W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 01:39 am GMT

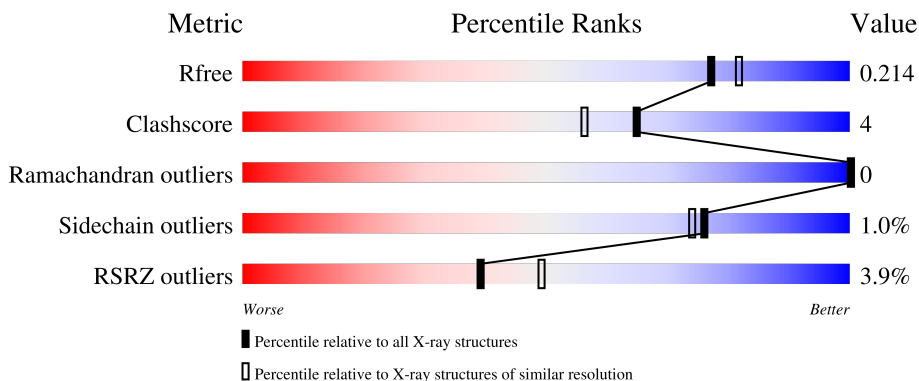|		
PDB ID	:	8BEO
Title	:	Crystal structure of E. coli glyoxylate carboligase mutant I393A with MAP
Authors	:	Shaanan, B.; Binshtein, E.
Deposited on	:	2022-10-21
Resolution	:	1.96 Å(reported)

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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 1.96 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	Percentile Ranks	Value
Rfree		0.214
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		3.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	616	89% 6% •
1	B	616	2% 90% 6% •
1	C	616	4% 90% 6% •
1	D	616	5% 89% 7% •
1	E	616	4% 89% 7% •

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Mol	Chain	Length	Quality of chain
1	F	616	7% ▬▬▬ 89% ▬▬▬▬▬▬▬▬▬ 7% •

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
12	DTU	E	605	-	-	X	-
5	ALU	D	605	-	-	X	-
7	PEG	A	608	-	-	X	-
8	DTT	A	609	-	-	X	-
8	DTT	B	607	-	-	X	-

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 58232 atoms, of which 27977 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 Glyoxylate carboligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	592	Total 9117	C 2879	H 4569	N 796	O 837	S 36	106	4	0
1	B	592	Total 9118	C 2880	H 4568	N 796	O 839	S 35	105	4	0
1	C	592	Total 9083	C 2870	H 4549	N 793	O 837	S 34	104	1	0
1	D	592	Total 9111	C 2878	H 4564	N 796	O 839	S 34	104	3	0
1	E	592	Total 9093	C 2873	H 4554	N 794	O 838	S 34	104	2	0
1	F	592	Total 9120	C 2880	H 4570	N 797	O 838	S 35	105	4	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P0AEP7
A	-21	GLY	-	expression tag	UNP P0AEP7
A	-20	SER	-	expression tag	UNP P0AEP7
A	-19	SER	-	expression tag	UNP P0AEP7
A	-18	HIS	-	expression tag	UNP P0AEP7
A	-17	HIS	-	expression tag	UNP P0AEP7
A	-16	HIS	-	expression tag	UNP P0AEP7
A	-15	HIS	-	expression tag	UNP P0AEP7
A	-14	HIS	-	expression tag	UNP P0AEP7
A	-13	HIS	-	expression tag	UNP P0AEP7
A	-12	SER	-	expression tag	UNP P0AEP7
A	-11	SER	-	expression tag	UNP P0AEP7
A	-10	GLY	-	expression tag	UNP P0AEP7
A	-9	LEU	-	expression tag	UNP P0AEP7
A	-8	VAL	-	expression tag	UNP P0AEP7
A	-7	PRO	-	expression tag	UNP P0AEP7
A	-6	ARG	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P0AEP7
A	-4	SER	-	expression tag	UNP P0AEP7
A	-3	HIS	-	expression tag	UNP P0AEP7
A	-2	MET	-	expression tag	UNP P0AEP7
A	-1	ALA	-	expression tag	UNP P0AEP7
A	0	SER	-	expression tag	UNP P0AEP7
A	393	ALA	ILE	engineered mutation	UNP P0AEP7
B	-22	MET	-	initiating methionine	UNP P0AEP7
B	-21	GLY	-	expression tag	UNP P0AEP7
B	-20	SER	-	expression tag	UNP P0AEP7
B	-19	SER	-	expression tag	UNP P0AEP7
B	-18	HIS	-	expression tag	UNP P0AEP7
B	-17	HIS	-	expression tag	UNP P0AEP7
B	-16	HIS	-	expression tag	UNP P0AEP7
B	-15	HIS	-	expression tag	UNP P0AEP7
B	-14	HIS	-	expression tag	UNP P0AEP7
B	-13	HIS	-	expression tag	UNP P0AEP7
B	-12	SER	-	expression tag	UNP P0AEP7
B	-11	SER	-	expression tag	UNP P0AEP7
B	-10	GLY	-	expression tag	UNP P0AEP7
B	-9	LEU	-	expression tag	UNP P0AEP7
B	-8	VAL	-	expression tag	UNP P0AEP7
B	-7	PRO	-	expression tag	UNP P0AEP7
B	-6	ARG	-	expression tag	UNP P0AEP7
B	-5	GLY	-	expression tag	UNP P0AEP7
B	-4	SER	-	expression tag	UNP P0AEP7
B	-3	HIS	-	expression tag	UNP P0AEP7
B	-2	MET	-	expression tag	UNP P0AEP7
B	-1	ALA	-	expression tag	UNP P0AEP7
B	0	SER	-	expression tag	UNP P0AEP7
B	393	ALA	ILE	engineered mutation	UNP P0AEP7
C	-22	MET	-	initiating methionine	UNP P0AEP7
C	-21	GLY	-	expression tag	UNP P0AEP7
C	-20	SER	-	expression tag	UNP P0AEP7
C	-19	SER	-	expression tag	UNP P0AEP7
C	-18	HIS	-	expression tag	UNP P0AEP7
C	-17	HIS	-	expression tag	UNP P0AEP7
C	-16	HIS	-	expression tag	UNP P0AEP7
C	-15	HIS	-	expression tag	UNP P0AEP7
C	-14	HIS	-	expression tag	UNP P0AEP7
C	-13	HIS	-	expression tag	UNP P0AEP7
C	-12	SER	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP P0AEP7
C	-10	GLY	-	expression tag	UNP P0AEP7
C	-9	LEU	-	expression tag	UNP P0AEP7
C	-8	VAL	-	expression tag	UNP P0AEP7
C	-7	PRO	-	expression tag	UNP P0AEP7
C	-6	ARG	-	expression tag	UNP P0AEP7
C	-5	GLY	-	expression tag	UNP P0AEP7
C	-4	SER	-	expression tag	UNP P0AEP7
C	-3	HIS	-	expression tag	UNP P0AEP7
C	-2	MET	-	expression tag	UNP P0AEP7
C	-1	ALA	-	expression tag	UNP P0AEP7
C	0	SER	-	expression tag	UNP P0AEP7
C	393	ALA	ILE	engineered mutation	UNP P0AEP7
D	-22	MET	-	initiating methionine	UNP P0AEP7
D	-21	GLY	-	expression tag	UNP P0AEP7
D	-20	SER	-	expression tag	UNP P0AEP7
D	-19	SER	-	expression tag	UNP P0AEP7
D	-18	HIS	-	expression tag	UNP P0AEP7
D	-17	HIS	-	expression tag	UNP P0AEP7
D	-16	HIS	-	expression tag	UNP P0AEP7
D	-15	HIS	-	expression tag	UNP P0AEP7
D	-14	HIS	-	expression tag	UNP P0AEP7
D	-13	HIS	-	expression tag	UNP P0AEP7
D	-12	SER	-	expression tag	UNP P0AEP7
D	-11	SER	-	expression tag	UNP P0AEP7
D	-10	GLY	-	expression tag	UNP P0AEP7
D	-9	LEU	-	expression tag	UNP P0AEP7
D	-8	VAL	-	expression tag	UNP P0AEP7
D	-7	PRO	-	expression tag	UNP P0AEP7
D	-6	ARG	-	expression tag	UNP P0AEP7
D	-5	GLY	-	expression tag	UNP P0AEP7
D	-4	SER	-	expression tag	UNP P0AEP7
D	-3	HIS	-	expression tag	UNP P0AEP7
D	-2	MET	-	expression tag	UNP P0AEP7
D	-1	ALA	-	expression tag	UNP P0AEP7
D	0	SER	-	expression tag	UNP P0AEP7
D	393	ALA	ILE	engineered mutation	UNP P0AEP7
E	-22	MET	-	initiating methionine	UNP P0AEP7
E	-21	GLY	-	expression tag	UNP P0AEP7
E	-20	SER	-	expression tag	UNP P0AEP7
E	-19	SER	-	expression tag	UNP P0AEP7
E	-18	HIS	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP P0AEP7
E	-16	HIS	-	expression tag	UNP P0AEP7
E	-15	HIS	-	expression tag	UNP P0AEP7
E	-14	HIS	-	expression tag	UNP P0AEP7
E	-13	HIS	-	expression tag	UNP P0AEP7
E	-12	SER	-	expression tag	UNP P0AEP7
E	-11	SER	-	expression tag	UNP P0AEP7
E	-10	GLY	-	expression tag	UNP P0AEP7
E	-9	LEU	-	expression tag	UNP P0AEP7
E	-8	VAL	-	expression tag	UNP P0AEP7
E	-7	PRO	-	expression tag	UNP P0AEP7
E	-6	ARG	-	expression tag	UNP P0AEP7
E	-5	GLY	-	expression tag	UNP P0AEP7
E	-4	SER	-	expression tag	UNP P0AEP7
E	-3	HIS	-	expression tag	UNP P0AEP7
E	-2	MET	-	expression tag	UNP P0AEP7
E	-1	ALA	-	expression tag	UNP P0AEP7
E	0	SER	-	expression tag	UNP P0AEP7
E	393	ALA	ILE	engineered mutation	UNP P0AEP7
F	-22	MET	-	initiating methionine	UNP P0AEP7
F	-21	GLY	-	expression tag	UNP P0AEP7
F	-20	SER	-	expression tag	UNP P0AEP7
F	-19	SER	-	expression tag	UNP P0AEP7
F	-18	HIS	-	expression tag	UNP P0AEP7
F	-17	HIS	-	expression tag	UNP P0AEP7
F	-16	HIS	-	expression tag	UNP P0AEP7
F	-15	HIS	-	expression tag	UNP P0AEP7
F	-14	HIS	-	expression tag	UNP P0AEP7
F	-13	HIS	-	expression tag	UNP P0AEP7
F	-12	SER	-	expression tag	UNP P0AEP7
F	-11	SER	-	expression tag	UNP P0AEP7
F	-10	GLY	-	expression tag	UNP P0AEP7
F	-9	LEU	-	expression tag	UNP P0AEP7
F	-8	VAL	-	expression tag	UNP P0AEP7
F	-7	PRO	-	expression tag	UNP P0AEP7
F	-6	ARG	-	expression tag	UNP P0AEP7
F	-5	GLY	-	expression tag	UNP P0AEP7
F	-4	SER	-	expression tag	UNP P0AEP7
F	-3	HIS	-	expression tag	UNP P0AEP7
F	-2	MET	-	expression tag	UNP P0AEP7
F	-1	ALA	-	expression tag	UNP P0AEP7
F	0	SER	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	393	ALA	ILE	engineered mutation	UNP P0AEP7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Mg 3	0	0
2	B	3	Total 3	Mg 3	0	0
2	C	2	Total 2	Mg 2	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
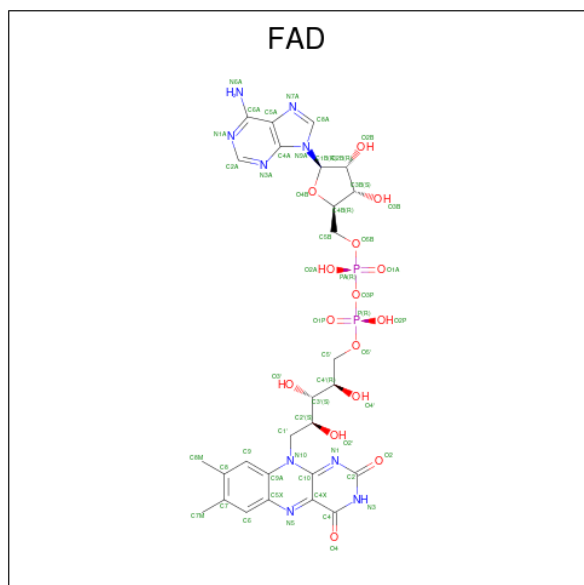
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 84	C 27	H 31	N 9	O 15	P 2	5	0
3	B	1	Total 84	C 27	H 31	N 9	O 15	P 2	5	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	P	5	0
			84	27	31	9	15	2		
3	D	1	Total	C	H	N	O	P	5	0
			84	27	31	9	15	2		
3	E	1	Total	C	H	N	O	P	5	0
			84	27	31	9	15	2		
3	F	1	Total	C	H	N	O	P	5	0
			84	27	31	9	15	2		

