



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2022 – 10:15 AM EST

PDB ID : 7MS9
Title : Crystal structure of E114D mutant of Cg10062 with a covalent intermediate of the hydration of acetylenecarboxylic acid
Authors : Nayebi, G.H.; Geiger, J.H.; Draths, K.
Deposited on : 2021-05-10
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	2.26
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)	:	2.26

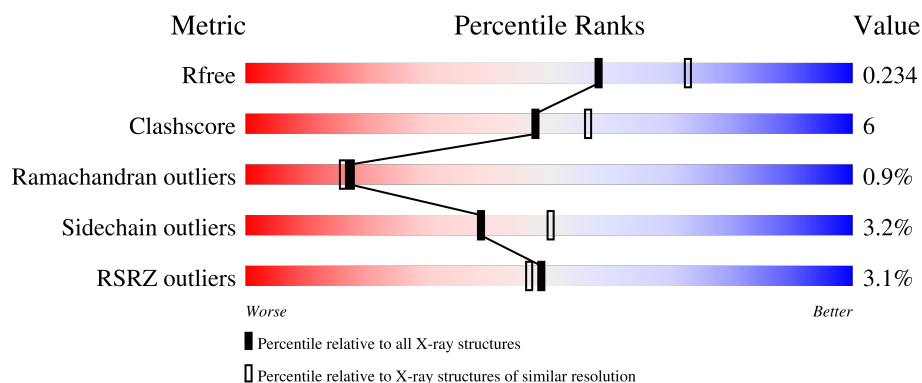
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	163	<div> <div>2%</div> <div>63% 12% 26%</div> </div>
1	B	163	<div> <div>2%</div> <div>62% 12% 26%</div> </div>
1	C	163	<div> <div>2%</div> <div>62% 12% 26%</div> </div>
1	D	163	<div> <div>0%</div> <div>63% 12% 26%</div> </div>
1	E	163	<div> <div>2%</div> <div>63% 10% 26%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	163	 58% 16% 26%
1	G	163	 59% 14% 26%
1	H	163	 58% 16% 26%
1	I	163	 61% 12% 26%
1	J	163	 60% 12% 26%
1	K	163	 60% 15% 26%
1	L	163	 61% 12% 26%

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	SO4	J	201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12493 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 4-oxalocrotonate tautomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	3	3	0
			1011	639	178	190	4			
1	B	121	Total	C	N	O	S	4	6	0
			1034	653	182	195	4			
1	C	121	Total	C	N	O	S	5	5	0
			1024	646	183	192	3			
1	D	121	Total	C	N	O	S	6	5	0
			1025	647	179	195	4			
1	E	121	Total	C	N	O	S	7	3	0
			1010	640	177	189	4			
1	F	121	Total	C	N	O	S	7	6	0
			1033	652	182	195	4			
1	G	121	Total	C	N	O	S	7	4	0
			1018	643	178	193	4			
1	H	121	Total	C	N	O	S	7	2	0
			1002	634	176	188	4			
1	I	121	Total	C	N	O	S	5	1	0
			996	631	175	187	3			
1	J	121	Total	C	N	O	S	5	2	0
			1007	637	179	188	3			
1	K	121	Total	C	N	O	S	7	2	0
			1002	634	176	188	4			
1	L	121	Total	C	N	O	S	11	1	0
			996	631	175	187	3			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
A	149	GLU	-	expression tag	UNP A0A0S2T163
A	150	ASN	-	expression tag	UNP A0A0S2T163
A	151	LEU	-	expression tag	UNP A0A0S2T163
A	152	TYR	-	expression tag	UNP A0A0S2T163

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Chain	Residue	Modelled	Actual	Comment	Reference
A	153	PHE	-	expression tag	UNP A0A0S2T163
A	154	GLN	-	expression tag	UNP A0A0S2T163
A	155	GLY	-	expression tag	UNP A0A0S2T163
A	156	LEU	-	expression tag	UNP A0A0S2T163
A	157	GLU	-	expression tag	UNP A0A0S2T163
A	158	HIS	-	expression tag	UNP A0A0S2T163
A	159	HIS	-	expression tag	UNP A0A0S2T163
A	160	HIS	-	expression tag	UNP A0A0S2T163
A	161	HIS	-	expression tag	UNP A0A0S2T163
A	162	HIS	-	expression tag	UNP A0A0S2T163
A	163	HIS	-	expression tag	UNP A0A0S2T163
B	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
B	149	GLU	-	expression tag	UNP A0A0S2T163
B	150	ASN	-	expression tag	UNP A0A0S2T163
B	151	LEU	-	expression tag	UNP A0A0S2T163
B	152	TYR	-	expression tag	UNP A0A0S2T163
B	153	PHE	-	expression tag	UNP A0A0S2T163
B	154	GLN	-	expression tag	UNP A0A0S2T163
B	155	GLY	-	expression tag	UNP A0A0S2T163
B	156	LEU	-	expression tag	UNP A0A0S2T163
B	157	GLU	-	expression tag	UNP A0A0S2T163
B	158	HIS	-	expression tag	UNP A0A0S2T163
B	159	HIS	-	expression tag	UNP A0A0S2T163
B	160	HIS	-	expression tag	UNP A0A0S2T163
B	161	HIS	-	expression tag	UNP A0A0S2T163
B	162	HIS	-	expression tag	UNP A0A0S2T163
B	163	HIS	-	expression tag	UNP A0A0S2T163
C	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
C	149	GLU	-	expression tag	UNP A0A0S2T163
C	150	ASN	-	expression tag	UNP A0A0S2T163
C	151	LEU	-	expression tag	UNP A0A0S2T163
C	152	TYR	-	expression tag	UNP A0A0S2T163
C	153	PHE	-	expression tag	UNP A0A0S2T163
C	154	GLN	-	expression tag	UNP A0A0S2T163
C	155	GLY	-	expression tag	UNP A0A0S2T163
C	156	LEU	-	expression tag	UNP A0A0S2T163
C	157	GLU	-	expression tag	UNP A0A0S2T163
C	158	HIS	-	expression tag	UNP A0A0S2T163
C	159	HIS	-	expression tag	UNP A0A0S2T163
C	160	HIS	-	expression tag	UNP A0A0S2T163
C	161	HIS	-	expression tag	UNP A0A0S2T163
C	162	HIS	-	expression tag	UNP A0A0S2T163

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Chain	Residue	Modelled	Actual	Comment	Reference
C	163	HIS	-	expression tag	UNP A0A0S2T163
D	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
D	149	GLU	-	expression tag	UNP A0A0S2T163
D	150	ASN	-	expression tag	UNP A0A0S2T163
D	151	LEU	-	expression tag	UNP A0A0S2T163
D	152	TYR	-	expression tag	UNP A0A0S2T163
D	153	PHE	-	expression tag	UNP A0A0S2T163
D	154	GLN	-	expression tag	UNP A0A0S2T163
D	155	GLY	-	expression tag	UNP A0A0S2T163
D	156	LEU	-	expression tag	UNP A0A0S2T163
D	157	GLU	-	expression tag	UNP A0A0S2T163
D	158	HIS	-	expression tag	UNP A0A0S2T163
D	159	HIS	-	expression tag	UNP A0A0S2T163
D	160	HIS	-	expression tag	UNP A0A0S2T163
D	161	HIS	-	expression tag	UNP A0A0S2T163
D	162	HIS	-	expression tag	UNP A0A0S2T163
D	163	HIS	-	expression tag	UNP A0A0S2T163
E	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
E	149	GLU	-	expression tag	UNP A0A0S2T163
E	150	ASN	-	expression tag	UNP A0A0S2T163
E	151	LEU	-	expression tag	UNP A0A0S2T163
E	152	TYR	-	expression tag	UNP A0A0S2T163
E	153	PHE	-	expression tag	UNP A0A0S2T163
E	154	GLN	-	expression tag	UNP A0A0S2T163
E	155	GLY	-	expression tag	UNP A0A0S2T163
E	156	LEU	-	expression tag	UNP A0A0S2T163
E	157	GLU	-	expression tag	UNP A0A0S2T163
E	158	HIS	-	expression tag	UNP A0A0S2T163
E	159	HIS	-	expression tag	UNP A0A0S2T163
E	160	HIS	-	expression tag	UNP A0A0S2T163
E	161	HIS	-	expression tag	UNP A0A0S2T163
E	162	HIS	-	expression tag	UNP A0A0S2T163
E	163	HIS	-	expression tag	UNP A0A0S2T163
F	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
F	149	GLU	-	expression tag	UNP A0A0S2T163
F	150	ASN	-	expression tag	UNP A0A0S2T163
F	151	LEU	-	expression tag	UNP A0A0S2T163
F	152	TYR	-	expression tag	UNP A0A0S2T163
F	153	PHE	-	expression tag	UNP A0A0S2T163
F	154	GLN	-	expression tag	UNP A0A0S2T163
F	155	GLY	-	expression tag	UNP A0A0S2T163
F	156	LEU	-	expression tag	UNP A0A0S2T163

