



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:50 PM UTC

PDB ID : 8OJE / pdb\_00008oje  
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 in complex with L-malate  
Authors : Haesaerts, S.; Loris, R.; Larsen, P.B.  
Deposited on : 2023-03-24  
Resolution : 3.14 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

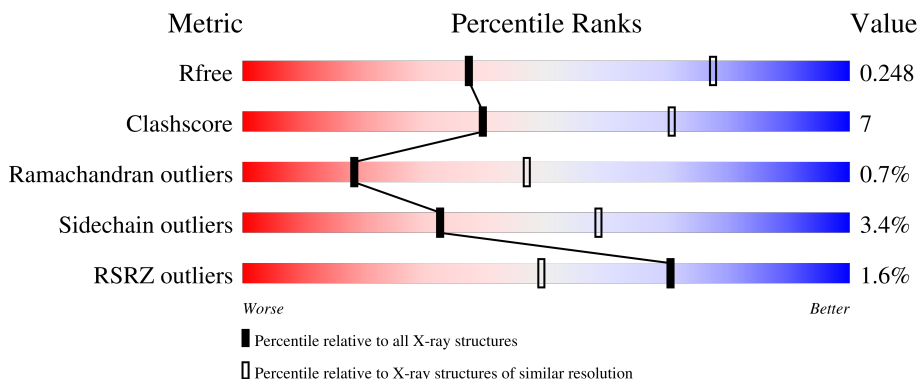
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	974	 2% 80% 14% . .
1	B	974	 2% 79% 16% . .
1	C	974	 % 78% 16% . .
1	D	974	 % 77% 17% . .
1	E	974	 2% 78% 16% . .

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Mol	Chain	Length	Quality of chain
1	F	974	 2% 79% 15% . .
1	G	974	 2% 79% 15% . .
1	H	974	 2% 76% 18% . .

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	PEG	A	1003	-	-	-	X
3	PEG	C	1003	-	-	-	X
3	PEG	E	1003	-	-	-	X
3	PEG	G	1003	-	-	-	X
4	CL	C	1009	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 59093 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 Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	932	7262	4622	1249	1362	29	0	2	0
1	B	932	7228	4603	1246	1350	29	0	2	2
1	C	932	7395	4696	1279	1390	30	0	3	1
1	D	933	7415	4709	1281	1395	30	0	4	0
1	E	933	7326	4658	1255	1383	30	0	3	0
1	F	933	7298	4642	1254	1372	30	0	4	0
1	G	933	7346	4662	1276	1378	30	0	2	1
1	H	933	7395	4694	1276	1395	30	0	4	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0

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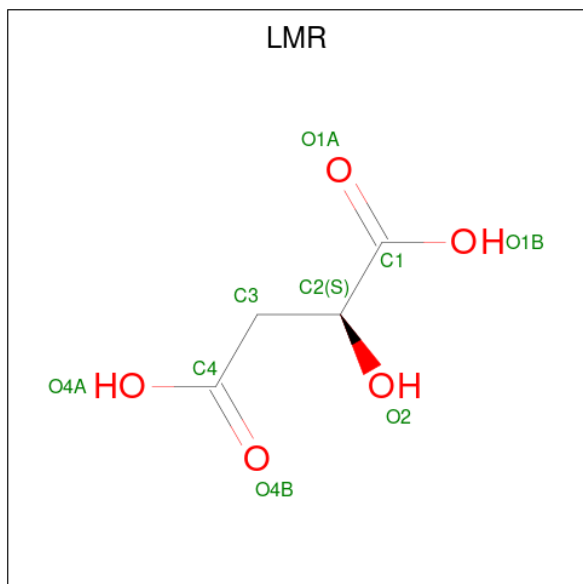
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0
D	-6	MET	-	initiating methionine	UNP Q9MAH0
D	-5	HIS	-	expression tag	UNP Q9MAH0
D	-4	HIS	-	expression tag	UNP Q9MAH0
D	-3	HIS	-	expression tag	UNP Q9MAH0
D	-2	HIS	-	expression tag	UNP Q9MAH0
D	-1	HIS	-	expression tag	UNP Q9MAH0
D	0	HIS	-	expression tag	UNP Q9MAH0
E	-6	MET	-	initiating methionine	UNP Q9MAH0
E	-5	HIS	-	expression tag	UNP Q9MAH0
E	-4	HIS	-	expression tag	UNP Q9MAH0
E	-3	HIS	-	expression tag	UNP Q9MAH0
E	-2	HIS	-	expression tag	UNP Q9MAH0
E	-1	HIS	-	expression tag	UNP Q9MAH0
E	0	HIS	-	expression tag	UNP Q9MAH0
F	-6	MET	-	initiating methionine	UNP Q9MAH0
F	-5	HIS	-	expression tag	UNP Q9MAH0
F	-4	HIS	-	expression tag	UNP Q9MAH0
F	-3	HIS	-	expression tag	UNP Q9MAH0
F	-2	HIS	-	expression tag	UNP Q9MAH0
F	-1	HIS	-	expression tag	UNP Q9MAH0
F	0	HIS	-	expression tag	UNP Q9MAH0
G	-6	MET	-	initiating methionine	UNP Q9MAH0
G	-5	HIS	-	expression tag	UNP Q9MAH0
G	-4	HIS	-	expression tag	UNP Q9MAH0
G	-3	HIS	-	expression tag	UNP Q9MAH0
G	-2	HIS	-	expression tag	UNP Q9MAH0
G	-1	HIS	-	expression tag	UNP Q9MAH0
G	0	HIS	-	expression tag	UNP Q9MAH0
H	-6	MET	-	initiating methionine	UNP Q9MAH0
H	-5	HIS	-	expression tag	UNP Q9MAH0
H	-4	HIS	-	expression tag	UNP Q9MAH0
H	-3	HIS	-	expression tag	UNP Q9MAH0
H	-2	HIS	-	expression tag	UNP Q9MAH0
H	-1	HIS	-	expression tag	UNP Q9MAH0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP Q9MAH0

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0
2	D	1	Total C O 9 4 5	0	0
2	E	1	Total C O 9 4 5	0	0
2	F	1	Total C O 9 4 5	0	0
2	G	1	Total C O 9 4 5	0	0
2	H	1	Total C O 9 4 5	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C 2 2	0	0
3	A	1	Total C 2 2	0	0
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C 2 2	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C 2 2	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C 2 2	0	0
3	C	1	Total C 2 2	0	0
3	C	1	Total C O 6 4 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 2 2	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C 2 2	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C 2 2	0	0
3	E	1	Total C O 6 4 2	0	0
3	E	1	Total C O 6 4 2	0	0
3	E	1	Total C 2 2	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C 2 2	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	G	1	Total C 2 2	0	0
3	G	1	Total C 2 2	0	0
3	G	1	Total C O 6 4 2	0	0
3	G	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 2 2	0	0
3	G	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	4	Total Cl 4 4	0	0
4	C	4	Total Cl 4 4	0	0
4	D	4	Total Cl 4 4	0	0
4	E	3	Total Cl 3 3	0	0
4	F	2	Total Cl 2 2	0	0
4	G	2	Total Cl 2 2	0	0
4	H	2	Total Cl 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	17	Total O 17 17	0	0
5	C	27	Total O 27 27	0	0
5	D	19	Total O 19 19	0	0

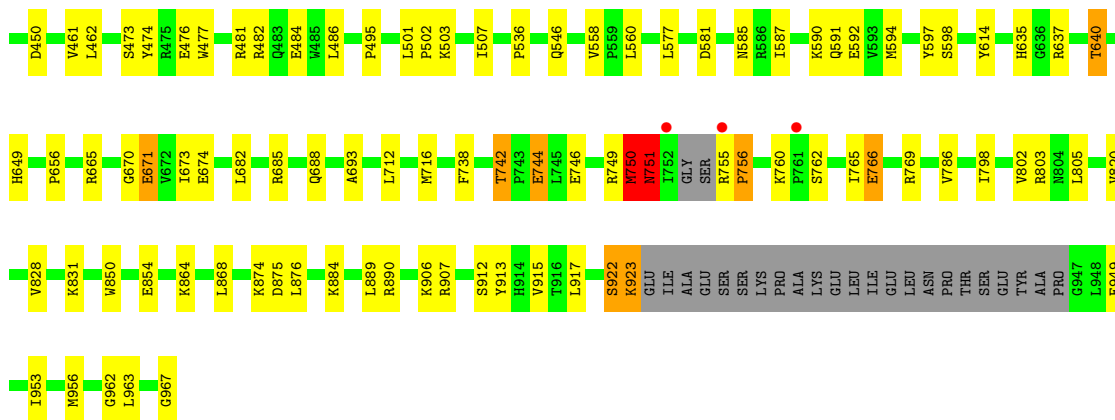
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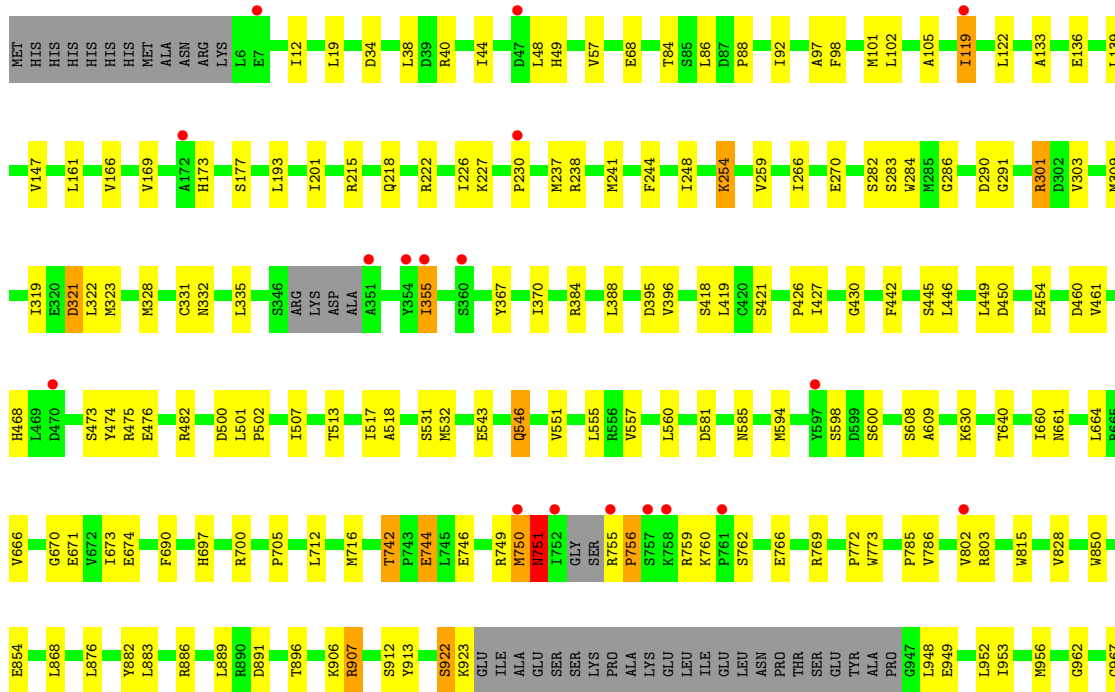
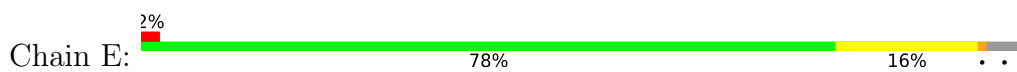
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	E	18	Total O 18 18	0	0
5	F	18	Total O 18 18	0	0
5	G	12	Total O 12 12	0	0
5	H	17	Total O 17 17	0	0