- Molecule 4 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-{(1S)-1-HYDROXY-1-[(R)-HYDROXY(METHOXY)PHOSPHORYL]ETHYL}-5-(2-{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDK) (formula: $C_{15}H_{26}N_4O_{11}P_3S$) (labeled as "Ligand of Interest" by depositor).
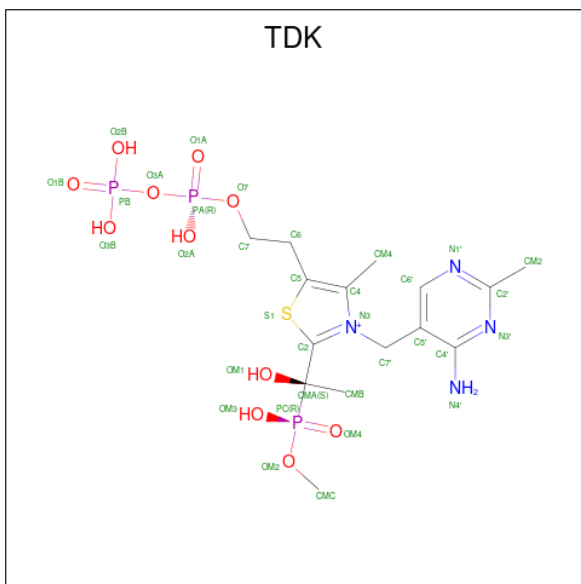
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	B	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	C	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	D	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	E	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	F	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		

- Molecule 5 is METHYL HYDROGEN (S)-ACETYLPHOSPHONATE (three-letter code: ALU) (formula: $C_3H_7O_4P$).
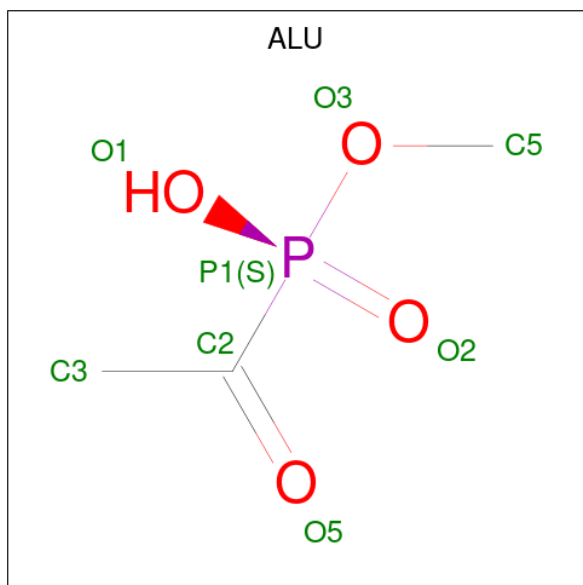
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	P	0	0
			14	3	6	4	1		
5	B	1	Total	C	H	O	P	0	0
			14	3	6	4	1		
5	C	1	Total	C	H	O	P	0	0
			14	3	6	4	1		
5	D	1	Total	C	H	O	P	0	0
			14	3	6	4	1		

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-1,4-BENZOQUINONE (three-letter code: UQ0) (formula: $C_9H_{10}O_4$).
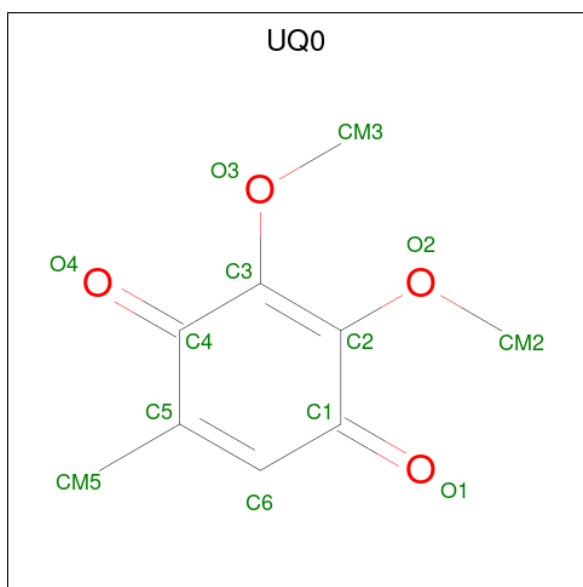
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 22	C 9	H 9	O 4	0	1
6	B	1	Total 22	C 9	H 9	O 4	0	0
6	C	1	Total 22	C 9	H 9	O 4	0	0
6	D	1	Total 22	C 9	H 9	O 4	0	0
6	E	1	Total 22	C 9	H 9	O 4	0	0
6	F	1	Total 22	C 9	H 9	O 4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4

OH O4

O2

O

C3

C1

HO

C2

O1

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 17	C 4	H 10	O 3	1	0
7	A	1	Total 17	C 4	H 10	O 3	1	0
7	A	1	Total 17	C 4	H 10	O 3	1	0
7	A	1	Total 17	C 4	H 10	O 3	1	0
7	A	1	Total 19	C 4	H 11	O 4	2	1
7	B	1	Total 17	C 4	H 10	O 3	1	0
7	C	1	Total 17	C 4	H 10	O 3	1	0
7	F	1	Total 17	C 4	H 10	O 3	1	0

- Molecule 8 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).

W O R L D W I D E
PDB
PROTEIN DATA BANK

DTT

O3   S4
HO   SH

C3(R)   C4

C1   C2(R)

HS
S1

OH
O2

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	O	S	3	0
			18	4	10	2	2		
8	A	1	Total	C	H	O	S	3	0
			18	4	10	2	2		
8	B	1	Total	C	H	O	S	3	0
			18	4	10	2	2		

- Molecule 9 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

FMT

C

OH O2

O
O1

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 10	C 2	H 4	O 4	2	1
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	C	1	Total 5	C 1	H 2	O 2	1	0
9	C	1	Total 5	C 1	H 2	O 2	1	0
9	C	1	Total 5	C 1	H 2	O 2	1	0
9	C	1	Total 5	C 1	H 2	O 2	1	0
9	D	1	Total 5	C 1	H 2	O 2	1	0

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

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE

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

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	Na 1	0	0
11	B	4	Total 4	Na 4	0	0
11	C	2	Total 2	Na 2	0	0
11	D	3	Total 3	Na 3	0	0
11	E	4	Total 4	Na 4	0	0
11	F	1	Total 1	Na 1	0	0

- Molecule 12 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: $C_4H_{10}O_2S_2$).

