



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:05 AM UTC

PDB ID : 6QCL / pdb_00006qcl
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

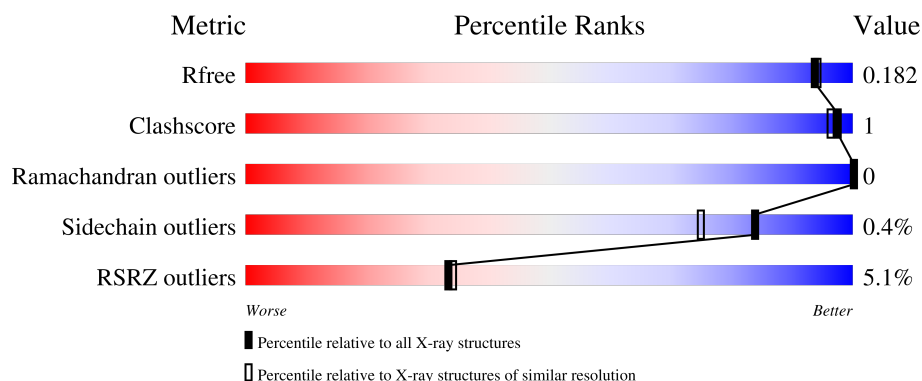
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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.



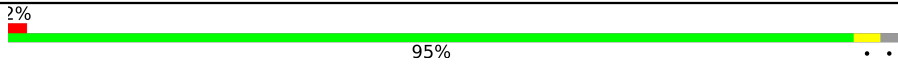
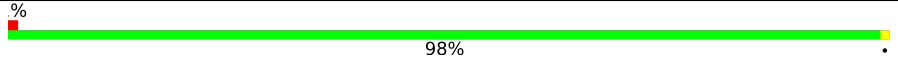
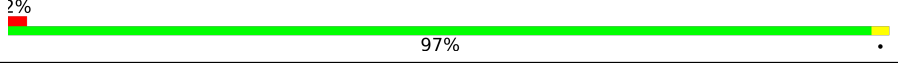
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 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	262	 7% 81% 18%
1	B	262	 13% 89% 9%
1	C	262	 10% 98% 2%
1	D	262	 3% 95% 2%
1	E	262	 2% 96% 2%

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Mol	Chain	Length	Quality of chain
1	F	262	
1	G	262	
1	H	262	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMR	F	1000	-	X	-	-
3	LMR	G	1000	-	X	-	-

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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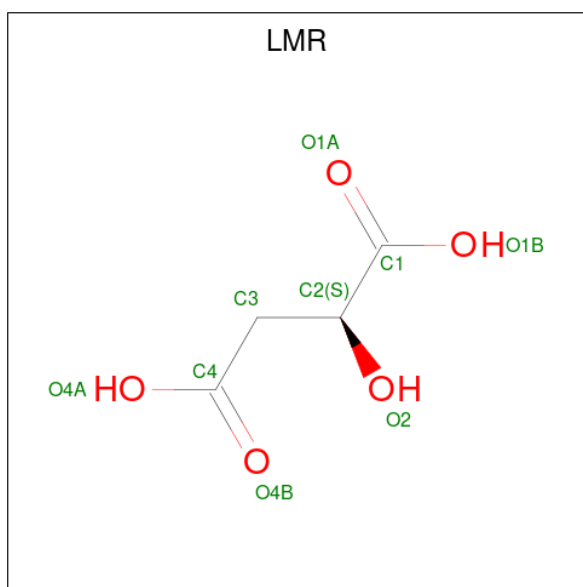
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Chain	Residue	Modelled	Actual	Comment	Reference
D	348	SER	-	expression tag	UNP Q9AJC4
D	349	HIS	-	expression tag	UNP Q9AJC4
D	350	MET	-	expression tag	UNP Q9AJC4
E	347	GLY	-	expression tag	UNP Q9AJC4
E	348	SER	-	expression tag	UNP Q9AJC4
E	349	HIS	-	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 (CCD ID: CA) (formula: Ca).

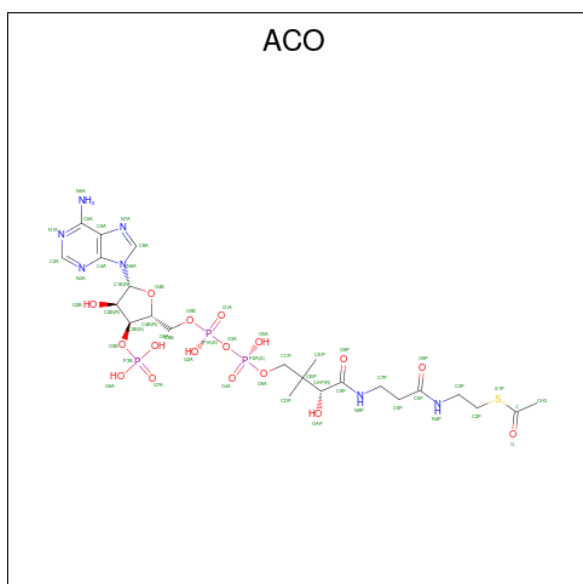
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅) (labeled as "Ligand of Interest" by depositor).



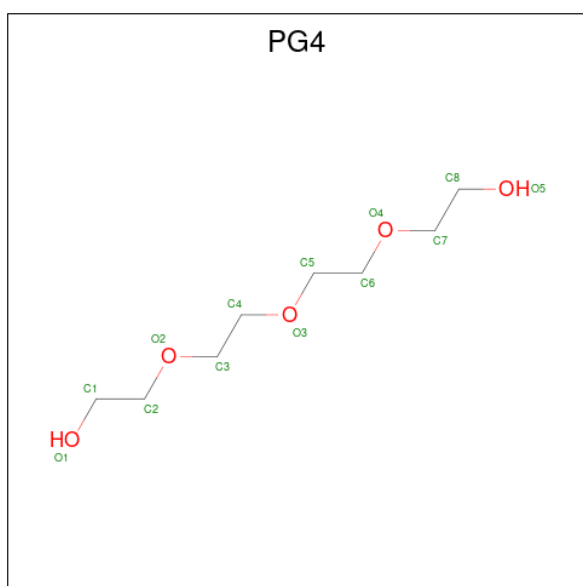
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 13	C 4	H 4	O 5	0	0
3	F	1	Total 13	C 4	H 4	O 5	0	0
3	G	1	Total 13	C 4	H 4	O 5	0	0
3	H	1	Total 13	C 4	H 4	O 5	0	0

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



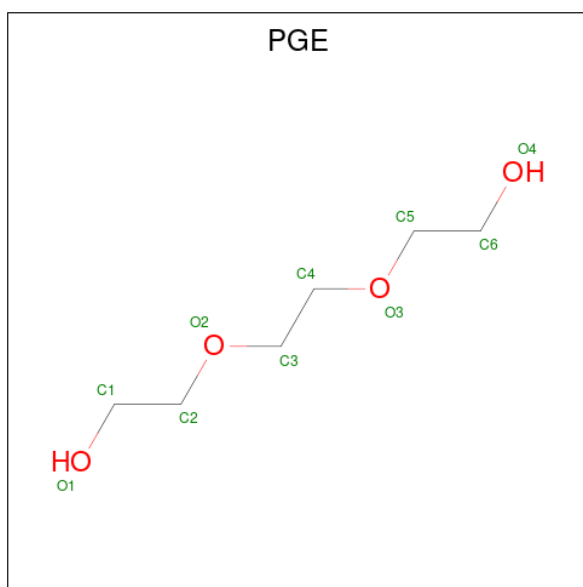
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	F	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	G	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		
4	H	1	Total	C	H	N	O	P	S	0	0
			89	23	38	7	17	3	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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		

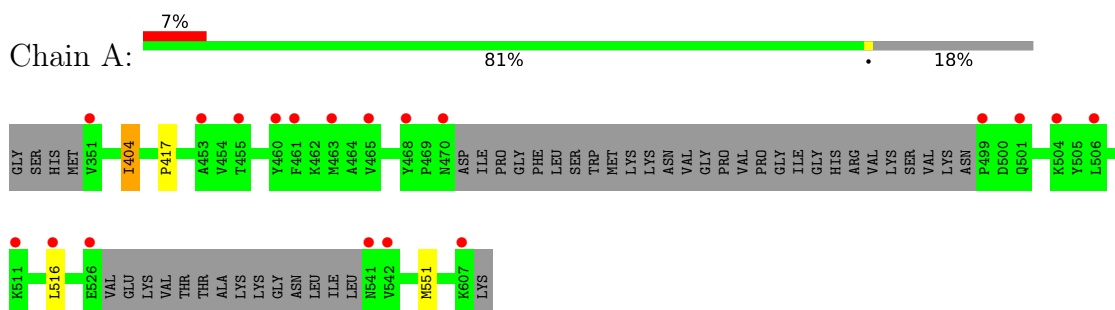
- Molecule 7 is water.

