



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:33 pm BST

PDB ID : 6QCL  
Title : Citryl-CoA lyase core module of Chlorobium limicola ATP citrate lyase in complex with acetyl-CoA and L-malate  
Authors : Verstraete, K.; Verschueren, K.  
Deposited on : 2018-12-28  
Resolution : 1.60 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	:	2.11
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)	:	2.11

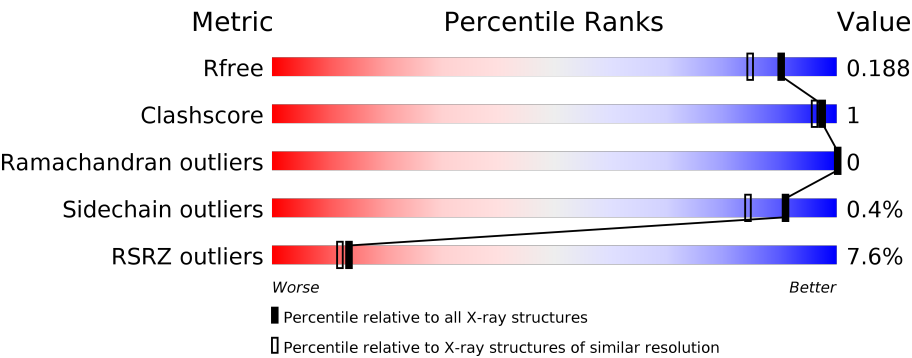
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	262	<div><div>9%</div><div><div></div><div>81%</div><div></div><div>18%</div></div><div></div></div>
1	B	262	<div><div>19%</div><div><div></div><div>90%</div><div></div><div>9%</div></div><div></div></div>
1	C	262	<div><div>23%</div><div><div></div><div>99%</div><div></div></div><div></div></div>
1	D	262	<div><div>6%</div><div><div></div><div>97%</div><div></div></div><div></div></div>
1	E	262	<div><div></div><div><div></div><div>96%</div><div></div></div><div></div></div>
1	F	262	<div><div>%</div><div><div></div><div>96%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	262	<div><div></div><div>98%</div><div>.</div></div>
1	H	262	<div>%<div><div></div><div>98%</div><div>.</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33116 atoms, of which 16022 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 ATP-citrate lyase alpha-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	4	0
			3341	1067	1660	282	321	11			
1	B	239	Total	C	H	N	O	S	0	3	0
			3750	1198	1872	317	351	12			
1	C	261	Total	C	H	N	O	S	0	3	0
			4065	1291	2036	346	379	13			
1	D	261	Total	C	H	N	O	S	0	3	0
			4065	1291	2036	346	379	13			
1	E	256	Total	C	H	N	O	S	0	4	0
			4043	1283	2031	344	373	12			
1	F	256	Total	C	H	N	O	S	0	5	0
			4051	1284	2034	345	376	12			
1	G	261	Total	C	H	N	O	S	0	4	0
			4101	1302	2057	349	380	13			
1	H	261	Total	C	H	N	O	S	0	7	0
			4114	1305	2064	350	382	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLY	-	expression tag	UNP Q9AJC4
A	348	SER	-	expression tag	UNP Q9AJC4
A	349	HIS	-	expression tag	UNP Q9AJC4
A	350	MET	-	expression tag	UNP Q9AJC4
B	347	GLY	-	expression tag	UNP Q9AJC4
B	348	SER	-	expression tag	UNP Q9AJC4
B	349	HIS	-	expression tag	UNP Q9AJC4
B	350	MET	-	expression tag	UNP Q9AJC4
C	347	GLY	-	expression tag	UNP Q9AJC4
C	348	SER	-	expression tag	UNP Q9AJC4
C	349	HIS	-	expression tag	UNP Q9AJC4
C	350	MET	-	expression tag	UNP Q9AJC4
D	347	GLY	-	expression tag	UNP Q9AJC4

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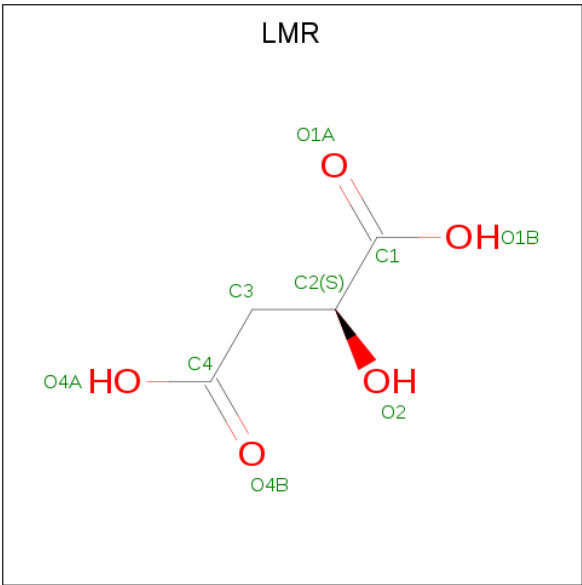
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Chain	Residue	Modelled	Actual	Comment	Reference
D	348	SER	-	expression tag	UNP Q9AJC4
D	349	HIS	-	expression tag	UNP Q9AJC4
D	350	MET	-	expression tag	UNP Q9AJC4
E	347	GLY	-	expression tag	UNP Q9AJC4
E	348	SER	-	expression tag	UNP Q9AJC4
E	349	HIS	-	expression tag	UNP Q9AJC4
E	350	MET	-	expression tag	UNP Q9AJC4
F	347	GLY	-	expression tag	UNP Q9AJC4
F	348	SER	-	expression tag	UNP Q9AJC4
F	349	HIS	-	expression tag	UNP Q9AJC4
F	350	MET	-	expression tag	UNP Q9AJC4
G	347	GLY	-	expression tag	UNP Q9AJC4
G	348	SER	-	expression tag	UNP Q9AJC4
G	349	HIS	-	expression tag	UNP Q9AJC4
G	350	MET	-	expression tag	UNP Q9AJC4
H	347	GLY	-	expression tag	UNP Q9AJC4
H	348	SER	-	expression tag	UNP Q9AJC4
H	349	HIS	-	expression tag	UNP Q9AJC4
H	350	MET	-	expression tag	UNP Q9AJC4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

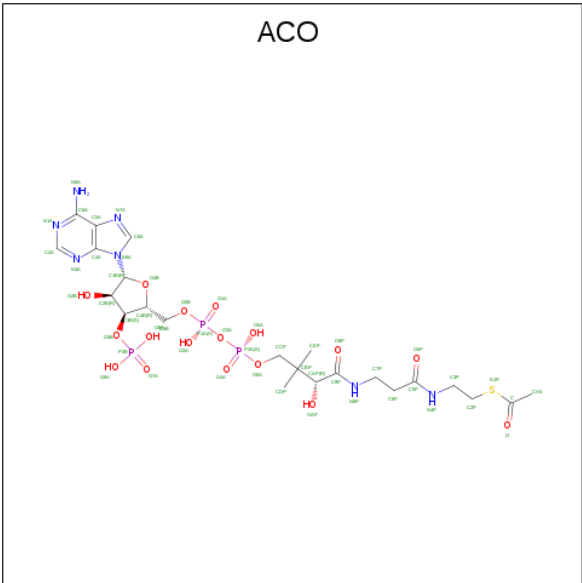
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by author).



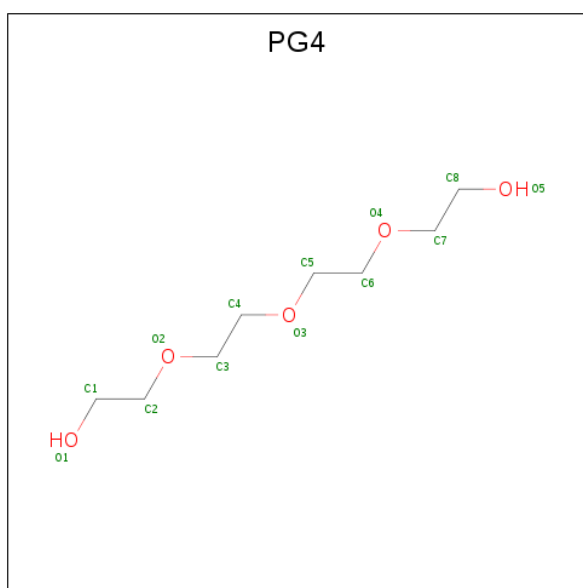
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			13	4	4	5		
3	F	1	Total	C	H	O	0	0
			13	4	4	5		
3	G	1	Total	C	H	O	0	0
			13	4	4	5		
3	H	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 4 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by author).