DTU

O3
HO

S4
SH

C4

C3(R)

C2(S)

C1

HS
S1

OH
O2

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	E	1	Total 18	C 4	H 10	O 2	S 2	0	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	E	1	Total 1	Cl 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	409	Total 409	O 409	0	0
14	B	416	Total 416	O 416	0	0
14	C	339	Total 339	O 339	0	0
14	D	346	Total 346	O 346	0	0
14	E	322	Total 322	O 322	0	0
14	F	287	Total 287	O 287	0	0

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3 Residue-property plots ⓘ

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: Glyoxylate carboligase
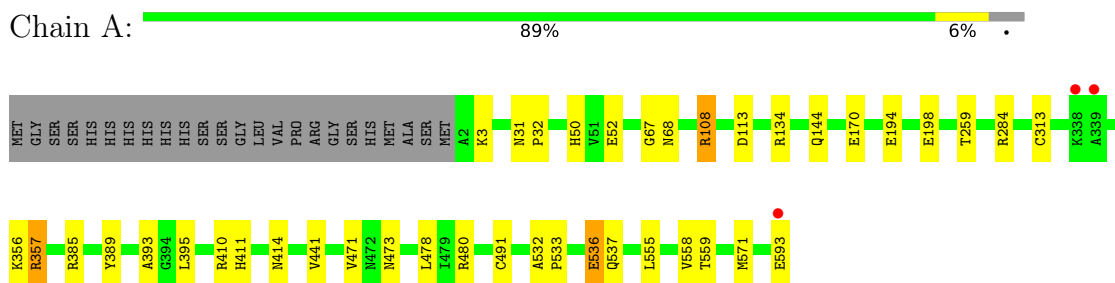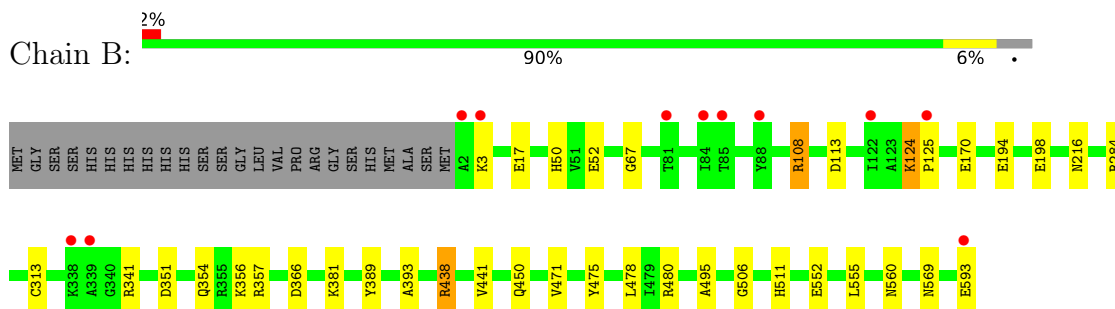
• Molecule 1: Glyoxylate carboligase

• Molecule 1: Glyoxylate carboligase

• Molecule 1: Glyoxylate carboligase

• Molecule 1: Glyoxylate carboligase

Chain E:

• Molecule 1: Glyoxylate carboligase

Chain F:
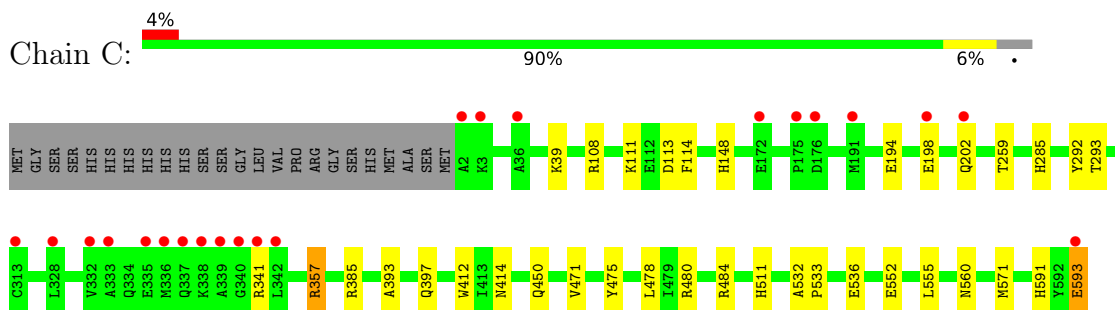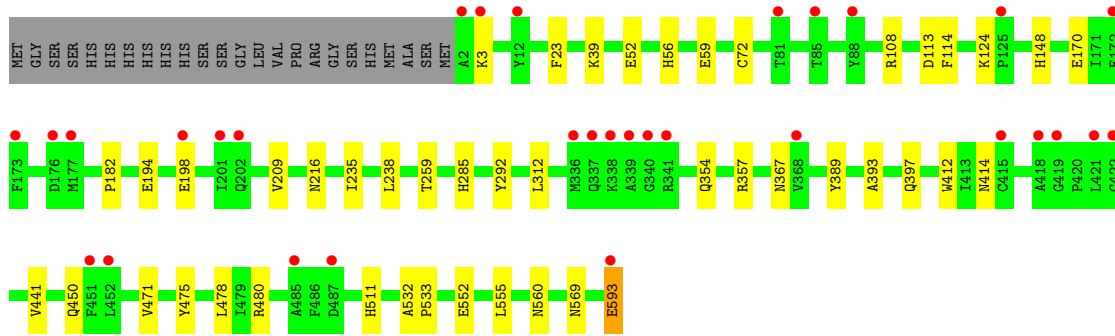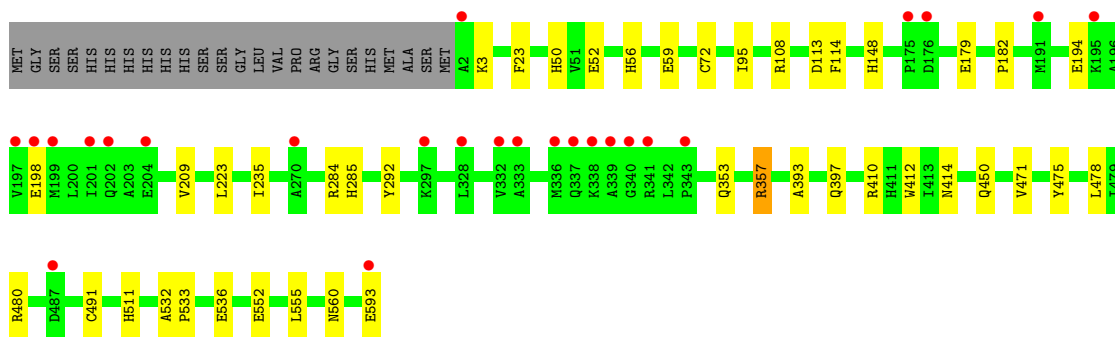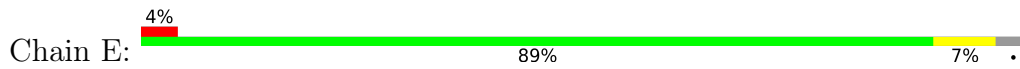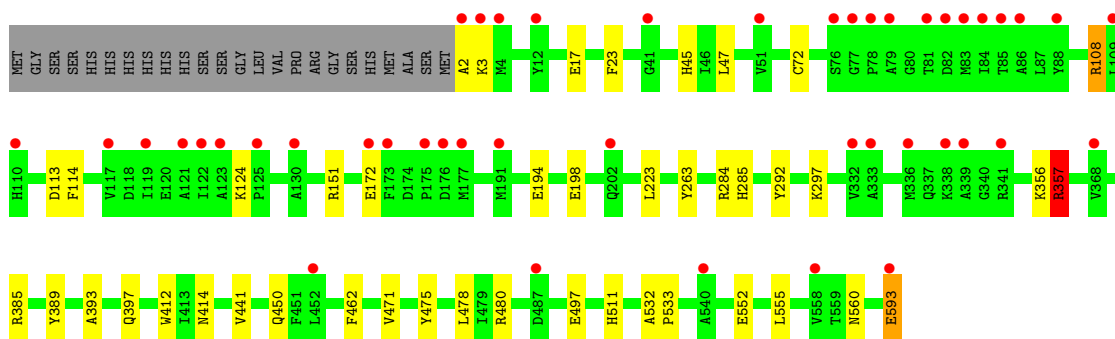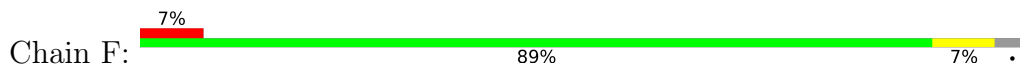
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.64Å 188.64Å 246.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.96 48.30 – 1.96	Depositor EDS
% Data completeness (in resolution range)	88.3 (48.35-1.96) 88.3 (48.30-1.96)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.88 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.176 , 0.204 0.190 , 0.214	Depositor DCC
R_{free} test set	8395 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 46.8	EDS
L-test for twinning [2]	$<|L|> = 0.53$, $<L^2> = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	58232	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.13 % 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 5.4097e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: CSO, UQ0, FMT, PGE, DTU, TDK, PEG, NA, MG, ALU, FAD, DTT, 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	0.54	1/4644 (0.0%)	0.79	2/6301 (0.0%)
1	B	0.52	1/4646 (0.0%)	0.76	2/6304 (0.0%)
1	C	0.52	1/4621 (0.0%)	0.77	4/6270 (0.1%)
1	D	0.52	0/4640	0.76	6/6295 (0.1%)
1	E	0.53	2/4629 (0.0%)	0.74	2/6281 (0.0%)
1	F	0.50	2/4646 (0.0%)	0.74	6/6304 (0.1%)
All	All	0.52	7/27826 (0.0%)	0.76	22/37755 (0.1%)

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	2
1	B	0	1
1	C	0	2
1	E	0	2
1	F	0	1
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	179	GLU	CD-OE2	-8.11	1.16	1.25
1	E	179	GLU	CD-OE1	-5.96	1.19	1.25
1	A	536	GLU	CD-OE2	5.75	1.31	1.25
1	C	536	GLU	CD-OE2	5.57	1.31	1.25
1	B	17	GLU	CD-OE2	5.42	1.31	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	ARG	NE-CZ-NH2	-13.12	113.74	120.30
1	C	357	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	E	357	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	D	593	GLU	CB-CA-C	-10.08	90.23	110.40
1	D	593	GLU	CG-CD-OE2	-7.93	102.43	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	357	ARG	Sidechain
1	B	341	ARG	Sidechain
1	C	341	ARG	Sidechain
1	C	357	ARG	Sidechain

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	4548	4569	4556	39	2
1	B	4550	4568	4555	33	0
1	C	4534	4549	4533	23	3
1	D	4547	4564	4550	34	1
1	E	4539	4554	4539	43	0
1	F	4550	4570	4557	32	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	53	31	31	1	0
3	B	53	31	31	0	0
3	C	53	31	31	3	0
3	D	53	31	31	3	0
3	E	53	31	31	1	0
3	F	53	31	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	34	22	22	6	0
4	B	34	22	22	8	0
4	C	34	22	22	4	0
4	D	34	22	22	4	0
4	E	34	22	22	8	0
4	F	34	22	22	7	0
5	A	8	6	7	1	0
5	B	8	6	7	0	0
5	C	8	6	7	1	0
5	D	8	6	7	6	0
6	A	13	9	0	2	0
6	B	13	9	0	0	0
6	C	13	9	0	0	0
6	D	13	9	0	0	0
6	E	13	9	0	1	0
6	F	13	9	0	0	0
7	A	36	51	46	14	0
7	B	7	10	10	1	0
7	C	7	10	10	2	0
7	F	7	10	10	0	0
8	A	16	20	20	8	0
8	B	8	10	10	4	0
9	A	24	16	14	1	0
9	B	30	20	15	1	0
9	C	12	8	6	0	0
9	D	9	6	4	1	0
9	E	15	10	7	0	0
9	F	18	12	6	0	0
10	A	10	14	14	1	0
11	A	1	0	0	0	0
11	B	4	0	0	0	0
11	C	2	0	0	0	0
11	D	3	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
12	E	8	10	10	9	0
13	E	1	0	0	0	0
14	A	409	0	0	8	0
14	B	416	0	0	7	1
14	C	339	0	0	4	0
14	D	346	0	0	2	0
14	E	322	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	287	0	0	2	0
All	All	30255	27977	27818	228	4

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 4.

