



Full wwPDB X-ray Structure Validation 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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

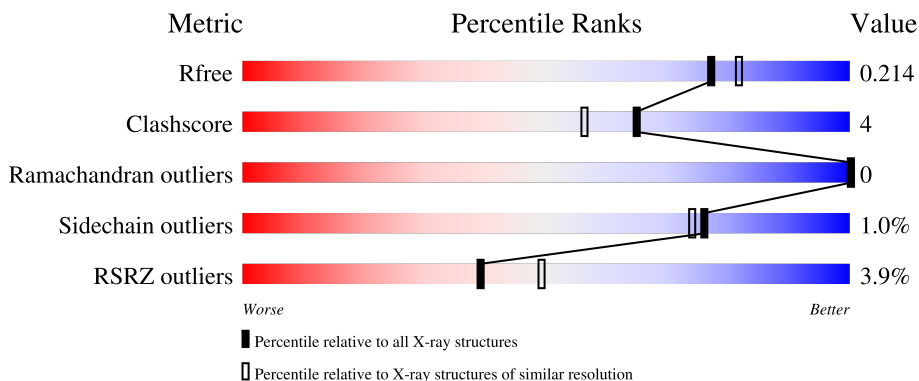
1 Overall quality at a glance

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	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 $\leq 5\%$. 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	616	89% 6% .
1	B	616	2% 89% 6% .
1	C	616	4% 89% 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	

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 [i](#)

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
			Total	C	H	N	O	S			
1	A	592	9117	2879	4569	796	837	36	106	4	0
1	B	592	9118	2880	4568	796	839	35	105	4	0
1	C	592	9083	2870	4549	793	837	34	104	1	0
1	D	592	9111	2878	4564	796	839	34	104	3	0
1	E	592	9093	2873	4554	794	838	34	104	2	0
1	F	592	9120	2880	4570	797	838	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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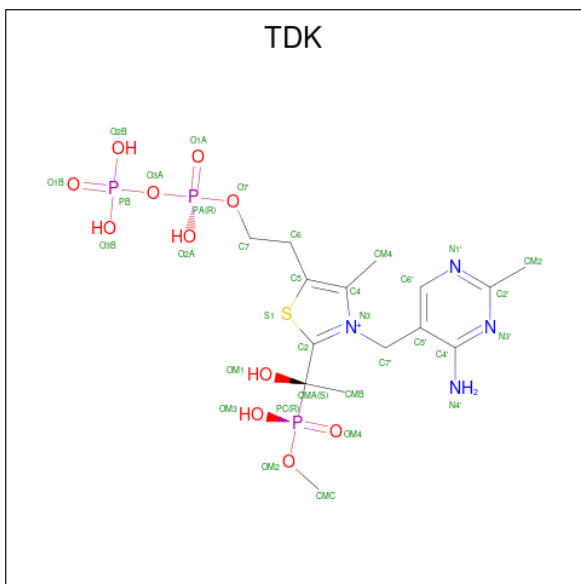
Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP P0AEP7
E	-16	HIS	-	expression tag	UNP P0AEP7
E	-15	HIS	-	expression tag	UNP P0AEP7
E	-14	HIS	-	expression tag	UNP P0AEP7
E	-13	HIS	-	expression tag	UNP P0AEP7
E	-12	SER	-	expression tag	UNP P0AEP7
E	-11	SER	-	expression tag	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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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
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(PHOSPHONOXY)PHOSPHORYL]OXY)ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDK) (formula: C₁₅H₂₆N₄O₁₁P₃S) (labeled as "Ligand of Interest" by depositor).



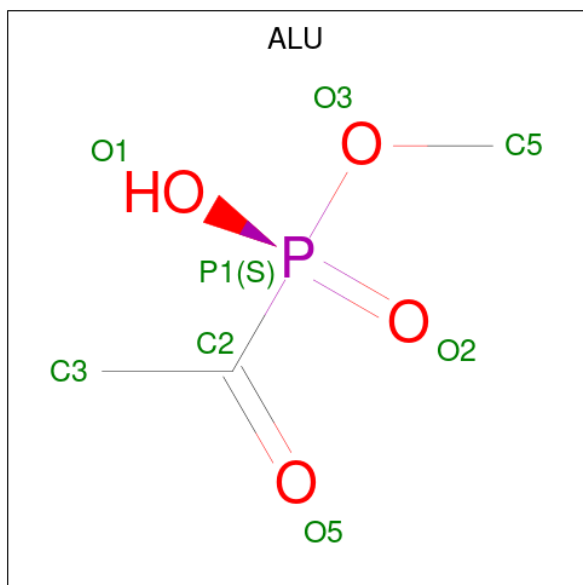
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	H	N	O	P			S
4	A	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	B	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	C	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	D	1	Total	C	H	N	O	P	S	3	0
			56	15	22	4	11	3	1		
4	E	1	Total	C	H	N	O	P	S	3	0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

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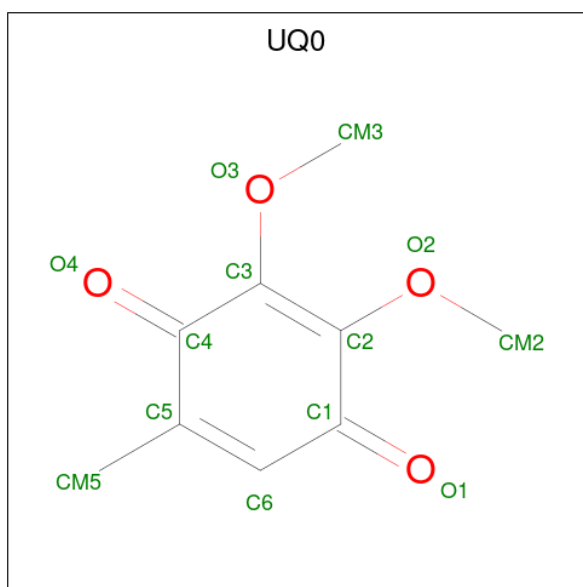
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	H	N	O	P			S
4	F	1	56	15	22	4	11	3	1	3	0

- Molecule 5 is METHYL HYDROGEN (S)-ACETYLPHOSPHONATE (three-letter code: ALU) (formula: C₃H₇O₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
5	A	1	14	3	6	4	1	0	0
5	B	1	14	3	6	4	1	0	0
5	C	1	14	3	6	4	1	0	0
5	D	1	14	3	6	4	1	0	0

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-1,4-BENZOQUINONE (three-letter code: UQ0) (formula: C₉H₁₀O₄).