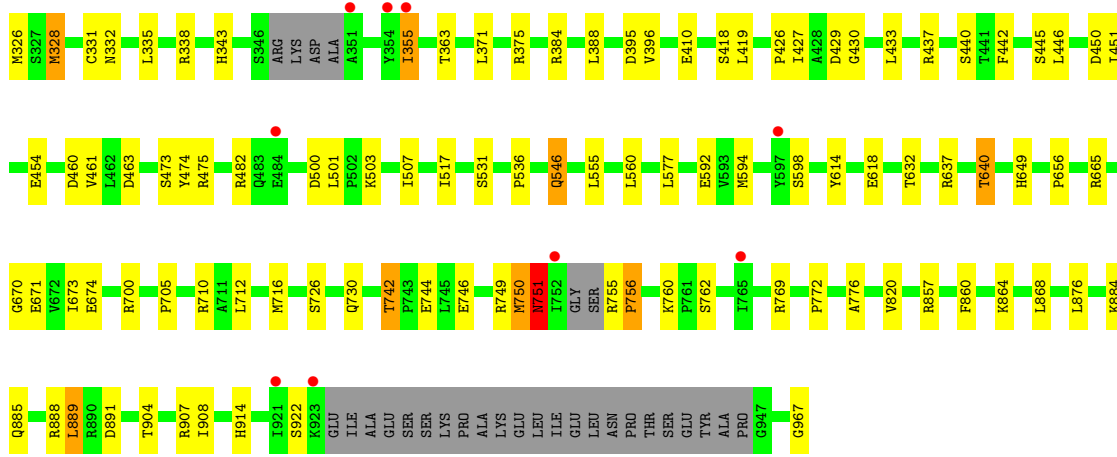




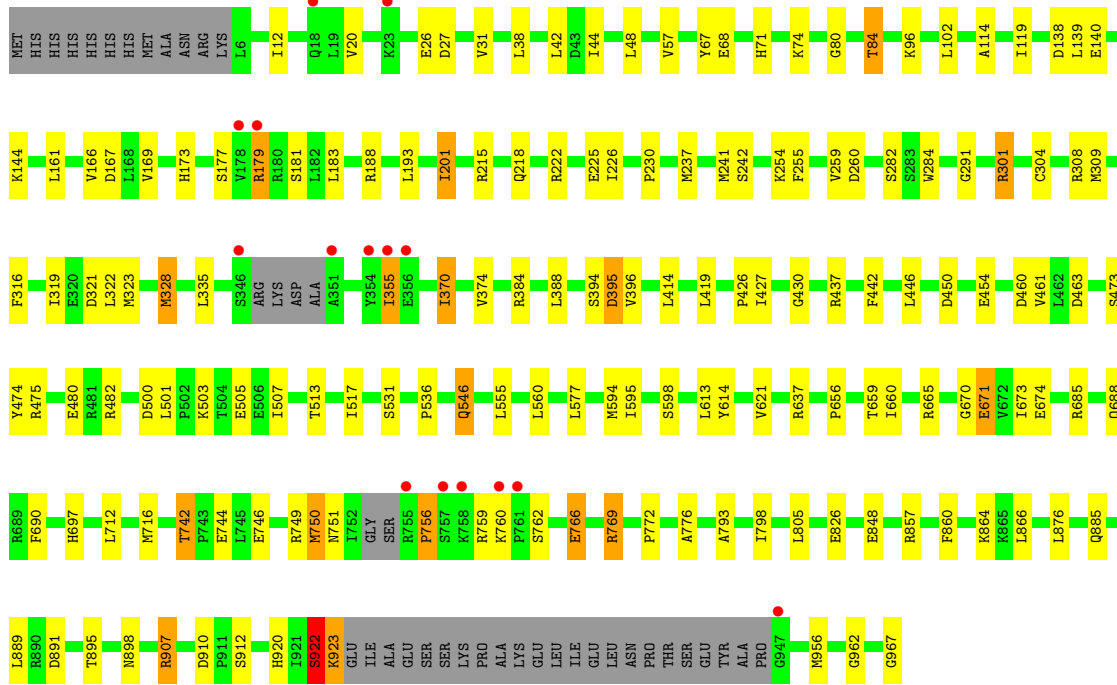
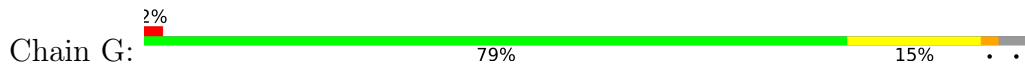


• Molecule 1: Phosphoenolpyruvate carboxylase 1

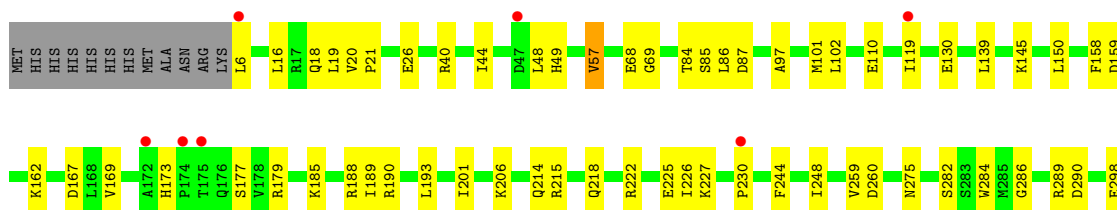
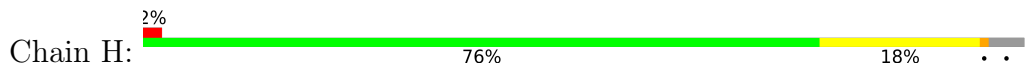


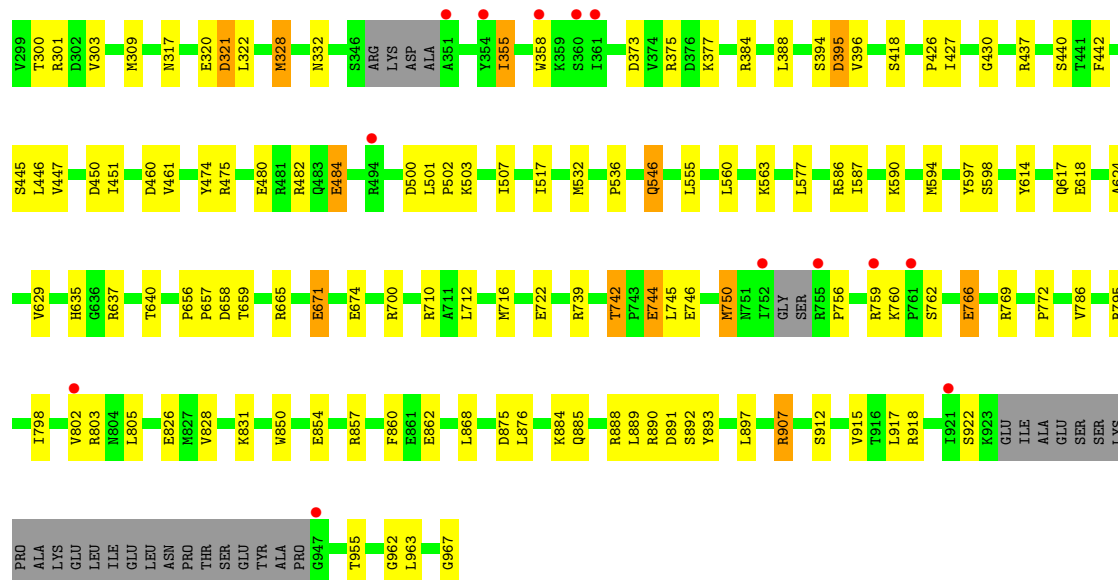


• Molecule 1: Phosphoenolpyruvate carboxylase 1



• Molecule 1: Phosphoenolpyruvate carboxylase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.08Å 352.20Å 176.04Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	48.93 – 3.14 48.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.93-3.14) 99.2 (48.93-3.14)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.202 , 0.240 0.212 , 0.248	Depositor DCC
$R_{free}$ test set	11875 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	59093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.14 % 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 8.3954e-04. 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: LMR, PEG, CL

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	0.26	0/7426	0.47	0/10091
1	B	0.25	0/7391	0.47	0/10047
1	C	0.28	0/7563	0.50	0/10257
1	D	0.29	0/7586	0.51	0/10287
1	E	0.28	0/7494	0.50	1/10178 (0.0%)
1	F	0.27	0/7469	0.49	0/10148
1	G	0.27	0/7510	0.48	0/10195
1	H	0.26	0/7566	0.49	0/10265
All	All	0.27	0/60005	0.49	1/81468 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	266	ILE	N-CA-C	-5.67	107.22	112.43

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	750	MET	Peptide
1	D	750	MET	Peptide
1	E	750	MET	Peptide

## 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	7262	0	6975	91	0
1	B	7228	0	6951	92	0
1	C	7395	0	7240	105	0
1	D	7415	0	7261	113	0
1	E	7326	0	7095	103	0
1	F	7298	0	7044	92	0
1	G	7346	0	7136	102	0
1	H	7395	0	7200	111	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	1	0
2	D	9	0	4	1	0
2	E	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	H	9	0	4	1	0
3	A	33	0	35	0	0
3	B	16	0	18	1	0
3	C	26	0	26	0	0
3	D	23	0	27	1	0
3	E	30	0	32	0	0
3	F	23	0	27	2	0
3	G	33	0	35	0	0
3	H	16	0	18	2	0
4	A	2	0	0	0	0
4	B	4	0	0	1	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0
4	G	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	1	0
5	A	5	0	0	0	0
5	B	17	0	0	2	0
5	C	27	0	0	0	0
5	D	19	0	0	0	0
5	E	18	0	0	1	0
5	F	18	0	0	0	0
5	G	12	0	0	0	0
5	H	17	0	0	0	0
All	All	59093	0	57152	774	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 7.