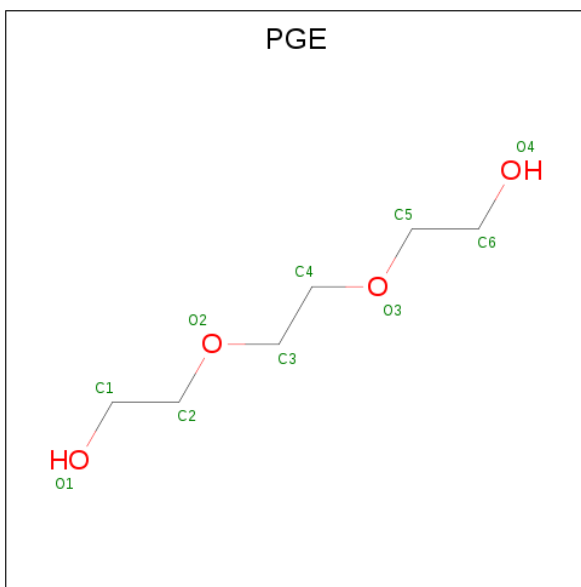
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	F	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	G	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	H	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			31	8	18	5		
5	F	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			24	6	14	4		
6	H	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 7 is water.

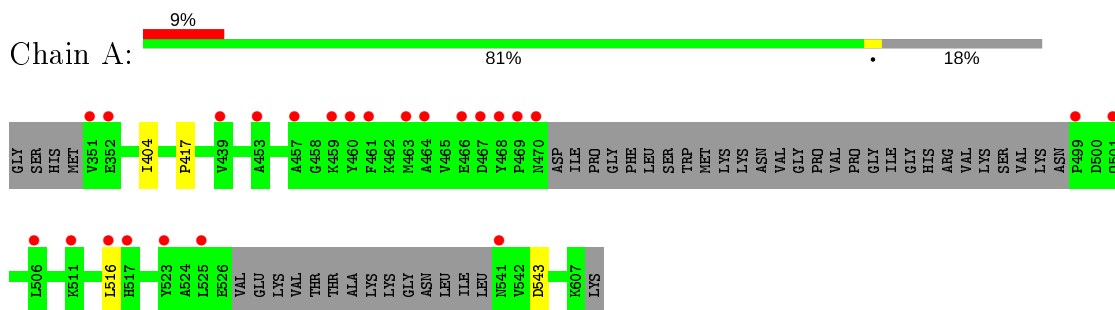
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	100	Total	O	0	0
			100	100		
7	B	108	Total	O	0	0
			108	108		
7	C	107	Total	O	0	0
			107	107		
7	D	136	Total	O	0	0
			136	136		
7	E	151	Total	O	0	0
			151	151		
7	F	137	Total	O	0	0
			137	137		
7	G	182	Total	O	0	0
			182	182		
7	H	145	Total	O	0	0
			145	145		



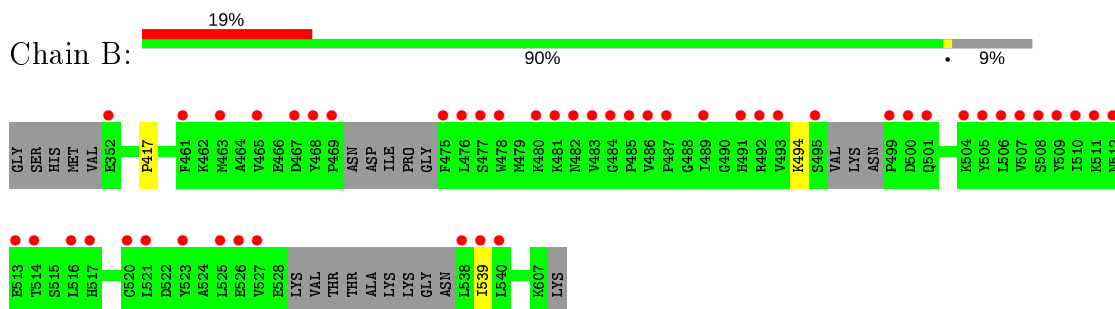
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

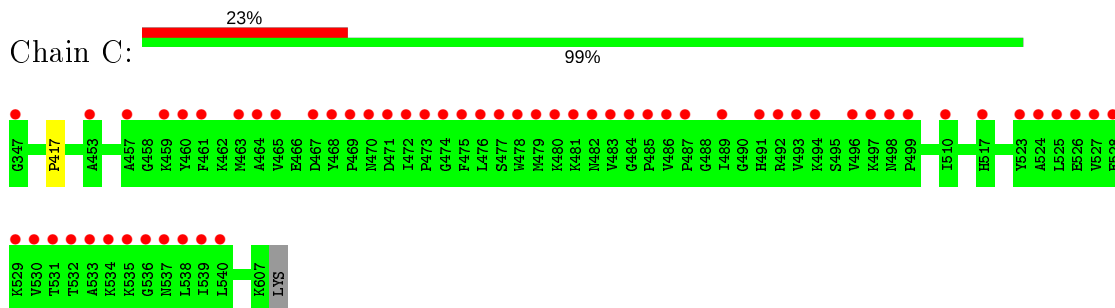
- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit

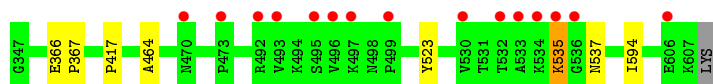


- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit





- Molecule 1: ATP-citrate lyase alpha-subunit

Chain E: 96% ..



- Molecule 1: ATP-citrate lyase alpha-subunit

Chain F: 96% ..



- Molecule 1: ATP-citrate lyase alpha-subunit

Chain G: 98% .



- Molecule 1: ATP-citrate lyase alpha-subunit

Chain H: 98% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.73Å 100.82Å 105.01Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	45.62 – 1.60 45.62 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.62-1.60) 98.9 (45.62-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.157 , 0.177 0.169 , 0.188	Depositor DCC
$R_{free}$ test set	13820 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, PGE, ACO, PG4, CA

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	0.53	0/1731	0.61	0/2344
1	B	0.51	0/1917	0.60	0/2593
1	C	0.51	0/2081	0.60	0/2819
1	D	0.51	0/2081	0.62	0/2819
1	E	0.50	0/2055	0.59	0/2785
1	F	0.49	0/2060	0.61	0/2791
1	G	0.52	0/2088	0.60	0/2830
1	H	0.51	0/2108	0.62	0/2857
All	All	0.51	0/16121	0.61	0/21838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	1660	1638	4	0
1	B	1878	1872	1868	3	0
1	C	2029	2036	2025	3	0
1	D	2029	2036	2025	5	0
1	E	2012	2031	2027	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2017	2034	2027	2	0
1	G	2044	2057	2053	4	0
1	H	2050	2064	2050	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	E	9	4	4	1	0
3	F	9	4	4	1	0
3	G	9	4	4	1	0
3	H	9	4	4	0	0
4	E	51	38	34	1	0
4	F	51	38	34	1	0
4	G	51	38	34	1	0
4	H	51	38	34	0	0
5	E	13	18	18	0	0
5	F	13	18	18	1	0
6	G	10	14	14	0	0
6	H	10	14	14	0	0
7	A	100	0	0	1	0
7	B	108	0	0	1	0
7	C	107	0	0	1	0
7	D	136	0	0	0	0
7	E	151	0	0	0	0
7	F	137	0	0	1	0
7	G	182	0	0	0	0
7	H	145	0	0	0	0
All	All	17094	16022	15929	27	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 1.