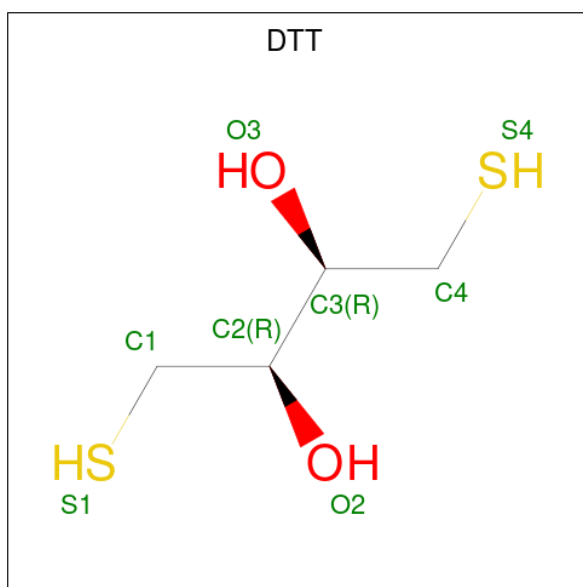
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	Total	C	H	O	0	1
			22	9	9	4		
6	B	1	Total	C	H	O	0	0
			22	9	9	4		
6	C	1	Total	C	H	O	0	0
			22	9	9	4		
6	D	1	Total	C	H	O	0	0
			22	9	9	4		
6	E	1	Total	C	H	O	0	0
			22	9	9	4		
6	F	1	Total	C	H	O	0	0
			22	9	9	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



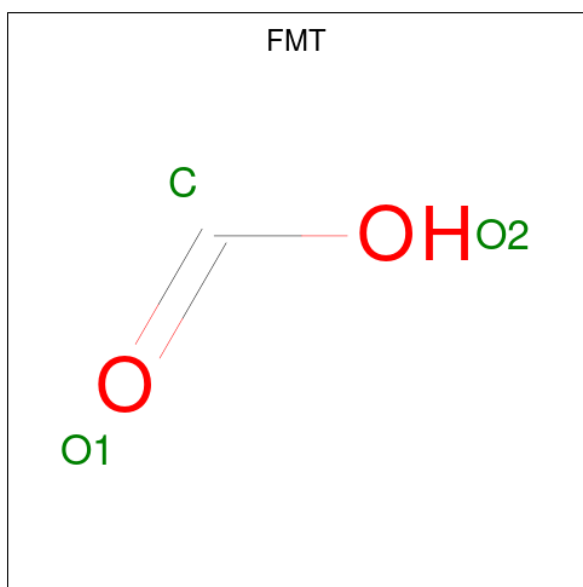
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	17	4	10	3	1	0
7	A	1	17	4	10	3	1	0
7	A	1	17	4	10	3	1	0
7	A	1	17	4	10	3	1	0
7	A	1	19	4	11	4	2	1
7	B	1	17	4	10	3	1	0
7	C	1	17	4	10	3	1	0
7	F	1	17	4	10	3	1	0

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



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

- Molecule 9 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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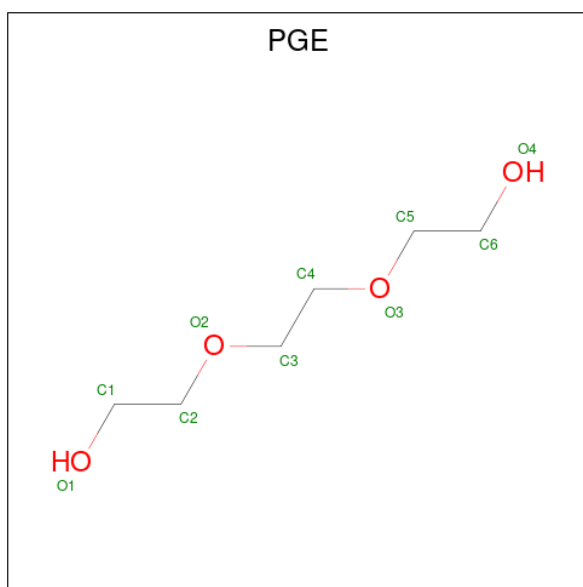
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	A	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	H 2	O 2	1	0
9	B	1	Total 5	C 1	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: C₆H₁₄O₄).

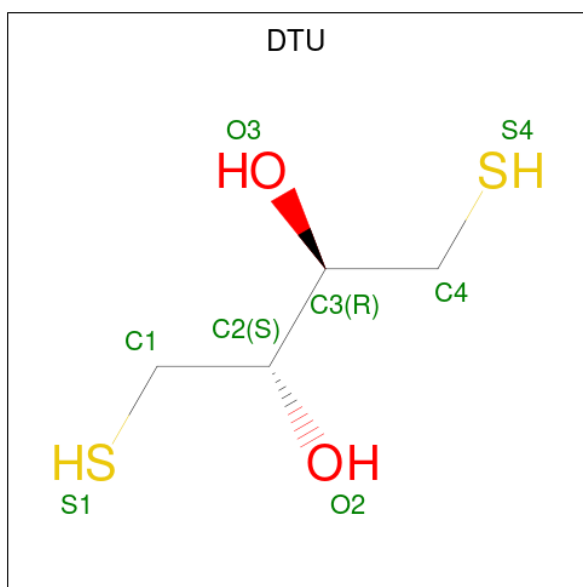


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	A	1	24	6	14	4	1	0

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

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

- Molecule 12 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C₄H₁₀O₂S₂).



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

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

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

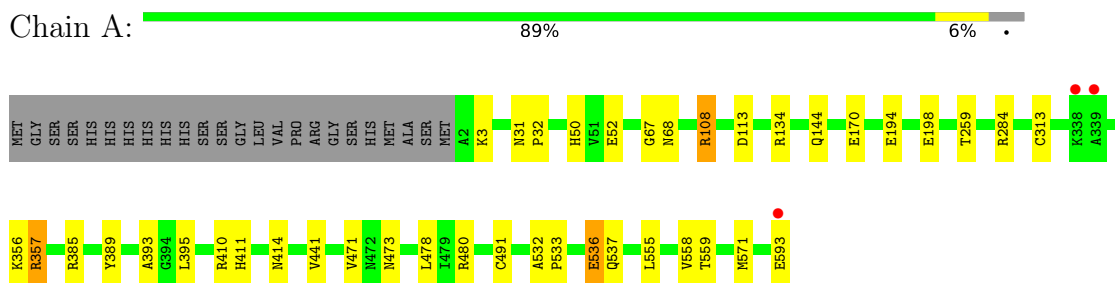
- Molecule 14 is water.