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		

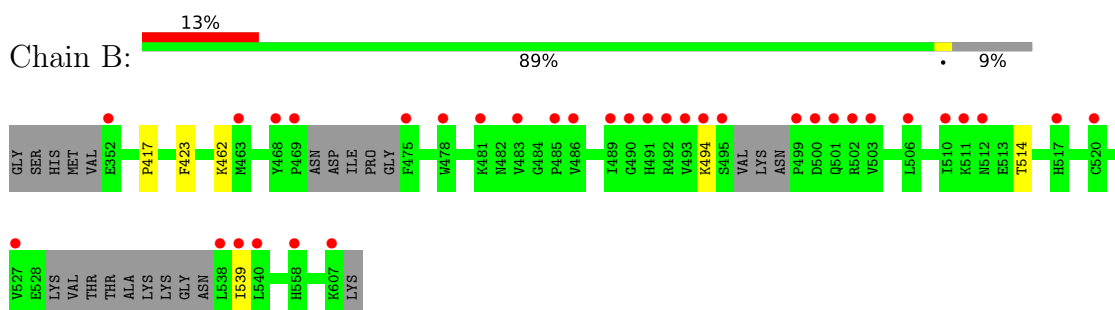
3 Residue-property plots [i](#)

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.

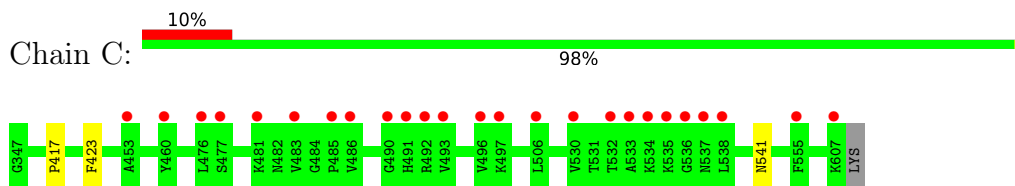
- Molecule 1: ATP-citrate lyase alpha-subunit



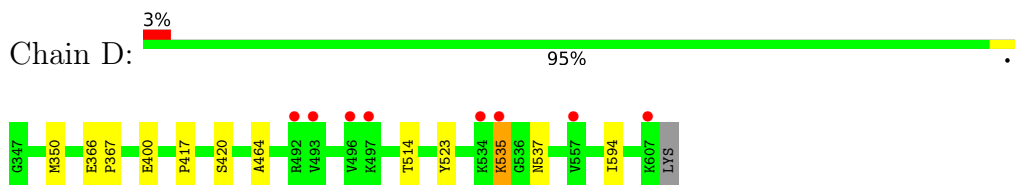
- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit



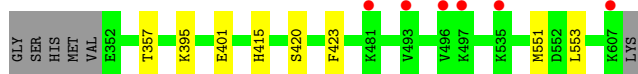
- Molecule 1: ATP-citrate lyase alpha-subunit



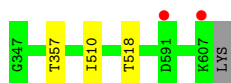
- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit



- Molecule 1: ATP-citrate lyase alpha-subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.8 (45.62-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.157 , 0.177 0.159 , 0.182	Depositor DCC
R_{free} test set	13821 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: ACO, PGE, LMR, 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	0.84	2/1731 (0.1%)	0.97	0/2344
1	B	0.82	0/1917	0.97	1/2593 (0.0%)
1	C	0.82	0/2081	1.00	2/2819 (0.1%)
1	D	0.84	1/2081 (0.0%)	1.00	2/2819 (0.1%)
1	E	0.79	1/2055 (0.0%)	0.95	0/2785
1	F	0.79	1/2060 (0.0%)	0.96	2/2791 (0.1%)
1	G	0.79	0/2088	0.93	0/2830
1	H	0.79	0/2108	0.95	1/2857 (0.0%)
All	All	0.81	5/16121 (0.0%)	0.97	8/21838 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	350	MET	SD-CE	-8.74	1.57	1.79
1	A	404	ILE	CG1-CD1	-7.23	1.23	1.51
1	A	551	MET	SD-CE	-5.71	1.65	1.79
1	F	551	MET	SD-CE	-5.60	1.65	1.79
1	E	551	MET	SD-CE	-5.08	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	423	PHE	CA-CB-CG	6.61	120.41	113.80
1	F	423	PHE	CA-CB-CG	5.44	119.24	113.80
1	D	420	SER	N-CA-C	5.39	117.16	111.28
1	D	400	GLU	CB-CG-CD	5.30	121.60	112.60
1	C	541	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	423	PHE	CA-CB-CG	-5.12	108.68	113.80
1	C	423	PHE	CA-CB-CG	-5.12	108.68	113.80
1	F	420	SER	N-CA-C	5.08	116.81	111.28

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	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
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
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
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%)	183 (100%)	0	100	100
1	B	203/219 (93%)	201 (99%)	2 (1%)	68	50
1	C	221/219 (101%)	221 (100%)	0	100	100
1	D	221/219 (101%)	219 (99%)	2 (1%)	70	55
1	E	218/219 (100%)	218 (100%)	0	100	100
1	F	219/219 (100%)	217 (99%)	2 (1%)	70	55
1	G	222/219 (101%)	222 (100%)	0	100	100
1	H	225/219 (103%)	224 (100%)	1 (0%)	84	75
All	All	1712/1752 (98%)	1705 (100%)	7 (0%)	84	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	462	LYS
1	B	514	THR
1	D	514	THR
1	D	535	LYS
1	F	395	LYS
1	F	415	HIS
1	H	514	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	512	ASN
1	B	580	ASN
1	C	580	ASN
1	D	349	HIS
1	D	498	ASN
1	D	580	ASN
1	E	580	ASN
1	E	602	GLN
1	F	501	GLN
1	G	517	HIS
1	G	580	ASN
1	H	349	HIS
1	H	580	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	H	1000	-	8,8,8	1.46	2 (25%)	10,10,10	2.57	3 (30%)
4	ACO	E	1001	-	51,53,53	0.61	1 (1%)	73,79,79	0.52	0
6	PGE	G	1002	-	9,9,9	0.15	0	8,8,8	0.20	0
6	PGE	H	1002	-	9,9,9	0.19	0	8,8,8	0.13	0
3	LMR	F	1000	-	8,8,8	1.98	4 (50%)	10,10,10	2.71	5 (50%)
5	PG4	E	1002	-	12,12,12	0.17	0	11,11,11	0.25	0
3	LMR	G	1000	-	8,8,8	1.96	4 (50%)	10,10,10	2.86	5 (50%)
5	PG4	F	1002	-	12,12,12	0.33	0	11,11,11	0.84	1 (9%)
4	ACO	H	1001	-	51,53,53	0.54	1 (1%)	73,79,79	0.56	0
4	ACO	F	1001	-	51,53,53	0.59	1 (1%)	73,79,79	0.60	0
4	ACO	G	1001	-	51,53,53	0.59	1 (1%)	73,79,79	0.50	0
3	LMR	E	1000	-	8,8,8	0.39	0	10,10,10	1.11	1 (10%)

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	H	1000	-	-	4/8/8/8	-
4	ACO	E	1001	-	-	4/51/67/67	0/3/3/3
6	PGE	G	1002	-	-	0/7/7/7	-
6	PGE	H	1002	-	-	4/7/7/7	-
3	LMR	F	1000	-	-	2/8/8/8	-
5	PG4	E	1002	-	-	2/10/10/10	-
3	LMR	G	1000	-	-	2/8/8/8	-
5	PG4	F	1002	-	-	5/10/10/10	-
4	ACO	H	1001	-	-	2/51/67/67	0/3/3/3
4	ACO	F	1001	-	-	3/51/67/67	0/3/3/3
4	ACO	G	1001	-	-	4/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMR	E	1000	-	-	5/8/8/8	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1000	LMR	O4B-C4	3.65	1.34	1.22
4	F	1001	ACO	P3B-O3B	3.54	1.65	1.59
3	H	1000	LMR	O1A-C1	3.33	1.32	1.22
3	G	1000	LMR	O1A-C1	3.28	1.31	1.22
4	E	1001	ACO	P3B-O3B	3.18	1.65	1.59
3	G	1000	LMR	O4B-C4	3.05	1.32	1.22
4	H	1001	ACO	P3B-O3B	2.87	1.64	1.59
3	F	1000	LMR	O1A-C1	2.73	1.30	1.22
4	G	1001	ACO	P3B-O3B	2.58	1.64	1.59
3	F	1000	LMR	O4A-C4	-2.31	1.23	1.30
3	G	1000	LMR	O4A-C4	-2.28	1.23	1.30
3	G	1000	LMR	O1B-C1	-2.28	1.23	1.30
3	H	1000	LMR	O1B-C1	-2.27	1.23	1.30
3	F	1000	LMR	O1B-C1	-2.24	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1000	LMR	O1A-C1-C2	-5.59	111.43	122.60
3	F	1000	LMR	O1A-C1-C2	-5.59	111.44	122.60
3	H	1000	LMR	O1A-C1-C2	-5.43	111.75	122.60
3	H	1000	LMR	O1B-C1-C2	5.36	124.06	112.74
3	G	1000	LMR	O1B-C1-C2	5.29	123.93	112.74
3	F	1000	LMR	O1B-C1-C2	5.00	123.31	112.74
3	E	1000	LMR	C2-C3-C4	2.50	118.63	112.08
3	G	1000	LMR	O4B-C4-C3	-2.45	115.33	122.84
3	G	1000	LMR	O4A-C4-C3	2.41	121.49	114.00
3	G	1000	LMR	C2-C3-C4	2.29	118.06	112.08
3	H	1000	LMR	C2-C3-C4	2.25	117.97	112.08
3	F	1000	LMR	O4A-C4-C3	2.10	120.53	114.00
3	F	1000	LMR	O4B-C4-C3	-2.10	116.40	122.84
5	F	1002	PG4	O3-C4-C3	2.09	119.87	110.35
3	F	1000	LMR	C2-C3-C4	2.06	117.46	112.08