All (27) 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:417:PRO:HB3	1:H:357[B]:THR:HG21	1.86	0.58
1:B:417:PRO:CB	1:H:357[B]:THR:HG21	2.34	0.57
1:D:535:LYS:HD2	1:D:537:ASN:OD1	2.04	0.57
7:C:728:HOH:O	1:E:357[B]:THR:HG22	2.05	0.56
1:A:417:PRO:CB	1:G:357[B]:THR:HG21	2.35	0.56
1:C:417:PRO:CB	1:E:357[B]:THR:HG21	2.38	0.53
7:B:823:HOH:O	1:H:357[B]:THR:HG22	2.08	0.53
1:E:419[B]:VAL:HG21	1:E:450:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419[B]:VAL:CG2	1:E:450:PHE:CE1	2.94	0.51
1:A:404:ILE:CD1	1:A:516:LEU:CD1	2.92	0.48
1:A:417:PRO:HB3	1:G:357[B]:THR:HG21	1.95	0.48
7:A:833:HOH:O	1:G:357[B]:THR:HG22	2.14	0.47
1:B:494:LYS:HB2	1:B:539:ILE:HD11	1.96	0.47
1:C:417:PRO:HG3	1:E:357[B]:THR:HG21	1.97	0.47
1:G:510:ILE:HG21	1:G:518:THR:HG21	1.97	0.47
1:D:366:GLU:HB2	1:D:367:PRO:HD2	1.98	0.46
1:C:417:PRO:HB3	1:E:357[B]:THR:HG21	1.99	0.45
3:F:1000:LMR:C1	4:F:1001:ACO:HH32	2.47	0.45
1:F:401:GLU:HG2	1:F:553:LEU:HD22	1.99	0.44
1:D:417:PRO:HG3	1:F:357[A]:THR:HG21	2.00	0.43
5:F:1002:PG4:H42	7:F:1161:HOH:O	2.18	0.43
1:D:464:ALA:HB1	1:D:523:TYR:CE1	2.54	0.43
1:A:404:ILE:CD1	1:A:516:LEU:HD12	2.48	0.43
1:H:510:ILE:HG21	1:H:518:THR:HG21	2.01	0.42
1:D:594:ILE:HD11	1:H:418:ALA:HB2	2.02	0.42
3:G:1000:LMR:C1	4:G:1001:ACO:HH32	2.51	0.41
3:E:1000:LMR:C1	4:E:1001:ACO:HH32	2.52	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	213/262 (81%)	212 (100%)	1 (0%)	0	100	100
1	B	234/262 (89%)	234 (100%)	0	0	100	100
1	C	262/262 (100%)	259 (99%)	3 (1%)	0	100	100
1	D	262/262 (100%)	261 (100%)	1 (0%)	0	100	100
1	E	258/262 (98%)	254 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	259/262 (99%)	255 (98%)	4 (2%)	0	100	100
1	G	263/262 (100%)	258 (98%)	5 (2%)	0	100	100
1	H	266/262 (102%)	260 (98%)	6 (2%)	0	100	100
All	All	2017/2096 (96%)	1993 (99%)	24 (1%)	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	183/219 (84%)	182 (100%)	1 (0%)	88	80
1	B	203/219 (93%)	203 (100%)	0	100	100
1	C	221/219 (101%)	221 (100%)	0	100	100
1	D	221/219 (101%)	220 (100%)	1 (0%)	88	80
1	E	218/219 (100%)	216 (99%)	2 (1%)	78	65
1	F	219/219 (100%)	218 (100%)	1 (0%)	88	80
1	G	222/219 (101%)	222 (100%)	0	100	100
1	H	225/219 (103%)	224 (100%)	1 (0%)	91	84
All	All	1712/1752 (98%)	1706 (100%)	6 (0%)	91	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	ASP
1	D	535	LYS
1	E	395	LYS
1	E	517	HIS
1	F	415	HIS
1	H	514	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	LMR	F	1000	-	2,8,8	0.30	0	3,10,10	1.57	1 (33%)
4	ACO	F	1001	-	45,53,53	0.70	1 (2%)	56,79,79	0.71	0
5	PG4	F	1002	-	12,12,12	0.33	0	11,11,11	0.84	1 (9%)
4	ACO	H	1001	-	45,53,53	0.69	1 (2%)	56,79,79	0.69	0
4	ACO	G	1001	-	45,53,53	0.75	1 (2%)	56,79,79	0.64	1 (1%)
3	LMR	G	1000	-	2,8,8	0.02	0	3,10,10	1.91	1 (33%)
3	LMR	E	1000	-	2,8,8	0.36	0	3,10,10	1.79	1 (33%)
3	LMR	H	1000	-	2,8,8	0.32	0	3,10,10	1.46	0
4	ACO	E	1001	-	45,53,53	0.72	1 (2%)	56,79,79	0.65	0
5	PG4	E	1002	-	12,12,12	0.17	0	11,11,11	0.25	0
6	PGE	H	1002	-	9,9,9	0.20	0	8,8,8	0.13	0
6	PGE	G	1002	-	9,9,9	0.14	0	8,8,8	0.21	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
3	LMR	F	1000	-	-	1/2/8/8	-
4	ACO	F	1001	-	-	3/47/67/67	0/3/3/3
5	PG4	F	1002	-	-	5/10/10/10	-
4	ACO	H	1001	-	-	2/47/67/67	0/3/3/3
4	ACO	G	1001	-	-	3/47/67/67	0/3/3/3
3	LMR	G	1000	-	-	1/2/8/8	-
3	LMR	E	1000	-	-	1/2/8/8	-
3	LMR	H	1000	-	-	0/2/8/8	-
4	ACO	E	1001	-	-	3/47/67/67	0/3/3/3
5	PG4	E	1002	-	-	2/10/10/10	-
6	PGE	H	1002	-	-	4/7/7/7	-
6	PGE	G	1002	-	-	0/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1001	ACO	P3B-O3B	3.40	1.65	1.59
4	E	1001	ACO	P3B-O3B	3.06	1.65	1.59
4	H	1001	ACO	P3B-O3B	2.78	1.64	1.59
4	G	1001	ACO	P3B-O3B	2.51	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1000	LMR	O2-C2-C3	2.66	114.34	108.50
3	F	1000	LMR	O2-C2-C3	2.40	113.78	108.50
3	G	1000	LMR	O2-C2-C3	2.34	113.63	108.50
5	F	1002	PG4	O3-C4-C3	2.10	119.87	110.39
4	G	1001	ACO	C5A-C6A-N6A	2.00	123.39	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1002	PG4	O2-C3-C4-O3
5	E	1002	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	H	1002	PGE	O1-C1-C2-O2
3	F	1000	LMR	C1-C2-C3-C4
6	H	1002	PGE	O2-C3-C4-O3
5	F	1002	PG4	C8-C7-O4-C6
5	E	1002	PG4	C8-C7-O4-C6
6	H	1002	PGE	C6-C5-O3-C4
4	E	1001	ACO	CAP-CBP-CCP-O6A
3	G	1000	LMR	C1-C2-C3-C4
3	E	1000	LMR	C1-C2-C3-C4
4	E	1001	ACO	CDP-CBP-CCP-O6A
5	F	1002	PG4	O3-C5-C6-O4
4	E	1001	ACO	CEP-CBP-CCP-O6A
5	F	1002	PG4	C4-C3-O2-C2
4	G	1001	ACO	O-C-S1P-C2P
5	F	1002	PG4	C6-C5-O3-C4
4	F	1001	ACO	C3B-O3B-P3B-O9A
4	G	1001	ACO	C3B-O3B-P3B-O8A
4	F	1001	ACO	O4B-C4B-C5B-O5B
4	H	1001	ACO	P2A-O3A-P1A-O2A
4	G	1001	ACO	P2A-O3A-P1A-O1A
6	H	1002	PGE	C4-C3-O2-C2
4	F	1001	ACO	C3B-C4B-C5B-O5B
4	H	1001	ACO	O-C-S1P-C2P

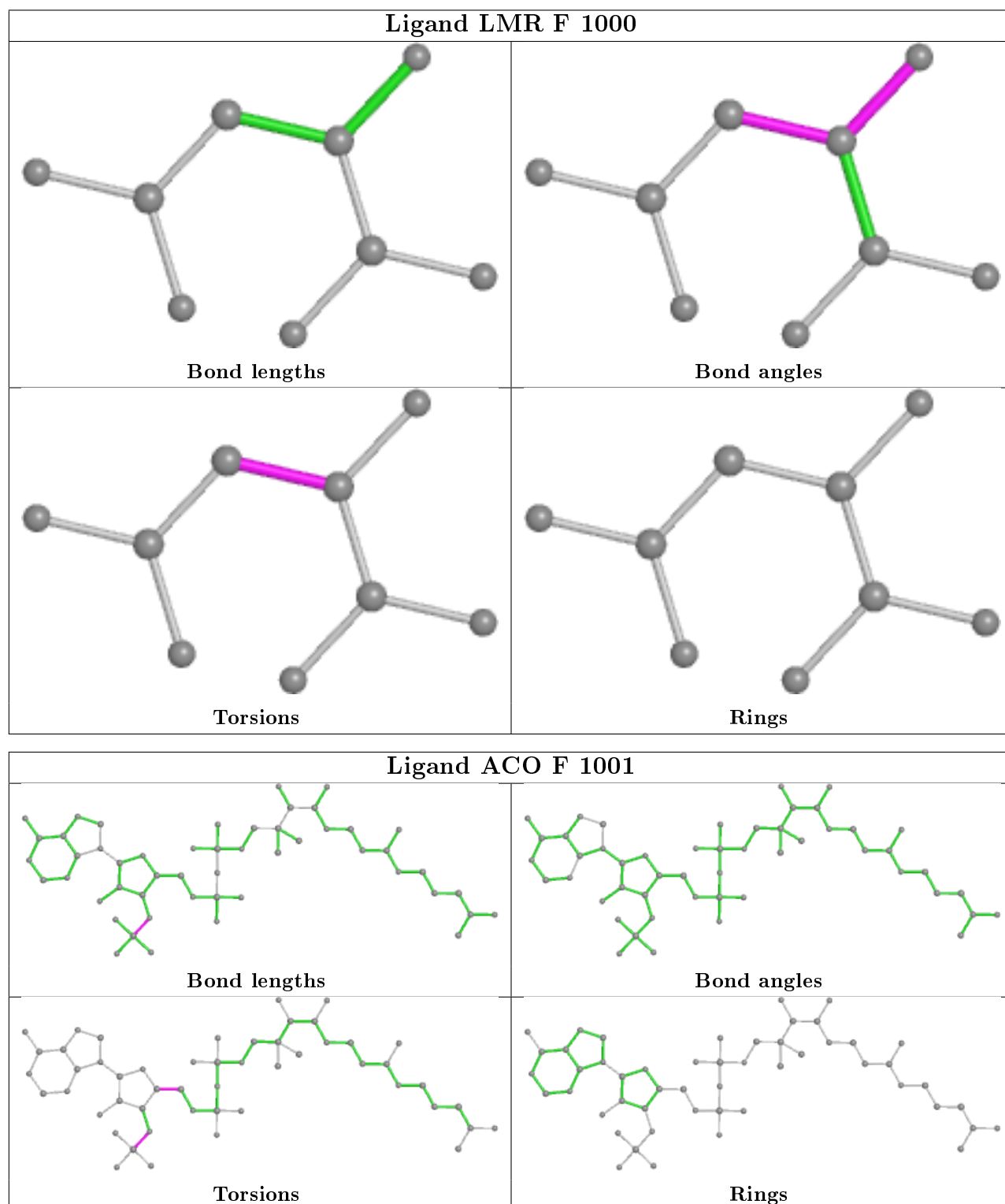
There are no ring outliers.