The worst 5 of 228 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)
4:E:603:TDK:HMC1	14:E:982:HOH:O	1.33	1.28
4:B:604:TDK:HMC1	14:B:1051:HOH:O	1.43	1.17
4:A:604:TDK:HMC1	14:A:1064:HOH:O	1.48	1.13
1:A:313[A]:CYS:SG	14:A:1060:HOH:O	2.23	0.96
1:B:366:ASP:HB2	14:B:1059:HOH:O	1.73	0.88

All (4) 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)
1:A:571:MET:SD	1:C:571:MET:CE[5_555]	1.94	0.26
1:C:591:HIS:HD1	1:D:354:GLN:HE22[3_545]	1.34	0.26
14:B:778:HOH:O	14:B:1031:HOH:O[7_555]	2.10	0.10
1:A:571:MET:SD	1:C:571:MET:HE3[5_555]	1.54	0.06

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	593/616 (96%)	584 (98%)	9 (2%)	0	100	100
1	B	593/616 (96%)	584 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	590/616 (96%)	582 (99%)	8 (1%)	0	100	100
1	D	592/616 (96%)	582 (98%)	10 (2%)	0	100	100
1	E	591/616 (96%)	578 (98%)	13 (2%)	0	100	100
1	F	593/616 (96%)	584 (98%)	9 (2%)	0	100	100
All	All	3552/3696 (96%)	3494 (98%)	58 (2%)	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	476/492 (97%)	473 (99%)	3 (1%)	86	85
1	B	476/492 (97%)	469 (98%)	7 (2%)	65	60
1	C	473/492 (96%)	470 (99%)	3 (1%)	86	85
1	D	475/492 (96%)	471 (99%)	4 (1%)	81	80
1	E	474/492 (96%)	471 (99%)	3 (1%)	86	85
1	F	476/492 (97%)	469 (98%)	7 (2%)	65	60
All	All	2850/2952 (96%)	2823 (99%)	27 (1%)	76	77

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	LYS
1	E	3	LYS
1	F	297	LYS
1	D	475	TYR
1	E	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	511	HIS
1	F	560	ASN
1	E	560	ASN
1	F	414	ASN
1	C	560	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CSO	D	344	1	3,6,7	0.66	0	0,6,8	-	-
1	CSO	C	344	1	3,6,7	0.61	0	0,6,8	-	-
1	CSO	E	344	1	3,6,7	0.78	0	0,6,8	-	-
1	CSO	F	344	1	3,6,7	0.85	0	0,6,8	-	-
1	CSO	A	344	1	3,6,7	0.64	0	0,6,8	-	-
1	CSO	B	344	1	3,6,7	0.71	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	D	344	1	-	1/1/5/7	-
1	CSO	C	344	1	-	0/1/5/7	-
1	CSO	E	344	1	-	1/1/5/7	-
1	CSO	F	344	1	-	0/1/5/7	-
1	CSO	A	344	1	-	0/1/5/7	-
1	CSO	B	344	1	-	0/1/5/7	-

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There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	344	CSO	N-CA-CB-SG
1	E	344	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 101 ligands modelled in this entry, 29 are monoatomic - leaving 72 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
4	TDK	C	603	2	29,35,35	2.71	6 (20%)	36,55,55	1.83	6 (16%)
9	FMT	B	611	-	2,2,2	1.32	0	1,1,1	0.24	0
9	FMT	D	606	-	2,2,2	1.12	0	1,1,1	0.30	0
5	ALU	C	606	-	4,7,7	2.68	2 (50%)	3,10,10	2.33	1 (33%)
9	FMT	A	615	-	2,2,2	1.17	0	1,1,1	0.21	0
3	FAD	B	603	-	53,58,58	0.88	2 (3%)	68,89,89	0.96	4 (5%)
9	FMT	A	620	-	2,2,2	1.41	0	1,1,1	0.09	0
9	FMT	B	609	-	2,2,2	0.86	0	1,1,1	0.43	0
6	UQ0	C	604	1	13,13,13	1.00	0	16,18,18	1.46	2 (12%)
9	FMT	B	614[A]	-	2,2,2	0.88	0	1,1,1	0.29	0
9	FMT	B	612	-	2,2,2	1.40	0	1,1,1	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	FMT	C	609	-	2,2,2	1.12	0	1,1,1	0.25	0
7	PEG	A	614	-	6,6,6	0.22	0	5,5,5	0.14	0
3	FAD	D	602	-	53,58,58	0.94	2 (3%)	68,89,89	0.95	3 (4%)
4	TDK	F	604	2	29,35,35	2.74	6 (20%)	36,55,55	2.59	6 (16%)
9	FMT	F	610	-	2,2,2	1.07	0	1,1,1	0.30	0
9	FMT	A	618	-	2,2,2	2.33	1 (50%)	1,1,1	0.06	0
9	FMT	F	611	-	2,2,2	1.13	0	1,1,1	0.25	0
3	FAD	F	603	-	53,58,58	1.00	2 (3%)	68,89,89	0.98	4 (5%)
9	FMT	F	609	-	2,2,2	1.13	0	1,1,1	0.20	0
5	ALU	D	605	-	4,7,7	2.01	1 (25%)	3,10,10	0.21	0
9	FMT	A	623	-	2,2,2	3.09	1 (50%)	1,1,1	0.55	0
7	PEG	A	621[B]	-	6,6,6	0.38	0	5,5,5	1.56	1 (20%)
9	FMT	D	607	-	2,2,2	0.92	0	1,1,1	0.33	0
7	PEG	B	610	-	6,6,6	0.20	0	5,5,5	0.22	0
9	FMT	B	617	-	2,2,2	1.22	0	1,1,1	0.26	0
9	FMT	F	608	-	2,2,2	1.10	0	1,1,1	0.25	0
7	PEG	A	608	-	6,6,6	1.25	1 (16%)	5,5,5	0.99	0
9	FMT	E	608	-	2,2,2	0.94	0	1,1,1	0.36	0
3	FAD	C	602	-	53,58,58	0.72	0	68,89,89	0.96	4 (5%)
4	TDK	B	604	2	29,35,35	2.75	5 (17%)	36,55,55	4.08	6 (16%)
6	UQ0	B	606	1	13,13,13	1.08	1 (7%)	16,18,18	0.94	1 (6%)
7	PEG	A	607	-	6,6,6	0.59	0	5,5,5	0.57	0
9	FMT	A	612	-	2,2,2	1.41	0	1,1,1	0.09	0
4	TDK	D	603	2	29,35,35	2.64	5 (17%)	36,55,55	1.82	5 (13%)
5	ALU	B	605	-	4,7,7	2.14	1 (25%)	3,10,10	1.94	1 (33%)
9	FMT	A	619	-	2,2,2	1.51	1 (50%)	1,1,1	0.03	0
9	FMT	B	618	-	2,2,2	0.76	0	1,1,1	0.33	0
9	FMT	D	608	-	2,2,2	1.31	0	1,1,1	0.25	0
9	FMT	F	613	-	2,2,2	1.13	0	1,1,1	0.20	0
6	UQ0	F	605	1	13,13,13	1.05	1 (7%)	16,18,18	1.05	1 (6%)
9	FMT	B	614[B]	-	2,2,2	1.22	0	1,1,1	0.30	0
9	FMT	E	609	-	2,2,2	0.99	0	1,1,1	0.31	0
9	FMT	B	608	-	2,2,2	1.03	0	1,1,1	0.25	0
4	TDK	E	603	2	29,35,35	2.49	6 (20%)	36,55,55	2.84	6 (16%)
9	FMT	E	607	-	2,2,2	1.48	1 (50%)	1,1,1	0.13	0
7	PEG	C	607	-	6,6,6	0.42	0	5,5,5	0.26	0
8	DTT	B	607	-	7,7,7	0.66	0	4,8,8	1.29	1 (25%)
4	TDK	A	604	2	29,35,35	3.03	6 (20%)	36,55,55	3.24	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	UQ0	E	604	1	13,13,13	1.03	0	16,18,18	0.85	0
9	FMT	A	617	-	2,2,2	1.09	0	1,1,1	0.26	0
12	DTU	E	605	-	7,7,7	0.39	0	4,8,8	0.80	0
9	FMT	B	620	-	2,2,2	2.13	1 (50%)	1,1,1	0.02	0
5	ALU	A	605	-	4,7,7	2.79	2 (50%)	3,10,10	1.20	0
8	DTT	A	609	-	7,7,7	0.41	0	4,8,8	1.37	1 (25%)
9	FMT	B	613	-	2,2,2	0.93	0	1,1,1	0.28	0
7	PEG	A	621[A]	-	6,6,6	0.33	0	5,5,5	1.58	1 (20%)
6	UQ0	A	606[A]	1	13,13,13	0.97	0	16,18,18	1.02	1 (6%)
7	PEG	F	606	-	6,6,6	0.15	0	5,5,5	0.22	0
9	FMT	C	608	-	2,2,2	1.24	0	1,1,1	0.17	0
10	PGE	A	613	-	9,9,9	0.57	0	8,8,8	0.43	0
6	UQ0	D	604	1	13,13,13	1.03	1 (7%)	16,18,18	0.89	1 (6%)
9	FMT	E	606	-	2,2,2	0.82	0	1,1,1	0.30	0
9	FMT	A	611	-	2,2,2	1.02	0	1,1,1	0.24	0
9	FMT	F	607	-	2,2,2	1.01	0	1,1,1	0.31	0
7	PEG	A	616	-	6,6,6	0.27	0	5,5,5	0.12	0
9	FMT	E	612	-	2,2,2	1.19	0	1,1,1	0.18	0
8	DTT	A	610	-	7,7,7	0.27	0	4,8,8	0.77	0
3	FAD	A	603	-	53,58,58	0.88	1 (1%)	68,89,89	0.97	4 (5%)
3	FAD	E	602	-	53,58,58	0.86	2 (3%)	68,89,89	0.92	3 (4%)
9	FMT	C	611	-	2,2,2	1.12	0	1,1,1	0.25	0
9	FMT	C	612	-	2,2,2	1.25	0	1,1,1	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TDK	C	603	2	-	14/26/35/35	0/2/2/2
5	ALU	C	606	-	-	0/2/9/9	-
3	FAD	B	603	-	-	4/30/50/50	0/6/6/6
6	UQ0	C	604	1	-	1/4/24/24	0/1/1/1
7	PEG	A	614	-	-	1/4/4/4	-
3	FAD	D	602	-	-	4/30/50/50	0/6/6/6
4	TDK	F	604	2	-	11/26/35/35	0/2/2/2
3	FAD	F	603	-	-	7/30/50/50	0/6/6/6
5	ALU	D	605	-	-	1/2/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	A	621[B]	-	-	2/4/4/4	-
7	PEG	B	610	-	-	1/4/4/4	-
7	PEG	A	608	-	-	1/4/4/4	-
3	FAD	C	602	-	-	5/30/50/50	0/6/6/6
4	TDK	B	604	2	-	12/26/35/35	0/2/2/2
6	UQ0	B	606	1	-	1/4/24/24	0/1/1/1
7	PEG	A	607	-	-	1/4/4/4	-
4	TDK	D	603	2	-	11/26/35/35	0/2/2/2
5	ALU	B	605	-	-	2/2/9/9	-
6	UQ0	F	605	1	-	0/4/24/24	0/1/1/1
4	TDK	E	603	2	-	9/26/35/35	0/2/2/2
7	PEG	C	607	-	-	1/4/4/4	-
8	DTT	B	607	-	-	5/8/8/8	-
4	TDK	A	604	2	-	9/26/35/35	0/2/2/2
6	UQ0	E	604	1	-	0/4/24/24	0/1/1/1
12	DTU	E	605	-	-	2/8/8/8	-
5	ALU	A	605	-	-	1/2/9/9	-
8	DTT	A	609	-	-	5/8/8/8	-
7	PEG	A	621[A]	-	-	3/4/4/4	-
6	UQ0	A	606[A]	1	-	2/4/24/24	0/1/1/1
7	PEG	F	606	-	-	3/4/4/4	-
10	PGE	A	613	-	-	6/7/7/7	-
6	UQ0	D	604	1	-	0/4/24/24	0/1/1/1
7	PEG	A	616	-	-	0/4/4/4	-
8	DTT	A	610	-	-	8/8/8/8	-
3	FAD	A	603	-	-	5/30/50/50	0/6/6/6
3	FAD	E	602	-	-	3/30/50/50	0/6/6/6