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Chain	Residue	Modelled	Actual	Comment	Reference
F	157	GLU	-	expression tag	UNP A0A0S2T163
F	158	HIS	-	expression tag	UNP A0A0S2T163
F	159	HIS	-	expression tag	UNP A0A0S2T163
F	160	HIS	-	expression tag	UNP A0A0S2T163
F	161	HIS	-	expression tag	UNP A0A0S2T163
F	162	HIS	-	expression tag	UNP A0A0S2T163
F	163	HIS	-	expression tag	UNP A0A0S2T163
G	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
G	149	GLU	-	expression tag	UNP A0A0S2T163
G	150	ASN	-	expression tag	UNP A0A0S2T163
G	151	LEU	-	expression tag	UNP A0A0S2T163
G	152	TYR	-	expression tag	UNP A0A0S2T163
G	153	PHE	-	expression tag	UNP A0A0S2T163
G	154	GLN	-	expression tag	UNP A0A0S2T163
G	155	GLY	-	expression tag	UNP A0A0S2T163
G	156	LEU	-	expression tag	UNP A0A0S2T163
G	157	GLU	-	expression tag	UNP A0A0S2T163
G	158	HIS	-	expression tag	UNP A0A0S2T163
G	159	HIS	-	expression tag	UNP A0A0S2T163
G	160	HIS	-	expression tag	UNP A0A0S2T163
G	161	HIS	-	expression tag	UNP A0A0S2T163
G	162	HIS	-	expression tag	UNP A0A0S2T163
G	163	HIS	-	expression tag	UNP A0A0S2T163
H	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
H	149	GLU	-	expression tag	UNP A0A0S2T163
H	150	ASN	-	expression tag	UNP A0A0S2T163
H	151	LEU	-	expression tag	UNP A0A0S2T163
H	152	TYR	-	expression tag	UNP A0A0S2T163
H	153	PHE	-	expression tag	UNP A0A0S2T163
H	154	GLN	-	expression tag	UNP A0A0S2T163
H	155	GLY	-	expression tag	UNP A0A0S2T163
H	156	LEU	-	expression tag	UNP A0A0S2T163
H	157	GLU	-	expression tag	UNP A0A0S2T163
H	158	HIS	-	expression tag	UNP A0A0S2T163
H	159	HIS	-	expression tag	UNP A0A0S2T163
H	160	HIS	-	expression tag	UNP A0A0S2T163
H	161	HIS	-	expression tag	UNP A0A0S2T163
H	162	HIS	-	expression tag	UNP A0A0S2T163
H	163	HIS	-	expression tag	UNP A0A0S2T163
I	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
I	149	GLU	-	expression tag	UNP A0A0S2T163
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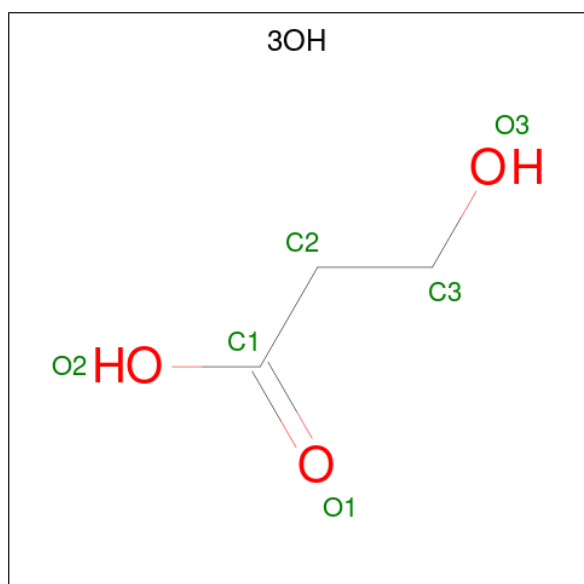
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I	152	TYR	-	expression tag	UNP A0A0S2T163
I	153	PHE	-	expression tag	UNP A0A0S2T163
I	154	GLN	-	expression tag	UNP A0A0S2T163
I	155	GLY	-	expression tag	UNP A0A0S2T163
I	156	LEU	-	expression tag	UNP A0A0S2T163
I	157	GLU	-	expression tag	UNP A0A0S2T163
I	158	HIS	-	expression tag	UNP A0A0S2T163
I	159	HIS	-	expression tag	UNP A0A0S2T163
I	160	HIS	-	expression tag	UNP A0A0S2T163
I	161	HIS	-	expression tag	UNP A0A0S2T163
I	162	HIS	-	expression tag	UNP A0A0S2T163
I	163	HIS	-	expression tag	UNP A0A0S2T163
J	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
J	149	GLU	-	expression tag	UNP A0A0S2T163
J	150	ASN	-	expression tag	UNP A0A0S2T163
J	151	LEU	-	expression tag	UNP A0A0S2T163
J	152	TYR	-	expression tag	UNP A0A0S2T163
J	153	PHE	-	expression tag	UNP A0A0S2T163
J	154	GLN	-	expression tag	UNP A0A0S2T163
J	155	GLY	-	expression tag	UNP A0A0S2T163
J	156	LEU	-	expression tag	UNP A0A0S2T163
J	157	GLU	-	expression tag	UNP A0A0S2T163
J	158	HIS	-	expression tag	UNP A0A0S2T163
J	159	HIS	-	expression tag	UNP A0A0S2T163
J	160	HIS	-	expression tag	UNP A0A0S2T163
J	161	HIS	-	expression tag	UNP A0A0S2T163
J	162	HIS	-	expression tag	UNP A0A0S2T163
J	163	HIS	-	expression tag	UNP A0A0S2T163
K	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
K	149	GLU	-	expression tag	UNP A0A0S2T163
K	150	ASN	-	expression tag	UNP A0A0S2T163
K	151	LEU	-	expression tag	UNP A0A0S2T163
K	152	TYR	-	expression tag	UNP A0A0S2T163
K	153	PHE	-	expression tag	UNP A0A0S2T163
K	154	GLN	-	expression tag	UNP A0A0S2T163
K	155	GLY	-	expression tag	UNP A0A0S2T163
K	156	LEU	-	expression tag	UNP A0A0S2T163
K	157	GLU	-	expression tag	UNP A0A0S2T163
K	158	HIS	-	expression tag	UNP A0A0S2T163
K	159	HIS	-	expression tag	UNP A0A0S2T163
K	160	HIS	-	expression tag	UNP A0A0S2T163

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Chain	Residue	Modelled	Actual	Comment	Reference
K	161	HIS	-	expression tag	UNP A0A0S2T163
K	162	HIS	-	expression tag	UNP A0A0S2T163
K	163	HIS	-	expression tag	UNP A0A0S2T163
L	114	ASP	GLU	engineered mutation	UNP A0A0S2T163
L	149	GLU	-	expression tag	UNP A0A0S2T163
L	150	ASN	-	expression tag	UNP A0A0S2T163
L	151	LEU	-	expression tag	UNP A0A0S2T163
L	152	TYR	-	expression tag	UNP A0A0S2T163
L	153	PHE	-	expression tag	UNP A0A0S2T163
L	154	GLN	-	expression tag	UNP A0A0S2T163
L	155	GLY	-	expression tag	UNP A0A0S2T163
L	156	LEU	-	expression tag	UNP A0A0S2T163
L	157	GLU	-	expression tag	UNP A0A0S2T163
L	158	HIS	-	expression tag	UNP A0A0S2T163
L	159	HIS	-	expression tag	UNP A0A0S2T163
L	160	HIS	-	expression tag	UNP A0A0S2T163
L	161	HIS	-	expression tag	UNP A0A0S2T163
L	162	HIS	-	expression tag	UNP A0A0S2T163
L	163	HIS	-	expression tag	UNP A0A0S2T163

- Molecule 2 is 3-HYDROXY-PROPANOIC ACID (three-letter code: 3OH) (formula: C₃H₆O₃) (labeled as "Ligand of Interest" by depositor).