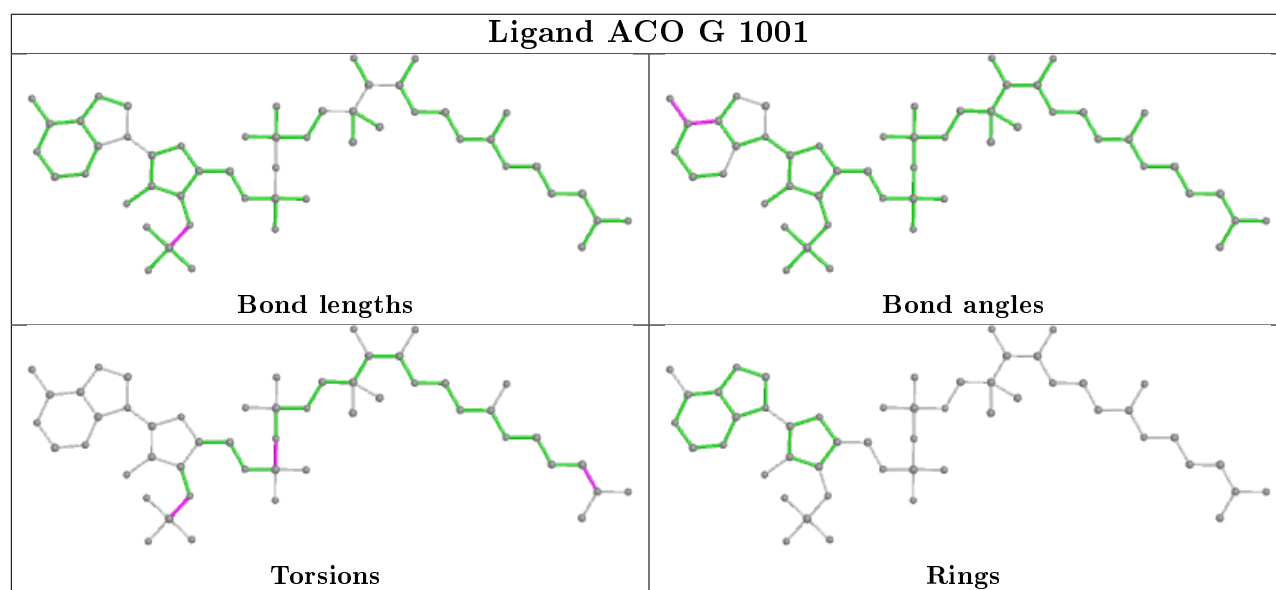
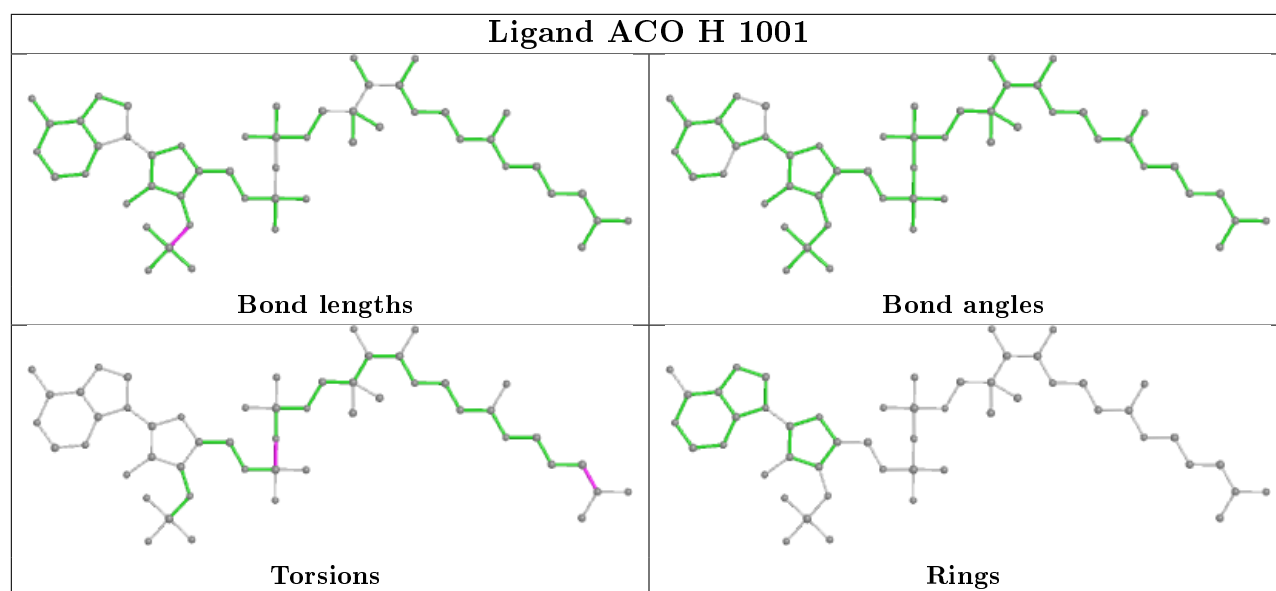
7 monomers are involved in 4 short contacts:

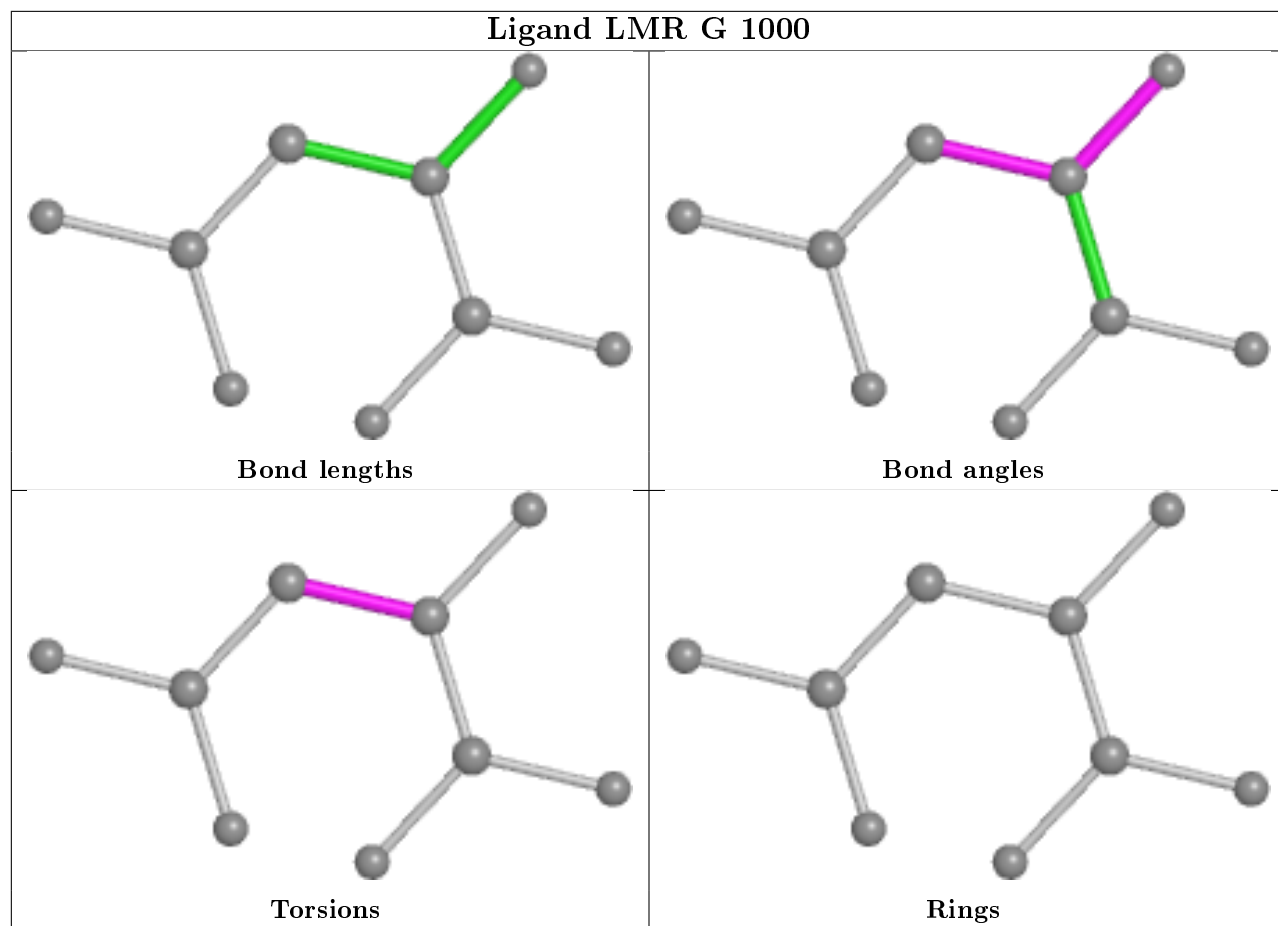
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1000	LMR	1	0
4	F	1001	ACO	1	0
5	F	1002	PG4	1	0
4	G	1001	ACO	1	0
3	G	1000	LMR	1	0
3	E	1000	LMR	1	0
4	E	1001	ACO	1	0