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

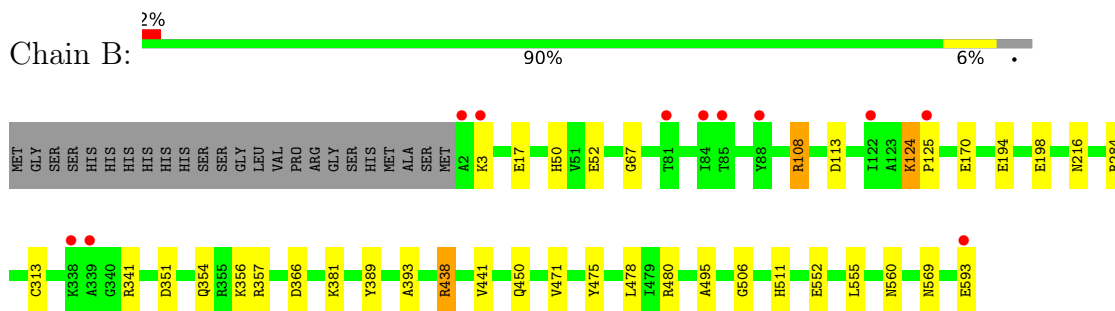
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

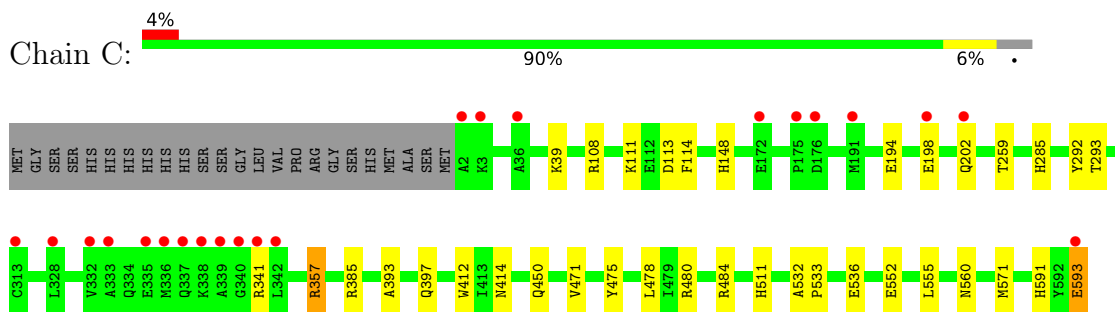
- Molecule 1: Glyoxylate carboligase



- Molecule 1: Glyoxylate carboligase

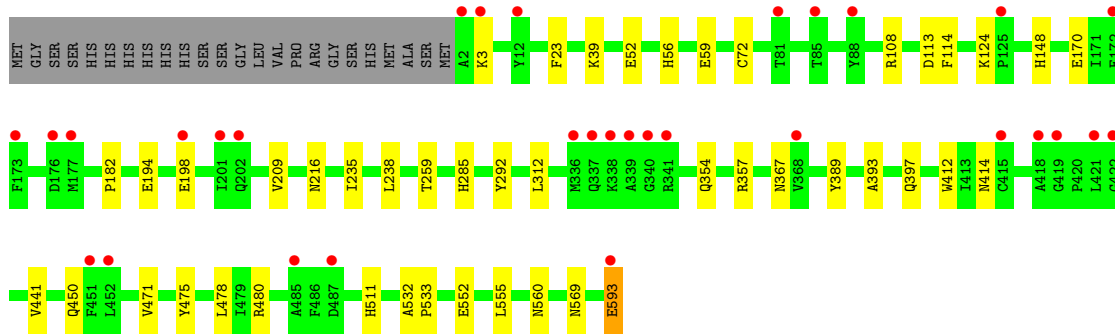


- Molecule 1: Glyoxylate carboligase

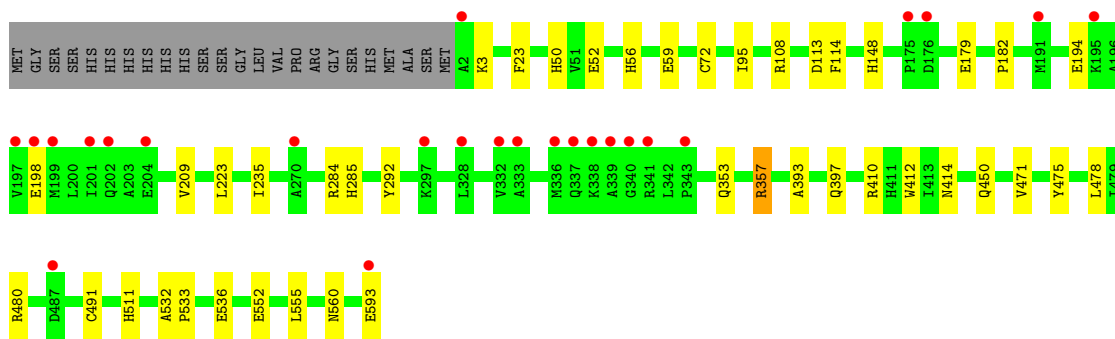
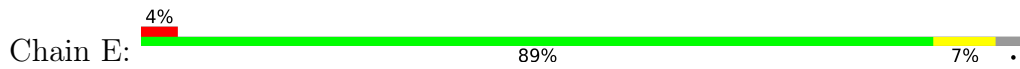


- Molecule 1: Glyoxylate carboligase

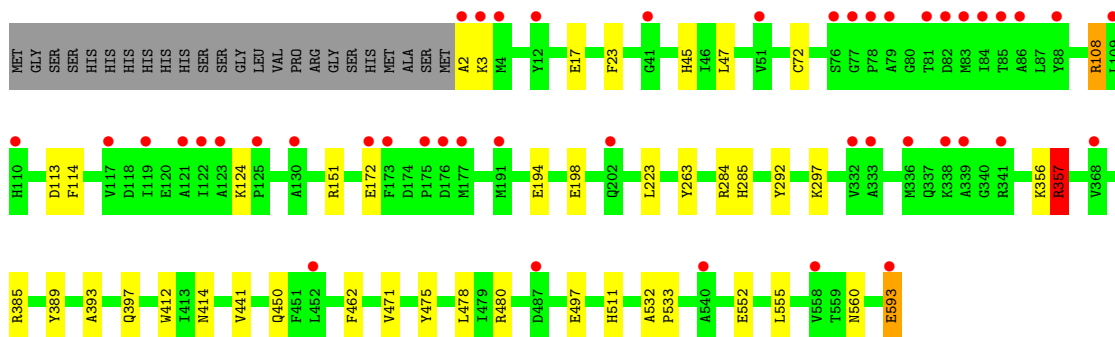
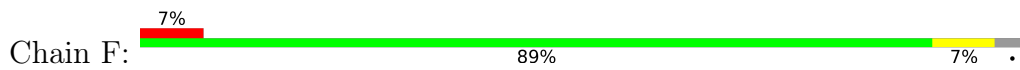