The worst 5 of 774 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:301[A]:ARG:NH2	1:B:388:LEU:O	2.11	0.84
1:F:169:VAL:HG22	1:F:282:SER:HB2	1.64	0.80
1:H:461:VAL:HG22	1:H:507:ILE:HG23	1.65	0.78
1:A:301:ARG:NH2	1:A:388:LEU:O	2.17	0.78
1:H:206:LYS:HE3	3:H:1003:PEG:H31	1.67	0.76

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	926/974 (95%)	885 (96%)	34 (4%)	7 (1%)	16 44
1	B	926/974 (95%)	882 (95%)	38 (4%)	6 (1%)	21 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	927/974 (95%)	882 (95%)	37 (4%)	8 (1%)	14	41
1	D	929/974 (95%)	882 (95%)	38 (4%)	9 (1%)	12	38
1	E	928/974 (95%)	882 (95%)	39 (4%)	7 (1%)	16	44
1	F	929/974 (95%)	884 (95%)	38 (4%)	7 (1%)	16	44
1	G	927/974 (95%)	882 (95%)	40 (4%)	5 (0%)	24	54
1	H	929/974 (95%)	884 (95%)	40 (4%)	5 (0%)	24	54
All	All	7421/7792 (95%)	7063 (95%)	304 (4%)	54 (1%)	18	47

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	395	ASP
1	B	227	LYS
1	B	395	ASP
1	B	922	SER
1	C	395	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	743/849 (88%)	718 (97%)	25 (3%)	32	58
1	B	738/849 (87%)	718 (97%)	20 (3%)	39	63
1	C	784/849 (92%)	754 (96%)	30 (4%)	29	56
1	D	787/849 (93%)	759 (96%)	28 (4%)	31	58
1	E	767/849 (90%)	742 (97%)	25 (3%)	33	59
1	F	757/849 (89%)	732 (97%)	25 (3%)	33	59
1	G	769/849 (91%)	739 (96%)	30 (4%)	28	56
1	H	780/849 (92%)	750 (96%)	30 (4%)	29	56
All	All	6125/6792 (90%)	5912 (96%)	213 (4%)	32	58

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	421	SER
1	F	637	ARG
1	H	546	GLN
1	E	671	GLU
1	F	57	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	869	GLN
1	H	438	GLN
1	F	964	GLN
1	G	783	HIS
1	H	964	GLN

### 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 71 ligands modelled in this entry, 23 are monoatomic - leaving 48 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	PEG	B	1002	3	6,6,6	0.49	0	5,5,5	0.45	0
3	PEG	A	1004	3	1,1,6	0.33	0	-		
3	PEG	D	1004	3	1,1,6	0.37	0	-		
3	PEG	F	1005	3	6,6,6	0.50	0	5,5,5	0.41	0
3	PEG	E	1004	3	5,5,6	0.33	0	4,4,5	2.61	1 (25%)
2	LMR	G	1001	-	8,8,8	1.50	1 (12%)	10,10,10	1.62	1 (10%)
2	LMR	C	1001	-	8,8,8	1.44	1 (12%)	10,10,10	1.66	1 (10%)
2	LMR	F	1001	-	8,8,8	1.62	1 (12%)	10,10,10	1.61	2 (20%)
3	PEG	D	1002	3	6,6,6	0.48	0	5,5,5	0.40	0
3	PEG	A	1002	3	6,6,6	0.51	0	5,5,5	0.51	0
3	PEG	H	1002	3	6,6,6	0.48	0	5,5,5	0.42	0
3	PEG	E	1002	3	6,6,6	0.52	0	5,5,5	0.41	0
3	PEG	E	1007	-	6,6,6	0.47	0	5,5,5	0.28	0
3	PEG	A	1007	3	1,1,6	0.38	0	-		
3	PEG	G	1007	3	1,1,6	0.40	0	-		
3	PEG	G	1006	3	6,6,6	0.51	0	5,5,5	0.45	0
3	PEG	C	1004	3	1,1,6	0.37	0	-		
3	PEG	C	1002	3	6,6,6	0.49	0	5,5,5	0.37	0
3	PEG	A	1008	-	6,6,6	0.50	0	5,5,5	0.36	0
3	PEG	F	1002	3	6,6,6	0.49	0	5,5,5	0.43	0
3	PEG	C	1007	-	6,6,6	0.50	0	5,5,5	0.46	0
3	PEG	H	1003	3	6,6,6	0.46	0	5,5,5	0.51	0
3	PEG	A	1005	-	5,5,6	0.58	0	4,4,5	0.43	0
3	PEG	H	1004	3	1,1,6	0.33	0	-		
2	LMR	E	1001	-	8,8,8	1.50	1 (12%)	10,10,10	1.59	2 (20%)
3	PEG	E	1005	3	5,5,6	0.72	0	4,4,5	1.26	0
3	PEG	C	1005	-	5,5,6	0.56	0	4,4,5	0.58	0
3	PEG	E	1006	3	1,1,6	0.54	0	-		
3	PEG	C	1006	3	1,1,6	0.43	0	-		
3	PEG	G	1004	3	1,1,6	0.29	0	-		
3	PEG	A	1003	3	1,1,6	0.35	0	-		
3	PEG	D	1003	3	6,6,6	0.47	0	5,5,5	0.63	0
3	PEG	F	1004	3	1,1,6	0.33	0	-		
3	PEG	G	1003	3	1,1,6	0.40	0	-		
3	PEG	A	1006	3	6,6,6	0.49	0	5,5,5	0.31	0
2	LMR	B	1001	-	8,8,8	1.53	1 (12%)	10,10,10	1.43	1 (10%)
2	LMR	H	1001	-	8,8,8	1.51	1 (12%)	10,10,10	1.62	1 (10%)
2	LMR	D	1001	-	8,8,8	1.44	1 (12%)	10,10,10	1.53	1 (10%)
3	PEG	G	1002	3	6,6,6	0.51	0	5,5,5	0.64	0
3	PEG	B	1004	3	1,1,6	0.39	0	-		
3	PEG	E	1003	3	1,1,6	0.39	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	C	1003	3	1,1,6	0.46	0	-		
3	PEG	D	1005	3	6,6,6	0.51	0	5,5,5	0.42	0
3	PEG	F	1003	3	6,6,6	0.48	0	5,5,5	0.51	0
3	PEG	G	1005	-	5,5,6	0.56	0	4,4,5	0.48	0
3	PEG	G	1008	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	B	1003	3	6,6,6	0.48	0	5,5,5	0.49	0
2	LMR	A	1001	-	8,8,8	1.45	1 (12%)	10,10,10	1.51	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	PEG	B	1002	3	-	0/4/4/4	-
3	PEG	F	1005	3	-	2/4/4/4	-
3	PEG	E	1004	3	-	3/3/3/4	-
2	LMR	G	1001	-	-	0/8/8/8	-
2	LMR	C	1001	-	-	3/8/8/8	-
2	LMR	F	1001	-	-	6/8/8/8	-
3	PEG	D	1002	3	-	2/4/4/4	-
3	PEG	A	1002	3	-	3/4/4/4	-
3	PEG	B	1003	3	-	3/4/4/4	-
3	PEG	H	1002	3	-	0/4/4/4	-
3	PEG	E	1002	3	-	2/4/4/4	-
3	PEG	E	1007	-	-	2/4/4/4	-
3	PEG	G	1006	3	-	3/4/4/4	-
3	PEG	C	1002	3	-	2/4/4/4	-
3	PEG	A	1008	-	-	2/4/4/4	-
3	PEG	F	1002	3	-	1/4/4/4	-
3	PEG	C	1007	-	-	3/4/4/4	-
3	PEG	H	1003	3	-	3/4/4/4	-
3	PEG	A	1005	-	-	2/3/3/4	-
2	LMR	E	1001	-	-	1/8/8/8	-
3	PEG	E	1005	3	-	3/3/3/4	-
3	PEG	D	1003	3	-	4/4/4/4	-
3	PEG	A	1006	3	-	2/4/4/4	-
2	LMR	B	1001	-	-	1/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMR	H	1001	-	-	1/8/8/8	-
2	LMR	D	1001	-	-	2/8/8/8	-
3	PEG	G	1002	3	-	2/4/4/4	-
3	PEG	D	1005	3	-	2/4/4/4	-
3	PEG	F	1003	3	-	3/4/4/4	-
3	PEG	G	1005	-	-	2/3/3/4	-
3	PEG	G	1008	-	-	2/4/4/4	-
3	PEG	C	1005	-	-	2/3/3/4	-
2	LMR	A	1001	-	-	3/8/8/8	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	LMR	C2-C1	-3.29	1.47	1.52
2	E	1001	LMR	C2-C1	-3.13	1.47	1.52
2	G	1001	LMR	C2-C1	-2.96	1.48	1.52
2	C	1001	LMR	C2-C1	-2.94	1.48	1.52
2	H	1001	LMR	C2-C1	-2.91	1.48	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1004	PEG	C2-O2-C3	4.95	130.44	113.06
2	G	1001	LMR	O1B-C1-C2	3.65	120.46	112.74
2	H	1001	LMR	O1B-C1-C2	3.58	120.31	112.74
2	C	1001	LMR	O1B-C1-C2	3.51	120.16	112.74
2	D	1001	LMR	O1B-C1-C2	3.36	119.84	112.74

