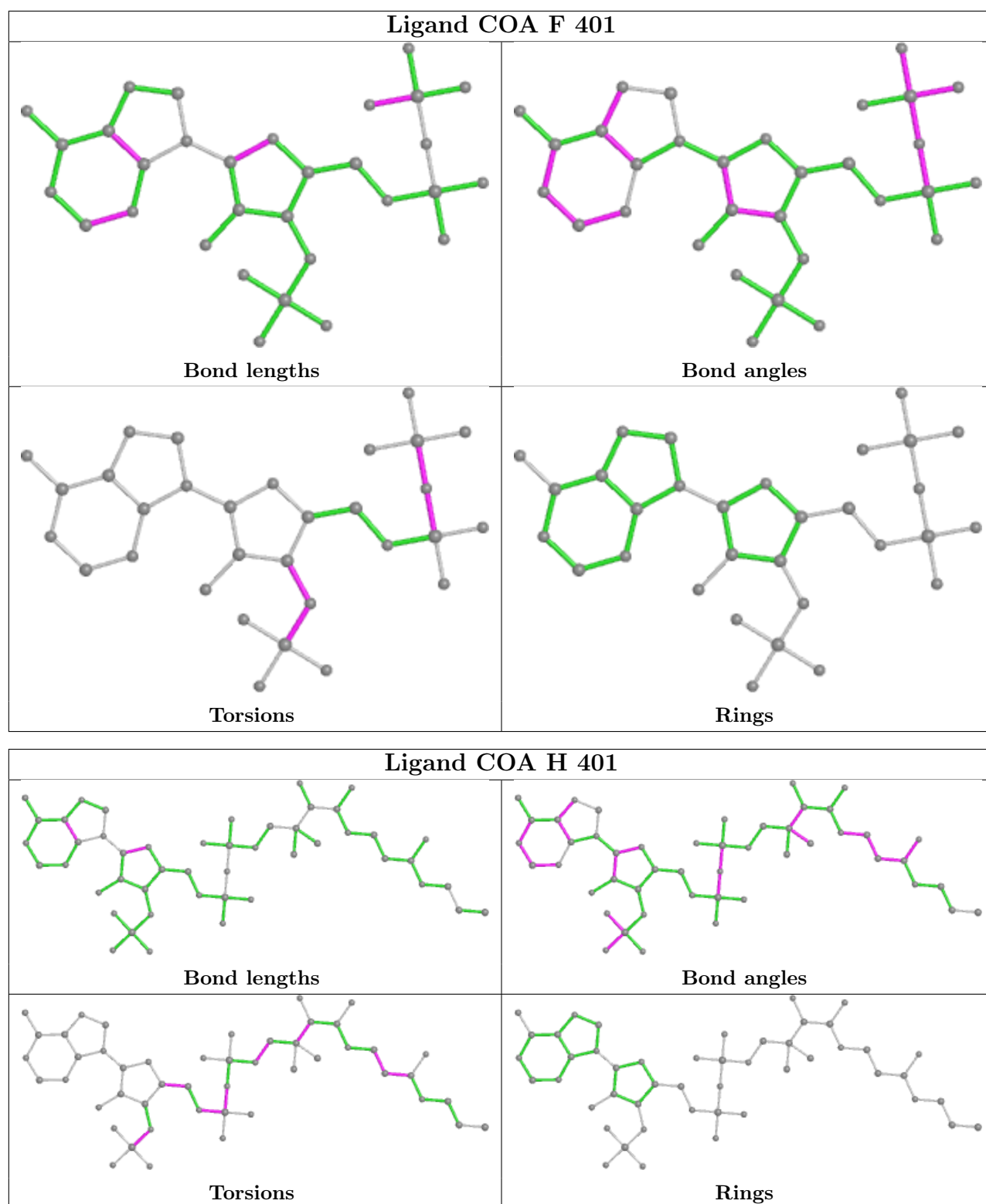
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	358/362 (98%)	-0.03	0 <span>100</span> <span>100</span>	28, 44, 71, 86	0
1	B	358/362 (98%)	-0.07	2 (0%) <span>89</span> <span>88</span>	24, 40, 69, 78	0
1	C	358/362 (98%)	-0.06	1 (0%) <span>94</span> <span>93</span>	27, 43, 63, 70	0
1	E	359/362 (99%)	-0.02	5 (1%) <span>75</span> <span>73</span>	29, 45, 69, 84	0
1	F	358/362 (98%)	-0.13	2 (0%) <span>89</span> <span>88</span>	23, 40, 61, 83	0
1	G	358/362 (98%)	-0.04	2 (0%) <span>89</span> <span>88</span>	29, 45, 70, 93	0
1	H	357/362 (98%)	-0.02	2 (0%) <span>89</span> <span>88</span>	25, 42, 66, 76	0
2	D	359/362 (99%)	-0.07	2 (0%) <span>89</span> <span>88</span>	21, 39, 61, 74	0
All	All	2865/2896 (98%)	-0.05	16 (0%) <span>89</span> <span>88</span>	21, 42, 67, 93	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.3
1	E	4	CYS	3.6
1	E	29	LEU	3.4
1	G	342	ASP	3.0
1	C	240	LEU	2.8
1	E	335	ASP	2.6
1	H	28	PHE	2.6
2	D	29	LEU	2.6
2	D	311[A]	PHE	2.6
1	E	150	THR	2.4
1	F	153	ASP	2.3
1	H	29	LEU	2.3
1	G	311[A]	PHE	2.2
1	B	240	LEU	2.2
1	B	342	ASP	2.0
1	F	150	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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(Å <sup>2</sup> )	Q<0.9
1	SCY	G	113	9/10	0.88	0.13	37,39,42,43	0
1	SCY	H	113	9/10	0.88	0.12	37,40,44,48	0
1	SCY	C	113	9/10	0.93	0.12	36,39,47,48	0
1	SCY	E	113	9/10	0.94	0.10	39,42,46,48	0
1	SCY	B	113	9/10	0.95	0.13	32,34,44,47	0
1	SCY	A	113	9/10	0.96	0.11	33,37,46,49	0
1	SCY	F	113	9/10	0.96	0.08	31,33,40,40	0