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	TDK	PC-CMA	13.74	2.06	1.84
4	F	604	TDK	PC-CMA	12.14	2.04	1.84
4	C	603	TDK	PC-CMA	12.13	2.04	1.84
4	B	604	TDK	PC-CMA	12.10	2.04	1.84
4	D	603	TDK	PC-CMA	12.04	2.03	1.84

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	604	TDK	OM4-PC-CMA	19.16	133.03	113.53
4	A	604	TDK	OM4-PC-CMA	13.62	127.39	113.53
4	B	604	TDK	OM2-PC-OM4	-13.59	85.17	114.58
4	E	603	TDK	OM4-PC-CMA	10.98	124.71	113.53
4	A	604	TDK	OM2-PC-OM4	-10.77	91.28	114.58

There are no chirality outliers.

5 of 141 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	FAD	C5B-O5B-PA-O1A
3	A	603	FAD	C5B-O5B-PA-O3P
3	B	603	FAD	C5B-O5B-PA-O1A
3	B	603	FAD	C5B-O5B-PA-O3P
3	C	602	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

30 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	TDK	4	0
5	C	606	ALU	1	0
9	B	612	FMT	1	0
3	D	602	FAD	3	0
4	F	604	TDK	7	0
3	F	603	FAD	3	0
5	D	605	ALU	6	0
9	A	623	FMT	1	0
9	D	607	FMT	1	0
7	B	610	PEG	1	0
7	A	608	PEG	7	0
3	C	602	FAD	3	0
4	B	604	TDK	8	0
7	A	607	PEG	3	0
4	D	603	TDK	4	0
4	E	603	TDK	8	0
7	C	607	PEG	2	0
8	B	607	DTT	4	0
4	A	604	TDK	6	0
6	E	604	UQ0	1	0
12	E	605	DTU	9	0
5	A	605	ALU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	609	DTT	7	0
7	A	621[A]	PEG	3	0
6	A	606[A]	UQ0	2	0
10	A	613	PGE	1	0
7	A	616	PEG	3	0
8	A	610	DTT	1	0
3	A	603	FAD	1	0
3	E	602	FAD	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 then 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.

Ligand TDK C 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TDK F 604

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TDK B 604

Bond lengths

Bond angles

Torsions

Rings

Ligand TDK D 603

Bond lengths

Bond angles

Torsions

Rings

Ligand TDK E 603

Bond lengths

Bond angles

Torsions

Rings

Ligand TDK A 604

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 602

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	591/616 (95%)	-0.26	3 (0%)	91	94	16, 24, 42, 66	0
1	B	591/616 (95%)	-0.01	11 (1%)	66	74	16, 25, 44, 69	0
1	C	591/616 (95%)	0.08	22 (3%)	41	51	24, 32, 50, 78	0
1	D	591/616 (95%)	0.20	31 (5%)	27	37	24, 32, 52, 73	0
1	E	591/616 (95%)	0.07	25 (4%)	36	45	24, 34, 53, 73	0
1	F	591/616 (95%)	0.36	45 (7%)	13	21	25, 34, 53, 82	0
All	All	3546/3696 (95%)	0.07	137 (3%)	39	49	16, 31, 50, 82	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	6.9
1	F	2	ALA	5.9
1	F	3	LYS	5.3
1	C	338	LYS	4.7
1	C	3	LYS	4.0

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

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(Å^2)	Q<0.9
1	CSO	D	344	7/8	0.88	0.17	50,55,61,64	1
1	CSO	E	344	7/8	0.89	0.26	55,57,67,69	1
1	CSO	F	344	7/8	0.89	0.11	55,56,65,66	1
1	CSO	A	344	7/8	0.90	0.16	42,46,63,64	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	CSO	B	344	7/8	0.90	0.13	43,45,56,58	1
1	CSO	C	344	7/8	0.90	0.16	48,51,65,67	1