- Molecule 1: Glyoxylate carboligase



- Molecule 1: Glyoxylate carboligase



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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.97Å)	Xtrriage
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	Xtrriage
Anisotropy	0.001	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: 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

All (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
1	F	17	GLU	CD-OE1	5.38	1.31	1.25
1	F	497	GLU	CD-OE1	5.30	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	357	ARG	N-CA-CB	-7.75	96.65	110.60
1	C	357	ARG	N-CA-CB	-7.47	97.16	110.60
1	D	593	GLU	CB-CG-CD	-7.32	94.43	114.20
1	E	357	ARG	N-CA-CB	-7.31	97.45	110.60
1	F	151[A]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	F	151[B]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	F	357	ARG	CB-CA-C	-6.74	96.91	110.40
1	D	357	ARG	CB-CA-C	-6.25	97.90	110.40
1	D	593	GLU	OE1-CD-OE2	6.19	130.73	123.30
1	F	357	ARG	CB-CG-CD	-6.01	95.98	111.60
1	C	484	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	D	357	ARG	CB-CG-CD	-5.78	96.56	111.60
1	B	438	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	357	ARG	CB-CG-CD	-5.52	97.24	111.60
1	F	151[A]	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	F	151[B]	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	C	484	ARG	NE-CZ-NH1	-5.26	117.67	120.30

There are no chirality outliers.