## 6.3 Carbohydrates [i](#)

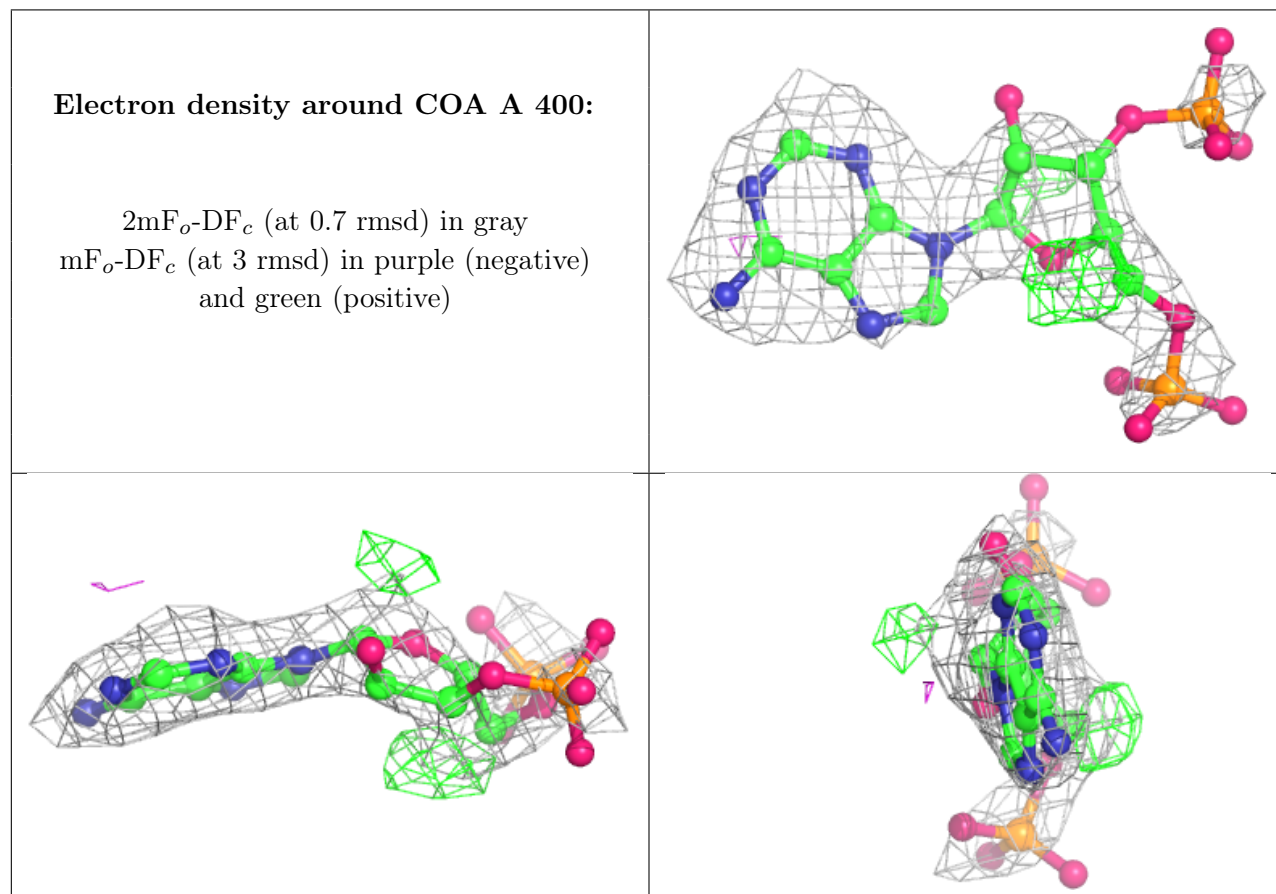
There are no monosaccharides in this entry.