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
9	FMT	C	608	3/3	0.52	0.30	53,59,70,72	1
5	ALU	A	605	8/8	0.56	0.31	42,56,66,72	14
5	ALU	C	606	8/8	0.57	0.34	48,58,67,70	14
9	FMT	B	608	3/3	0.61	0.21	51,54,56,57	1
5	ALU	D	605	8/8	0.66	0.29	38,46,53,54	14
7	PEG	A	621[A]	7/7	0.71	0.25	31,65,78,81	2
7	PEG	A	621[B]	7/7	0.71	0.25	33,65,78,81	2
6	UQ0	E	604	13/13	0.72	0.24	71,83,98,102	0
9	FMT	A	620	3/3	0.74	0.33	50,52,56,60	1
11	NA	E	611	1/1	0.75	0.35	68,68,68,68	0
7	PEG	A	607	7/7	0.76	0.29	54,62,64,67	1
8	DTT	B	607	8/8	0.77	0.23	49,56,61,61	18
12	DTU	E	605	8/8	0.77	0.32	42,45,50,57	18
9	FMT	A	618	3/3	0.78	0.28	31,32,47,56	1
9	FMT	F	607	3/3	0.78	0.15	58,64,67,67	1
10	PGE	A	613	10/10	0.79	0.22	33,43,48,52	24
5	ALU	B	605	8/8	0.80	0.29	45,57,73,76	14
9	FMT	C	611	3/3	0.80	0.32	56,62,67,69	1
9	FMT	E	612	3/3	0.81	0.33	65,69,76,81	1
9	FMT	B	612	3/3	0.81	0.18	45,51,55,55	1
6	UQ0	C	604	13/13	0.81	0.21	67,79,84,85	0
9	FMT	C	609	3/3	0.81	0.28	65,66,68,70	1
9	FMT	B	609	3/3	0.81	0.26	56,57,65,72	1
9	FMT	E	609	3/3	0.82	0.16	61,63,66,67	1
7	PEG	F	606	7/7	0.82	0.26	64,74,80,83	1
9	FMT	A	617	3/3	0.82	0.36	51,55,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
11	NA	D	611	1/1	0.83	0.17	57,57,57,57	0
9	FMT	A	611	3/3	0.83	0.19	54,56,61,64	1
7	PEG	A	614	7/7	0.83	0.15	34,43,47,49	17
9	FMT	A	623	3/3	0.84	0.28	25,26,38,50	1
7	PEG	B	610	7/7	0.84	0.26	64,68,74,75	1
9	FMT	B	618	3/3	0.84	0.20	53,54,55,60	1
9	FMT	F	613	3/3	0.84	0.32	52,52,58,62	1
9	FMT	F	609	3/3	0.85	0.13	55,57,59,60	1
9	FMT	B	620	3/3	0.85	0.22	35,44,47,55	1
9	FMT	E	608	3/3	0.86	0.28	52,59,62,64	1
9	FMT	F	608	3/3	0.86	0.38	53,57,61,64	1
9	FMT	A	619	3/3	0.87	0.18	49,50,56,59	1
9	FMT	F	610	3/3	0.87	0.37	51,54,61,62	1
9	FMT	F	611	3/3	0.87	0.19	52,54,56,57	1
11	NA	E	613	1/1	0.87	0.43	68,68,68,68	0
7	PEG	A	616	7/7	0.87	0.18	62,71,74,75	1
9	FMT	D	608	3/3	0.88	0.22	49,49,54,59	1
9	FMT	B	611	3/3	0.88	0.18	46,56,60,60	1
9	FMT	D	606	3/3	0.88	0.14	56,56,57,58	1
6	UQ0	A	606[A]	13/13	0.89	0.27	38,48,54,55	22
7	PEG	C	607	7/7	0.89	0.21	48,61,64,65	1
9	FMT	E	606	3/3	0.89	0.15	54,57,60,60	1
9	FMT	E	607	3/3	0.89	0.17	37,38,49,56	1
9	FMT	A	612	3/3	0.89	0.10	46,49,56,63	1
9	FMT	A	615	3/3	0.89	0.21	57,65,76,86	1
7	PEG	A	608	7/7	0.89	0.26	15,23,27,29	17
8	DTT	A	609	8/8	0.89	0.20	29,44,52,52	18
9	FMT	C	612	3/3	0.89	0.22	61,62,66,69	1
9	FMT	B	614[B]	3/3	0.91	0.40	22,25,27,28	5
8	DTT	A	610	8/8	0.91	0.17	54,67,106,109	3
9	FMT	B	614[A]	3/3	0.91	0.40	31,32,33,33	5
11	NA	B	619	1/1	0.91	0.88	70,70,70,70	1
9	FMT	D	607	3/3	0.93	0.22	31,33,43,50	5
9	FMT	B	617	3/3	0.93	0.14	39,45,52,58	1
2	MG	B	622	1/1	0.93	0.13	46,46,46,46	0
11	NA	D	609	1/1	0.93	0.11	47,47,47,47	0
11	NA	C	610	1/1	0.94	0.16	60,60,60,60	0
6	UQ0	F	605	13/13	0.94	0.12	48,56,60,61	0
2	MG	E	616	1/1	0.94	0.10	45,45,45,45	0
13	CL	E	610	1/1	0.94	0.35	73,73,73,73	0
9	FMT	B	613	3/3	0.95	0.09	50,52,55,56	1
4	TDK	F	604	34/34	0.95	0.14	26,39,81,93	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
6	UQ0	D	604	13/13	0.95	0.12	48,57,62,63	0
11	NA	E	615	1/1	0.96	0.12	50,50,50,50	0
4	TDK	E	603	34/34	0.96	0.13	30,41,91,93	3
4	TDK	D	603	34/34	0.96	0.16	25,39,78,97	3
4	TDK	C	603	34/34	0.97	0.11	23,36,79,103	3
3	FAD	E	602	53/53	0.97	0.11	22,31,35,36	5
11	NA	B	621	1/1	0.97	0.05	32,32,32,32	0
4	TDK	B	604	34/34	0.97	0.14	17,30,79,87	3
11	NA	C	613	1/1	0.97	0.07	35,35,35,35	0
6	UQ0	B	606	13/13	0.97	0.12	41,51,61,63	0
3	FAD	A	603	53/53	0.98	0.10	13,20,23,25	5
3	FAD	C	602	53/53	0.98	0.09	19,27,31,33	5
3	FAD	D	602	53/53	0.98	0.11	19,28,31,31	5
11	NA	D	610	1/1	0.98	0.05	34,34,34,34	0
2	MG	A	624	1/1	0.98	0.06	32,32,32,32	0
11	NA	A	622	1/1	0.98	0.05	33,33,33,33	0
11	NA	B	615	1/1	0.98	0.16	40,40,40,40	0
11	NA	E	614	1/1	0.98	0.11	59,59,59,59	0
11	NA	B	616	1/1	0.98	0.22	47,47,47,47	0
11	NA	F	612	1/1	0.98	0.11	41,41,41,41	0
3	FAD	F	603	53/53	0.98	0.11	21,29,32,32	5
4	TDK	A	604	34/34	0.98	0.11	15,26,72,84	3
2	MG	F	601	1/1	0.99	0.03	29,29,29,29	0
2	MG	F	602	1/1	0.99	0.16	24,24,24,24	0
2	MG	E	601	1/1	0.99	0.06	29,29,29,29	0
3	FAD	B	603	53/53	0.99	0.13	12,20,23,25	5
2	MG	B	602	1/1	0.99	0.21	20,20,20,20	1
2	MG	A	601	1/1	1.00	0.04	18,18,18,18	0
2	MG	C	601	1/1	1.00	0.06	25,25,25,25	0
2	MG	C	605	1/1	1.00	0.14	22,22,22,22	0
2	MG	D	601	1/1	1.00	0.05	28,28,28,28	0
2	MG	B	601	1/1	1.00	0.04	21,21,21,21	0
2	MG	A	602	1/1	1.00	0.13	21,21,21,21	1