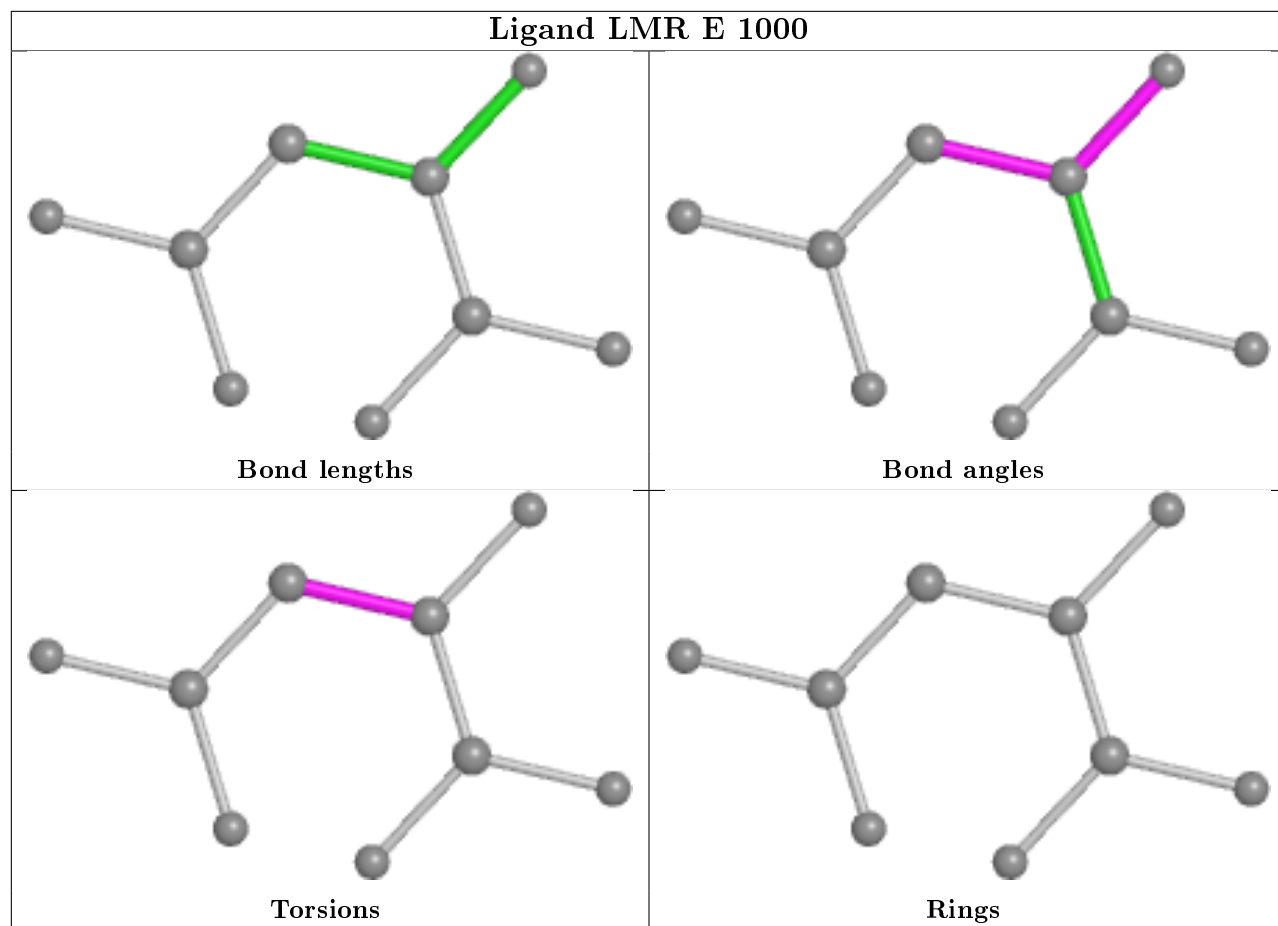
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