## 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, 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.

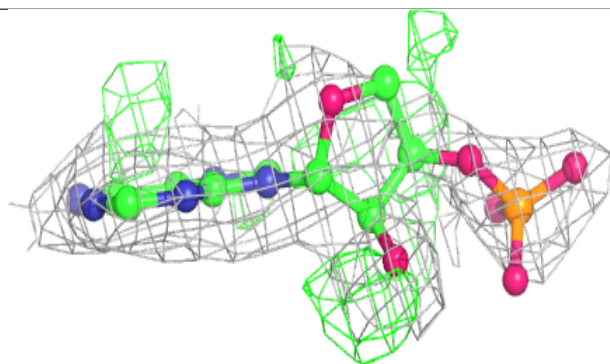
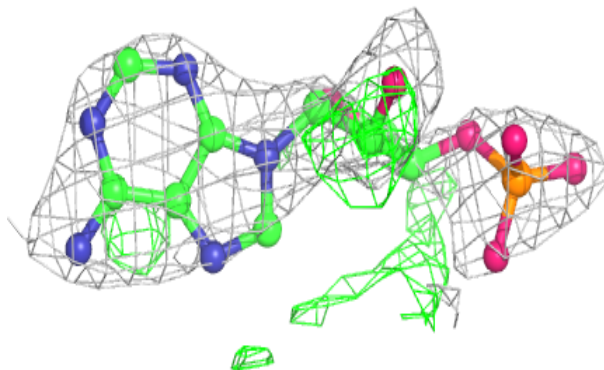
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	COA	A	400	27/48	0.66	0.28	55,74,88,91	27
3	COA	B	400	21/48	0.72	0.21	45,49,53,54	21
3	COA	D	400	21/48	0.75	0.23	39,48,59,66	21
3	COA	H	401	48/48	0.75	0.26	50,63,76,82	48
3	COA	E	400	27/48	0.83	0.19	48,51,56,59	27
5	MLI	G	403	7/7	0.84	0.14	66,67,71,71	0
3	COA	F	401	31/48	0.86	0.17	53,70,92,96	0
4	NA	H	402	1/1	0.87	0.08	45,45,45,45	0
3	COA	G	401	31/48	0.88	0.17	53,69,78,83	0
4	NA	B	401	1/1	0.97	0.07	32,32,32,32	0
4	NA	C	401	1/1	0.97	0.10	39,39,39,39	0
4	NA	A	401	1/1	0.98	0.07	42,42,42,42	0
4	NA	F	402	1/1	0.98	0.12	34,34,34,34	0
4	NA	D	401	1/1	0.99	0.05	36,36,36,36	0
4	NA	G	402	1/1	0.99	0.06	51,51,51,51	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.