There are no chirality outliers.

All (37) 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
6	H	1002	PGE	O1-C1-C2-O2
3	E	1000	LMR	O1B-C1-C2-C3
6	H	1002	PGE	O2-C3-C4-O3
5	E	1002	PG4	C8-C7-O4-C6
4	E	1001	ACO	CDP-CBP-CCP-O6A
6	H	1002	PGE	C6-C5-O3-C4
5	F	1002	PG4	C8-C7-O4-C6
4	E	1001	ACO	CAP-CBP-CCP-O6A
3	E	1000	LMR	C2-C3-C4-O4B
3	H	1000	LMR	C2-C3-C4-O4B
3	E	1000	LMR	O1A-C1-C2-C3
3	G	1000	LMR	O1A-C1-C2-C3
3	H	1000	LMR	O1A-C1-C2-C3
5	F	1002	PG4	O3-C5-C6-O4
4	G	1001	ACO	O-C-S1P-C2P
3	E	1000	LMR	C2-C3-C4-O4A
3	H	1000	LMR	C2-C3-C4-O4A
5	F	1002	PG4	C4-C3-O2-C2
3	F	1000	LMR	O1A-C1-C2-C3
3	F	1000	LMR	O1B-C1-C2-C3
3	G	1000	LMR	O1B-C1-C2-C3
3	H	1000	LMR	O1B-C1-C2-C3
4	H	1001	ACO	O-C-S1P-C2P
5	F	1002	PG4	C6-C5-O3-C4
4	G	1001	ACO	P2A-O3A-P1A-O1A
4	H	1001	ACO	P2A-O3A-P1A-O2A
4	F	1001	ACO	C3B-C4B-C5B-O5B
6	H	1002	PGE	C4-C3-O2-C2
4	E	1001	ACO	CEP-CBP-CCP-O6A
4	G	1001	ACO	CDP-CBP-CCP-O6A
4	F	1001	ACO	O4B-C4B-C5B-O5B
3	E	1000	LMR	O1B-C1-C2-O2
4	E	1001	ACO	P2A-O3A-P1A-O2A
4	F	1001	ACO	P2A-O3A-P1A-O2A
4	G	1001	ACO	P2A-O3A-P1A-O2A

There are no ring outliers.

7 monomers are involved in 4 short contacts:

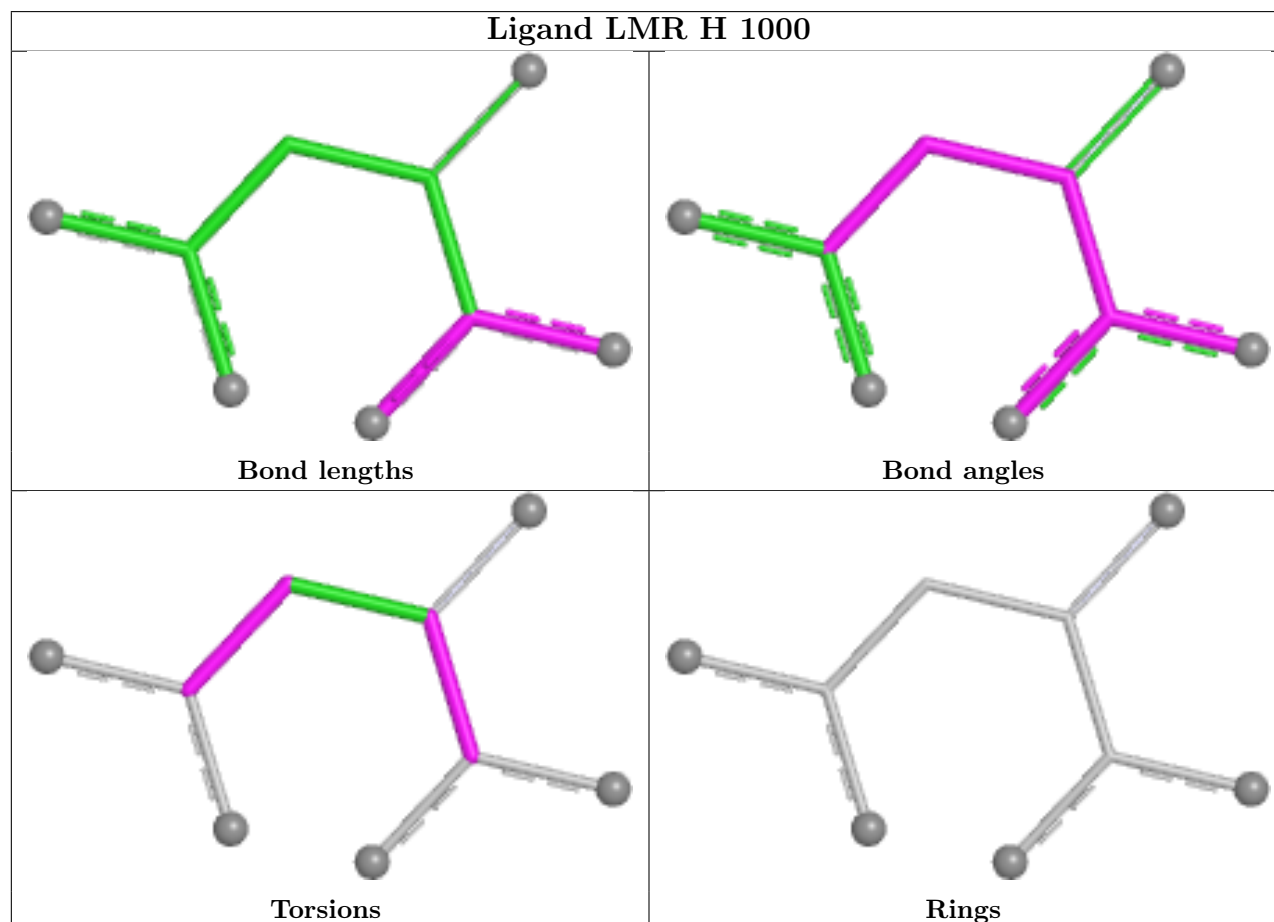
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1001	ACO	1	0