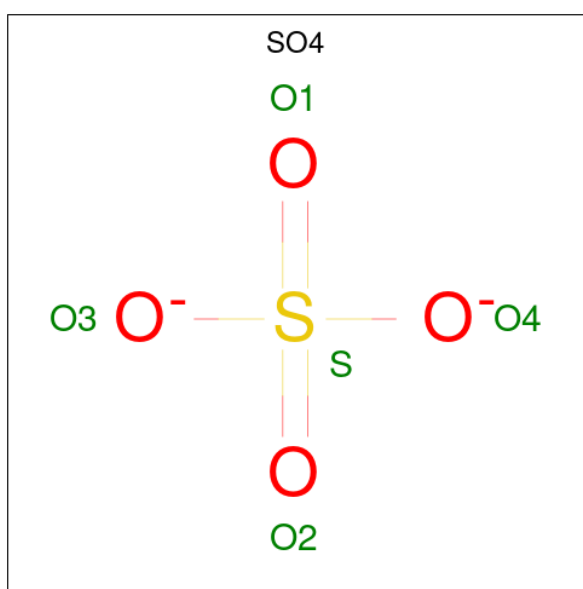
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			5	3	2		
2	H	1	Total	C	O	0	0
			5	3	2		
2	I	1	Total	C	O	0	0
			5	3	2		
2	K	1	Total	C	O	0	0
			5	3	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

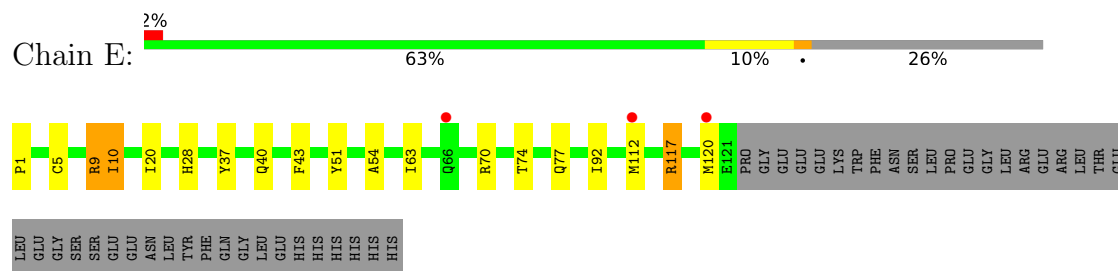
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	24	Total O 24 24	0	0
4	C	25	Total O 25 25	0	0
4	D	18	Total O 18 18	0	0
4	E	32	Total O 32 32	0	0
4	F	20	Total O 20 20	0	0
4	G	19	Total O 19 19	0	0
4	H	18	Total O 18 18	0	0
4	I	29	Total O 29 29	0	0
4	J	23	Total O 23 23	0	0
4	K	19	Total O 19 19	0	0
4	L	19	Total O 19 19	0	0

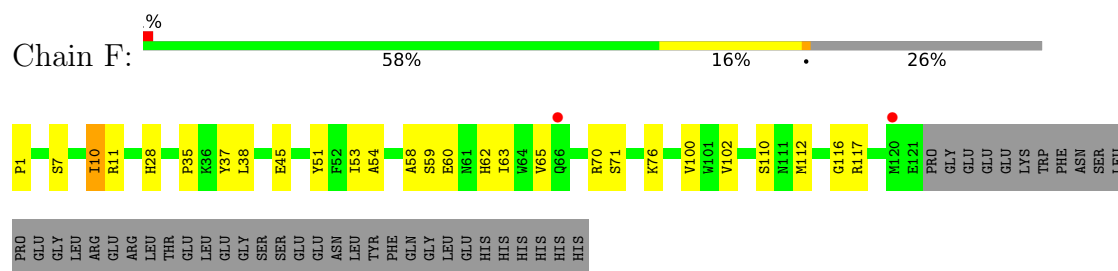
- Molecule 1: 4-oxalocrotonate tautomerase



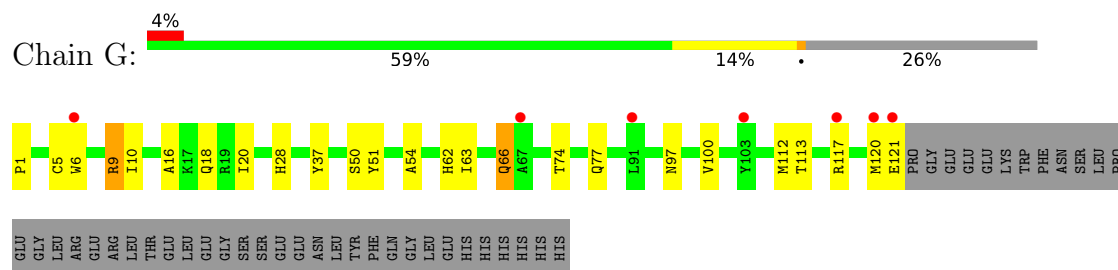
- Molecule 1: 4-oxalocrotonate tautomerase



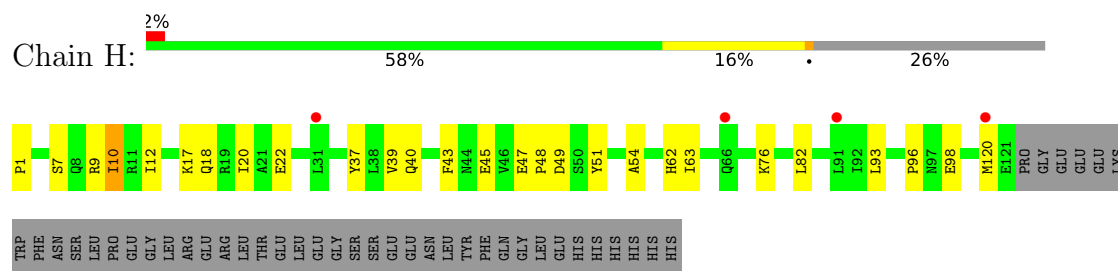
- Molecule 1: 4-oxalocrotonate tautomerase



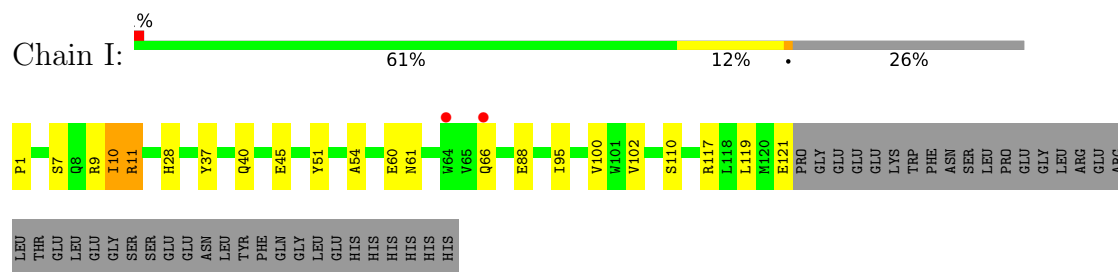
- Molecule 1: 4-oxalocrotonate tautomerase



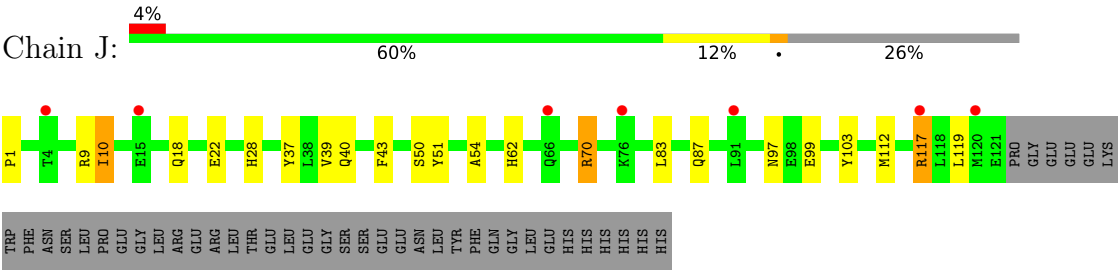
- Molecule 1: 4-oxalocrotonate tautomerase



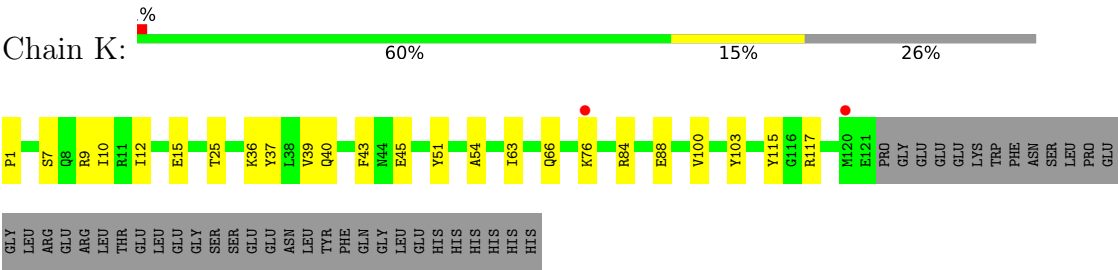
- Molecule 1: 4-oxalocrotonate tautomerase