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

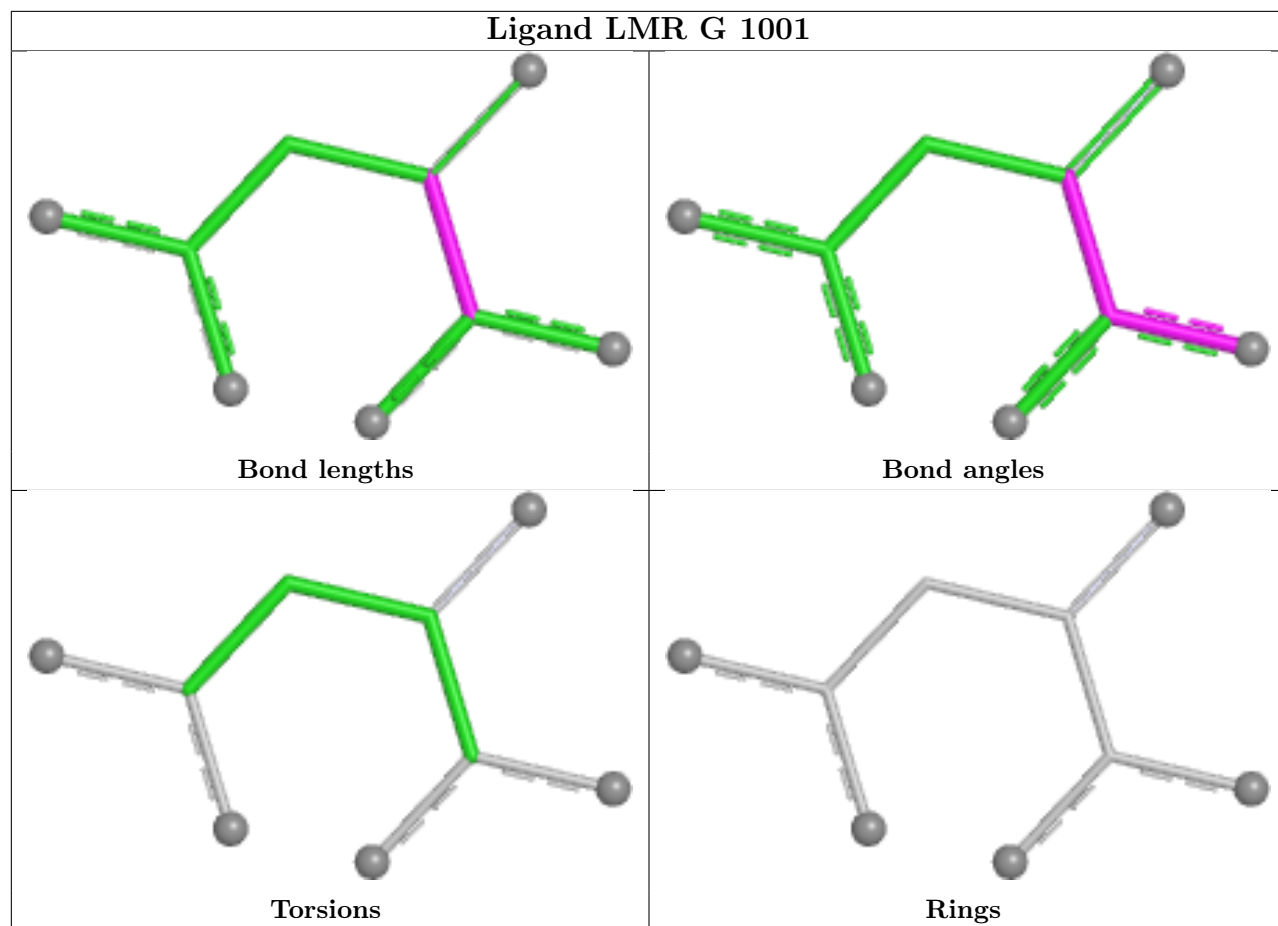
Mol	Chain	Res	Type	Atoms
2	F	1001	LMR	O1A-C1-C2-O2
2	F	1001	LMR	O1B-C1-C2-O2
3	E	1004	PEG	O2-C3-C4-O4
3	E	1007	PEG	O1-C1-C2-O2
3	A	1008	PEG	O2-C3-C4-O4

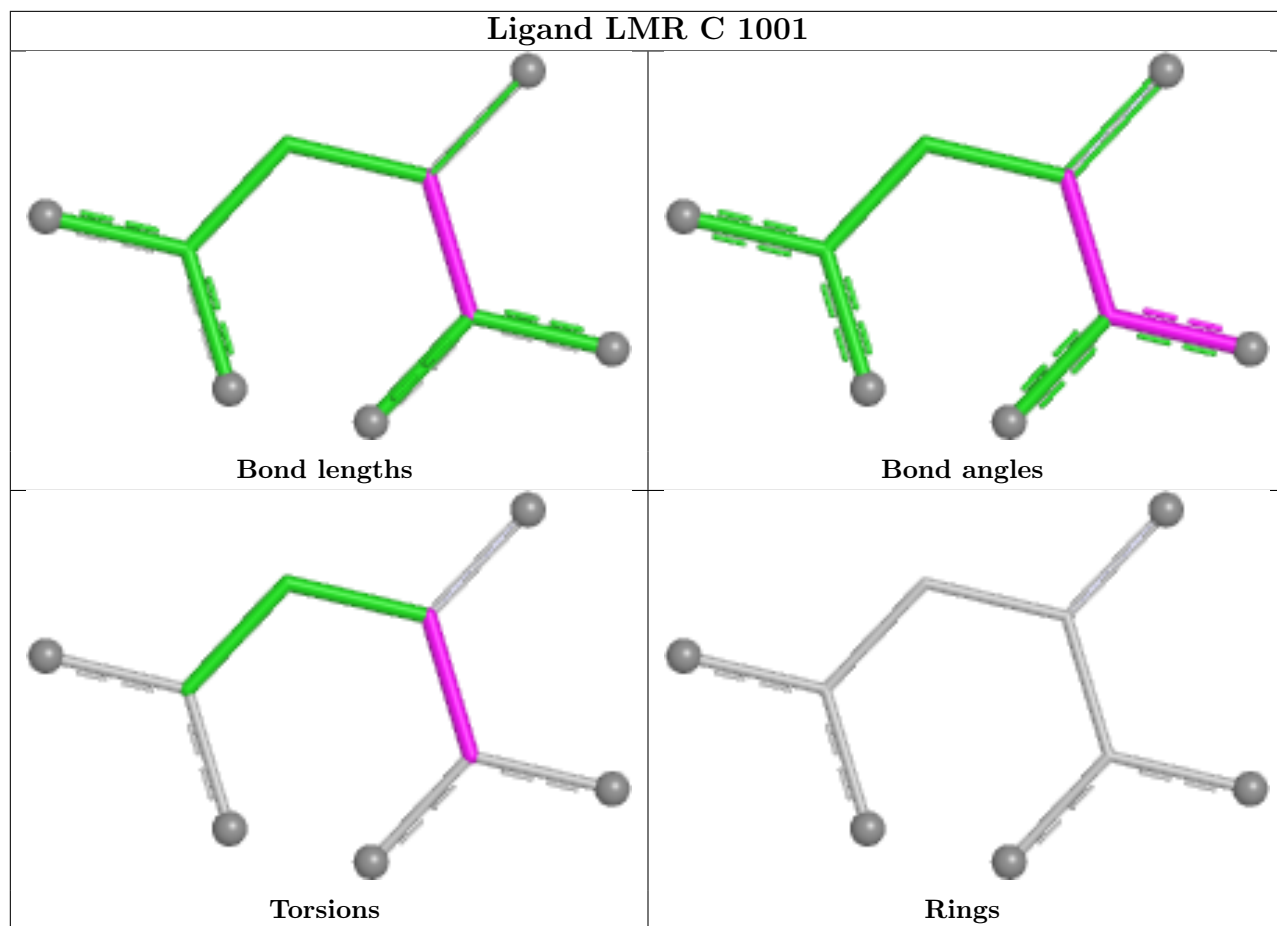
There are no ring outliers.

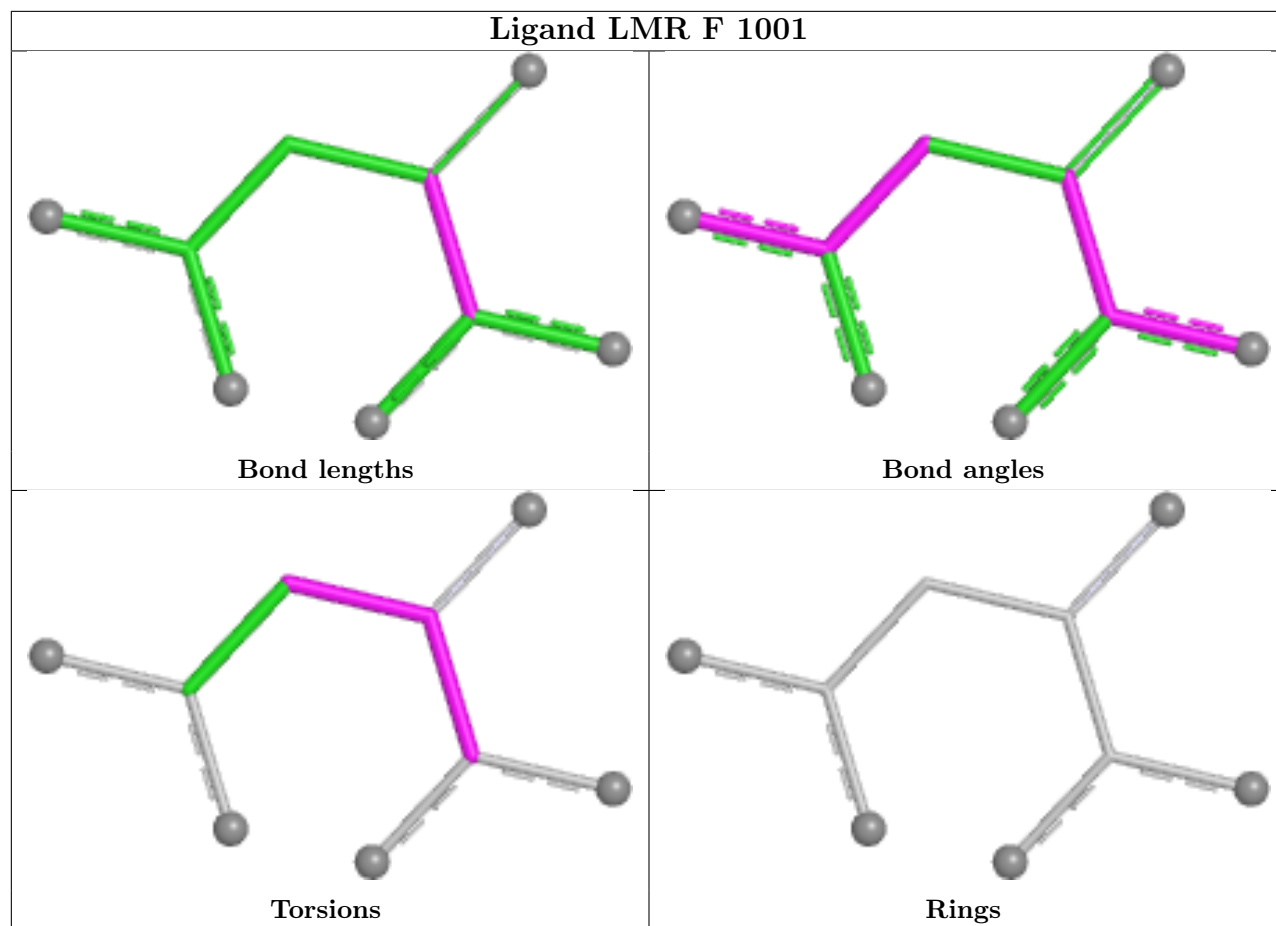
9 monomers are involved in 9 short contacts:

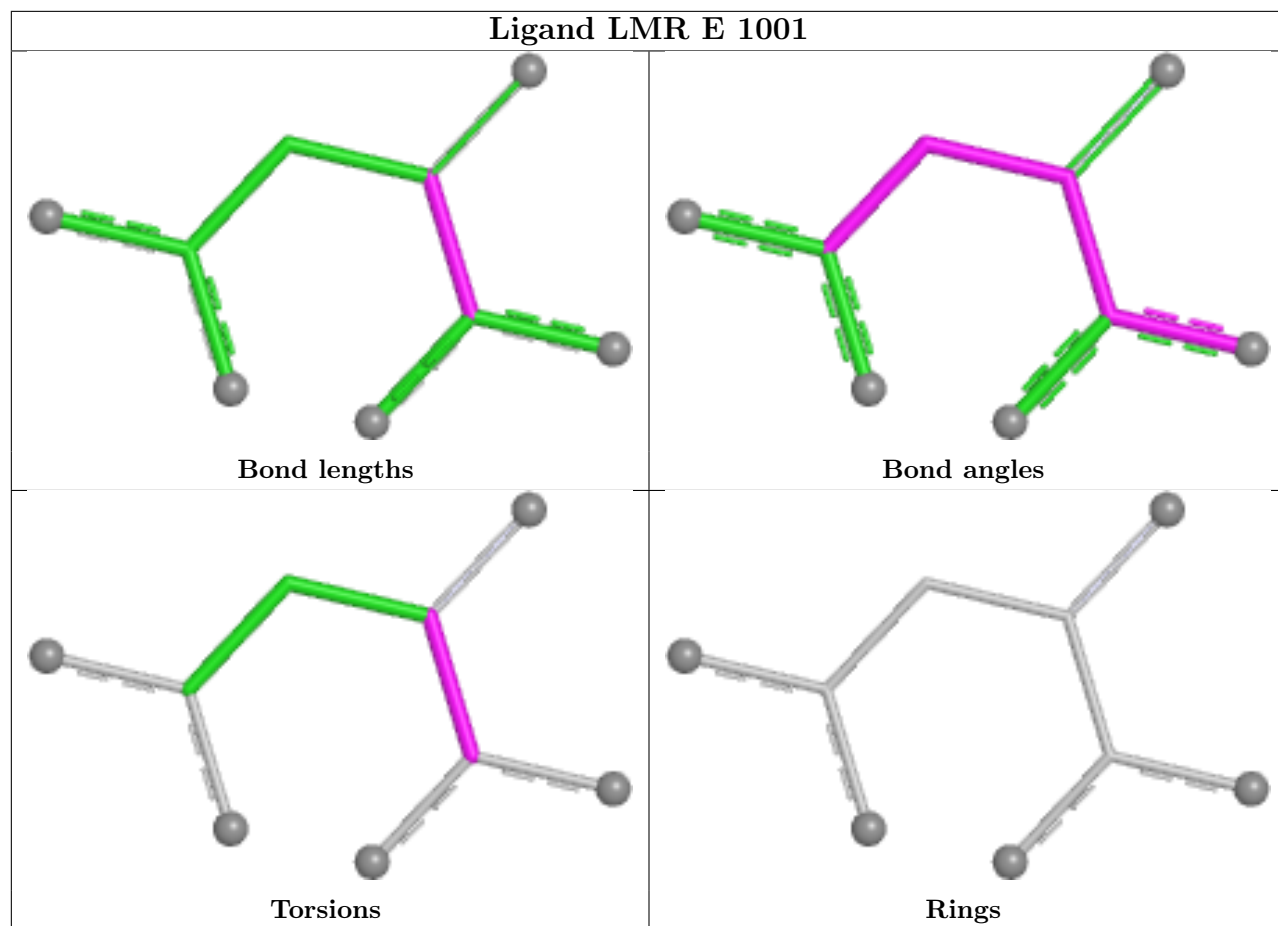
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	LMR	1	0
3	D	1002	PEG	1	0
3	H	1002	PEG	1	0
3	F	1002	PEG	1	0
3	H	1003	PEG	1	0
2	H	1001	LMR	1	0
2	D	1001	LMR	1	0
3	F	1003	PEG	1	0
3	B	1003	PEG	1	0

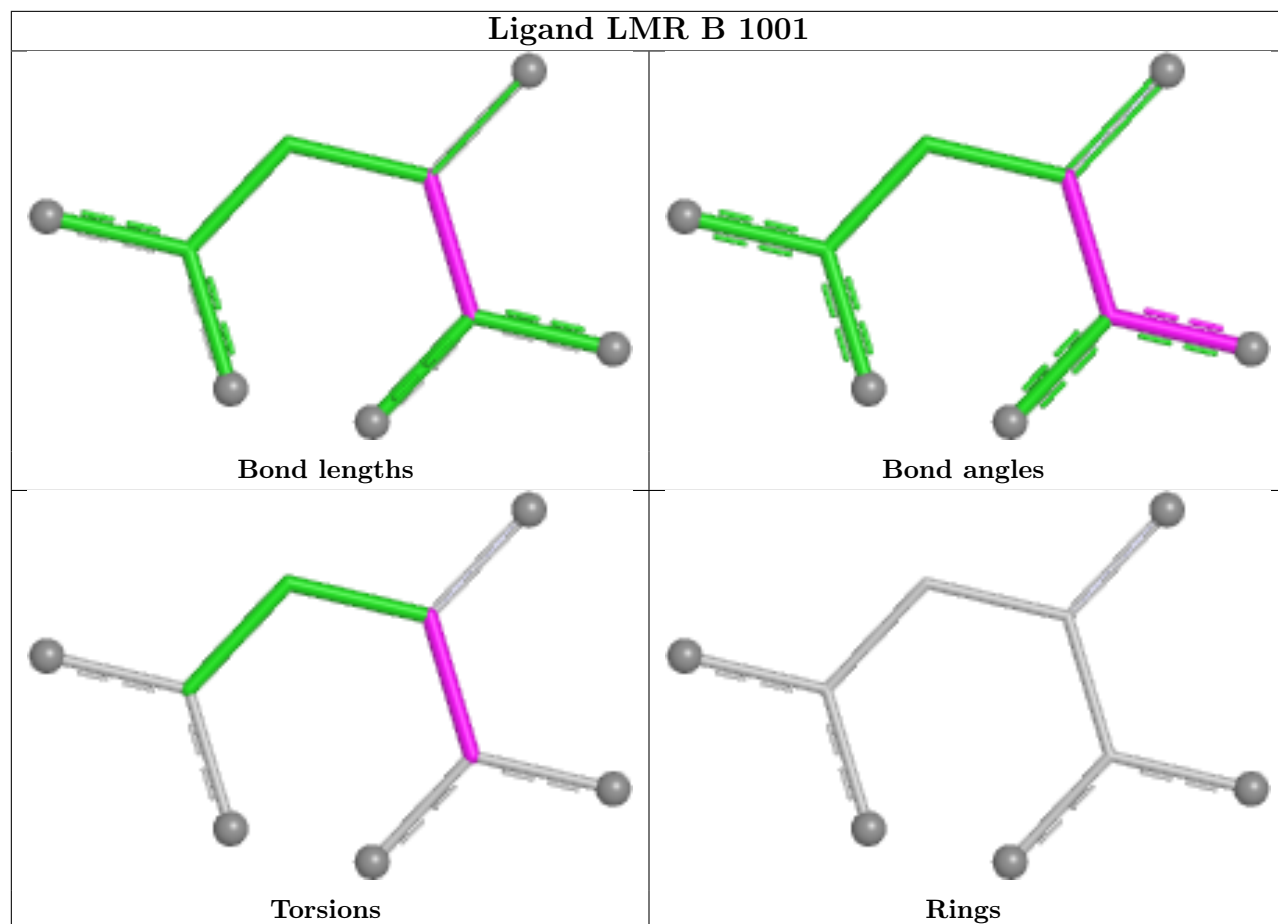
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