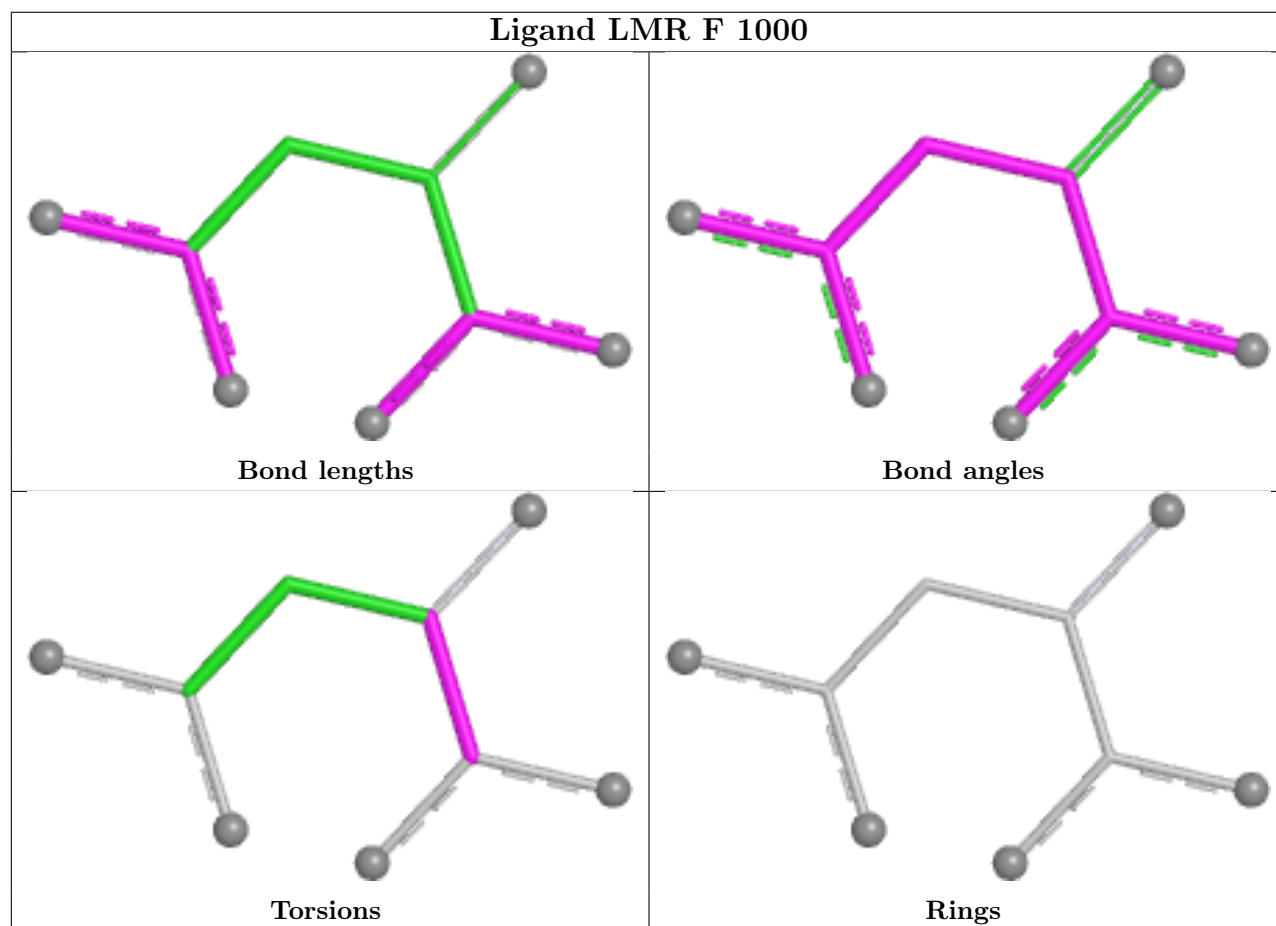
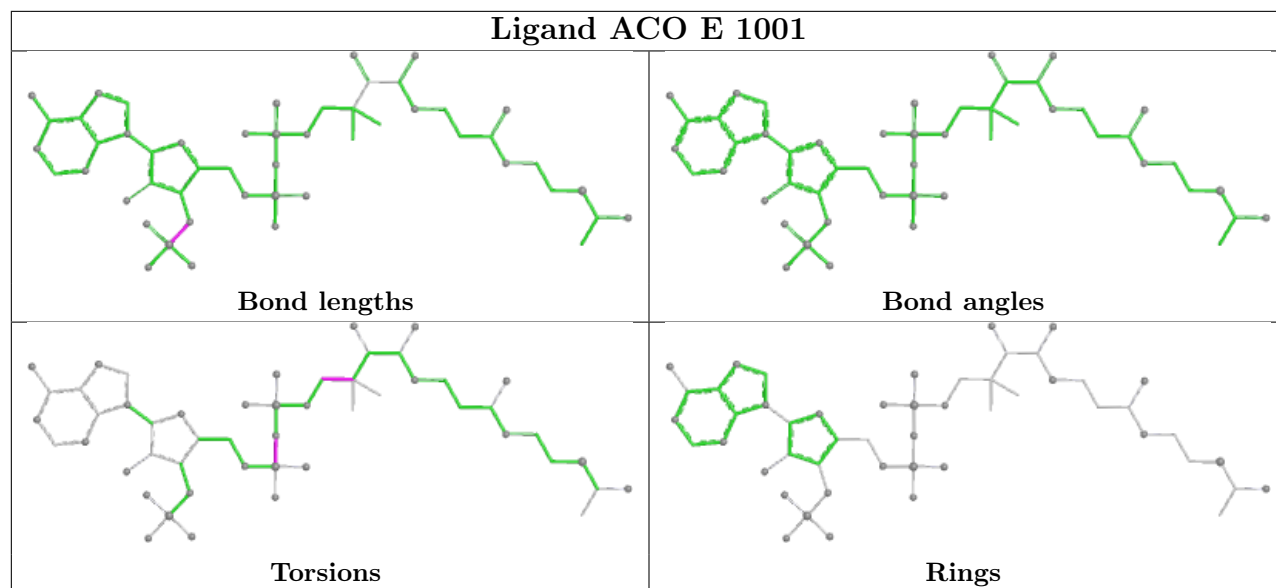
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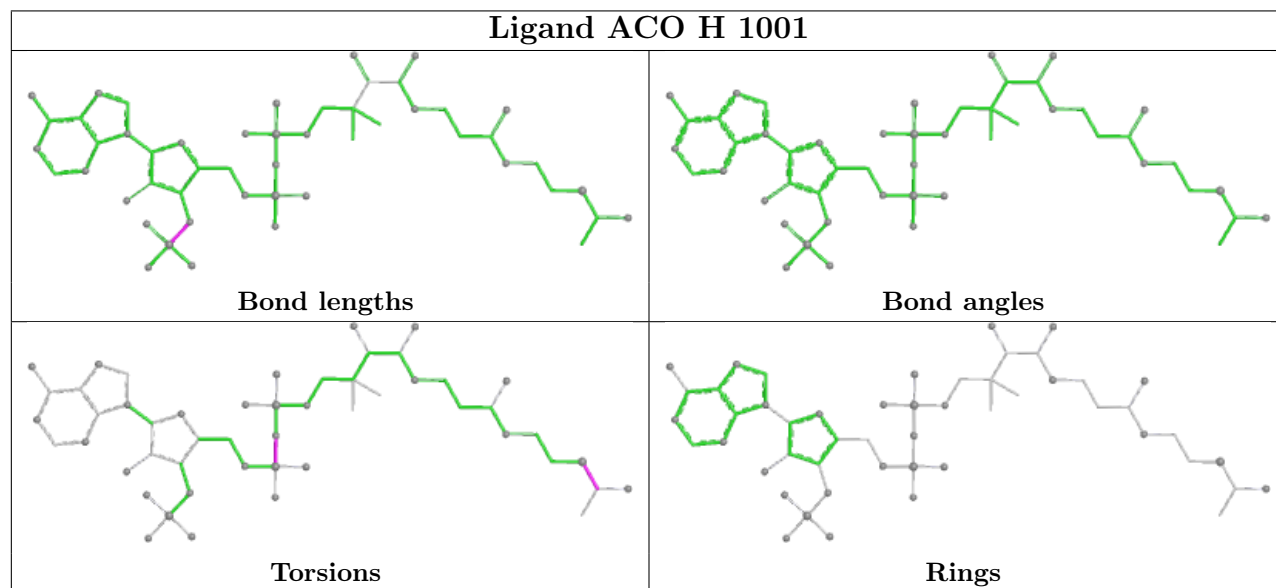
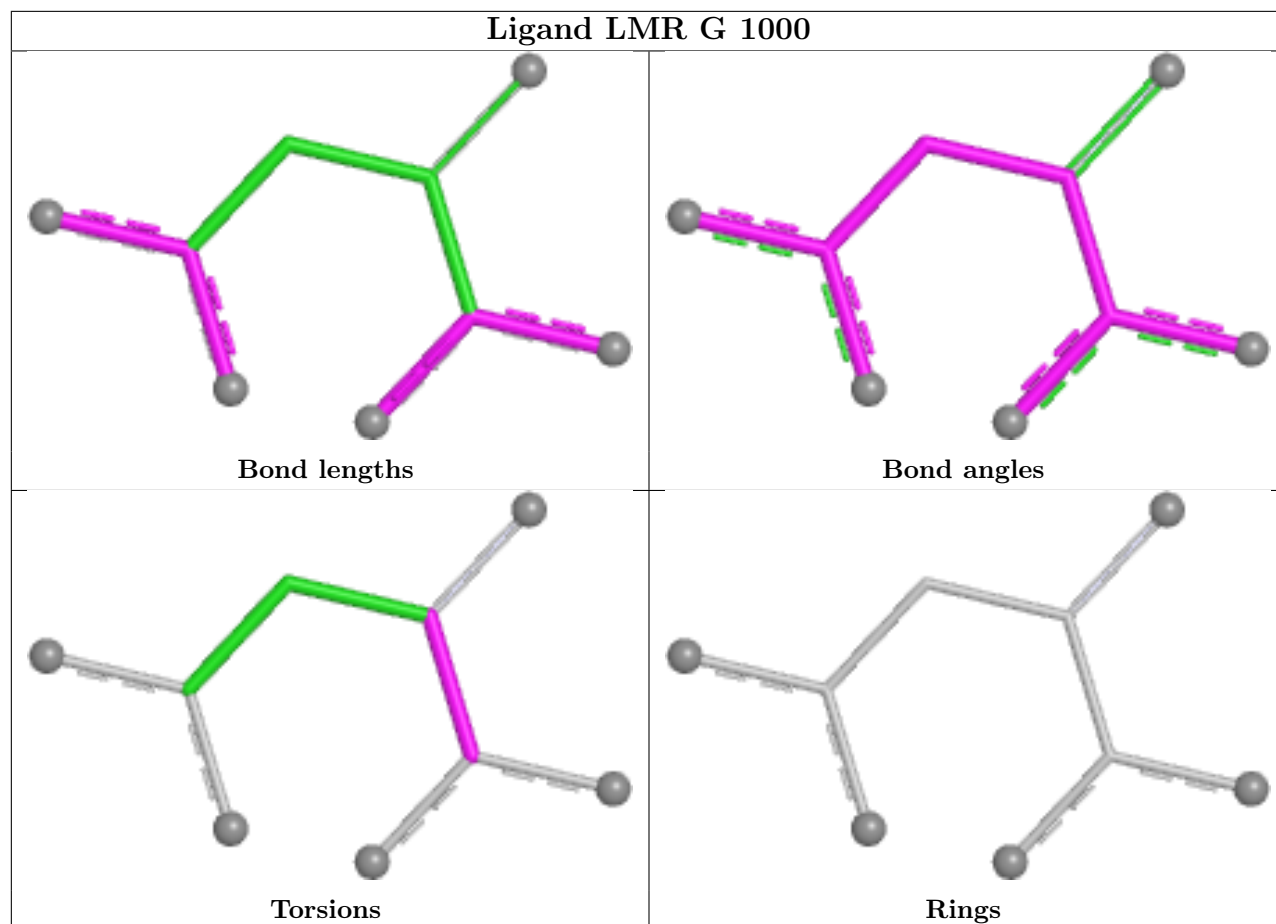
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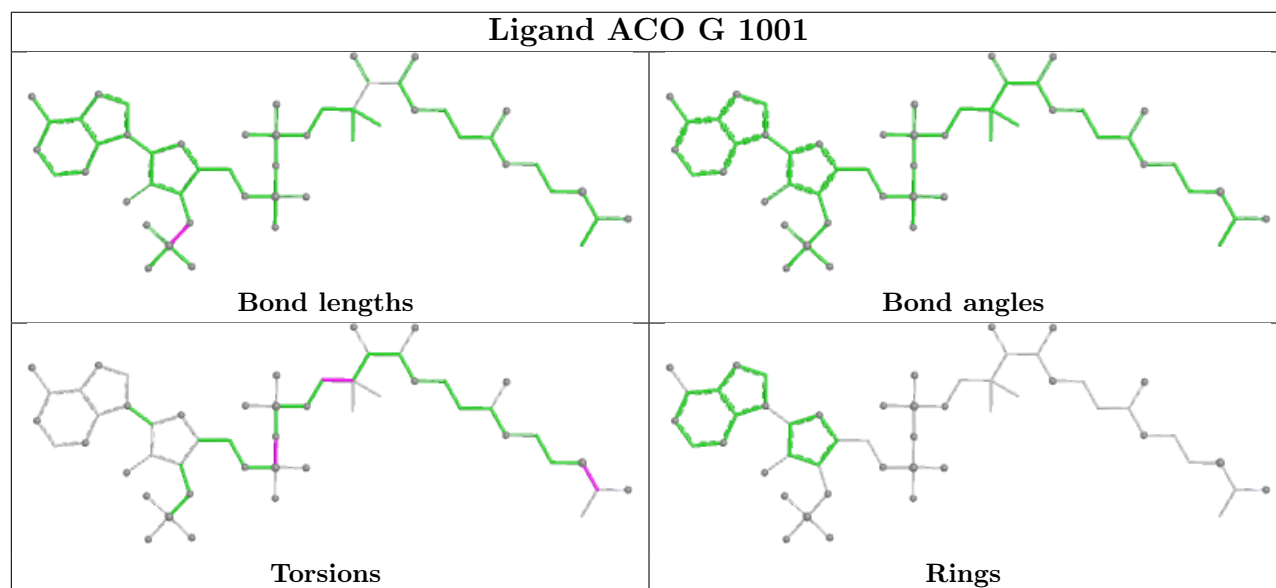
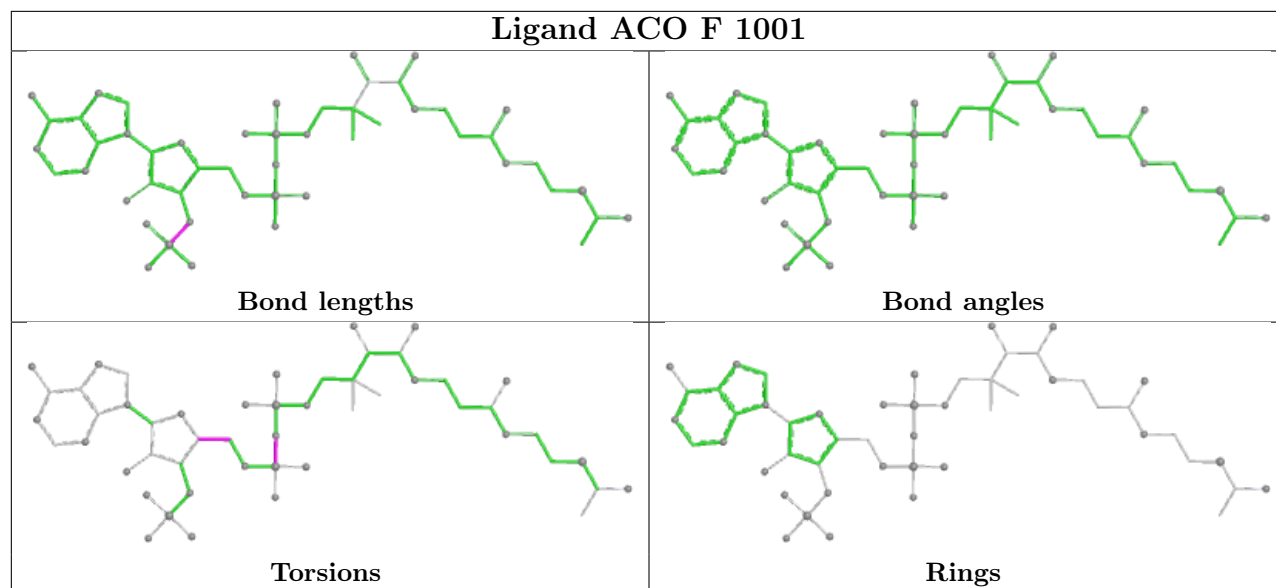
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1000	LMR	1	0
3	G	1000	LMR	1	0
5	F	1002	PG4	1	0
4	F	1001	ACO	1	0
4	G	1001	ACO	1	0
3	E	1000	LMR	1	0