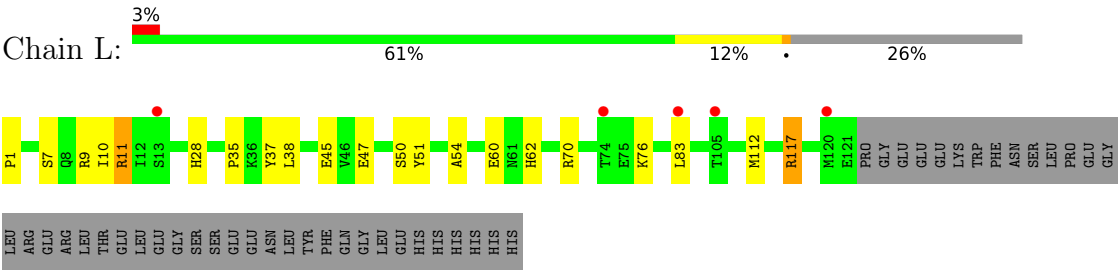
- Molecule 1: 4-oxalocrotonate tautomerase



• Molecule 1: 4-oxalocrotonate tautomerase



• Molecule 1: 4-oxalocrotonate tautomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.32Å 146.30Å 146.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.09 – 2.20 36.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.09-2.20) 99.4 (36.09-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.235 0.183 , 0.234	Depositor DCC
R_{free} test set	2004 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12493	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3OH, SO4

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	0.25	0/1032	0.54	0/1400
1	B	0.25	0/1055	0.53	0/1432
1	C	0.24	0/1045	0.52	0/1417
1	D	0.24	0/1046	0.53	0/1420
1	E	0.24	0/1031	0.51	0/1399
1	F	0.24	0/1054	0.51	0/1431
1	G	0.24	0/1039	0.52	0/1410
1	H	0.25	0/1023	0.53	0/1388
1	I	0.25	0/1017	0.52	0/1380
1	J	0.24	0/1028	0.54	0/1394
1	K	0.25	0/1023	0.52	0/1388
1	L	0.24	0/1017	0.52	0/1380
All	All	0.24	0/12410	0.52	0/16839

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	1011	0	1000	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1034	0	1022	11	0
1	C	1024	0	1014	14	0
1	D	1025	0	1012	13	0
1	E	1010	0	1004	13	0
1	F	1033	0	1022	15	0
1	G	1018	0	1005	17	0
1	H	1002	0	993	20	0
1	I	996	0	989	16	0
1	J	1007	0	1002	19	0
1	K	1002	0	993	13	0
1	L	996	0	990	13	0
2	A	5	0	2	1	0
2	B	5	0	2	1	0
2	H	5	0	2	0	0
2	I	5	0	2	1	0
2	K	5	0	2	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	J	5	0	0	2	0
3	L	5	0	0	0	0
4	A	29	0	0	1	0
4	B	24	0	0	0	0
4	C	25	0	0	1	1
4	D	18	0	0	3	1
4	E	32	0	0	0	0
4	F	20	0	0	0	0
4	G	19	0	0	4	1
4	H	18	0	0	0	0
4	I	29	0	0	1	0
4	J	23	0	0	2	1
4	K	19	0	0	1	0
4	L	19	0	0	0	0
All	All	12493	0	12056	147	2

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 6.

The worst 5 of 147 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:O	4:A:301:HOH:O	1.81	0.97
1:G:18:GLN:NE2	4:G:301:HOH:O	1.98	0.96
1:F:110:SER:HA	1:F:117[B]:ARG:HH12	1.46	0.79
1:C:47:GLU:OE2	1:E:9:ARG:NH2	2.17	0.78
1:J:103:TYR:OH	4:J:301:HOH:O	2.02	0.78

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:318:HOH:O	4:J:323:HOH:O[3_554]	2.13	0.07
4:C:323:HOH:O	4:D:318:HOH:O[4_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/163 (75%)	117 (96%)	4 (3%)	1 (1%)	19	19
1	B	125/163 (77%)	122 (98%)	2 (2%)	1 (1%)	19	19
1	C	123/163 (76%)	118 (96%)	4 (3%)	1 (1%)	19	19
1	D	124/163 (76%)	121 (98%)	3 (2%)	0	100	100
1	E	122/163 (75%)	117 (96%)	4 (3%)	1 (1%)	19	19
1	F	125/163 (77%)	121 (97%)	3 (2%)	1 (1%)	19	19
1	G	123/163 (76%)	116 (94%)	5 (4%)	2 (2%)	9	7
1	H	121/163 (74%)	116 (96%)	3 (2%)	2 (2%)	9	6
1	I	120/163 (74%)	116 (97%)	3 (2%)	1 (1%)	19	19
1	J	121/163 (74%)	116 (96%)	4 (3%)	1 (1%)	19	19
1	K	121/163 (74%)	117 (97%)	3 (2%)	1 (1%)	19	19
1	L	120/163 (74%)	114 (95%)	5 (4%)	1 (1%)	19	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1467/1956 (75%)	1411 (96%)	43 (3%)	13 (1%)	17 16

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	ILE
1	C	10	ILE
1	F	10	ILE
1	I	10	ILE
1	K	10	ILE

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	109/144 (76%)	104 (95%)	5 (5%)	27 34
1	B	112/144 (78%)	108 (96%)	4 (4%)	35 45
1	C	110/144 (76%)	108 (98%)	2 (2%)	59 72
1	D	111/144 (77%)	106 (96%)	5 (4%)	27 34
1	E	109/144 (76%)	104 (95%)	5 (5%)	27 34
1	F	112/144 (78%)	109 (97%)	3 (3%)	44 57
1	G	110/144 (76%)	106 (96%)	4 (4%)	35 45
1	H	108/144 (75%)	106 (98%)	2 (2%)	57 71
1	I	107/144 (74%)	104 (97%)	3 (3%)	43 56
1	J	108/144 (75%)	103 (95%)	5 (5%)	27 34
1	K	108/144 (75%)	102 (94%)	6 (6%)	21 25
1	L	107/144 (74%)	102 (95%)	5 (5%)	26 33
All	All	1311/1728 (76%)	1262 (96%)	49 (4%)	39 43

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	51	TYR
1	J	70[C]	ARG
1	H	76	LYS
1	I	66	GLN
1	J	117[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	8	GLN
1	L	56	GLN
1	F	28	HIS
1	G	8	GLN
1	J	87	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	201	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	G	201	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	L	201	-	4,4,4	0.20	0	6,6,6	0.23	0
2	3OH	K	201	1	1,4,5	2.66	1 (100%)	1,4,5	5.76	1 (100%)
2	3OH	A	201	1	1,4,5	2.63	1 (100%)	1,4,5	6.47	1 (100%)
3	SO4	E	201	-	4,4,4	0.13	0	6,6,6	0.08	0
2	3OH	B	201	1	1,4,5	2.66	1 (100%)	1,4,5	6.48	1 (100%)
3	SO4	D	201	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	J	201	-	4,4,4	0.14	0	6,6,6	0.07	0
2	3OH	I	201	1	1,4,5	2.63	1 (100%)	1,4,5	6.43	1 (100%)
2	3OH	H	201	1	1,4,5	2.68	1 (100%)	1,4,5	5.83	1 (100%)

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
2	3OH	K	201	1	-	0/0/2/3	-
2	3OH	A	201	1	-	0/0/2/3	-
2	3OH	B	201	1	-	0/0/2/3	-
2	3OH	I	201	1	-	0/0/2/3	-
2	3OH	H	201	1	-	0/0/2/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	3OH	C3-C2	-2.68	1.32	1.50
2	B	201	3OH	C3-C2	-2.66	1.32	1.50
2	K	201	3OH	C3-C2	-2.66	1.32	1.50
2	A	201	3OH	C3-C2	-2.63	1.32	1.50
2	I	201	3OH	C3-C2	-2.63	1.32	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	3OH	C3-C2-C1	6.48	121.55	112.59
2	A	201	3OH	C3-C2-C1	6.47	121.53	112.59
2	I	201	3OH	C3-C2-C1	6.43	121.48	112.59
2	H	201	3OH	C3-C2-C1	5.83	120.66	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	201	3OH	C3-C2-C1	5.76	120.55	112.59

There are no chirality outliers.