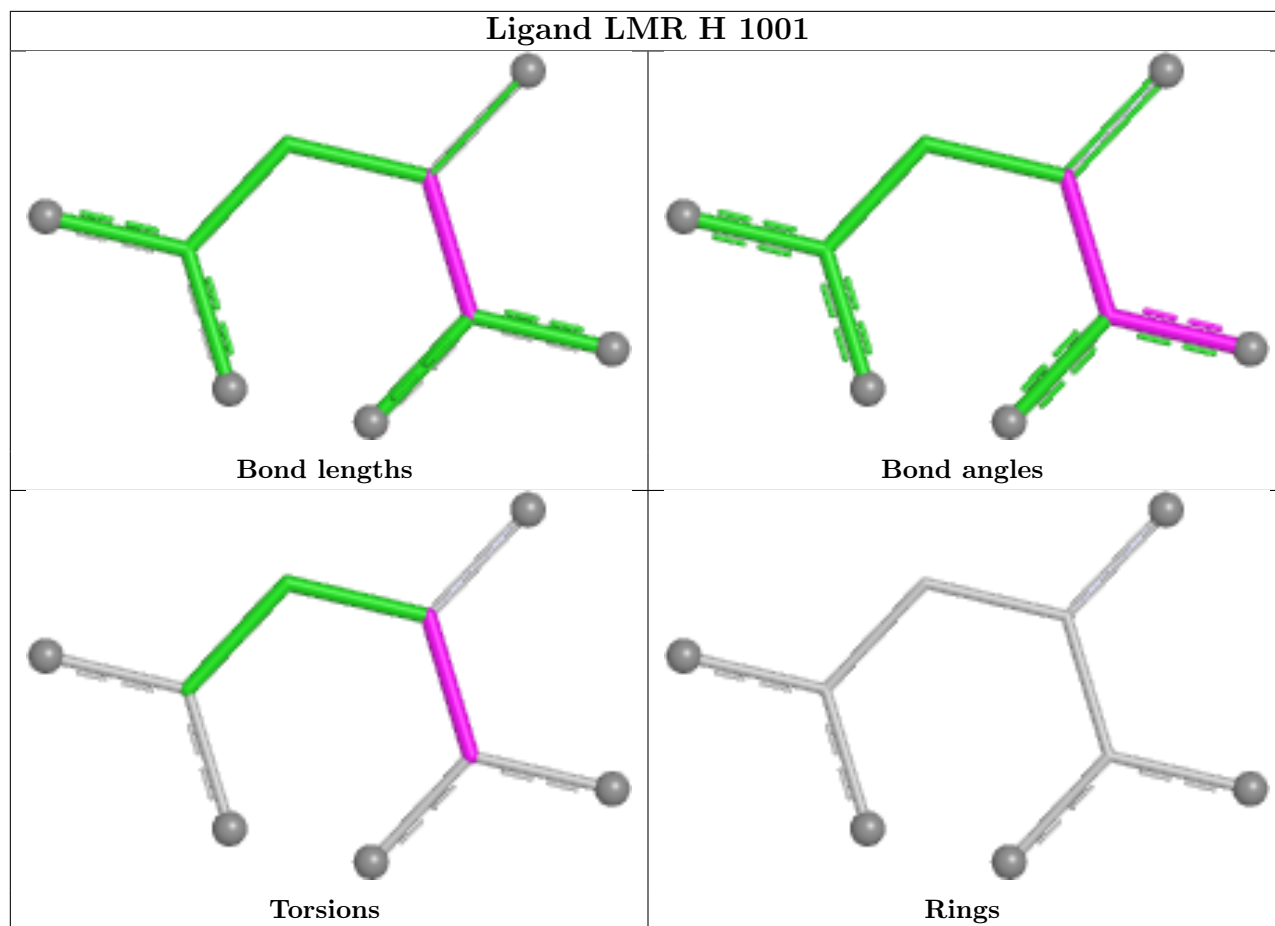


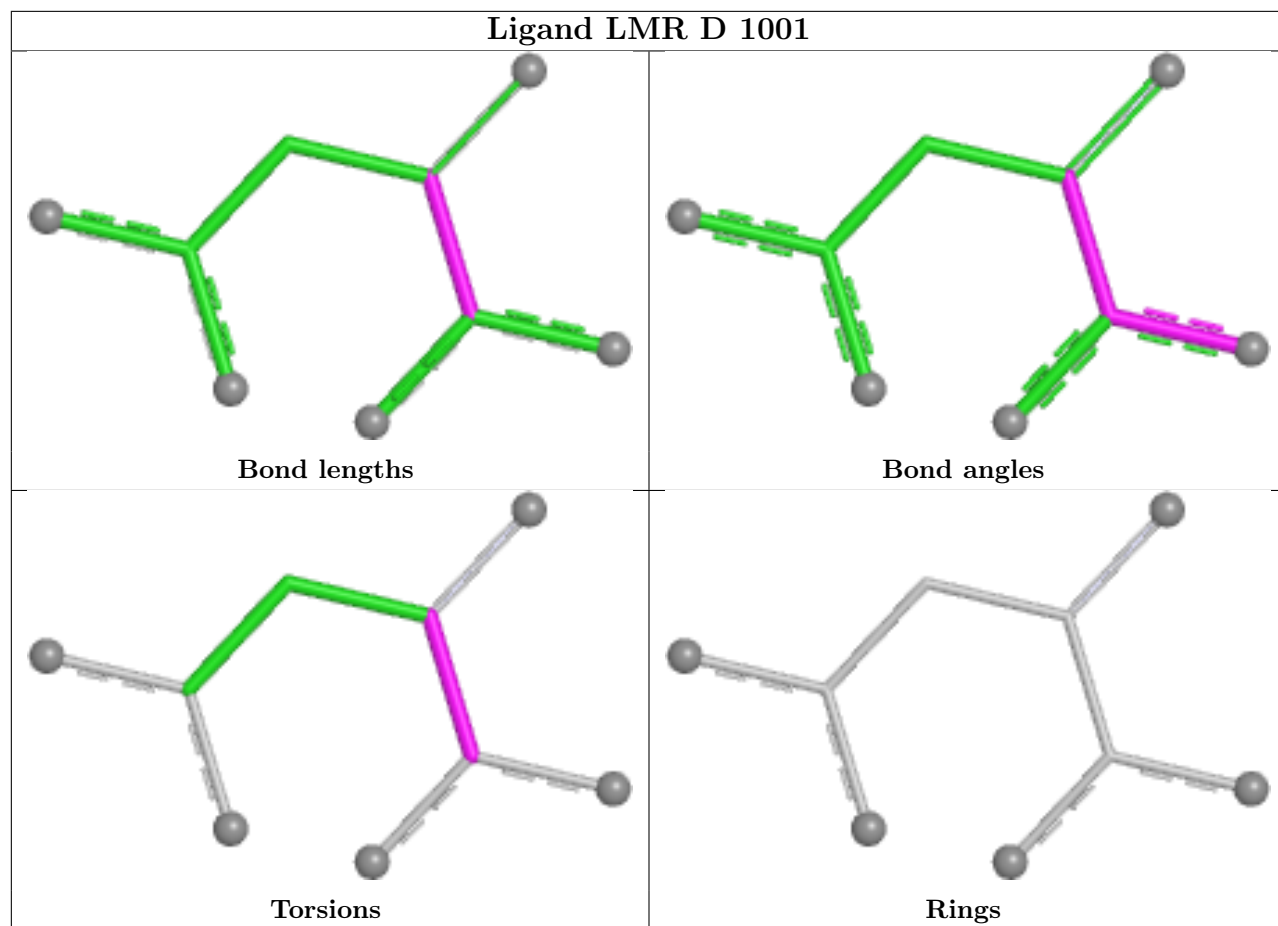


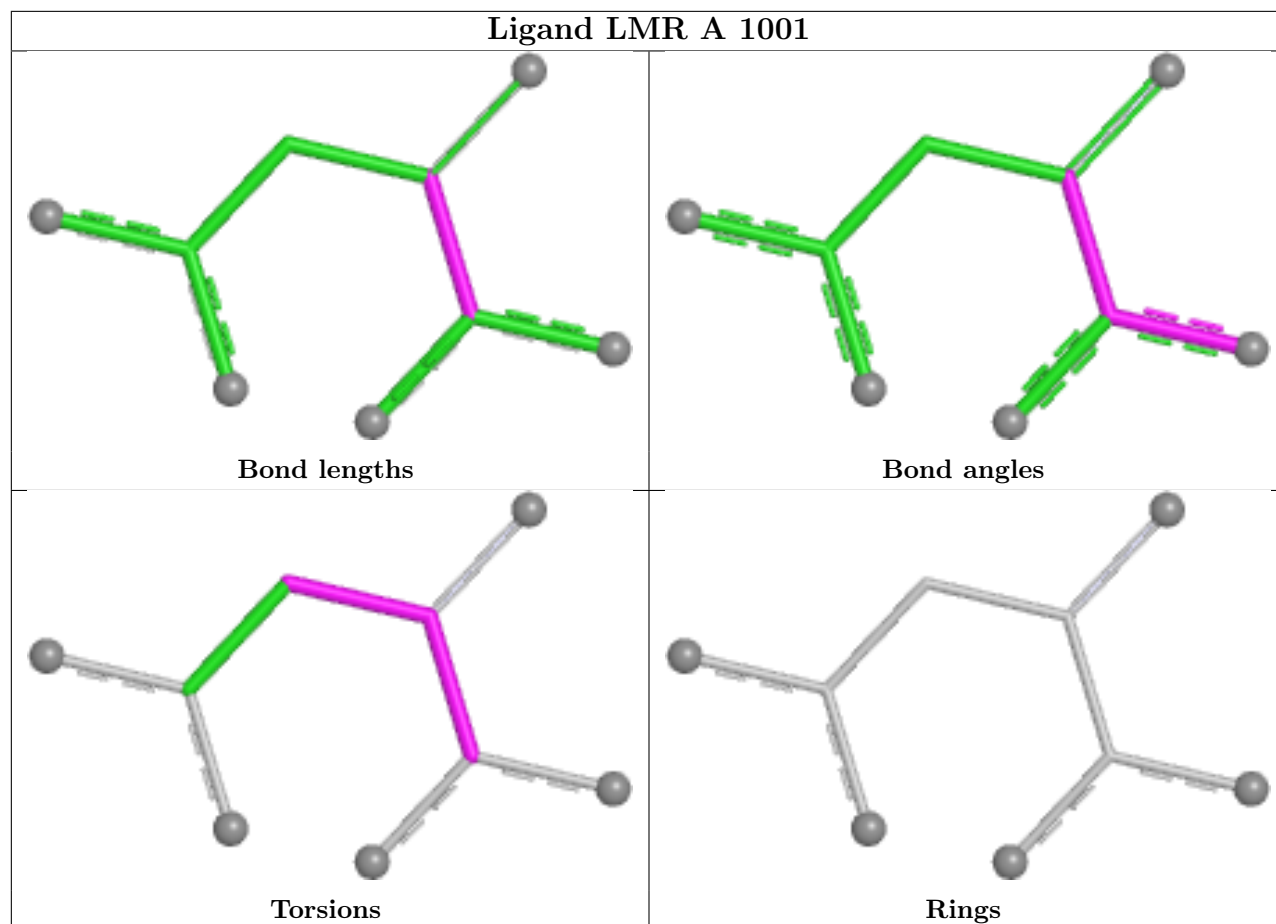












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	932/974 (95%)	-0.13	16 (1%) 69 48	36, 75, 125, 207	2 (0%)
1	B	932/974 (95%)	-0.12	17 (1%) 67 46	39, 78, 133, 226	2 (0%)
1	C	932/974 (95%)	-0.25	9 (0%) 79 61	33, 65, 116, 227	3 (0%)
1	D	933/974 (95%)	-0.29	10 (1%) 78 59	30, 64, 115, 209	4 (0%)
1	E	933/974 (95%)	-0.22	18 (1%) 66 45	32, 64, 119, 223	3 (0%)
1	F	933/974 (95%)	-0.17	17 (1%) 67 46	34, 68, 124, 217	4 (0%)
1	G	933/974 (95%)	-0.14	15 (1%) 70 49	44, 74, 130, 269	2 (0%)
1	H	933/974 (95%)	-0.15	20 (2%) 63 42	32, 73, 128, 227	4 (0%)
All	All	7461/7792 (95%)	-0.18	122 (1%) 70 49	30, 71, 124, 269	24 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	GLU	6.0
1	B	355	ILE	5.3
1	D	351	ALA	4.3
1	E	172	ALA	4.3
1	D	755	ARG	4.1