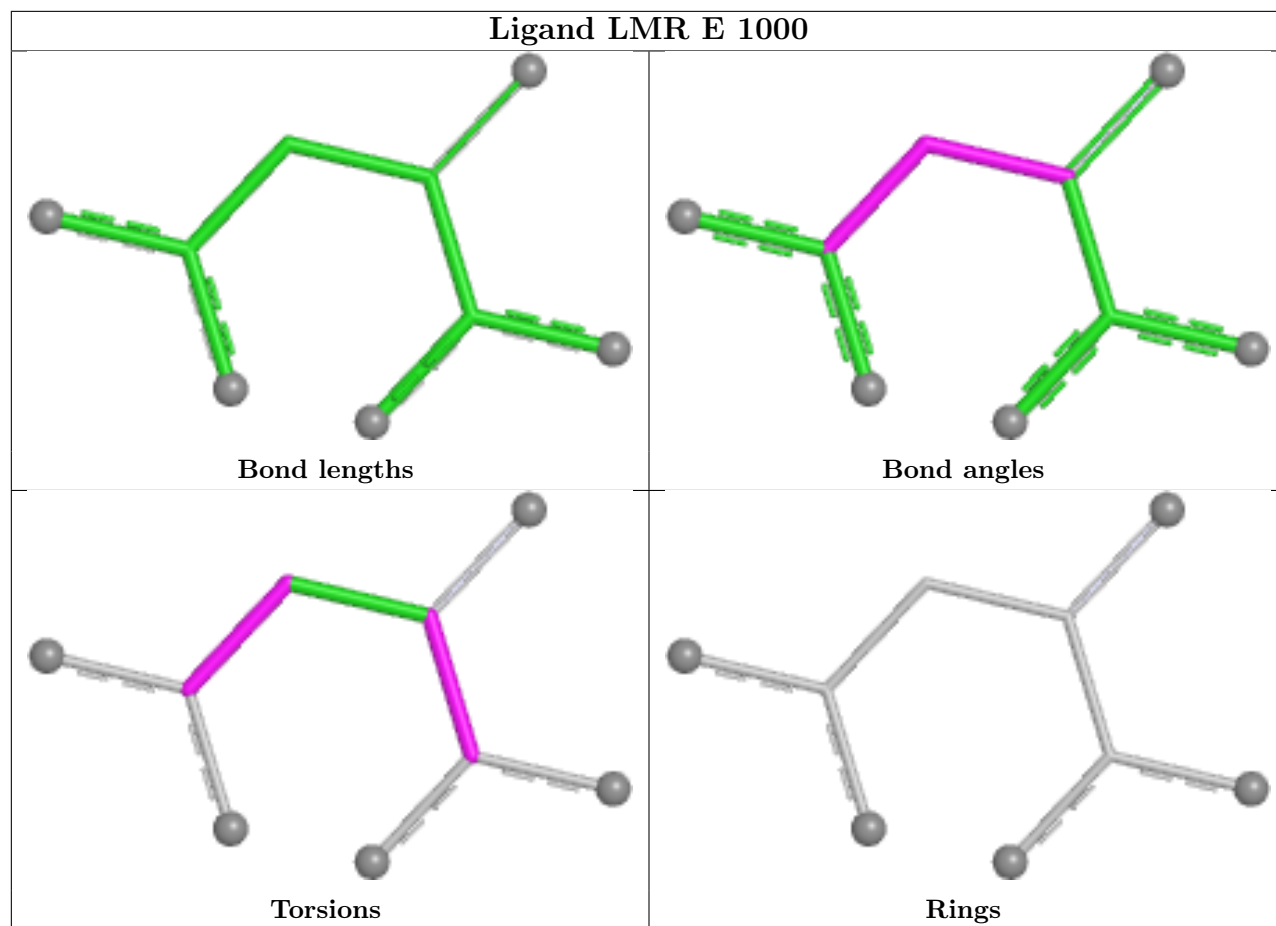
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	215/262 (82%)	0.08	19 (8%) 15 15	7, 22, 67, 97	2 (0%)
1	B	239/262 (91%)	0.37	34 (14%) 6 6	7, 27, 60, 79	3 (1%)
1	C	261/262 (99%)	0.31	25 (9%) 13 13	7, 27, 79, 118	2 (0%)
1	D	261/262 (99%)	-0.18	8 (3%) 51 54	8, 23, 47, 88	2 (0%)
1	E	256/262 (97%)	-0.28	4 (1%) 70 74	9, 22, 49, 88	4 (1%)
1	F	256/262 (97%)	-0.20	6 (2%) 61 64	6, 22, 50, 83	5 (1%)
1	G	261/262 (99%)	-0.49	2 (0%) 82 86	7, 18, 38, 80	4 (1%)
1	H	261/262 (99%)	-0.42	4 (1%) 72 76	7, 20, 42, 73	5 (1%)
All	All	2010/2096 (95%)	-0.11	102 (5%) 33 34	6, 22, 57, 118	27 (1%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	499	PRO	5.6
1	A	499	PRO	5.0
1	A	470	ASN	4.7
1	B	495	SER	4.7
1	E	607	LYS	4.6
1	B	538	LEU	4.5
1	B	493	VAL	4.3
1	G	607	LYS	4.3
1	C	483	VAL	4.2
1	C	497	LYS	4.1
1	C	496	VAL	4.1
1	H	607	LYS	3.9
1	B	469	PRO	3.9
1	C	493	VAL	3.9
1	F	607	LYS	3.9
1	A	506	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	506	LEU	3.7
1	B	478	TRP	3.7
1	C	453	ALA	3.7
1	A	351	VAL	3.6
1	C	535	LYS	3.6
1	A	461	PHE	3.5
1	B	489	ILE	3.3
1	B	483	VAL	3.3
1	A	607	LYS	3.3
1	D	607	LYS	3.2
1	B	539	ILE	3.2
1	B	486	VAL	3.2
1	C	536	GLY	3.1
1	B	491	HIS	3.1
1	E	496	VAL	3.1
1	F	496	VAL	3.1
1	B	485	PRO	3.0
1	B	490	GLY	3.0
1	D	493	VAL	3.0
1	C	537	ASN	3.0
1	A	542	VAL	3.0
1	A	463	MET	3.0
1	C	538	LEU	3.0
1	C	481	LYS	2.9
1	A	460	TYR	2.9
1	H	347	GLY	2.9
1	B	494	LYS	2.9
1	C	607	LYS	2.9
1	A	465	VAL	2.8
1	F	535	LYS	2.8
1	C	534	LYS	2.8
1	C	491	HIS	2.8
1	D	496	VAL	2.8
1	C	533	ALA	2.7
1	B	468	TYR	2.7
1	D	534	LYS	2.7
1	A	516	LEU	2.7
1	C	492	ARG	2.7
1	C	485	PRO	2.7
1	B	607	LYS	2.7
1	B	500	ASP	2.6
1	C	506	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	486	VAL	2.6
1	F	481	LYS	2.5
1	B	352	GLU	2.5
1	D	492	ARG	2.5
1	B	510	ILE	2.5
1	B	475	PHE	2.5
1	F	497	LYS	2.4
1	D	557	VAL	2.4
1	F	493	VAL	2.4
1	A	541	ASN	2.4
1	C	460	TYR	2.4
1	C	555	PHE	2.4
1	A	511	LYS	2.4
1	B	481	LYS	2.4
1	E	542[A]	VAL	2.4
1	D	497	LYS	2.3
1	B	520	CYS	2.3
1	B	517	HIS	2.3
1	B	512	ASN	2.3
1	C	532	THR	2.3
1	C	490	GLY	2.3
1	A	501	GLN	2.2
1	B	503	VAL	2.2
1	C	530	VAL	2.2
1	H	352	GLU	2.2
1	A	468	TYR	2.2
1	B	492	ARG	2.2
1	A	455	THR	2.2
1	A	504	LYS	2.1
1	A	526	GLU	2.1
1	B	502	ARG	2.1
1	A	453	ALA	2.1
1	B	527	VAL	2.1
1	B	511	LYS	2.1
1	D	535	LYS	2.1
1	B	540	LEU	2.1
1	B	501	GLN	2.1
1	G	591	ASP	2.1
1	H	350	MET	2.1
1	C	477	SER	2.1
1	C	476	LEU	2.1
1	E	555	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	463	MET	2.0
1	B	558	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