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 TDK F 604:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
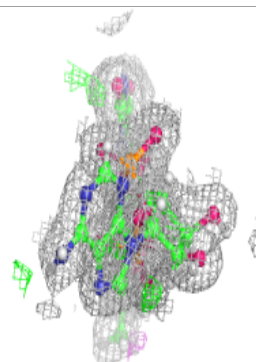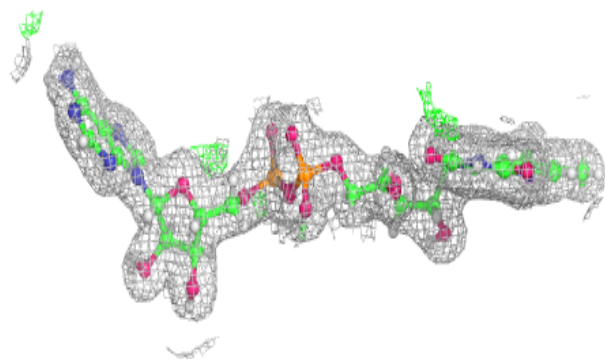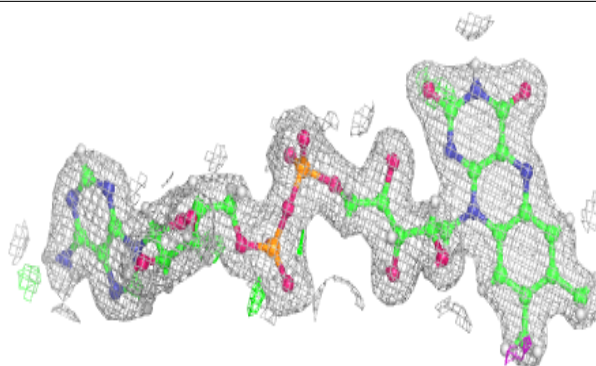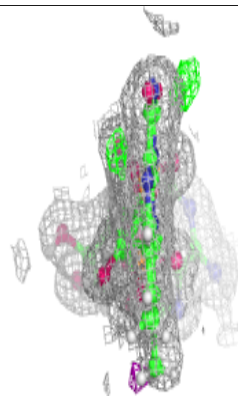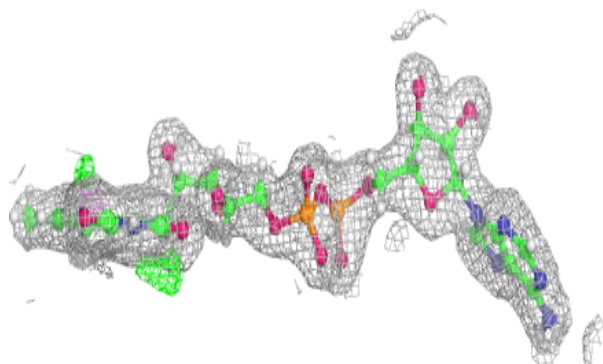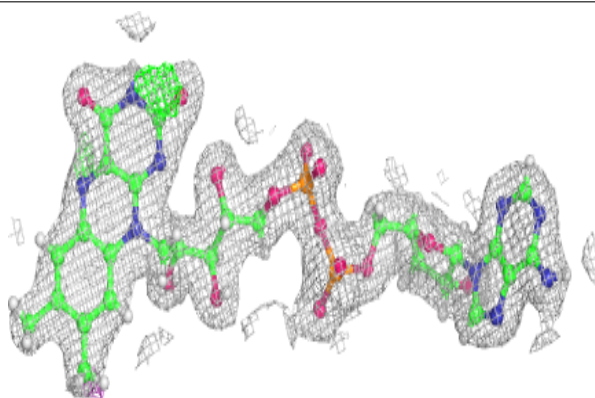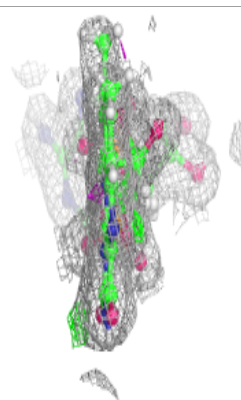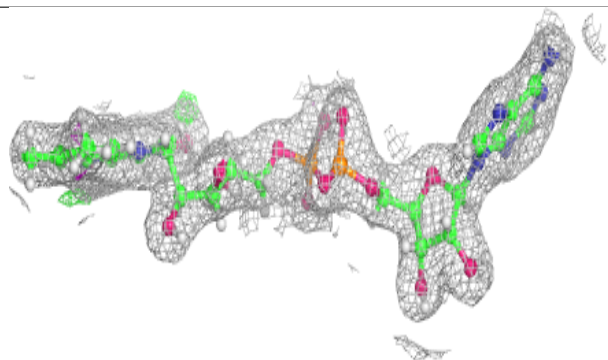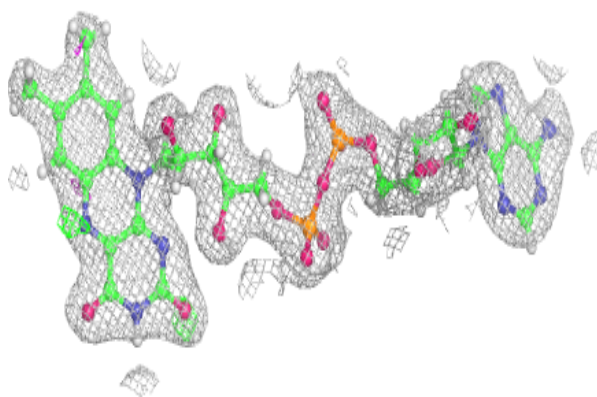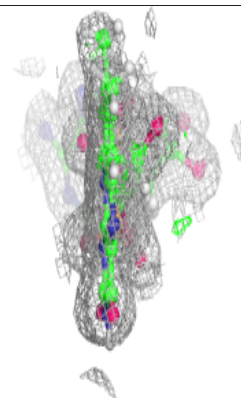$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
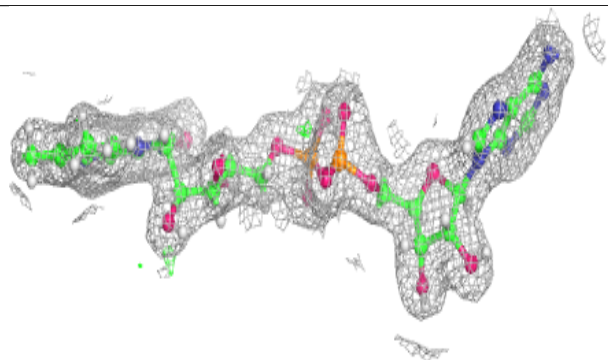and green (positive)
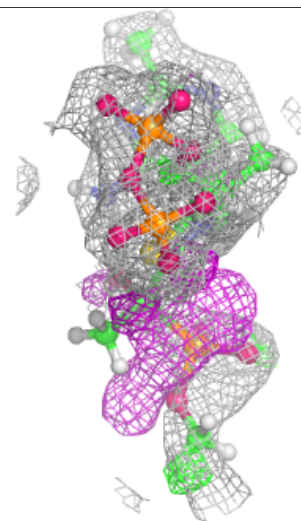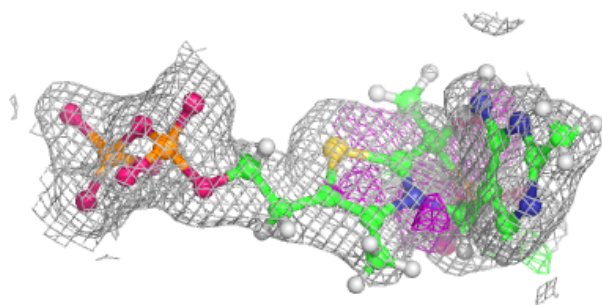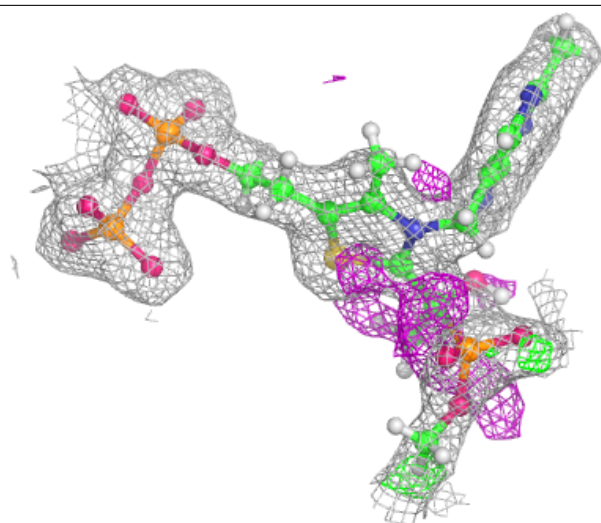
Electron density around TDK E 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
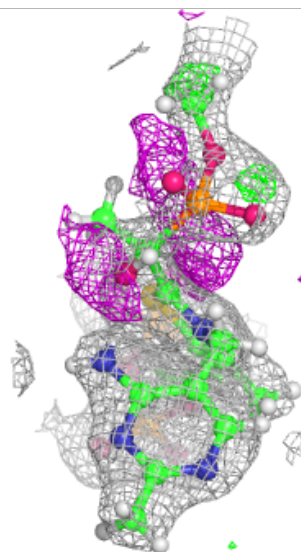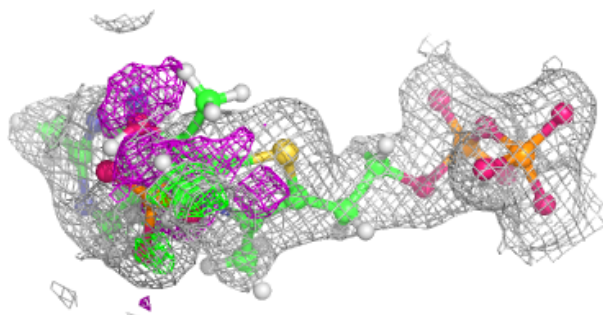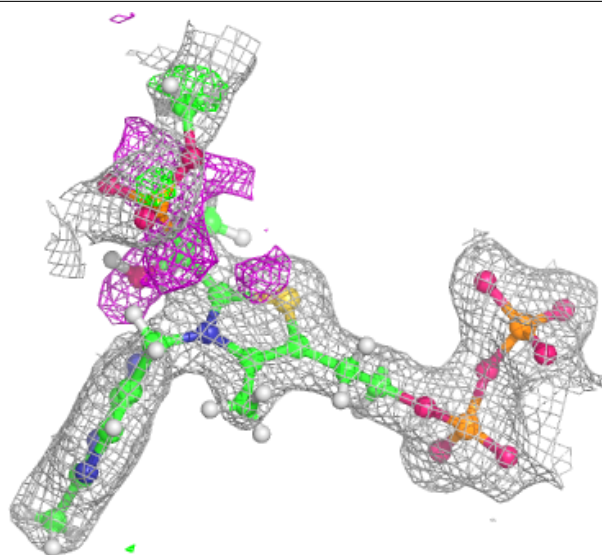
Electron density around TDK D 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
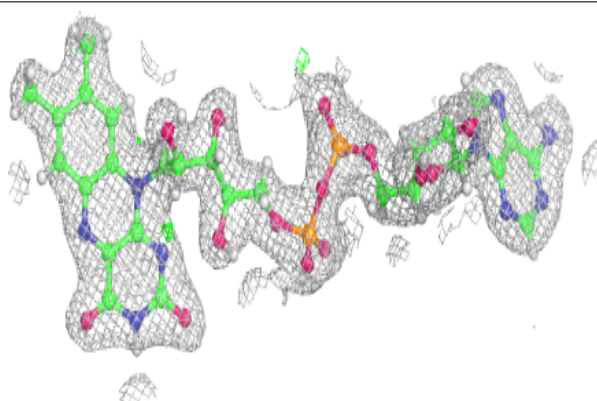and green (positive)
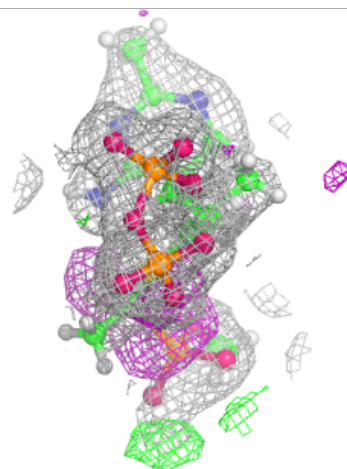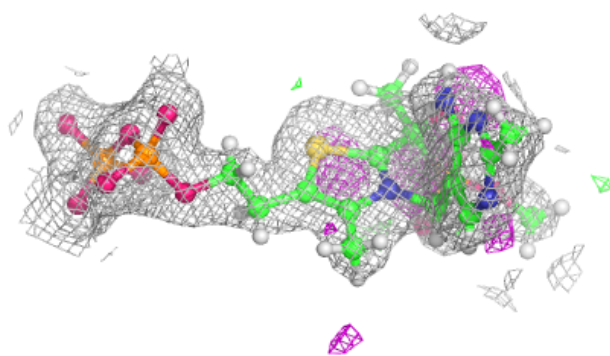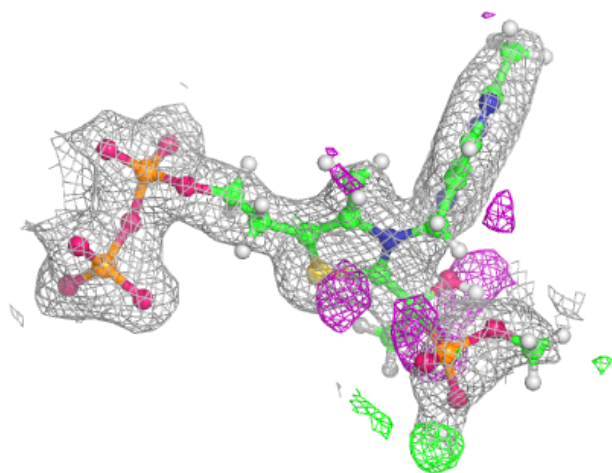
Electron density around TDK C 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
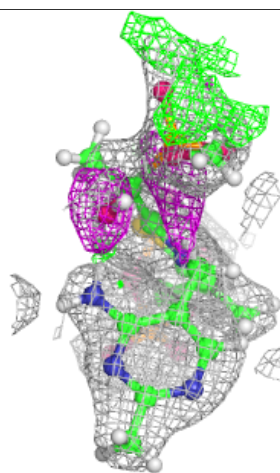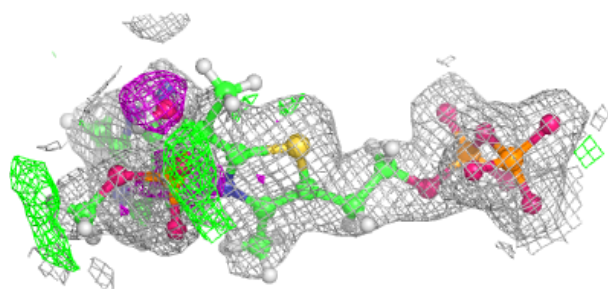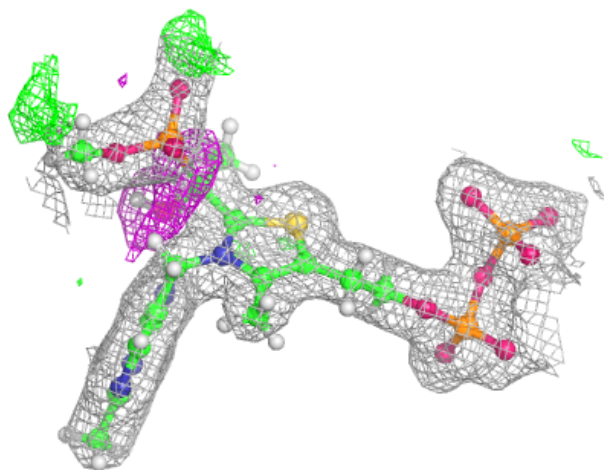
Electron density around FAD E 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
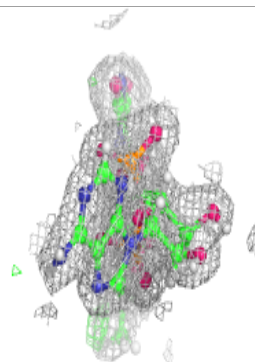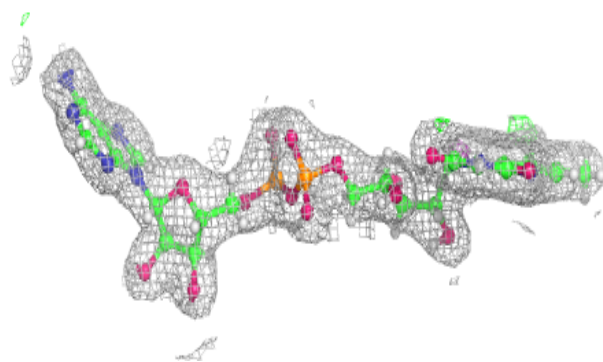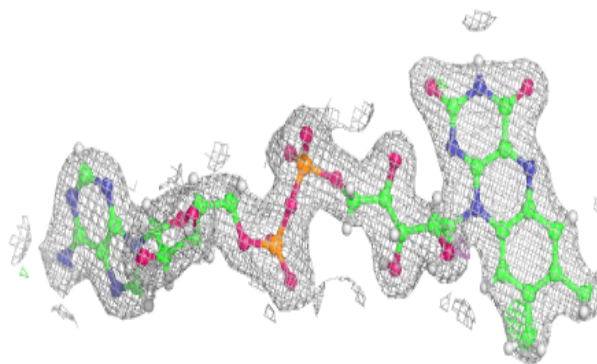
Electron density around TDK B 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
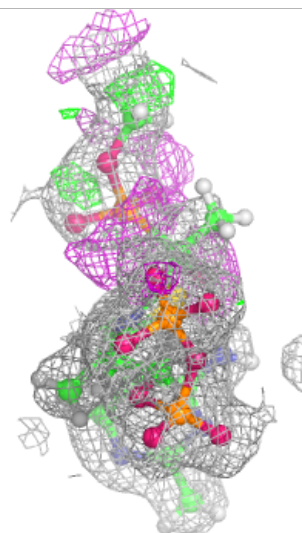mF_o-DF_c (at 3 rmsd) in purple (negative)
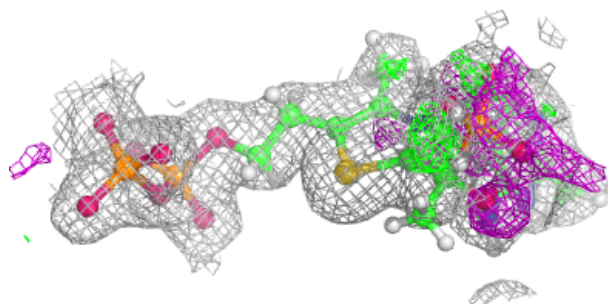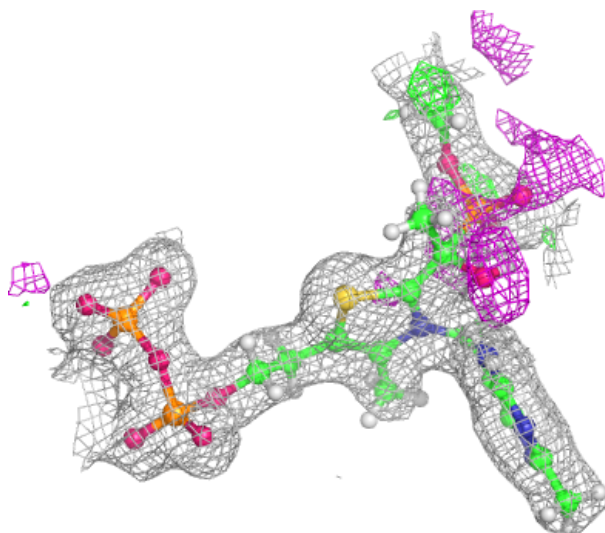and green (positive)
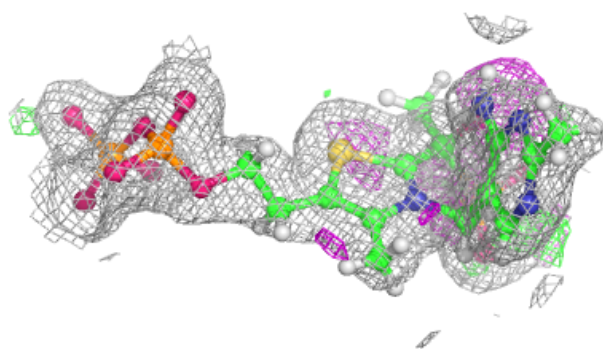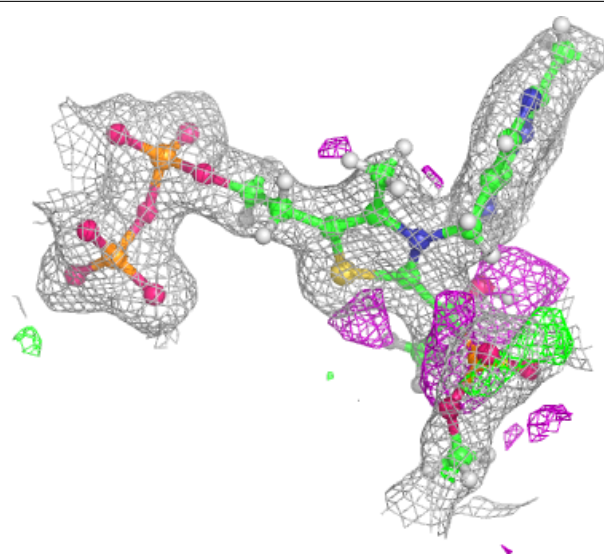
Electron density around FAD A 603:

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

Electron density around FAD C 602:

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

Electron density around FAD D 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
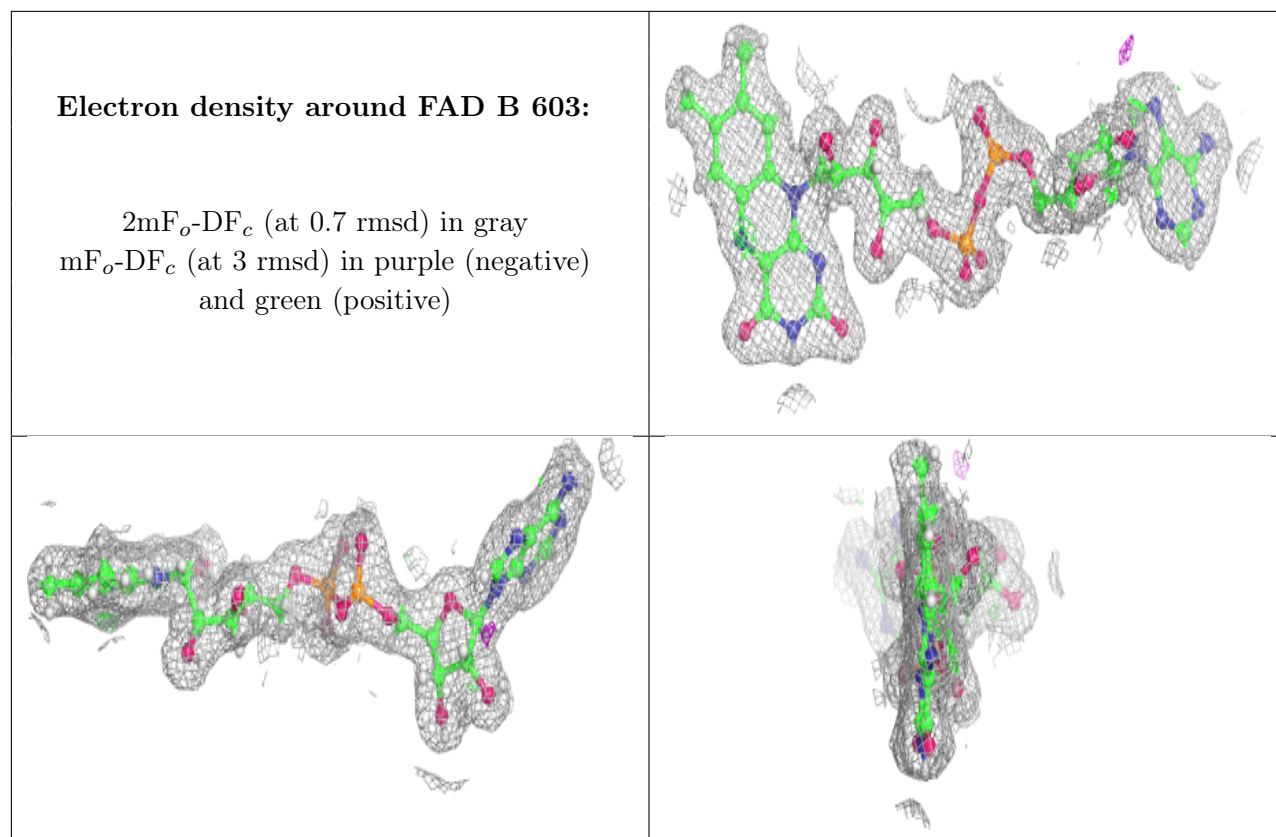and green (positive)

Electron density around FAD F 603:

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 TDK A 604:

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

Electron density around FAD B 603:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.