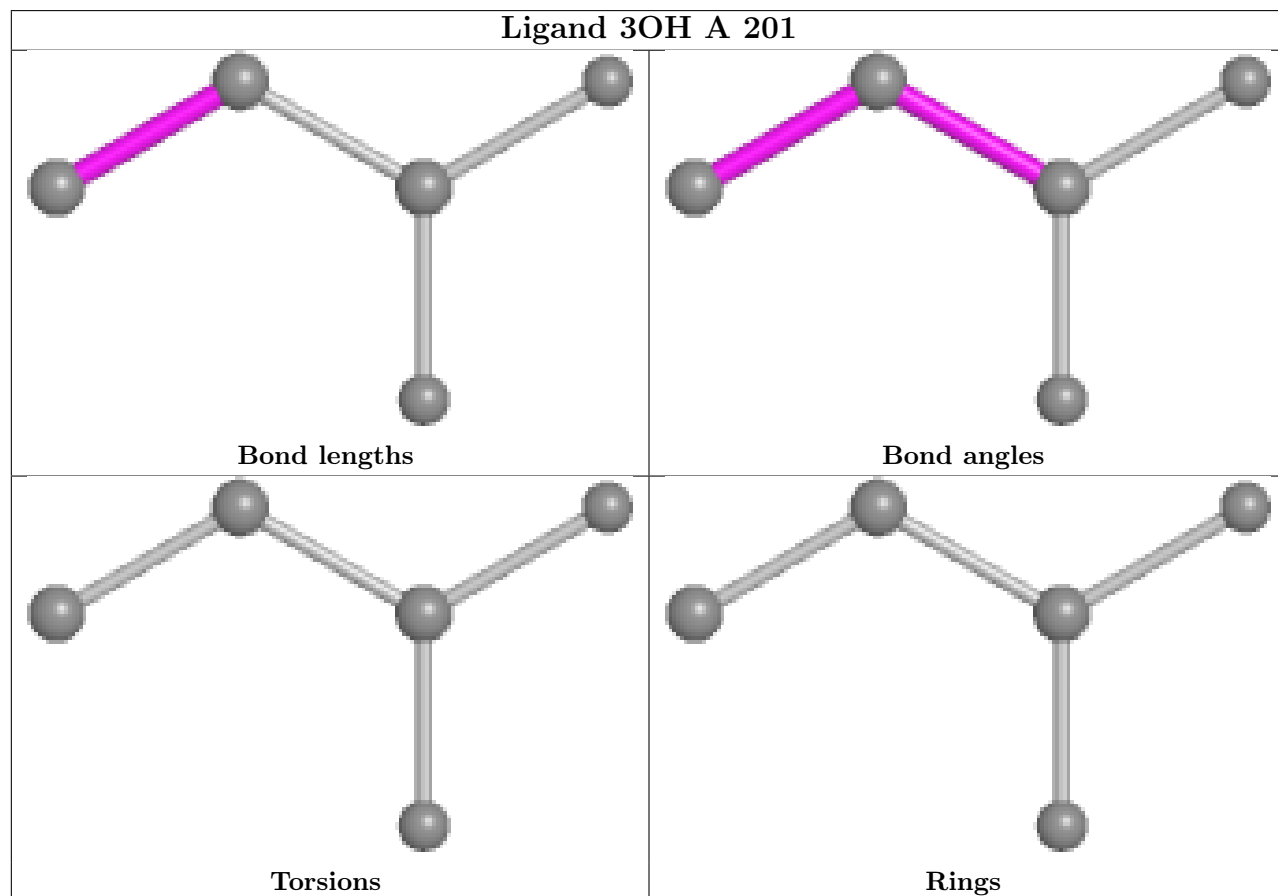
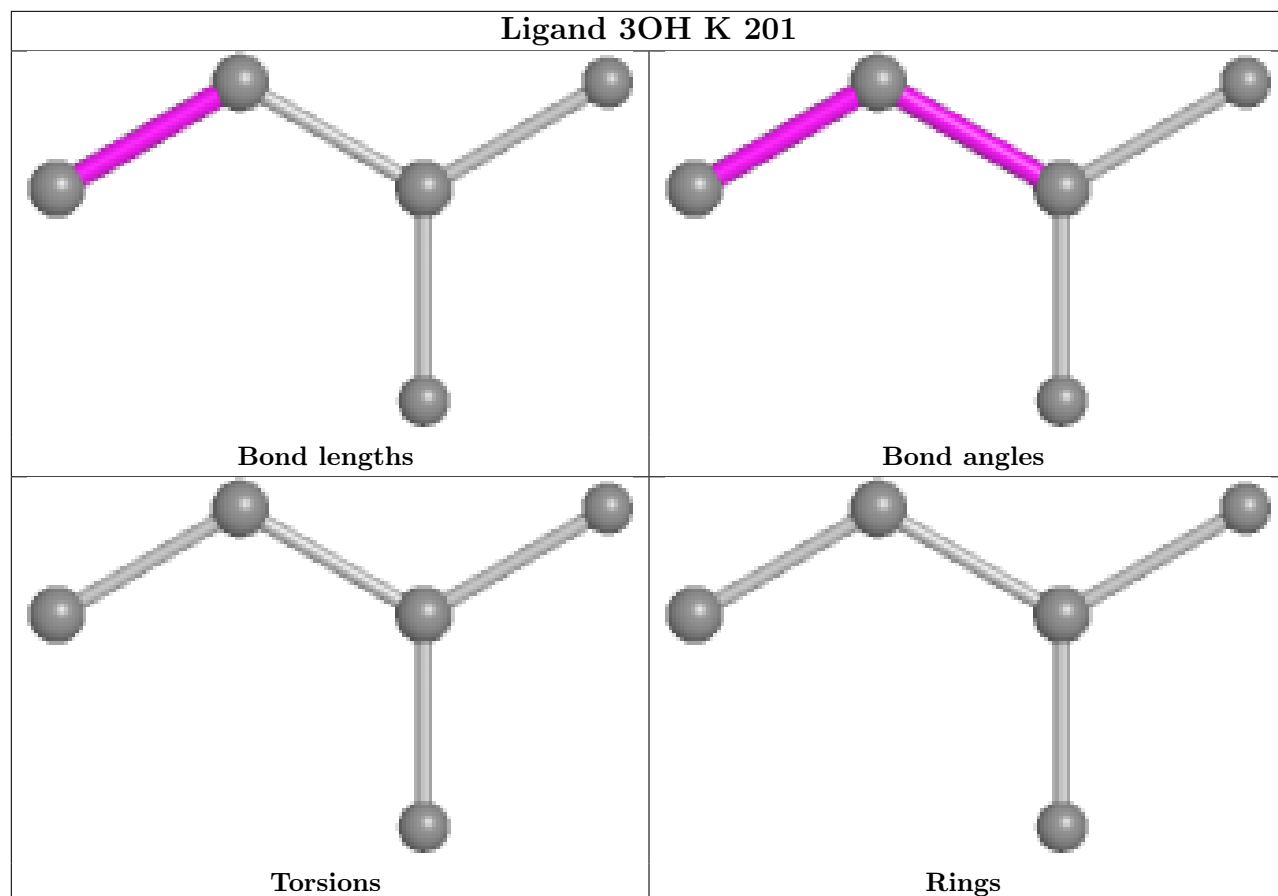
There are no torsion outliers.