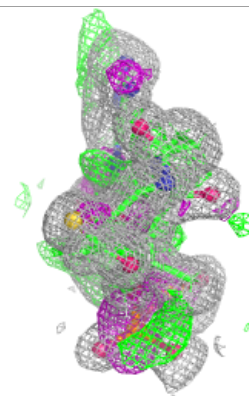
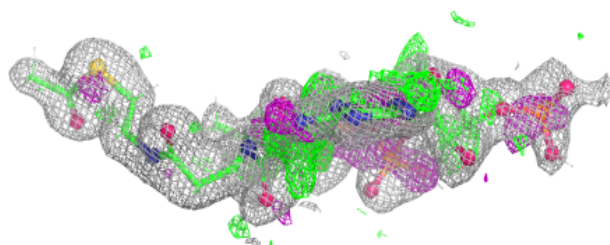
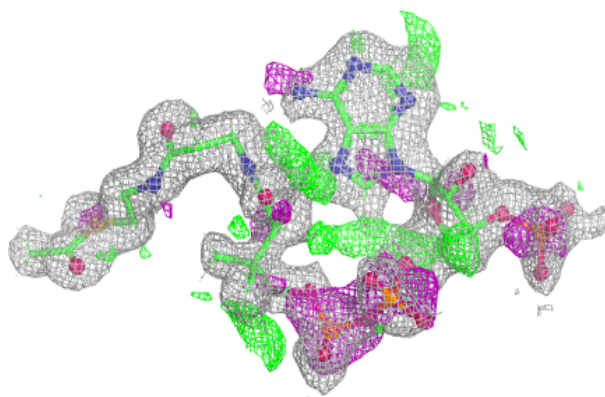
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACO	F	1001	51/51	0.83	0.14	20,32,58,63	0
5	PG4	E	1002	13/13	0.84	0.16	39,47,53,54	0
5	PG4	F	1002	13/13	0.89	0.12	30,37,42,45	0
3	LMR	F	1000	9/9	0.90	0.10	25,30,34,35	0
6	PGE	G	1002	10/10	0.90	0.13	39,43,50,52	0
6	PGE	H	1002	10/10	0.90	0.13	40,42,46,50	0
3	LMR	E	1000	9/9	0.94	0.07	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	0.06	17,20,22,23	0
4	ACO	G	1001	51/51	0.97	0.06	11,18,38,44	0
4	ACO	H	1001	51/51	0.97	0.06	12,20,39,48	0
3	LMR	G	1000	9/9	0.98	0.05	15,20,22,24	0
2	CA	B	701	1/1	0.99	0.03	15,15,15,15	0
2	CA	A	701	1/1	1.00	0.03	14,14,14,14	0