All (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
1	E	357	ARG	Sidechain
1	E	475	TYR	Peptide
1	F	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.39	0.87
1:E:410:ARG:HH22	12:E:605:DTU:H1C1	1.39	0.86
1:F:108:ARG:HG3	1:F:108:ARG:HH11	1.38	0.85
1:D:480:ARG:HH12	1:D:560:ASN:HD21	1.24	0.84
1:A:395:LEU:HD12	7:A:608:PEG:H31	1.60	0.83
1:B:67:GLY:H	8:B:607:DTT:H3	1.43	0.83
1:C:39:LYS:NZ	14:C:701:HOH:O	2.12	0.83
1:E:410:ARG:NH2	12:E:605:DTU:H1C1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ARG:HH12	1:B:560:ASN:HD21	1.22	0.82
4:B:604:TDK:N4'	4:B:604:TDK:OM1	2.11	0.82
1:A:410:ARG:HH22	8:A:609:DTT:C4	1.93	0.81
1:E:480:ARG:HH12	1:E:560:ASN:HD21	1.26	0.80
1:A:50:HIS:HD2	1:A:52:GLU:H	1.26	0.80
1:D:593:GLU:OXT	1:D:593:GLU:HG2	1.80	0.80
1:B:50:HIS:HD2	1:B:52:GLU:H	1.27	0.79
1:B:108:ARG:HG3	1:B:108:ARG:HH11	1.49	0.78
1:A:67:GLY:H	8:A:609:DTT:H2	1.45	0.78
1:F:480:ARG:HH12	1:F:560:ASN:HD21	1.27	0.78
1:E:410:ARG:HH12	12:E:605:DTU:H1C1	1.48	0.75
1:E:410:ARG:NH1	12:E:605:DTU:H1C1	2.01	0.75
1:D:478:LEU:HD23	4:D:603:TDK:HMB3	1.69	0.74
1:C:480:ARG:HH12	1:C:560:ASN:HD21	1.34	0.73
1:E:50:HIS:HD2	1:E:52:GLU:H	1.35	0.72
1:D:450:GLN:HE21	1:D:511:HIS:HE1	1.37	0.72
1:B:354:GLN:HG2	14:B:733:HOH:O	1.91	0.71
1:B:450:GLN:HE21	1:B:511:HIS:HE1	1.35	0.71
1:D:39:LYS:NZ	14:D:702:HOH:O	2.24	0.71
1:A:410:ARG:HH22	8:A:609:DTT:H42	1.56	0.70
1:D:393:ALA:HB1	4:D:603:TDK:HMB2	1.72	0.70
1:E:397:GLN:HE21	1:E:414:ASN:HD21	1.37	0.70
1:C:397:GLN:HE21	1:C:414:ASN:HD21	1.38	0.70
5:C:606:ALU:H5C2	1:E:491:CYS:SG	2.32	0.70
4:F:604:TDK:CMC	14:F:971:HOH:O	2.40	0.70
1:F:397:GLN:HE21	1:F:414:ASN:HD21	1.40	0.69
1:C:450:GLN:HE21	1:C:511:HIS:HE1	1.39	0.69
1:B:478:LEU:HD23	4:B:604:TDK:HMB3	1.73	0.69
4:A:604:TDK:OM1	4:A:604:TDK:N4'	2.27	0.68
1:A:411:HIS:HE2	8:A:610:DTT:HS2	1.40	0.68
1:F:478:LEU:HD23	4:F:604:TDK:HMB3	1.74	0.68
1:E:410:ARG:HH22	12:E:605:DTU:C1	2.06	0.68
1:F:108:ARG:HG3	1:F:108:ARG:NH1	2.08	0.68
4:F:604:TDK:OM1	4:F:604:TDK:N4'	2.27	0.67
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.07	0.67
1:C:393:ALA:HB1	4:C:603:TDK:HMB2	1.74	0.67
1:D:52:GLU:OE2	1:D:56:HIS:HE1	1.77	0.67
1:E:478:LEU:HD23	4:E:603:TDK:HMB3	1.77	0.66
1:F:108:ARG:HH11	1:F:108:ARG:CG	2.08	0.66
1:D:397:GLN:HE21	1:D:414:ASN:HD21	1.41	0.66
1:A:50:HIS:CD2	1:A:52:GLU:H	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ARG:CZ	12:E:605:DTU:H1C1	2.24	0.66
1:F:450:GLN:HE21	1:F:511:HIS:HE1	1.43	0.66
10:A:613:PGE:H6	14:A:986:HOH:O	1.94	0.66
1:E:108:ARG:HH11	1:E:108:ARG:HG3	1.61	0.66
7:A:607:PEG:H31	7:A:621[A]:PEG:H11	1.76	0.65
1:B:471:VAL:HB	1:B:555:LEU:HD11	1.78	0.65
1:B:50:HIS:CD2	1:B:52:GLU:H	2.12	0.65
1:A:108:ARG:HG3	1:A:108:ARG:NH1	2.09	0.65
1:E:284:ARG:HH12	4:E:603:TDK:HMC3	1.61	0.65
1:B:284:ARG:HH12	4:B:604:TDK:HMC3	1.60	0.65
1:E:393:ALA:HB1	4:E:603:TDK:HMB2	1.77	0.64
1:C:108:ARG:HG3	1:C:108:ARG:HH11	1.62	0.64
1:C:478:LEU:HD23	4:C:603:TDK:HMB3	1.79	0.64
1:B:284:ARG:HH22	4:B:604:TDK:HMC2	1.62	0.64
4:D:603:TDK:OM1	4:D:603:TDK:N4'	2.30	0.63
1:B:108:ARG:HH11	1:B:108:ARG:CG	2.11	0.63
1:B:393:ALA:HB1	4:B:604:TDK:HMB2	1.81	0.62
1:E:52:GLU:OE2	1:E:56:HIS:HE1	1.81	0.62
1:B:450:GLN:HE21	1:B:511:HIS:CE1	2.16	0.62
7:A:607:PEG:C3	7:A:621[A]:PEG:H11	2.29	0.62
1:A:68:ASN:O	8:A:609:DTT:H11	2.00	0.62
1:A:473:ASN:ND2	7:A:608:PEG:H11	2.15	0.62
1:D:450:GLN:HE21	1:D:511:HIS:CE1	2.17	0.62
1:A:478:LEU:HD23	4:A:604:TDK:HMB3	1.81	0.61
1:E:471:VAL:HB	1:E:555:LEU:HD11	1.81	0.61
1:A:144:GLN:HE22	7:A:621[A]:PEG:H12	1.65	0.61
1:D:108:ARG:HG3	1:D:108:ARG:HH11	1.65	0.61
1:D:478:LEU:CD2	4:D:603:TDK:HMB3	2.29	0.61
1:A:558:VAL:HA	7:A:608:PEG:H42	1.83	0.60
1:A:491:CYS:SG	5:A:605:ALU:O3	2.57	0.59
1:E:50:HIS:CD2	1:E:52:GLU:H	2.16	0.59
1:F:393:ALA:HB1	4:F:604:TDK:HMB2	1.84	0.59
1:F:471:VAL:HB	1:F:555:LEU:HD11	1.83	0.59
1:C:450:GLN:HE21	1:C:511:HIS:CE1	2.19	0.59
1:F:478:LEU:CD2	4:F:604:TDK:HMB3	2.32	0.58
1:A:537:GLN:HG3	14:A:1078:HOH:O	2.03	0.58
1:A:393:ALA:HB1	4:A:604:TDK:HMB2	1.84	0.58
1:A:410:ARG:HH22	8:A:609:DTT:H41	1.69	0.58
1:B:478:LEU:CD2	4:B:604:TDK:HMB3	2.33	0.58
1:C:471:VAL:HB	1:C:555:LEU:HD11	1.85	0.58
1:D:367:ASN:HD22	1:D:367:ASN:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:HIS:NE2	7:C:607:PEG:H21	2.19	0.57
1:E:450:GLN:HE21	1:E:511:HIS:HE1	1.53	0.57
1:D:471:VAL:HB	1:D:555:LEU:HD11	1.86	0.57
4:E:603:TDK:OM1	4:E:603:TDK:N4'	2.35	0.56
1:F:194:GLU:O	1:F:198:GLU:HG2	2.06	0.56
1:C:511:HIS:HD2	1:C:552:GLU:OE2	1.89	0.56
1:B:67:GLY:N	8:B:607:DTT:H3	2.17	0.56
1:D:114:PHE:CZ	3:F:603:FAD:HM82	2.41	0.56
1:F:511:HIS:HD2	1:F:552:GLU:OE2	1.89	0.56
1:F:450:GLN:HE21	1:F:511:HIS:CE1	2.23	0.55
1:B:108:ARG:HG3	1:B:108:ARG:NH1	2.14	0.55
3:C:602:FAD:HM82	1:E:114:PHE:CZ	2.42	0.55
1:D:511:HIS:HD2	1:D:552:GLU:OE2	1.90	0.55
5:D:605:ALU:O1	1:F:462:PHE:CZ	2.58	0.55
1:C:194:GLU:O	1:C:198:GLU:HG2	2.07	0.54
1:C:285:HIS:HE1	1:C:292:TYR:OH	1.90	0.54
1:C:412:TRP:HE1	1:C:414:ASN:HD22	1.53	0.54
1:A:284:ARG:HH22	4:A:604:TDK:HMC2	1.73	0.54