### 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, 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	PEG	C	1003	2/7	0.15	0.49	49,49,49,69	0
3	PEG	G	1003	2/7	0.21	0.59	62,62,62,78	0
4	CL	C	1009	1/1	0.38	0.54	233,233,233,233	0
3	PEG	A	1003	2/7	0.43	0.62	75,75,75,85	0
3	PEG	E	1003	2/7	0.52	0.43	56,56,56,69	0
3	PEG	C	1004	2/7	0.60	0.29	49,49,49,72	0
3	PEG	F	1004	2/7	0.70	0.23	46,46,46,69	0
3	PEG	B	1004	2/7	0.72	0.39	87,87,87,98	0
3	PEG	A	1005	6/7	0.74	0.26	77,88,90,92	0
3	PEG	G	1004	2/7	0.74	0.29	63,63,63,75	0
3	PEG	A	1004	2/7	0.74	0.30	64,64,64,77	0
3	PEG	C	1005	6/7	0.77	0.24	46,78,84,93	0
3	PEG	D	1004	2/7	0.79	0.19	56,56,56,79	0
4	CL	B	1006	1/1	0.80	0.30	125,125,125,125	0
3	PEG	E	1004	6/7	0.82	0.15	80,83,89,90	0
3	PEG	A	1006	7/7	0.83	0.29	66,80,102,102	0
3	PEG	G	1005	6/7	0.83	0.23	75,89,90,98	0
3	PEG	F	1005	7/7	0.83	0.24	56,58,66,73	0
3	PEG	E	1006	2/7	0.83	0.41	52,52,52,54	0
3	PEG	H	1002	7/7	0.85	0.18	77,83,95,98	0
3	PEG	E	1005	6/7	0.85	0.23	85,88,96,97	0
3	PEG	G	1007	2/7	0.85	0.32	58,58,58,65	0
3	PEG	B	1002	7/7	0.86	0.15	80,92,101,103	0
3	PEG	D	1002	7/7	0.87	0.14	66,74,84,85	0
3	PEG	G	1006	7/7	0.87	0.26	71,73,87,90	0
3	PEG	E	1002	7/7	0.87	0.17	60,68,77,77	0
3	PEG	F	1002	7/7	0.88	0.15	76,81,95,96	0
3	PEG	H	1004	2/7	0.88	0.20	48,48,48,64	0
3	PEG	A	1002	7/7	0.88	0.22	70,74,83,84	0
3	PEG	G	1008	7/7	0.88	0.15	72,75,82,85	0
4	CL	H	1006	1/1	0.88	0.16	83,83,83,83	0
4	CL	B	1008	1/1	0.89	0.14	67,67,67,67	0
3	PEG	C	1006	2/7	0.89	0.23	39,39,39,53	0
2	LMR	B	1001	9/9	0.89	0.12	89,93,97,101	0
3	PEG	G	1002	7/7	0.90	0.17	58,70,82,86	0
3	PEG	B	1003	7/7	0.91	0.18	79,82,84,86	0
4	CL	A	1010	1/1	0.91	0.09	81,81,81,81	0

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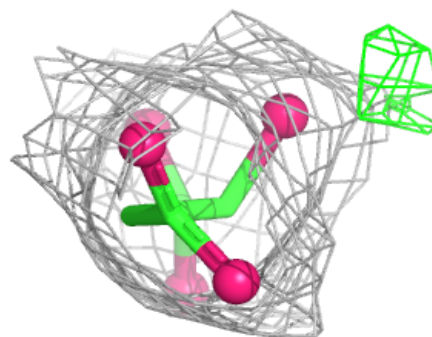
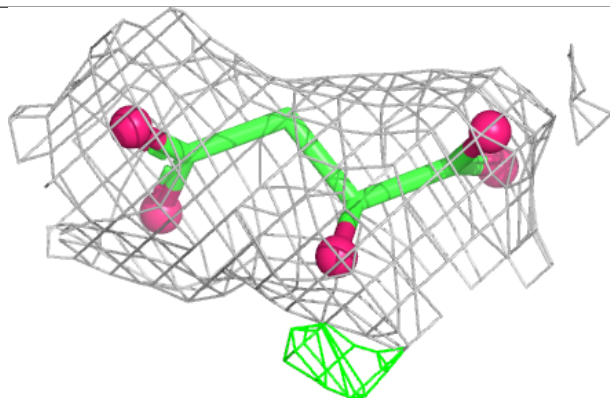
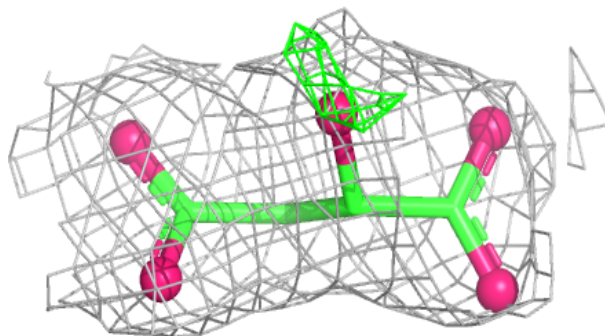
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	E	1010	1/1	0.91	0.07	76,76,76,76	0
3	PEG	C	1002	7/7	0.91	0.14	33,53,68,86	0
4	CL	C	1011	1/1	0.92	0.09	71,71,71,71	0
4	CL	E	1009	1/1	0.92	0.24	114,114,114,114	0
4	CL	D	1008	1/1	0.93	0.17	66,66,66,66	0
4	CL	D	1009	1/1	0.93	0.16	64,64,64,64	0
3	PEG	A	1007	2/7	0.93	0.28	43,43,43,56	0
3	PEG	D	1005	7/7	0.93	0.15	61,66,71,75	0
4	CL	F	1006	1/1	0.93	0.15	56,56,56,56	0
3	PEG	H	1003	7/7	0.93	0.10	63,64,75,84	0
2	LMR	D	1001	9/9	0.94	0.18	63,65,68,71	0
2	LMR	F	1001	9/9	0.94	0.09	64,71,76,79	0
2	LMR	A	1001	9/9	0.94	0.13	68,70,79,79	0
4	CL	G	1009	1/1	0.94	0.08	65,65,65,65	0
3	PEG	E	1007	7/7	0.94	0.08	56,58,66,75	0
4	CL	B	1007	1/1	0.95	0.16	71,71,71,71	0
4	CL	E	1008	1/1	0.95	0.21	64,64,64,64	0
3	PEG	D	1003	7/7	0.95	0.10	59,70,89,95	0
2	LMR	G	1001	9/9	0.95	0.11	71,76,80,81	0
3	PEG	C	1007	7/7	0.95	0.12	55,64,85,92	0
4	CL	D	1006	1/1	0.95	0.21	70,70,70,70	0
2	LMR	E	1001	9/9	0.95	0.10	57,61,69,69	0
2	LMR	C	1001	9/9	0.96	0.09	64,67,73,74	0
4	CL	B	1005	1/1	0.96	0.06	63,63,63,63	0
2	LMR	H	1001	9/9	0.96	0.11	74,79,84,84	0
4	CL	G	1010	1/1	0.96	0.05	57,57,57,57	0
3	PEG	F	1003	7/7	0.96	0.09	64,68,88,94	0
4	CL	C	1010	1/1	0.97	0.07	64,64,64,64	0
4	CL	D	1007	1/1	0.97	0.06	62,62,62,62	0
4	CL	H	1005	1/1	0.97	0.15	68,68,68,68	0
4	CL	F	1007	1/1	0.97	0.08	66,66,66,66	0
3	PEG	A	1008	7/7	0.98	0.07	70,70,72,79	0
4	CL	C	1008	1/1	0.98	0.13	53,53,53,53	0
4	CL	A	1009	1/1	0.98	0.16	66,66,66,66	0

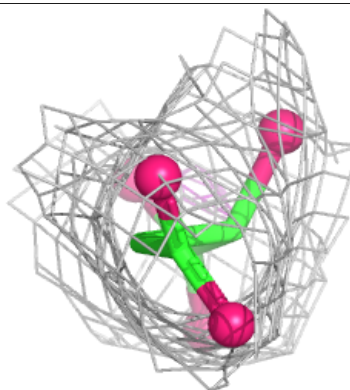
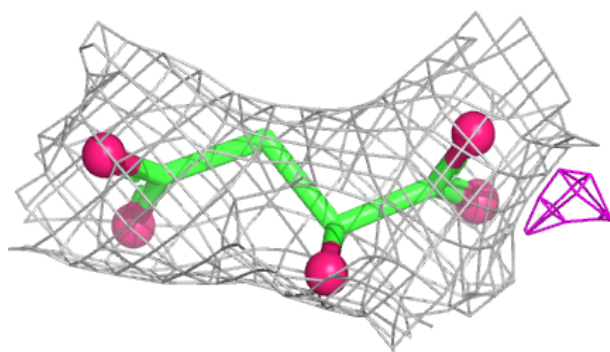
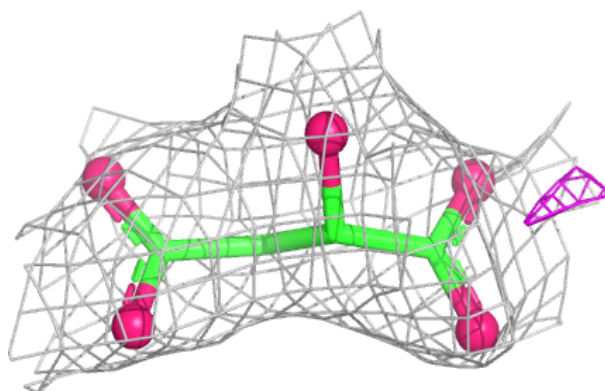
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMR B 1001:**

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

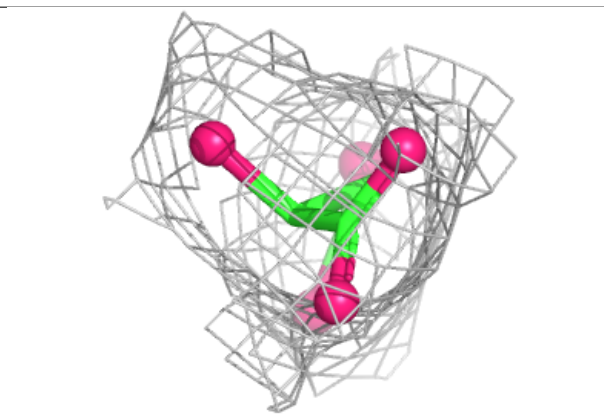
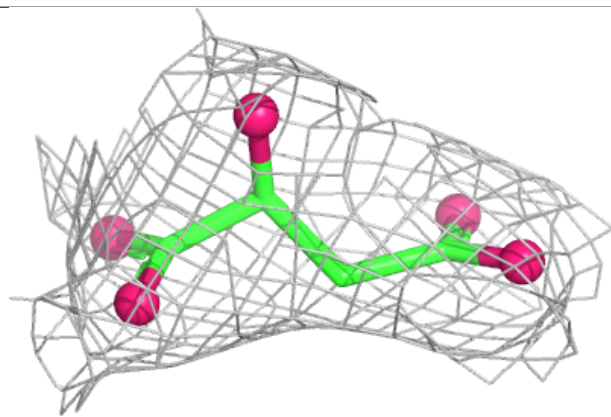
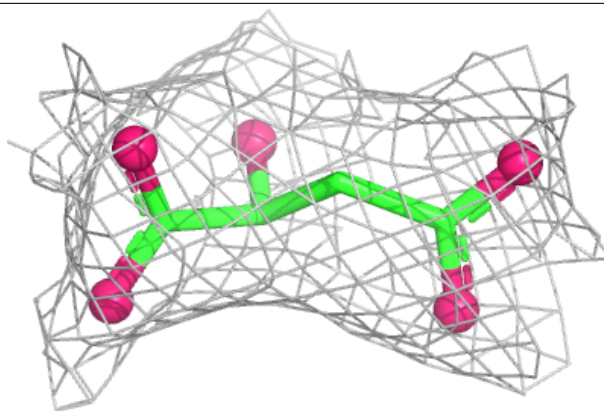
**Electron density around LMR D 1001:**