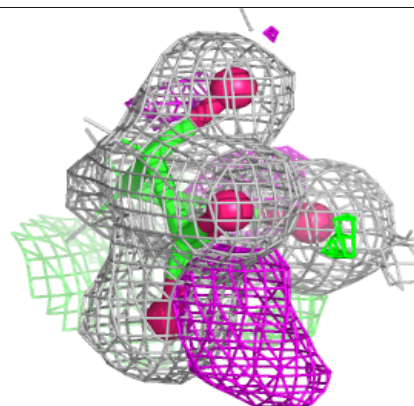
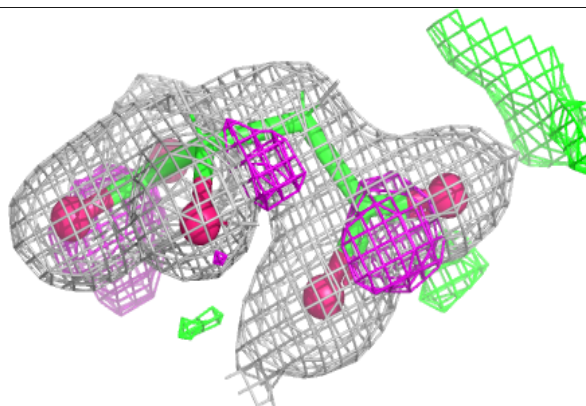
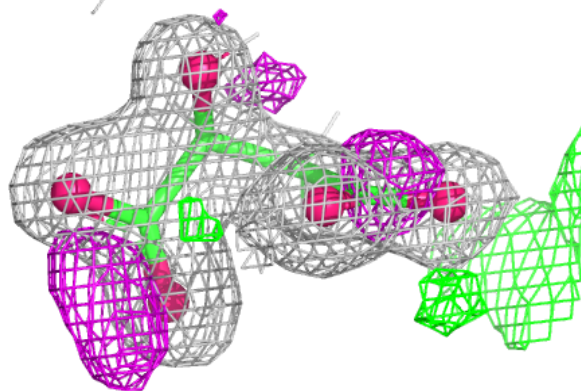
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO F 1001:

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

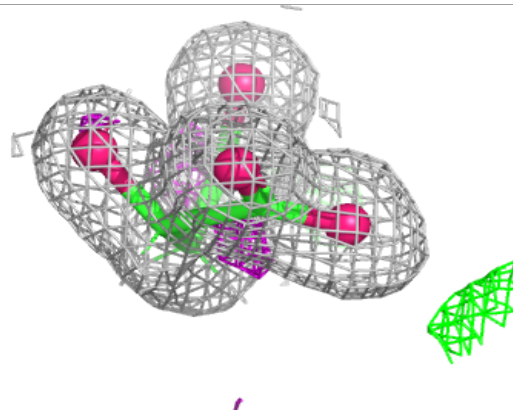
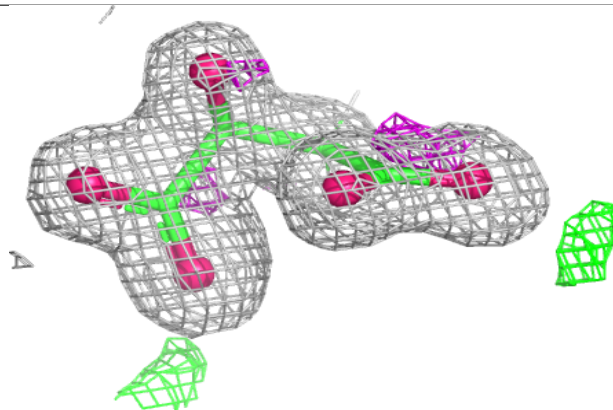
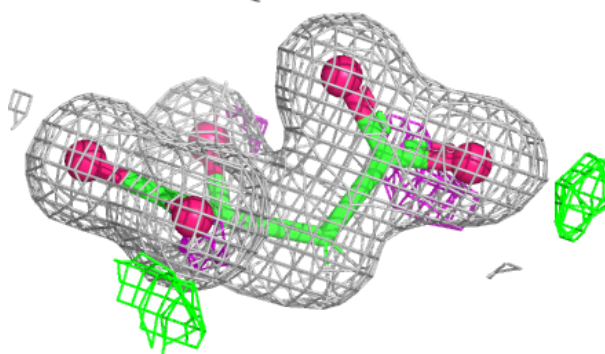
**Electron density around LMR F 1000:**

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

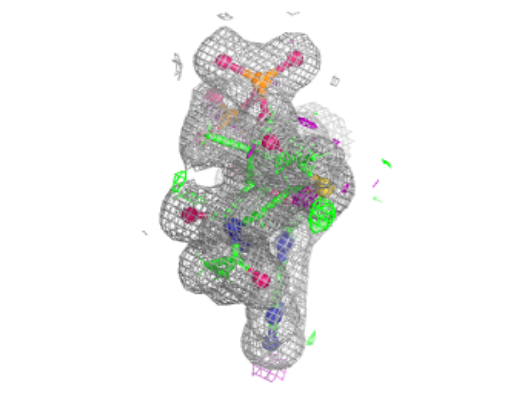
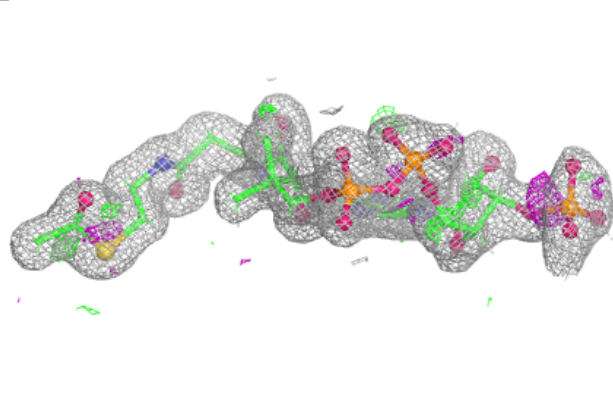
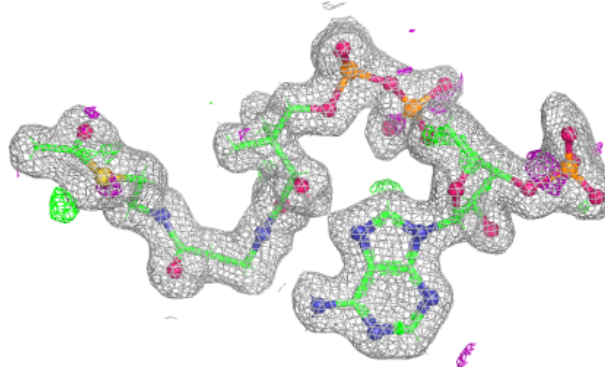


Electron density around LMR E 1000:

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

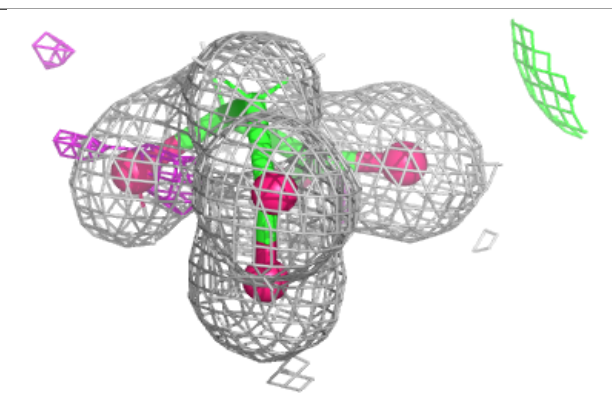
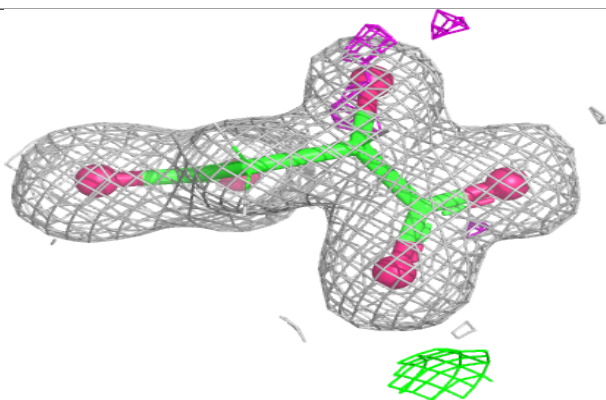
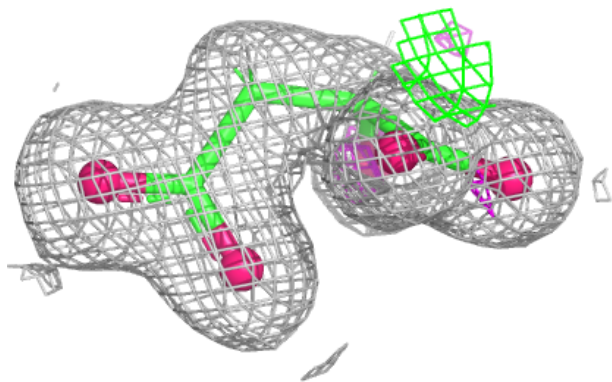
**Electron density around ACO E 1001:**