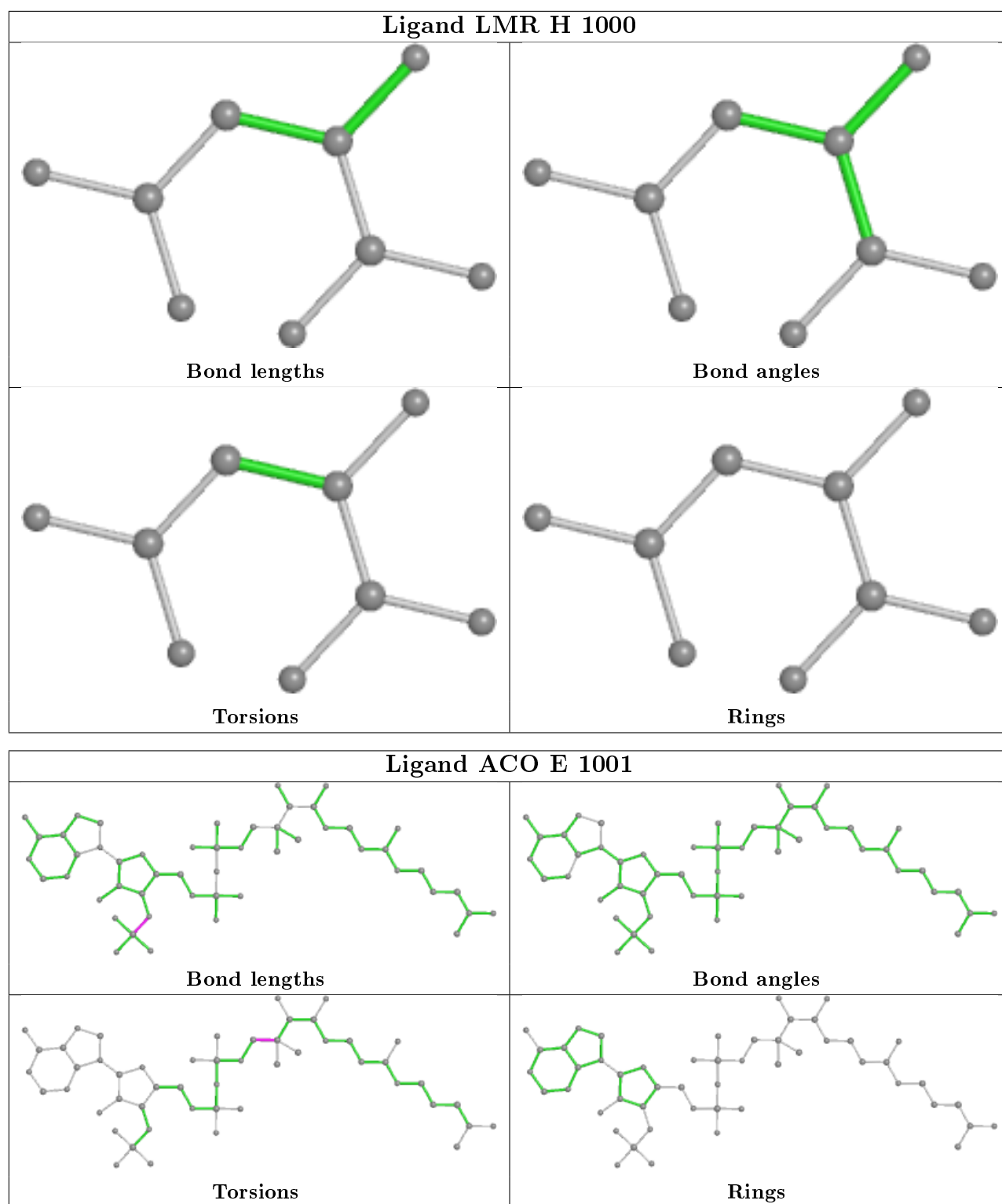
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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	215/262 (82%)	0.35	24 (11%) 5 4	12, 22, 68, 98	0
1	B	239/262 (91%)	0.79	49 (20%) 1 0	12, 27, 62, 79	0
1	C	261/262 (99%)	1.09	59 (22%) 0 0	11, 26, 78, 112	0
1	D	261/262 (99%)	0.14	15 (5%) 23 21	12, 23, 47, 83	0
1	E	256/262 (97%)	-0.16	1 (0%) 92 92	12, 22, 46, 88	0
1	F	256/262 (97%)	-0.15	2 (0%) 86 86	11, 22, 51, 85	0
1	G	261/262 (99%)	-0.25	1 (0%) 92 92	12, 18, 38, 78	0
1	H	261/262 (99%)	-0.27	2 (0%) 86 86	12, 20, 38, 72	0
All	All	2010/2096 (95%)	0.18	153 (7%) 13 12	11, 22, 57, 112	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	483	VAL	9.7
1	C	496	VAL	9.6
1	C	493	VAL	8.7
1	C	535	LYS	8.3
1	C	536	GLY	8.3
1	B	478	TRP	8.2
1	C	533	ALA	8.1
1	C	530	VAL	7.2
1	A	351	VAL	7.2
1	C	478	TRP	7.0
1	C	538	LEU	6.7
1	A	460	TYR	6.5
1	B	468	TYR	6.2
1	B	486	VAL	6.1
1	C	492	ARG	6.1
1	A	461	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	497	LYS	5.8
1	D	492	ARG	5.7
1	C	472	ILE	5.7
1	C	480	LYS	5.7
1	B	489	ILE	5.6
1	B	481	LYS	5.4
1	C	485	PRO	5.3
1	B	517	HIS	5.3
1	B	538	LEU	5.3
1	B	493	VAL	5.2
1	D	496	VAL	5.2
1	D	493	VAL	5.2
1	D	497	LYS	5.2
1	C	475	PHE	5.1
1	C	539	ILE	5.1
1	C	534	LYS	5.1
1	A	468	TYR	5.0
1	B	516	LEU	4.9
1	C	468	TYR	4.8
1	C	481	LYS	4.8
1	C	473	PRO	4.7
1	C	477	SER	4.7
1	C	476	LEU	4.7
1	C	537	ASN	4.6
1	B	495	SER	4.5
1	C	460	TYR	4.5
1	C	489	ILE	4.4
1	B	523	TYR	4.4
1	C	486	VAL	4.4
1	B	476	LEU	4.3
1	C	491	HIS	4.3
1	A	523	TYR	4.3
1	D	533	ALA	4.2
1	C	532	THR	4.2
1	A	463	MET	4.2
1	B	501	GLN	4.2
1	B	491	HIS	4.1
1	B	485	PRO	4.1
1	B	492	ARG	4.0
1	B	477	SER	4.0
1	B	539	ILE	3.9
1	B	499	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	469	PRO	3.8
1	C	482	ASN	3.8
1	C	461	PHE	3.8
1	C	517	HIS	3.7
1	B	475	PHE	3.6
1	B	540	LEU	3.6
1	C	527	VAL	3.5
1	B	484	GLY	3.4
1	C	529	LYS	3.4
1	B	461	PHE	3.4
1	C	484	GLY	3.3
1	C	525	LEU	3.3
1	C	470	ASN	3.3
1	A	467	ASP	3.3
1	C	471	ASP	3.2
1	C	469	PRO	3.2
1	C	474	GLY	3.2
1	B	504	LYS	3.2
1	B	526	GLU	3.2
1	B	527	VAL	3.2
1	B	506	LEU	3.2
1	B	525	LEU	3.1
1	C	540	LEU	3.1
1	C	467	ASP	3.1
1	C	459	LYS	3.1
1	A	525	LEU	3.1
1	A	511	LYS	3.1
1	D	535	LYS	3.1
1	B	469	PRO	3.1
1	C	464	ALA	3.1
1	A	470	ASN	3.0
1	A	501	GLN	3.0
1	B	512	ASN	3.0
1	C	499	PRO	3.0
1	B	352	GLU	3.0
1	C	494	LYS	3.0
1	C	465	VAL	2.9
1	B	521	LEU	2.9
1	B	510	ILE	2.9
1	B	507	VAL	2.9
1	C	510	ILE	2.9
1	C	526	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	453	ALA	2.8
1	C	523	TYR	2.7
1	A	506	LEU	2.7
1	C	453	ALA	2.7
1	B	482	ASN	2.7
1	D	534	LYS	2.7
1	C	531	THR	2.7
1	C	457	ALA	2.7
1	B	480	LYS	2.7
1	D	470	ASN	2.7
1	A	352	GLU	2.7
1	C	487	PRO	2.7
1	B	483	VAL	2.6
1	B	505	TYR	2.5
1	A	457	ALA	2.5
1	C	479	MET	2.5
1	D	606	GLU	2.5
1	B	465	VAL	2.5
1	B	467	ASP	2.5
1	A	466	GLU	2.5
1	A	464	ALA	2.4
1	B	511	LYS	2.4
1	B	500	ASP	2.4
1	D	499	PRO	2.4
1	B	508	SER	2.4
1	C	524	ALA	2.4
1	A	499	PRO	2.3
1	D	473	PRO	2.3
1	C	463	MET	2.3
1	B	487	PRO	2.3
1	B	513	GLU	2.3
1	E	470	ASN	2.3
1	F	517	HIS	2.2
1	C	528	GLU	2.2
1	C	498	ASN	2.2
1	B	514	THR	2.2
1	H	350	MET	2.2
1	D	530	VAL	2.2
1	H	347	GLY	2.1
1	G	365	GLU	2.1
1	F	535	LYS	2.1
1	B	463	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	347	GLY	2.1
1	D	495	SER	2.1
1	A	439	VAL	2.1
1	A	541	ASN	2.1
1	D	532	THR	2.1
1	A	459	LYS	2.1
1	B	509	TYR	2.0
1	A	516	LEU	2.0
1	A	517	HIS	2.0
1	B	520	CYS	2.0
1	D	536	GLY	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 carbohydrates 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.

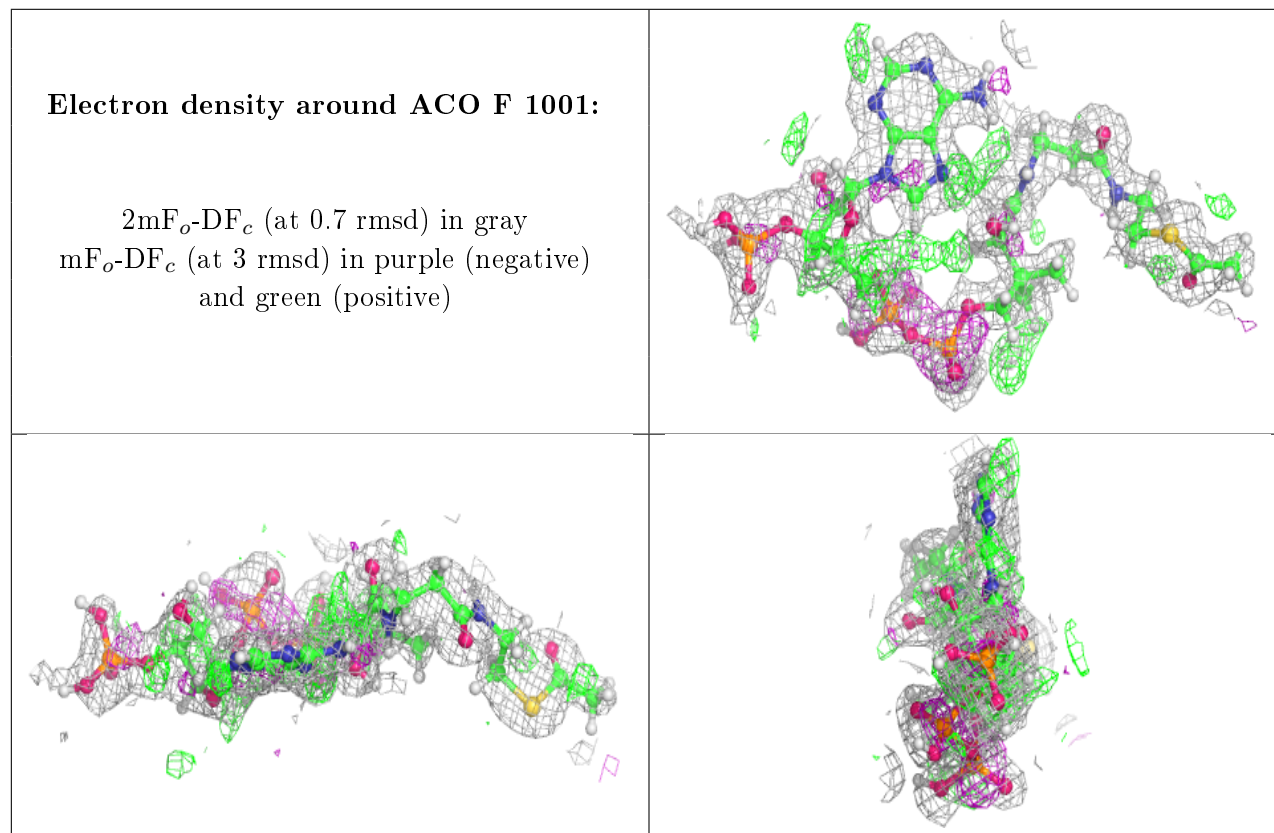
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PG4	E	1002	13/13	0.77	0.14	39,47,53,54	0
5	PG4	F	1002	13/13	0.81	0.12	30,37,42,45	0
4	ACO	F	1001	51/51	0.81	0.15	20,32,58,63	0
3	LMR	F	1000	9/9	0.88	0.15	25,30,34,35	0
6	PGE	G	1002	10/10	0.88	0.11	39,43,50,52	0
6	PGE	H	1002	10/10	0.90	0.11	40,42,46,50	0
3	LMR	E	1000	9/9	0.93	0.10	24,24,28,28	0
4	ACO	E	1001	51/51	0.95	0.08	12,24,43,46	0
3	LMR	H	1000	9/9	0.96	0.07	17,20,22,23	0
4	ACO	H	1001	51/51	0.97	0.07	12,20,39,48	0
4	ACO	G	1001	51/51	0.97	0.07	11,18,38,44	0
3	LMR	G	1000	9/9	0.98	0.07	15,20,22,24	0