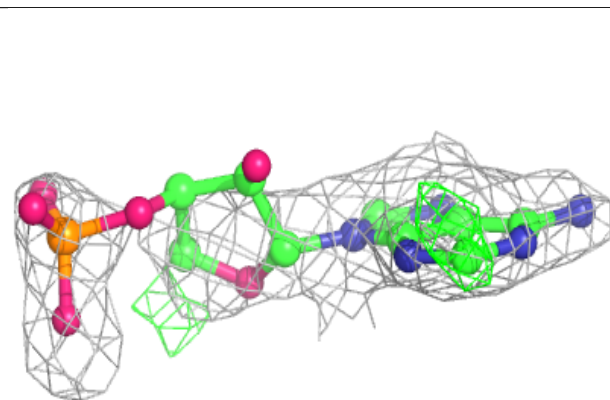
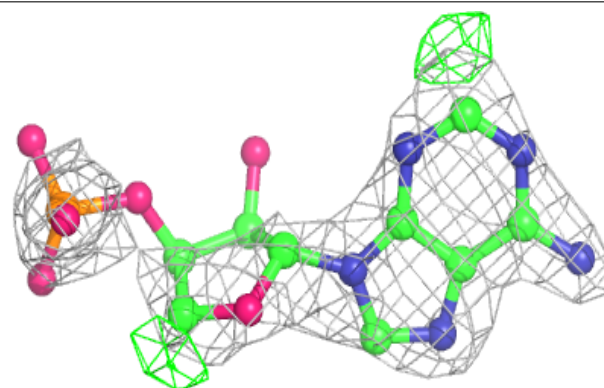


**Electron density around COA B 400:**

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

**Electron density around COA D 400:**

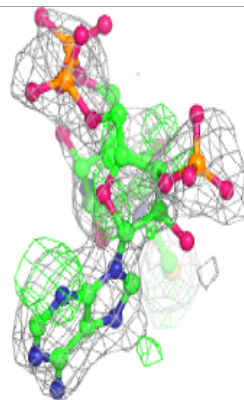
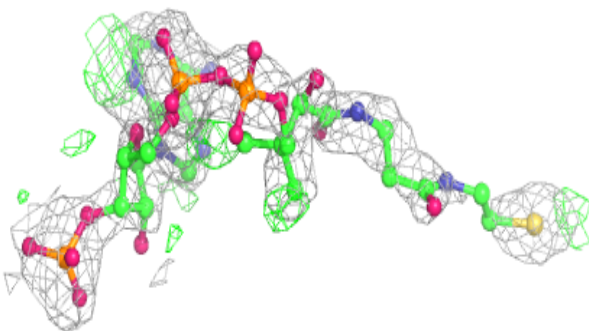
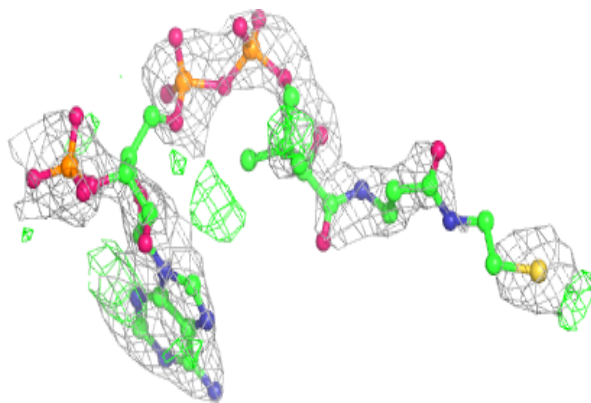
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



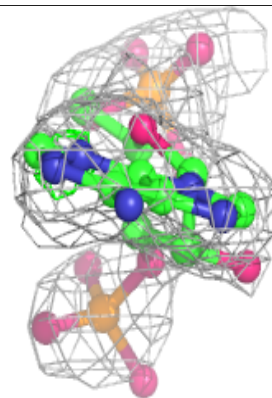
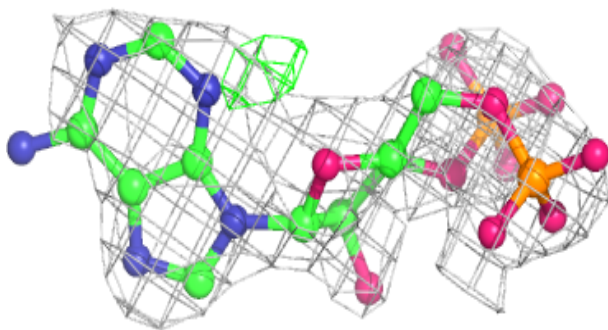
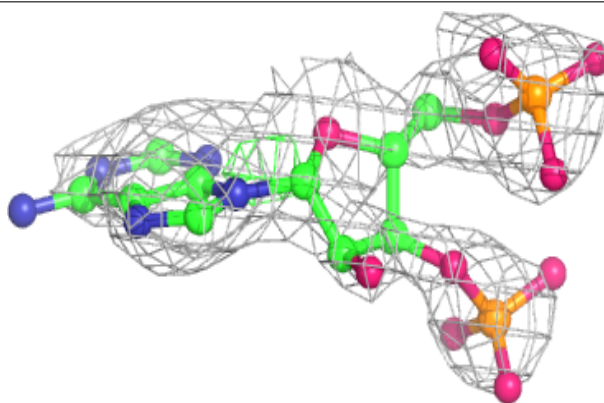