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

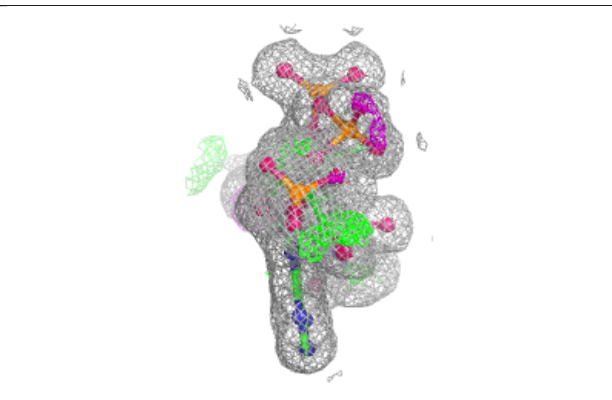
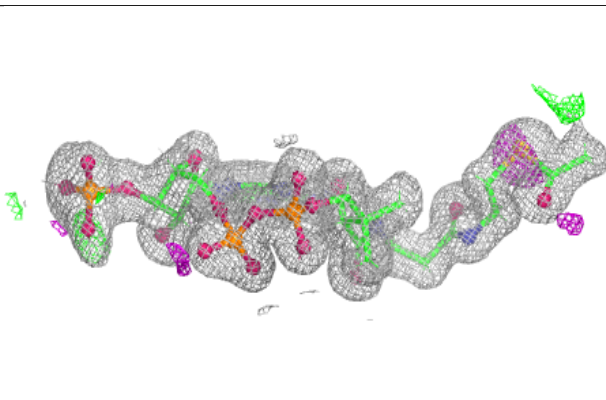
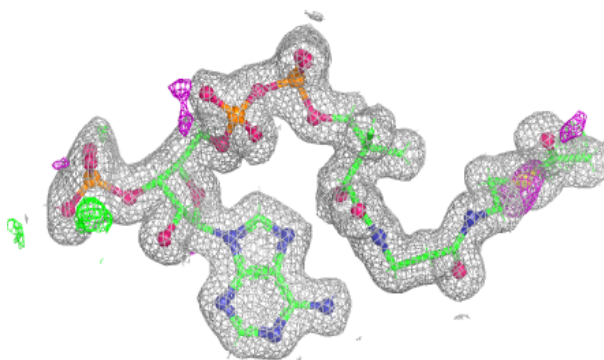


Electron density around LMR H 1000:

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

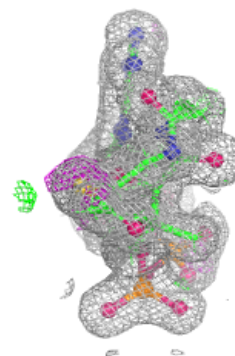
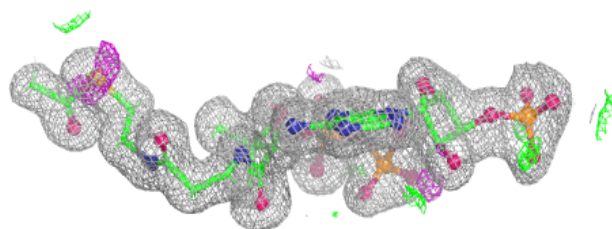
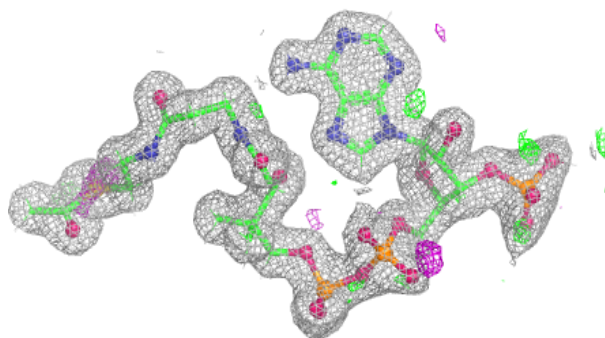
**Electron density around ACO G 1001:**

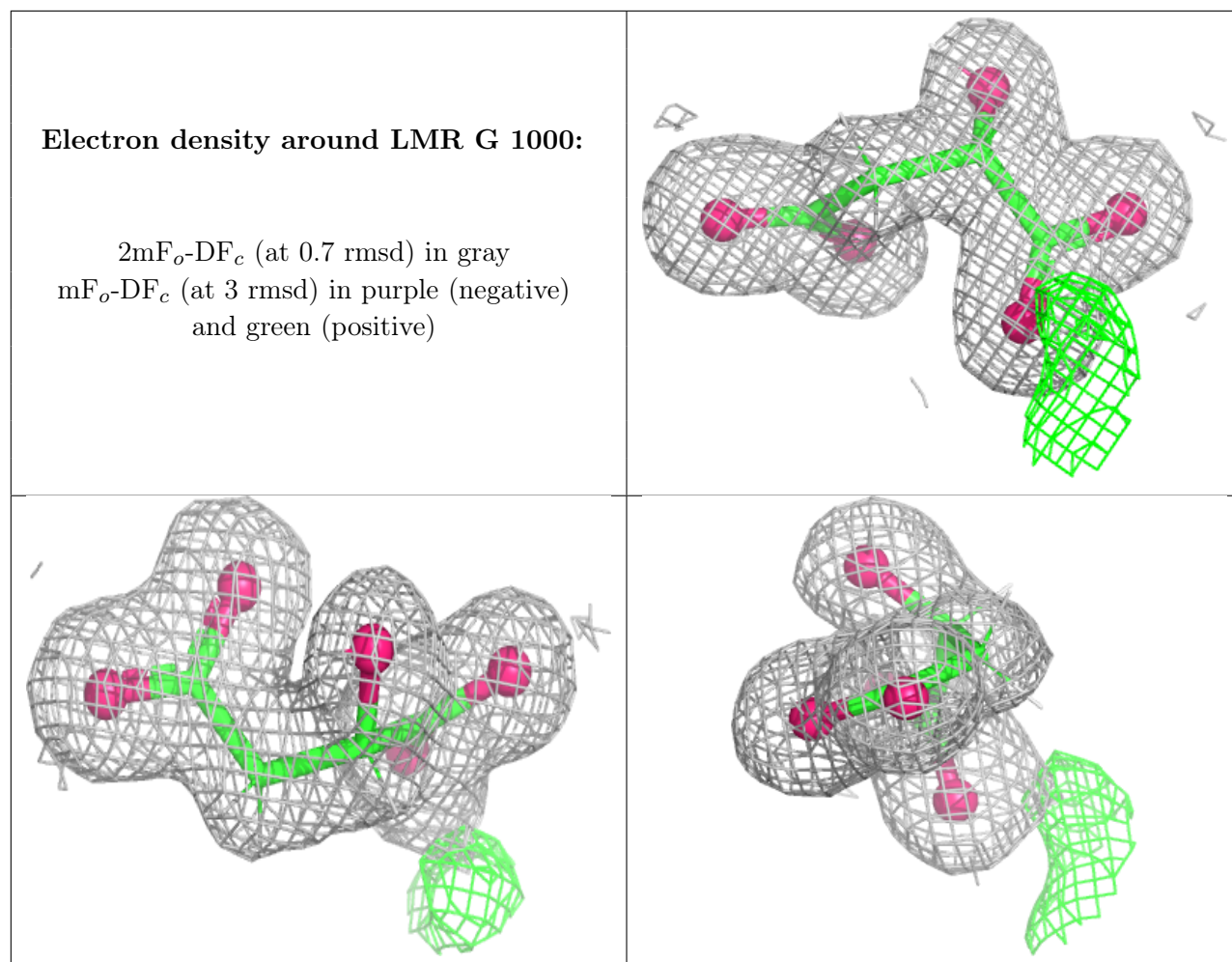
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.