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

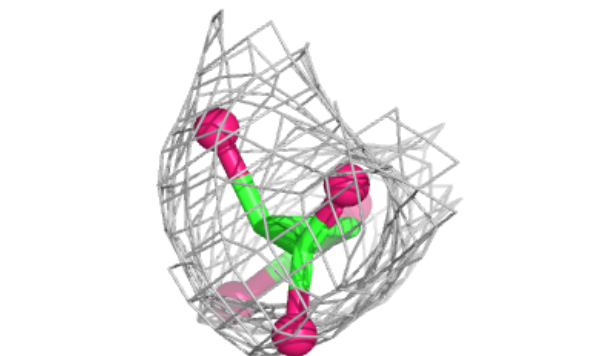
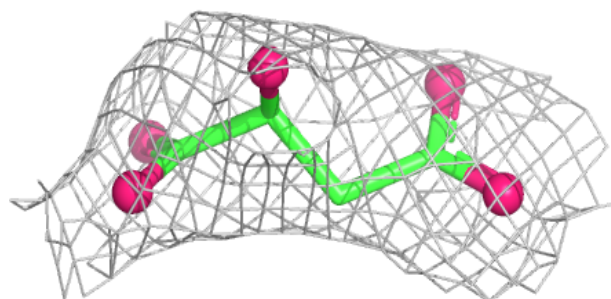
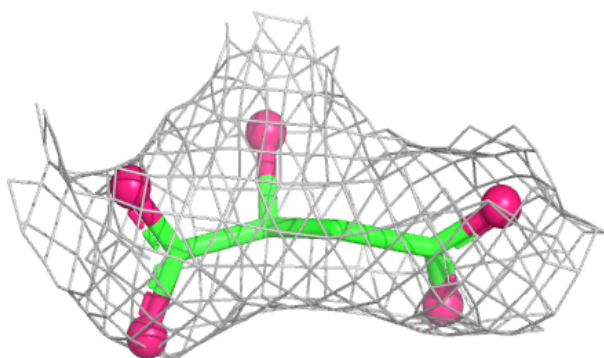


**Electron density around LMR F 1001:**

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

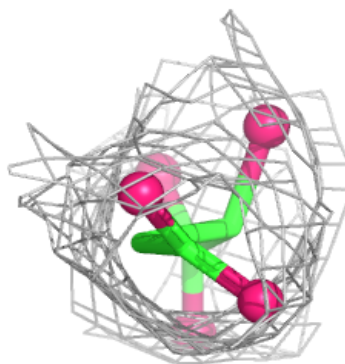
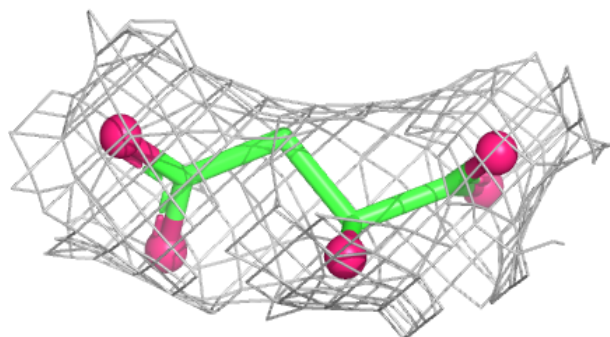
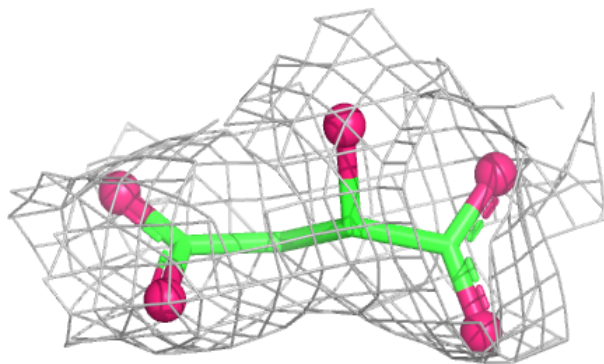
**Electron density around LMR A 1001:**

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

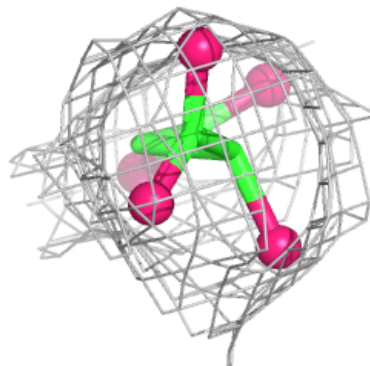
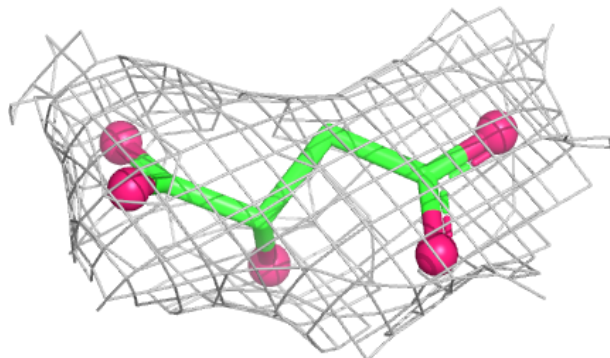
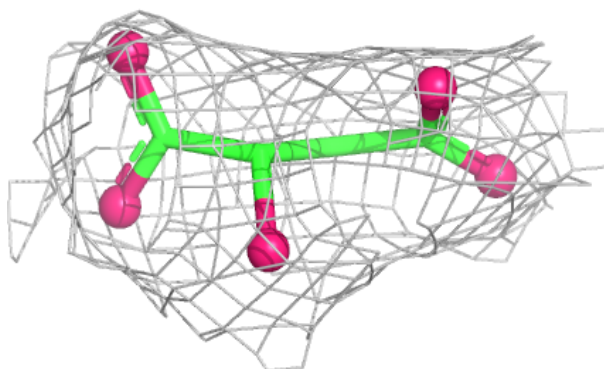


**Electron density around LMR G 1001:**

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

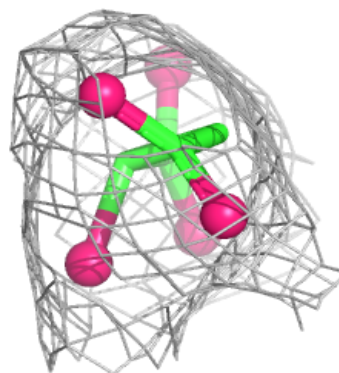
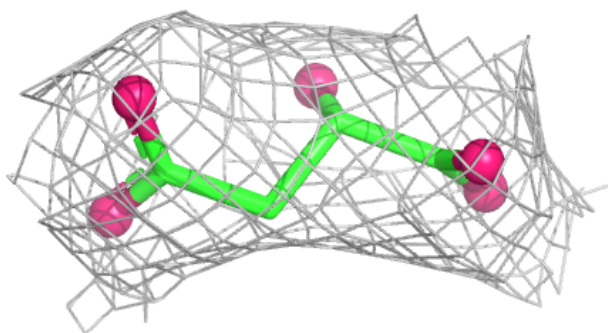
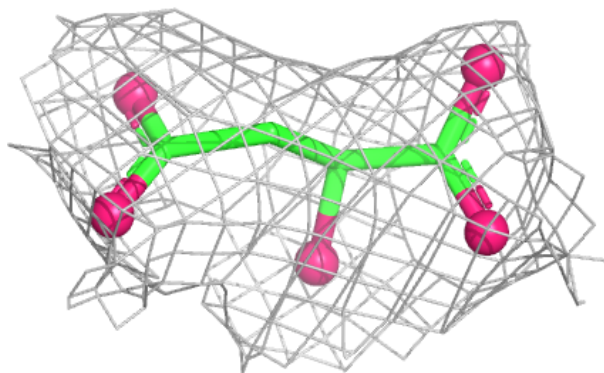
**Electron density around LMR E 1001:**

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

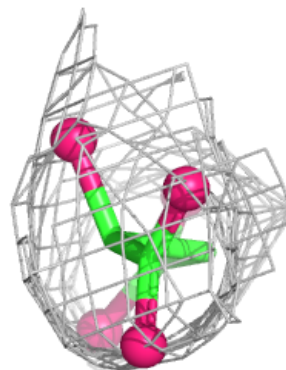
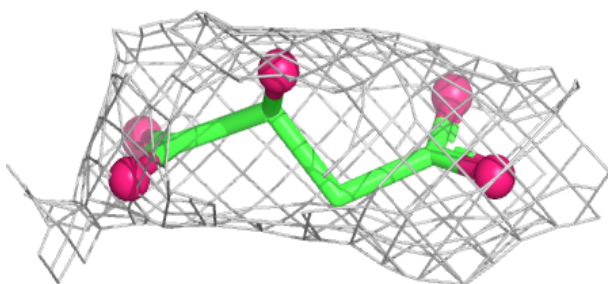
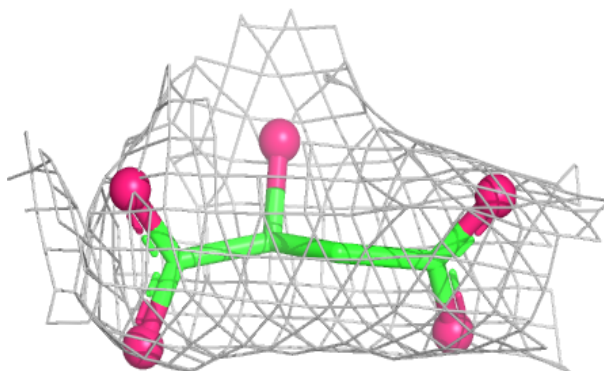


**Electron density around LMR C 1001:**

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

**Electron density around LMR H 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.