**Electron density around COA H 401:**

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

**Electron density around COA E 400:**

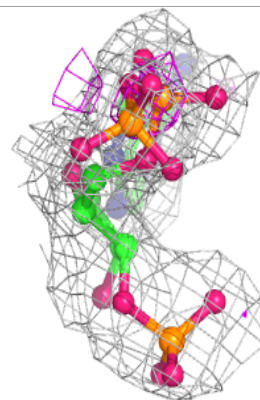
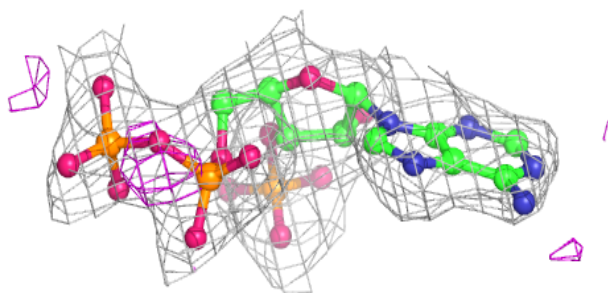
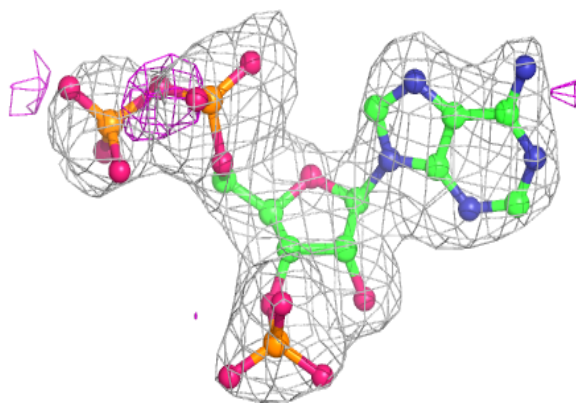
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



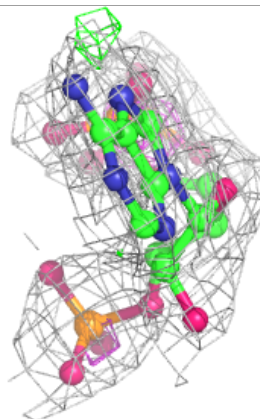
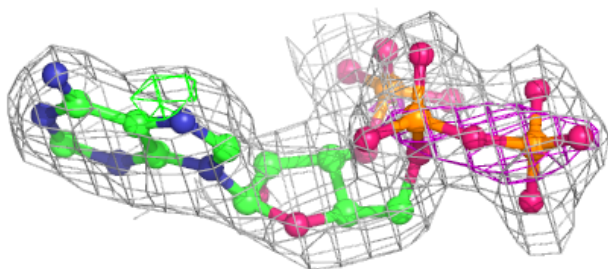
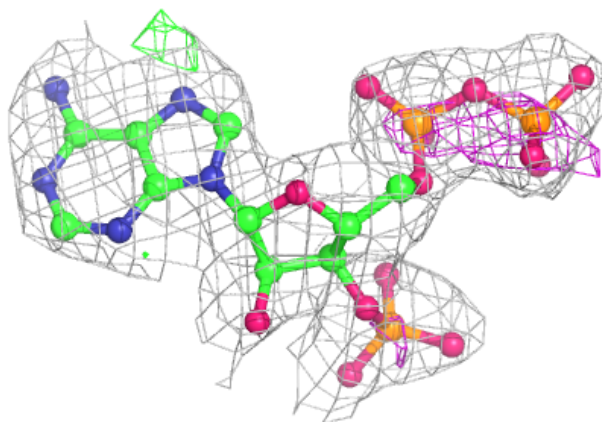


**Electron density around COA F 401:**

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

**Electron density around COA G 401:**

$2mF_o - DF_c$  (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.