1:A:410:ARG:NH2	8:A:609:DTT:H42	2.20	0.54
1:B:381:LYS:HE2	14:B:1062:HOH:O	2.07	0.54
1:D:194:GLU:O	1:D:198:GLU:HG2	2.07	0.54
1:B:511:HIS:HD2	1:B:552:GLU:OE2	1.92	0.53
1:E:108:ARG:HG3	1:E:108:ARG:NH1	2.22	0.53
1:B:284:ARG:HH12	4:B:604:TDK:CMC	2.21	0.53
1:E:412:TRP:HE1	1:E:414:ASN:HD22	1.56	0.53
1:C:108:ARG:HG3	1:C:108:ARG:NH1	2.21	0.52
1:E:56:HIS:HD2	1:E:59:GLU:OE2	1.91	0.52
1:B:194:GLU:O	1:B:198:GLU:HG2	2.09	0.52
3:D:602:FAD:HM82	1:F:114:PHE:CZ	2.45	0.52
1:D:593:GLU:OXT	1:D:593:GLU:CG	2.48	0.52
5:D:605:ALU:O1	1:F:462:PHE:HZ	1.93	0.52
1:D:3:LYS:HE3	1:D:170:GLU:OE1	2.09	0.52
1:F:285:HIS:HE1	1:F:292:TYR:OH	1.92	0.52
1:A:473:ASN:ND2	7:A:608:PEG:C1	2.72	0.52
1:A:385:ARG:H	1:A:593:GLU:HG3	1.75	0.52
1:D:56:HIS:HD2	1:D:59:GLU:OE2	1.93	0.52
4:C:603:TDK:OM1	4:C:603:TDK:N4'	2.39	0.51
1:F:385:ARG:H	1:F:593:GLU:HG3	1.75	0.51
1:E:194:GLU:O	1:E:198:GLU:HG2	2.11	0.51
1:E:410:ARG:HH12	12:E:605:DTU:C1	2.21	0.51
1:E:511:HIS:HD2	1:E:552:GLU:OE2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:TRP:HE1	1:F:414:ASN:HD22	1.58	0.50
1:E:148:HIS:HD2	1:E:182:PRO:O	1.94	0.50
1:E:450:GLN:HE21	1:E:511:HIS:CE1	2.29	0.50
1:A:558:VAL:HA	7:A:608:PEG:C4	2.42	0.50
1:D:480:ARG:HH12	1:D:560:ASN:ND2	2.03	0.50
1:E:480:ARG:HH22	1:E:560:ASN:ND2	2.09	0.50
1:E:536:GLU:HG3	14:E:1010:HOH:O	2.11	0.50
9:B:612:FMT:C	14:B:991:HOH:O	2.60	0.49
1:A:559:THR:H	7:A:608:PEG:C4	2.24	0.49
8:B:607:DTT:H41	14:B:995:HOH:O	2.13	0.49
1:E:353:GLN:HG2	6:E:604:UQ0:CM2	2.43	0.49
5:D:605:ALU:H1	1:F:462:PHE:HZ	1.55	0.49
1:C:114:PHE:CZ	3:E:602:FAD:HM82	2.47	0.49
14:A:1056:HOH:O	1:B:313[B]:CYS:SG	2.49	0.49
1:D:285:HIS:HE1	1:D:292:TYR:OH	1.94	0.49
1:D:412:TRP:HE1	1:D:414:ASN:HD22	1.60	0.49
1:A:532:ALA:HB3	1:A:533:PRO:HD3	1.95	0.48
7:C:607:PEG:H41	14:C:872:HOH:O	2.12	0.48
1:D:148:HIS:HD2	1:D:182:PRO:O	1.96	0.48
1:E:285:HIS:HE1	1:E:292:TYR:OH	1.96	0.48
1:A:194:GLU:O	1:A:198:GLU:HG2	2.14	0.48
5:D:605:ALU:H3C2	1:F:45:HIS:ND1	2.28	0.48
1:A:478:LEU:CD2	4:A:604:TDK:HMB3	2.44	0.48
1:E:532:ALA:HB3	1:E:533:PRO:HD3	1.96	0.47
1:A:480:ARG:HH21	7:A:608:PEG:H41	1.79	0.47
1:C:385:ARG:H	1:C:593:GLU:HG3	1.80	0.47
9:A:623:FMT:H	14:A:1015:HOH:O	2.14	0.47
1:E:95:ILE:HG21	12:E:605:DTU:S1	2.55	0.47
1:F:480:ARG:HH22	1:F:560:ASN:ND2	2.13	0.47
1:B:3:LYS:HE3	1:B:170:GLU:OE1	2.14	0.47
1:E:284:ARG:HH22	4:E:603:TDK:HMC2	1.79	0.47
4:F:604:TDK:HMC1	14:F:971:HOH:O	2.09	0.46
1:B:108:ARG:NH2	14:B:710:HOH:O	2.38	0.46
1:C:478:LEU:CD2	4:C:603:TDK:HMB3	2.44	0.46
1:D:532:ALA:HB3	1:D:533:PRO:HD3	1.98	0.46
1:F:532:ALA:HB3	1:F:533:PRO:HD3	1.97	0.46
1:A:356:LYS:NZ	7:A:616:PEG:O4	2.45	0.46
1:D:108:ARG:HG3	1:D:108:ARG:NH1	2.30	0.45
1:D:114:PHE:CE1	3:F:603:FAD:HM82	2.52	0.45
1:C:259:THR:OG1	3:C:602:FAD:C4X	2.64	0.45
9:D:607:FMT:C	14:D:703:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:605:ALU:H3C1	1:F:47:LEU:HB2	1.99	0.45
1:D:569:ASN:C	1:D:569:ASN:OD1	2.54	0.45
7:A:607:PEG:H11	7:A:607:PEG:H42	1.98	0.45
1:F:284:ARG:HH12	4:F:604:TDK:HMC1	1.82	0.45
1:C:532:ALA:HB3	1:C:533:PRO:HD3	1.98	0.44
3:C:602:FAD:HM82	1:E:114:PHE:CE1	2.53	0.44
1:A:108:ARG:HD3	14:A:1075:HOH:O	2.18	0.44
6:A:606[A]:UQ0:C5	7:A:616:PEG:H31	2.47	0.44
1:B:569:ASN:C	1:B:569:ASN:OD1	2.55	0.44
1:D:259:THR:OG1	3:D:602:FAD:C4X	2.66	0.44
1:E:95:ILE:CG2	12:E:605:DTU:S1	3.06	0.43
1:A:536:GLU:HG2	14:A:830:HOH:O	2.19	0.43
1:A:3:LYS:HD2	1:A:170:GLU:OE1	2.19	0.43
1:A:471:VAL:HB	1:A:555:LEU:HD11	2.00	0.43
1:B:495:ALA:HB1	1:B:506:GLY:O	2.18	0.43
1:E:284:ARG:HH12	4:E:603:TDK:CMC	2.31	0.42
1:A:31:ASN:N	1:A:32:PRO:CD	2.81	0.42
1:A:67:GLY:N	8:A:609:DTT:H2	2.24	0.42
1:B:389:TYR:HA	1:B:441:VAL:O	2.19	0.42
3:F:603:FAD:H9	3:F:603:FAD:H1'1	1.88	0.42
1:B:216:ASN:OD1	8:B:607:DTT:H11	2.18	0.42
1:D:312:LEU:O	1:D:312:LEU:HD12	2.19	0.42
1:D:389:TYR:HA	1:D:441:VAL:O	2.20	0.42
1:A:389:TYR:HA	1:A:441:VAL:O	2.20	0.42
1:B:480:ARG:HH22	1:B:560:ASN:ND2	2.18	0.42
1:B:480:ARG:HH12	1:B:560:ASN:ND2	2.02	0.42
1:C:293:THR:HB	14:C:702:HOH:O	2.20	0.42
1:E:478:LEU:CD2	4:E:603:TDK:HMB3	2.47	0.42
1:A:259:THR:OG1	3:A:603:FAD:C4X	2.68	0.41
1:D:23:PHE:O	1:D:72:CYS:HA	2.21	0.41
1:C:198:GLU:O	1:C:202:GLN:HG2	2.20	0.41
1:F:23:PHE:O	1:F:72:CYS:HA	2.20	0.41
1:F:389:TYR:HA	1:F:441:VAL:O	2.21	0.41
1:D:209:VAL:HA	1:D:235:ILE:O	2.21	0.41
1:D:312:LEU:HD12	1:D:312:LEU:C	2.41	0.41
5:D:605:ALU:C3	1:F:45:HIS:ND1	2.83	0.41
6:A:606[A]:UQ0:C4	7:A:616:PEG:H31	2.51	0.41
1:C:111:LYS:HE3	14:C:1013:HOH:O	2.20	0.41
1:E:209:VAL:HA	1:E:235:ILE:O	2.20	0.41
1:E:223:LEU:C	1:E:223:LEU:HD13	2.41	0.41
1:B:124:LYS:HB3	1:B:125:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:HZ3	7:B:610:PEG:H21	1.86	0.41
1:E:23:PHE:O	1:E:72:CYS:HA	2.21	0.41
1:F:2:ALA:HB1	1:F:172:GLU:OE1	2.21	0.41
1:D:238:LEU:HD21	1:D:414:ASN:ND2	2.36	0.40
3:D:602:FAD:H9	3:D:602:FAD:H1'1	1.93	0.40
1:F:223:LEU:HD13	1:F:223:LEU:C	2.42	0.40
1:E:52:GLU:OE2	1:E:56:HIS:CE1	2.68	0.40
1:F:263:TYR:CD1	1:F:356:LYS:HG2	2.55	0.40
1:E:536:GLU:HG2	14:E:730:HOH:O	2.20	0.40
1:F:357:ARG:NH1	1:F:357:ARG:HG3	2.37	0.40