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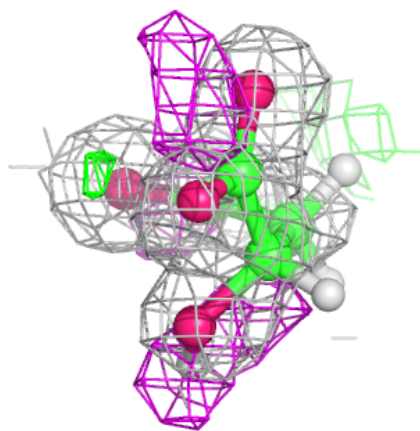
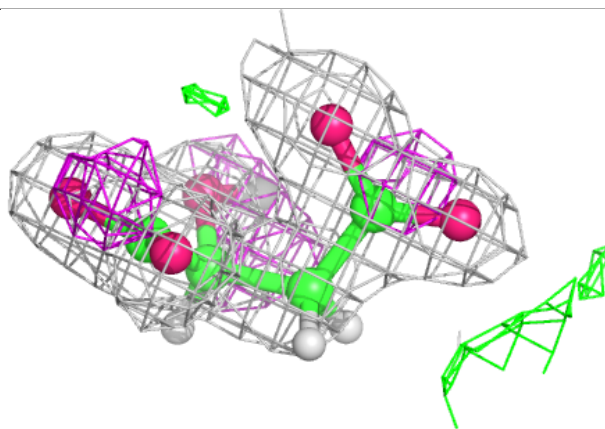
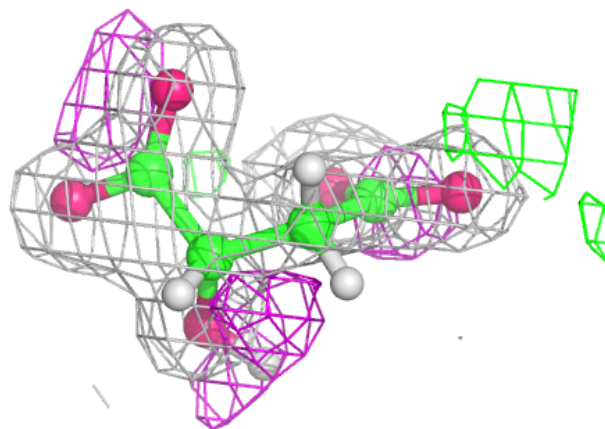
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	701	1/1	0.99	0.06	15,15,15,15	0
2	CA	A	701	1/1	1.00	0.06	14,14,14,14	0

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.



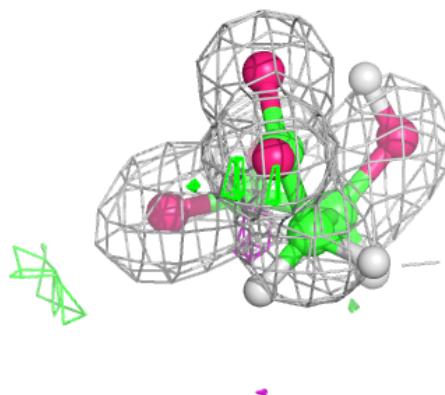
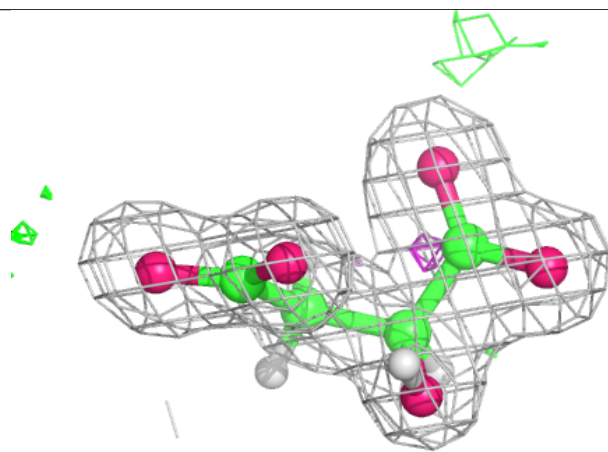
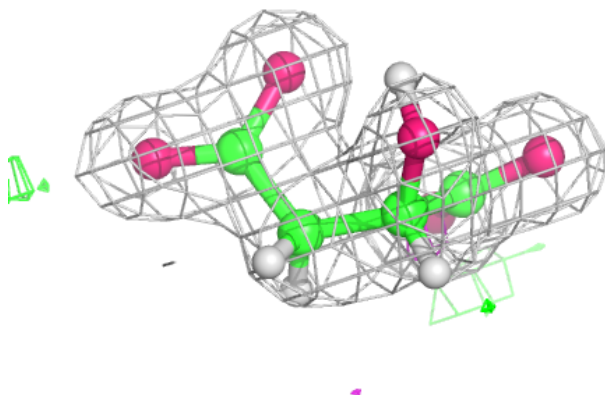
**Electron density around LMR F 1000:**

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



**Electron density around LMR E 1000:**

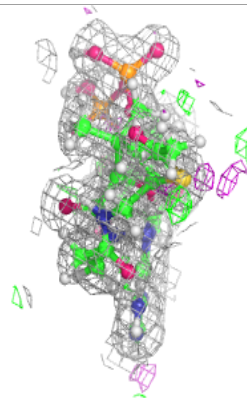
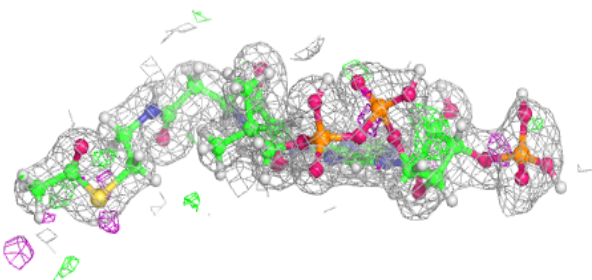
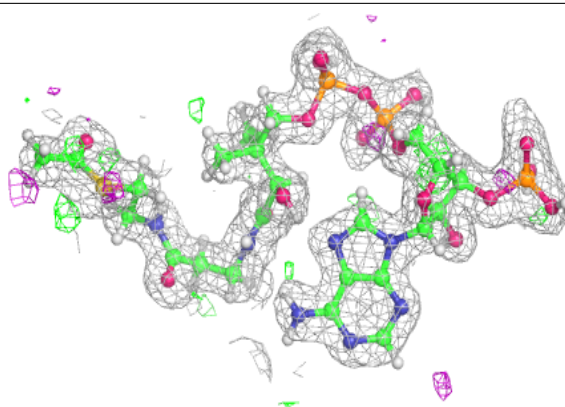
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