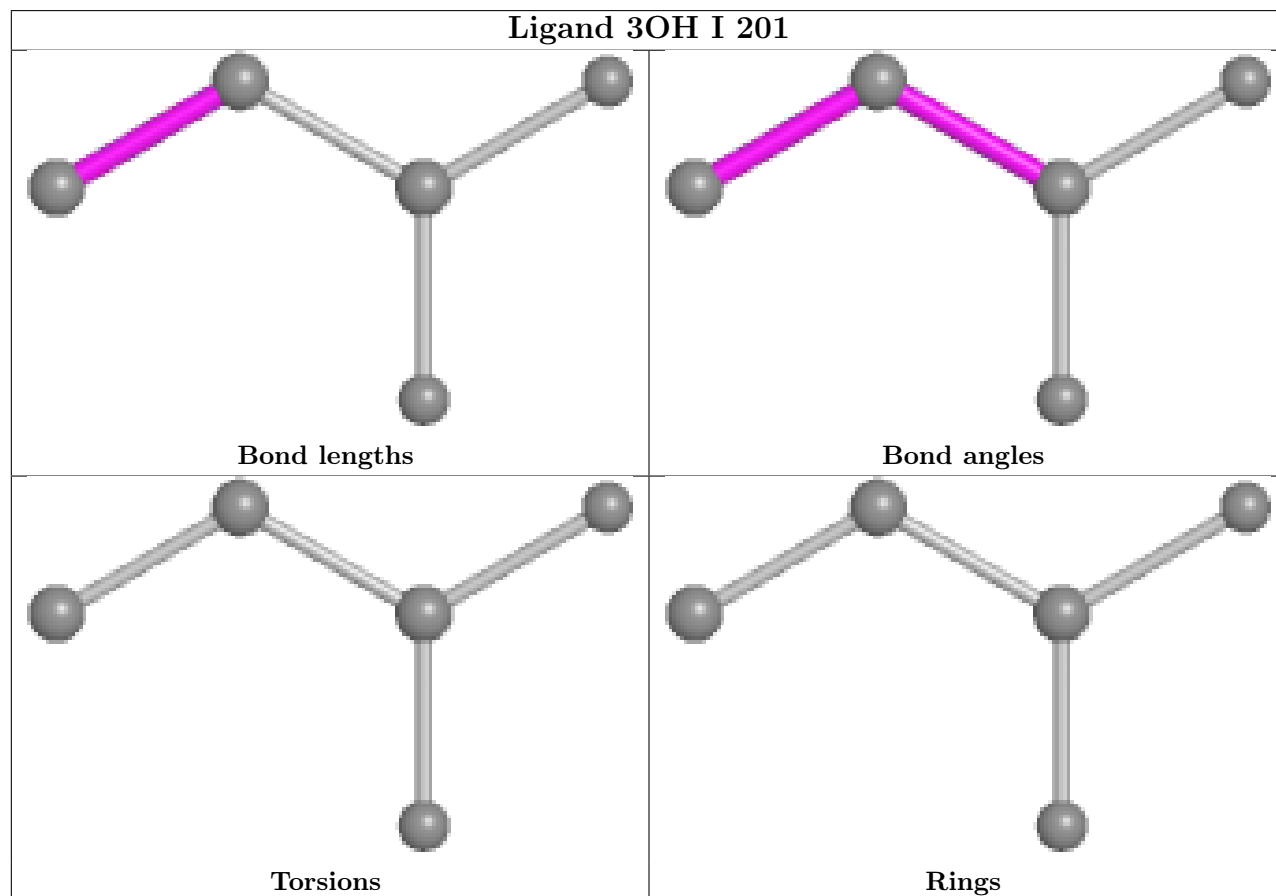
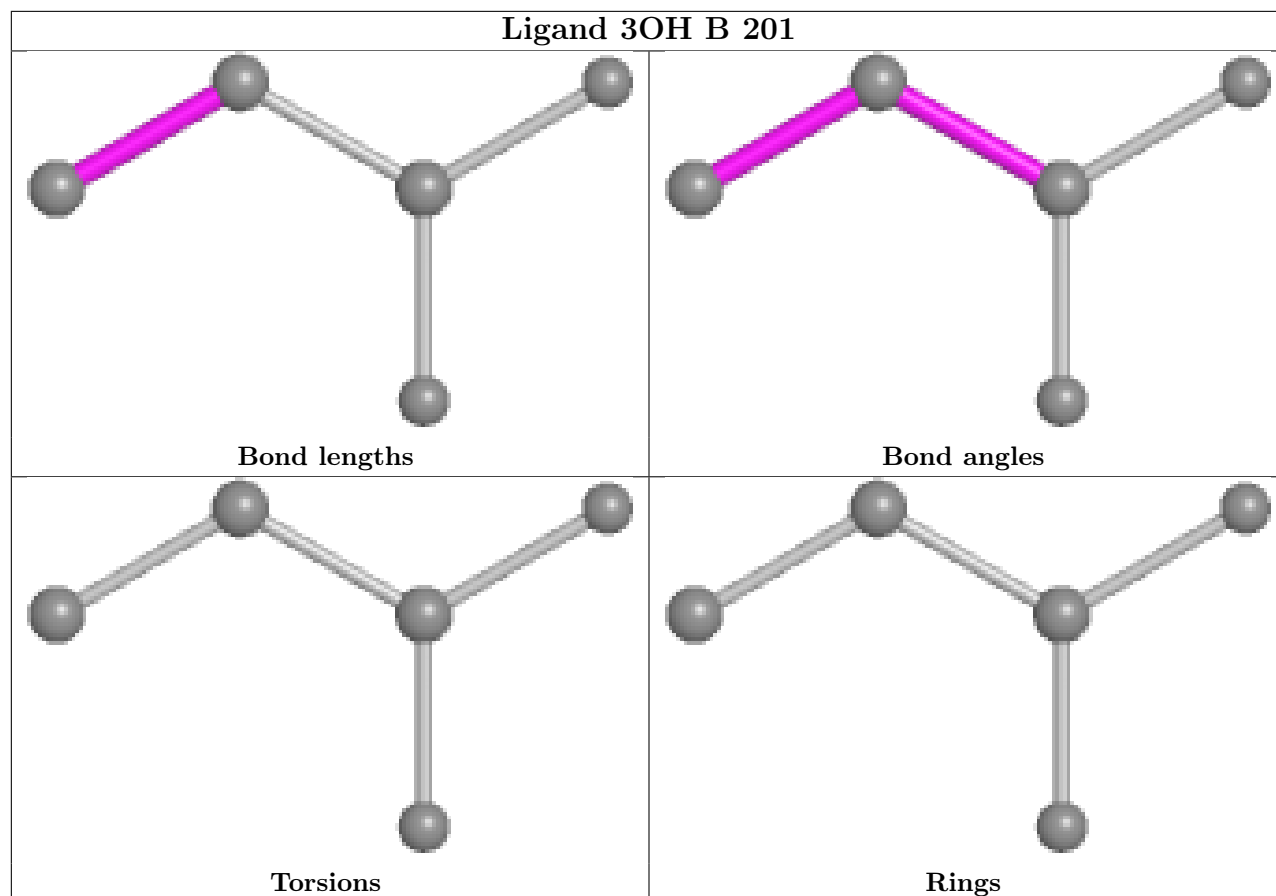
There are no ring outliers.

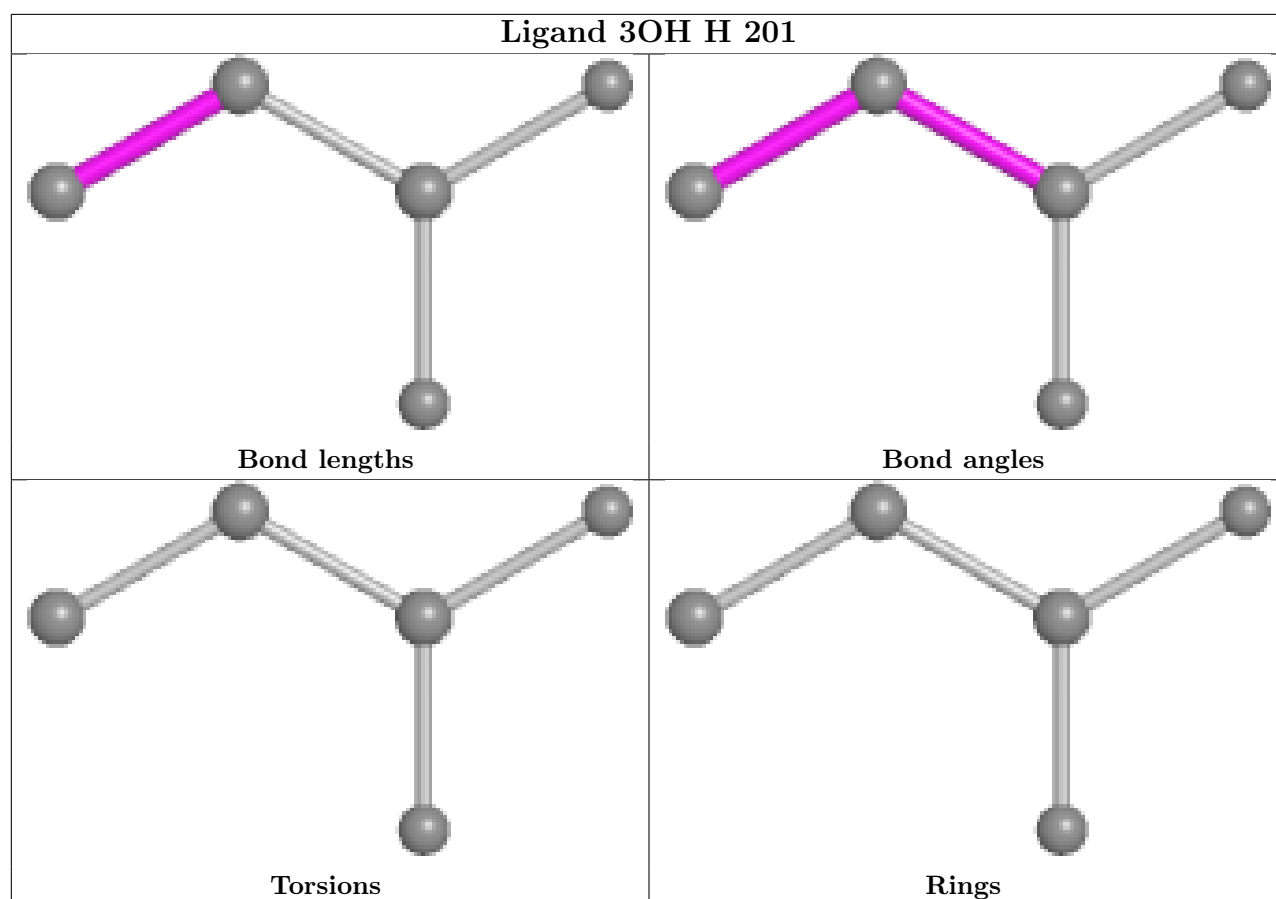
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	3OH	1	0
3	E	201	SO4	1	0
2	B	201	3OH	1	0
3	J	201	SO4	2	0
2	I	201	3OH	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	121/163 (74%)	0.08	4 (3%)	46	44	36, 47, 60, 93	92 (76%)
1	B	121/163 (74%)	-0.03	3 (2%)	57	55	37, 48, 58, 108	77 (63%)
1	C	121/163 (74%)	0.05	4 (3%)	46	44	37, 46, 57, 110	93 (76%)
1	D	121/163 (74%)	-0.01	2 (1%)	70	68	38, 48, 59, 108	86 (71%)
1	E	121/163 (74%)	-0.07	3 (2%)	57	55	34, 46, 58, 103	92 (76%)
1	F	121/163 (74%)	-0.07	2 (1%)	70	68	38, 48, 61, 107	90 (74%)
1	G	121/163 (74%)	0.19	7 (5%)	23	22	37, 50, 62, 101	84 (69%)
1	H	121/163 (74%)	0.11	4 (3%)	46	44	37, 48, 61, 94	94 (77%)
1	I	121/163 (74%)	0.04	2 (1%)	70	68	36, 46, 57, 95	93 (76%)
1	J	121/163 (74%)	0.26	7 (5%)	23	22	38, 50, 61, 93	97 (80%)
1	K	121/163 (74%)	0.07	2 (1%)	70	68	38, 47, 62, 95	84 (69%)
1	L	121/163 (74%)	0.22	5 (4%)	37	35	38, 51, 63, 116	93 (76%)
All	All	1452/1956 (74%)	0.07	45 (3%)	49	47	34, 48, 61, 116	1075 (74%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	120	MET	9.1
1	G	121	GLU	4.3
1	E	120	MET	3.9
1	J	91	LEU	3.9
1	H	120	MET	3.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