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	593/616 (96%)	584 (98%)	9 (2%)	0	100 100
1	B	593/616 (96%)	584 (98%)	9 (2%)	0	100 100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3552/3696 (96%)	3494 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	113	ASP
1	A	414	ASN
1	B	108	ARG
1	B	113	ASP
1	B	124	LYS
1	B	351	ASP
1	B	438	ARG
1	B	475	TYR
1	B	593	GLU
1	C	113	ASP
1	C	475	TYR
1	C	593	GLU
1	D	113	ASP

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Mol	Chain	Res	Type
1	D	124	LYS
1	D	216	ASN
1	D	475	TYR
1	E	3	LYS
1	E	113	ASP
1	E	593	GLU
1	F	3	LYS
1	F	108	ARG
1	F	113	ASP
1	F	124	LYS
1	F	297	LYS
1	F	475	TYR
1	F	593	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	115	GLN
1	A	334	GLN
1	A	354	GLN
1	B	50	HIS
1	B	334	GLN
1	B	511	HIS
1	B	560	ASN
1	C	285	HIS
1	C	414	ASN
1	C	500	ASN
1	C	511	HIS
1	C	560	ASN
1	D	31	ASN
1	D	56	HIS
1	D	148	HIS
1	D	285	HIS
1	D	367	ASN
1	D	414	ASN
1	D	500	ASN
1	D	511	HIS
1	D	560	ASN
1	E	50	HIS
1	E	56	HIS
1	E	148	HIS

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Mol	Chain	Res	Type
1	E	285	HIS
1	E	414	ASN
1	E	500	ASN
1	E	511	HIS
1	E	560	ASN
1	F	31	ASN
1	F	285	HIS
1	F	414	ASN
1	F	500	ASN
1	F	511	HIS
1	F	560	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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. '2' 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	-