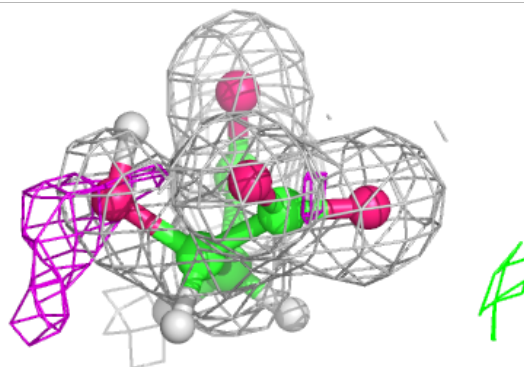
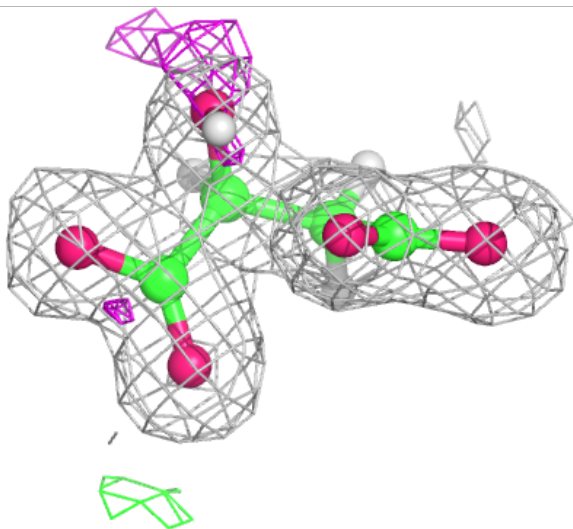
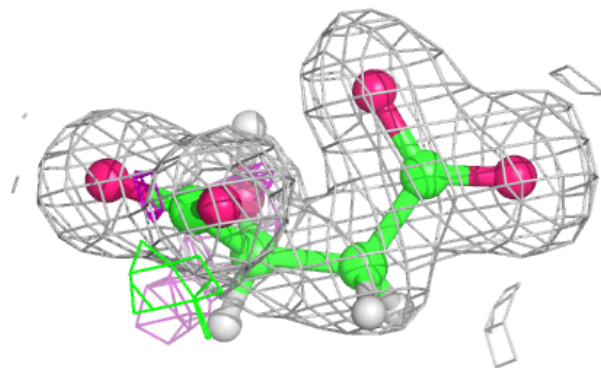
**Electron density around ACO E 1001:**

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



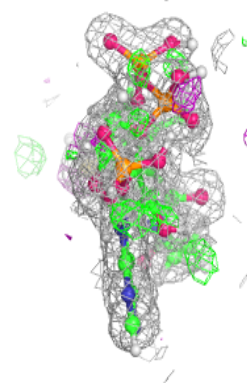
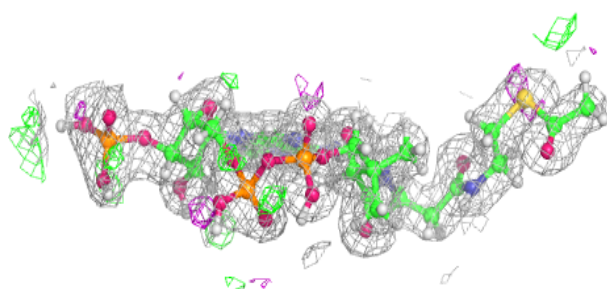
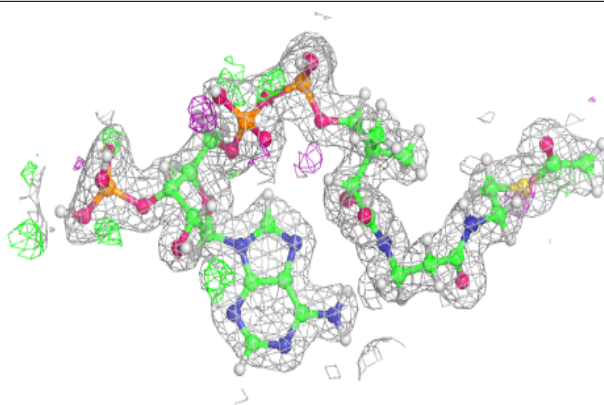
**Electron density around LMR H 1000:**

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

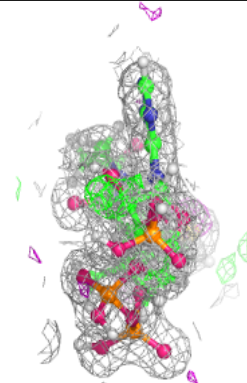
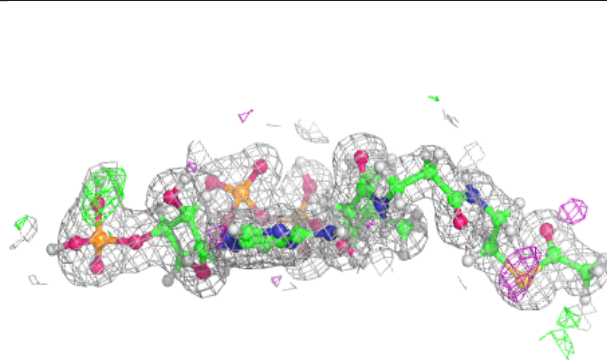
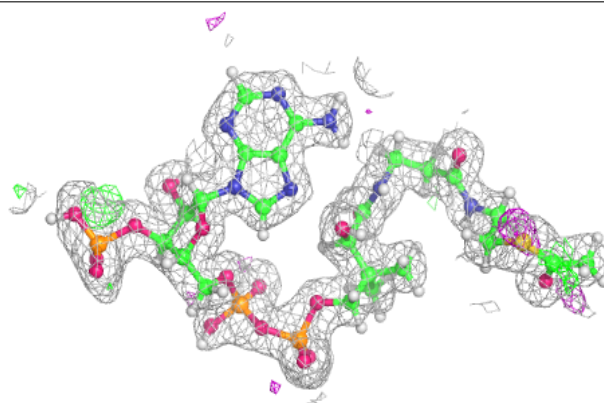


**Electron density around ACO H 1001:**

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

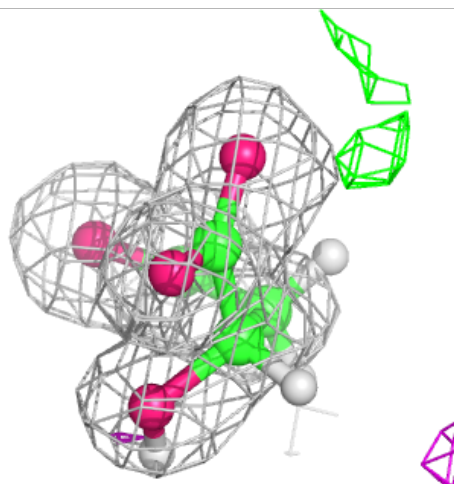
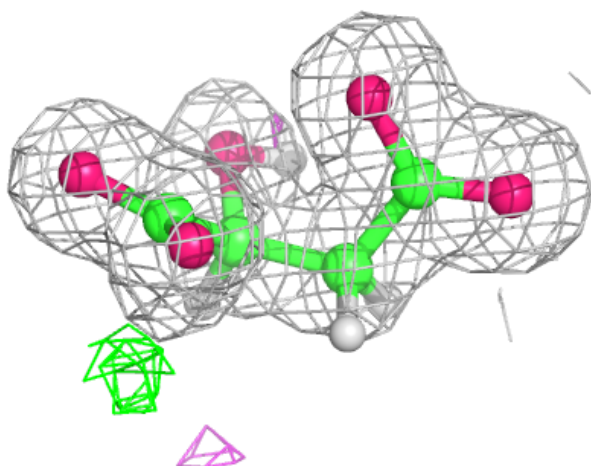
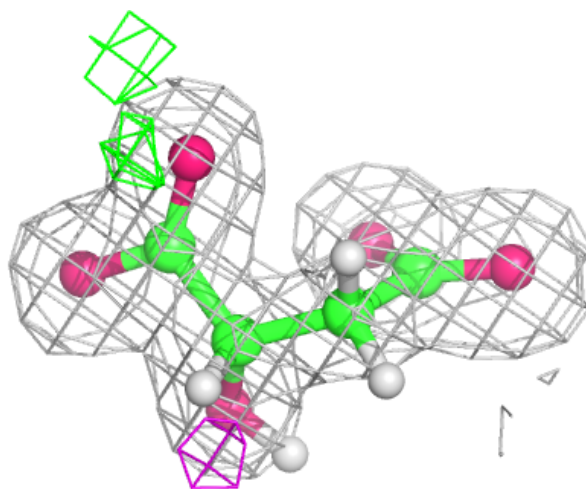
**Electron density around ACO G 1001:**

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



**Electron density around LMR G 1000:**

$2mF_o-DF_c$  (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.