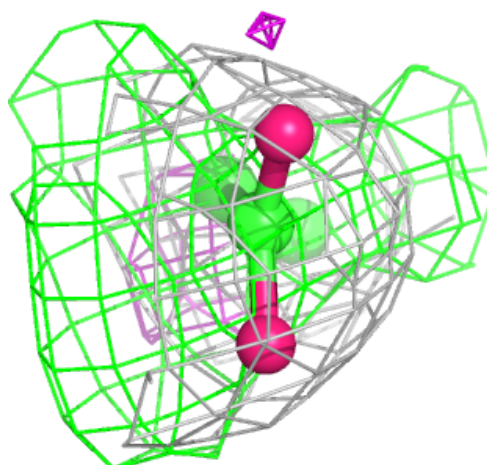
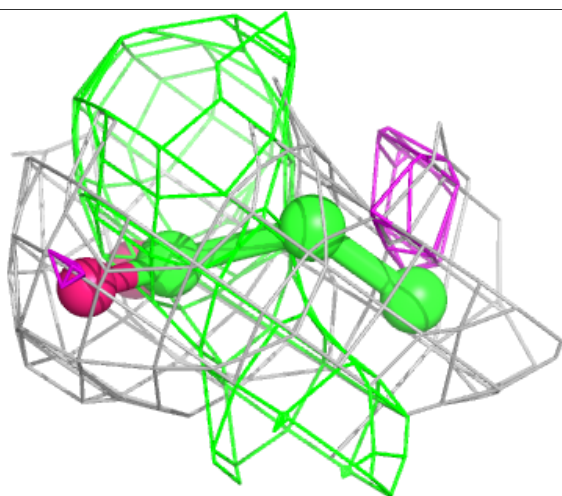
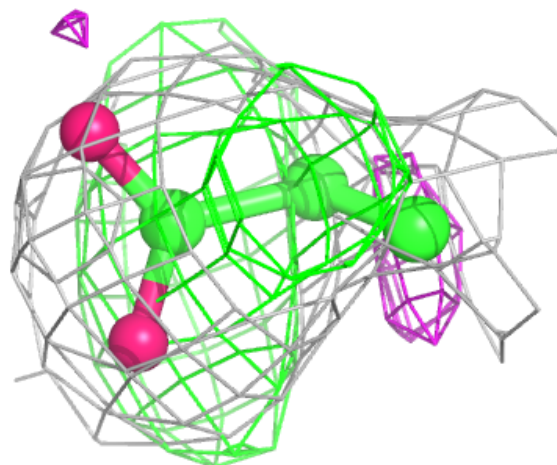
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	3OH	A	201	5/6	0.84	0.31	34,59,68,85	0
2	3OH	B	201	5/6	0.89	0.31	35,65,73,73	0
2	3OH	I	201	5/6	0.89	0.31	29,65,74,78	0
2	3OH	K	201	5/6	0.91	0.28	36,70,75,76	0
2	3OH	H	201	5/6	0.93	0.27	37,61,70,84	0
3	SO4	G	201	5/5	0.97	0.12	44,45,48,61	4
3	SO4	F	201	5/5	0.98	0.11	49,50,56,61	1
3	SO4	L	201	5/5	0.98	0.11	43,49,52,64	2
3	SO4	C	201	5/5	0.99	0.10	46,47,51,62	3
3	SO4	D	201	5/5	0.99	0.10	45,45,56,62	3
3	SO4	J	201	5/5	0.99	0.10	48,53,57,57	4
3	SO4	E	201	5/5	0.99	0.10	45,47,48,56	2

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.

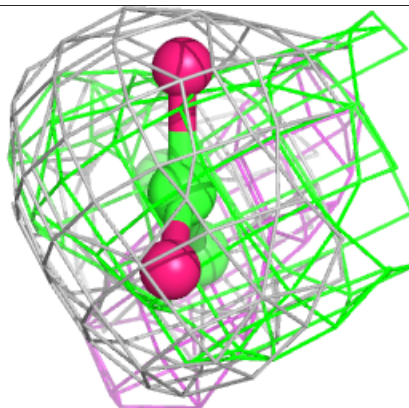
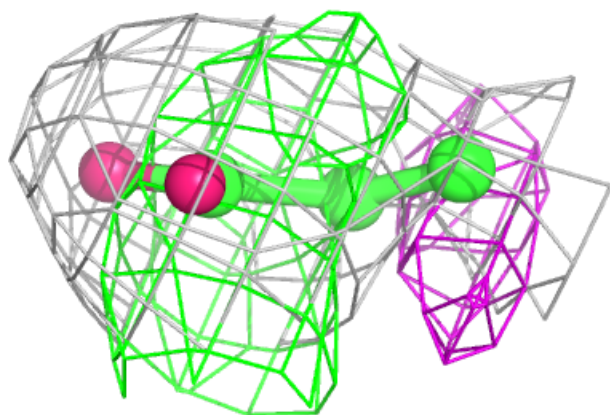
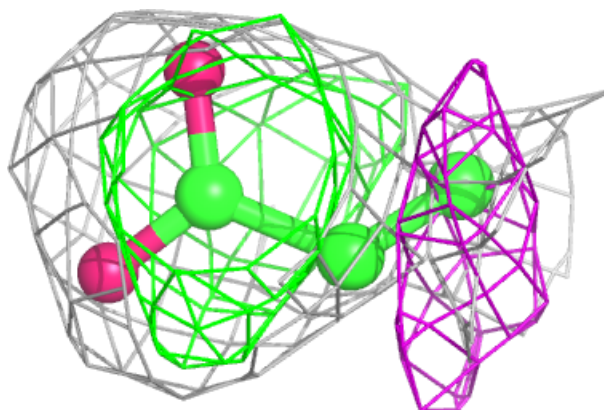
Electron density around 3OH A 201:

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



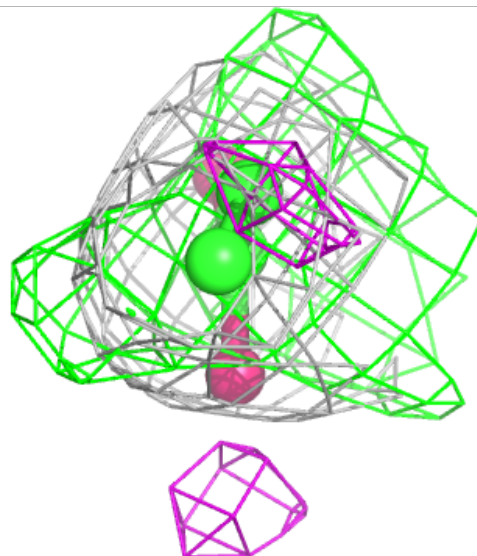
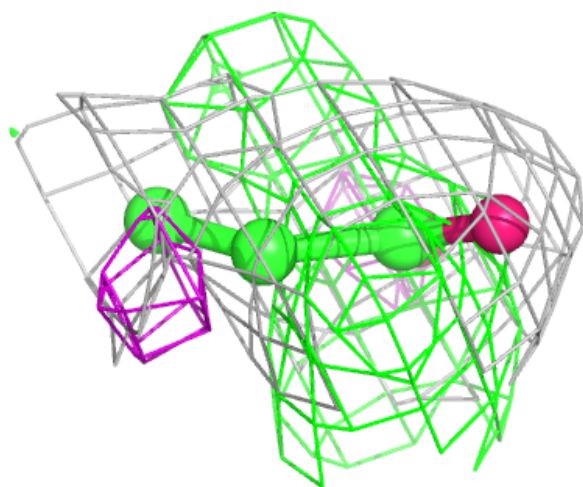
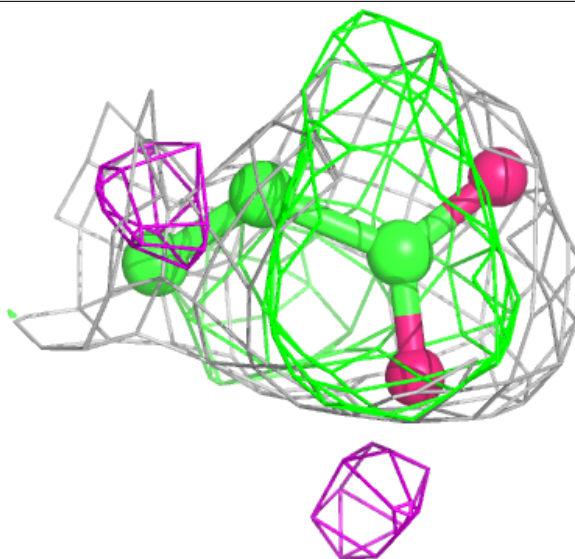
Electron density around 3OH B 201:

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



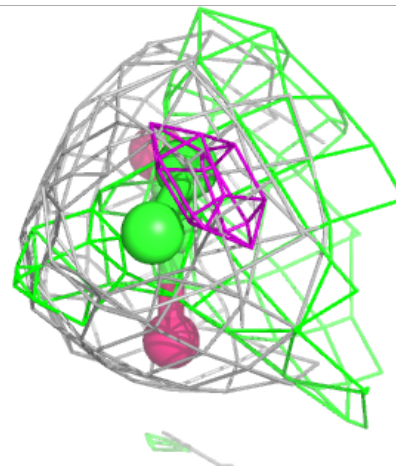
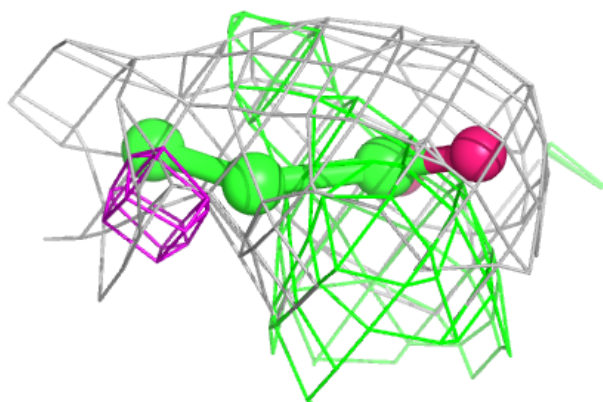
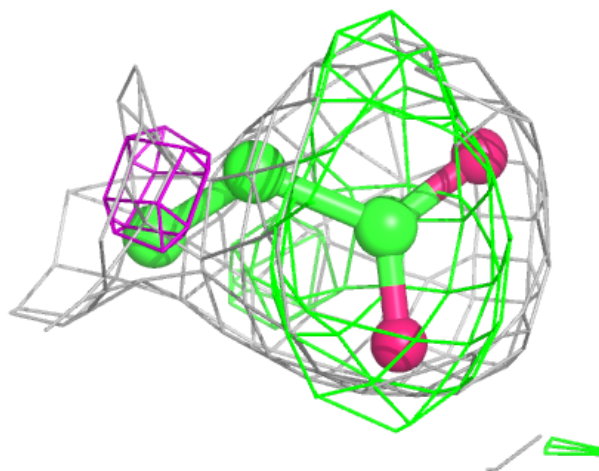
Electron density around 3OH I 201:

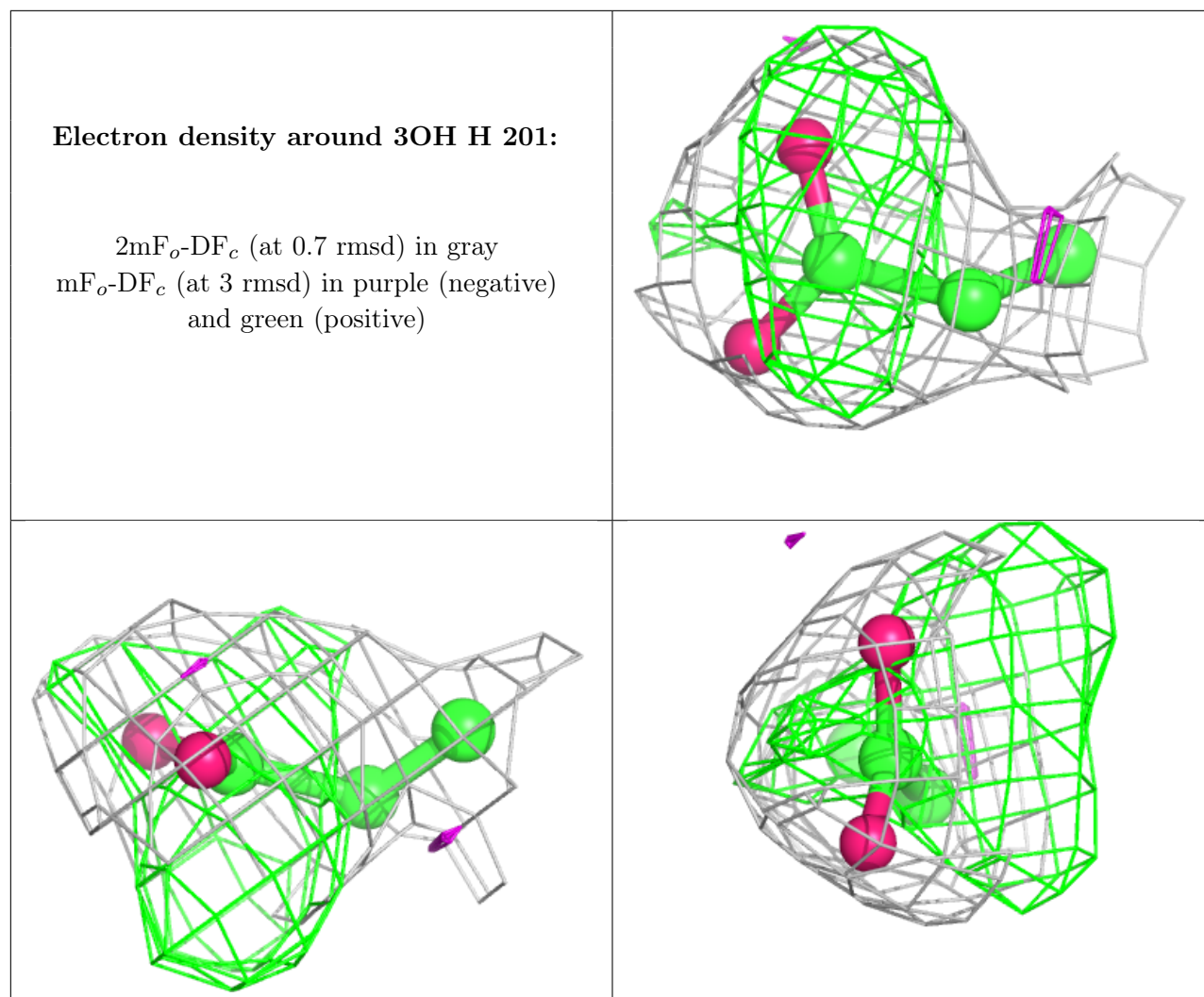
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3OH K 201:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.