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

All (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
4	E	603	TDK	PC-CMA	10.56	2.01	1.84
4	F	604	TDK	C6-C5	-5.72	1.48	1.50
4	A	604	TDK	C6-C5	-5.58	1.48	1.50
4	B	604	TDK	C6-C5	-5.45	1.48	1.50
4	E	603	TDK	C6-C5	-5.14	1.48	1.50
3	F	603	FAD	C1'-C2'	4.88	1.59	1.52
4	C	603	TDK	C6-C5	-4.87	1.48	1.50
4	D	603	TDK	C6-C5	-4.51	1.48	1.50
5	A	605	ALU	P1-O3	4.47	1.64	1.57
9	A	623	FMT	O2-C	4.33	1.50	1.28
5	B	605	ALU	P1-O3	4.10	1.63	1.57
3	D	602	FAD	C1'-C2'	4.00	1.58	1.52
5	C	606	ALU	P1-O3	3.92	1.63	1.57
3	B	603	FAD	C1'-C2'	3.71	1.57	1.52
3	E	602	FAD	C1'-C2'	3.68	1.57	1.52
5	D	605	ALU	P1-O3	3.59	1.63	1.57
5	C	606	ALU	O5-C2	3.44	1.26	1.21
3	A	603	FAD	C1'-C2'	3.39	1.57	1.52
4	A	604	TDK	PC-OM3	-3.34	1.49	1.56
9	A	618	FMT	O2-C	3.27	1.45	1.28
4	B	604	TDK	PC-OM3	-3.11	1.50	1.56
4	B	604	TDK	PC-OM2	3.09	1.62	1.57
4	F	604	TDK	PC-OM2	3.03	1.61	1.57
5	A	605	ALU	O5-C2	3.00	1.25	1.21
9	B	620	FMT	O2-C	2.99	1.43	1.28
4	A	604	TDK	PC-OM2	2.98	1.61	1.57
4	C	603	TDK	PC-OM3	-2.95	1.50	1.56
4	E	603	TDK	PC-OM3	-2.79	1.50	1.56
3	D	602	FAD	O2'-C2'	2.78	1.49	1.43
4	E	603	TDK	PB-O1B	2.67	1.59	1.50
4	E	603	TDK	PC-OM2	2.66	1.61	1.57
4	C	603	TDK	PC-OM2	2.52	1.61	1.57
7	A	608	PEG	O4-C4	2.52	1.55	1.42
3	F	603	FAD	O2'-C2'	2.50	1.48	1.43
4	F	604	TDK	C2-N3	2.50	1.40	1.35
4	D	603	TDK	C2-N3	2.45	1.40	1.35
4	D	603	TDK	PC-OM2	2.41	1.61	1.57
6	B	606	UQ0	O1-C1	2.35	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	TDK	C2-N3	2.34	1.40	1.35
4	D	603	TDK	PC-OM3	-2.32	1.51	1.56
4	E	603	TDK	C2-N3	2.32	1.40	1.35
4	F	604	TDK	PC-OM3	-2.26	1.51	1.56
3	B	603	FAD	O2'-C2'	2.26	1.48	1.43
3	E	602	FAD	O2'-C2'	2.23	1.48	1.43
4	A	604	TDK	C2-N3	2.22	1.40	1.35
6	D	604	UQ0	O1-C1	2.22	1.30	1.24
6	F	605	UQ0	O1-C1	2.15	1.30	1.24
9	A	619	FMT	O2-C	2.13	1.39	1.28
4	F	604	TDK	C4-N3	2.12	1.44	1.39
4	C	603	TDK	C5-S1	-2.10	1.70	1.74
9	E	607	FMT	O2-C	2.09	1.39	1.28
4	B	604	TDK	C2-N3	2.08	1.40	1.35
4	A	604	TDK	PB-O1B	2.03	1.57	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	E	603	TDK	OM2-PC-OM4	-9.73	93.53	114.58
4	F	604	TDK	OM4-PC-CMA	9.52	123.23	113.53
4	F	604	TDK	OM2-PC-OM4	-8.38	96.46	114.58
4	D	603	TDK	OM3-PC-CMA	8.09	120.28	106.27
4	C	603	TDK	OM3-PC-CMA	7.91	119.96	106.27
4	F	604	TDK	C6-C5-C4	-5.92	122.69	127.43
4	E	603	TDK	C6-C5-C4	-5.68	122.88	127.43
6	C	604	UQ0	O1-C1-C2	-4.15	115.48	121.55
4	A	604	TDK	OM3-PC-CMA	-3.99	99.35	106.27
5	C	606	ALU	O3-P1-O2	-3.83	100.00	114.51
4	C	603	TDK	C6-C5-C4	-3.55	124.58	127.43
4	A	604	TDK	C6-C5-C4	-3.55	124.59	127.43
4	D	603	TDK	OM2-PC-OM4	-3.43	107.16	114.58
7	A	621[A]	PEG	O1-C1-C2	-3.38	92.19	111.81
7	A	621[B]	PEG	O1-C1-C2	-3.34	92.45	111.81
5	B	605	ALU	O3-P1-O2	-3.17	102.50	114.51
6	F	605	UQ0	O1-C1-C2	-3.09	117.03	121.55
6	A	606[A]	UQ0	O1-C1-C2	-3.06	117.08	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	FAD	C5A-C6A-N6A	3.05	124.98	120.35
4	E	603	TDK	C5-C4-N3	2.90	113.72	107.66
4	F	604	TDK	C5-C4-N3	2.88	113.68	107.66
3	F	603	FAD	P-O3P-PA	2.83	142.52	132.83
4	D	603	TDK	C5-C4-N3	2.81	113.53	107.66
3	B	603	FAD	O4B-C1B-C2B	-2.81	102.82	106.93
4	A	604	TDK	N4'-C4'-N3'	-2.81	113.07	117.03
4	B	604	TDK	C5-C4-N3	2.78	113.46	107.66
4	C	603	TDK	C5-C4-N3	2.70	113.30	107.66
4	A	604	TDK	C5-C4-N3	2.62	113.13	107.66
6	B	606	UQ0	O1-C1-C2	-2.60	117.75	121.55
6	D	604	UQ0	O1-C1-C2	-2.54	117.83	121.55
3	D	602	FAD	C5A-C6A-N6A	2.54	124.21	120.35
3	C	602	FAD	C1B-N9A-C4A	-2.51	122.23	126.64
4	A	604	TDK	C5'-C4'-N4'	2.46	125.68	122.19
3	E	602	FAD	O2'-C2'-C1'	2.46	115.76	109.80
4	F	604	TDK	O3B-PB-O2B	2.46	117.02	107.64
4	B	604	TDK	OM3-PC-CMA	-2.43	102.05	106.27
3	E	602	FAD	O4B-C1B-C2B	-2.43	103.38	106.93
3	F	603	FAD	O2'-C2'-C1'	2.42	115.64	109.80
4	C	603	TDK	PC-OM2-CMC	2.41	127.97	122.17
3	B	603	FAD	P-O3P-PA	2.37	140.95	132.83
3	D	602	FAD	O2'-C2'-C1'	2.33	115.43	109.80
3	F	603	FAD	O4B-C1B-C2B	-2.28	103.60	106.93
4	B	604	TDK	O2A-PA-O1A	2.24	123.34	112.24
3	C	602	FAD	P-O3P-PA	2.21	140.41	132.83
3	A	603	FAD	O4'-C4'-C3'	2.21	114.46	109.10
4	D	603	TDK	PC-OM2-CMC	2.20	127.47	122.17
3	A	603	FAD	P-O3P-PA	2.18	140.32	132.83
8	A	609	DTT	O2-C2-C3	-2.17	105.27	109.72
4	F	604	TDK	O2A-PA-O1A	2.15	122.89	112.24
4	D	603	TDK	OM4-PC-CMA	-2.14	111.35	113.53
4	E	603	TDK	N4'-C4'-N3'	-2.14	114.01	117.03
8	B	607	DTT	O3-C3-C2	-2.11	105.40	109.72
6	C	604	UQ0	C6-C5-C4	-2.10	117.72	119.53
3	F	603	FAD	C5A-C6A-N6A	2.10	123.54	120.35
4	E	603	TDK	OM3-PC-CMA	-2.09	102.64	106.27
4	C	603	TDK	N4'-C4'-N3'	-2.09	114.08	117.03
3	A	603	FAD	C5A-C6A-N6A	2.08	123.51	120.35
4	A	604	TDK	O2A-PA-O1A	2.08	122.51	112.24
3	D	602	FAD	O4B-C1B-C2B	-2.07	103.89	106.93
3	C	602	FAD	C5A-C6A-N6A	2.05	123.47	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	FAD	C5A-C6A-N6A	2.05	123.47	120.35
4	A	604	TDK	CM2-C2'-N1'	2.04	119.38	117.14
4	C	603	TDK	O3B-PB-O2B	2.04	115.42	107.64
3	C	602	FAD	O4'-C4'-C3'	2.03	114.03	109.10
4	B	604	TDK	CM4-C4-N3	-2.02	120.14	122.69
3	B	603	FAD	C4X-C4-N3	2.02	118.33	113.19
3	A	603	FAD	C1B-N9A-C4A	-2.00	123.12	126.64

There are no chirality outliers.

All (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
3	C	602	FAD	C5B-O5B-PA-O3P
3	D	602	FAD	C5B-O5B-PA-O1A
3	D	602	FAD	C5B-O5B-PA-O3P
3	E	602	FAD	C5B-O5B-PA-O1A
3	F	603	FAD	C5B-O5B-PA-O1A
3	F	603	FAD	C5B-O5B-PA-O3P
4	A	604	TDK	C4-C5-C6-C7
4	A	604	TDK	C2-CMA-PC-OM2
4	A	604	TDK	C4'-C5'-C7'-N3
4	B	604	TDK	PA-O3A-PB-O2B
4	B	604	TDK	C4-C5-C6-C7
4	B	604	TDK	C2-CMA-PC-OM2
4	B	604	TDK	C2-CMA-PC-OM4
4	B	604	TDK	OM1-CMA-PC-OM2
4	B	604	TDK	OM1-CMA-PC-OM4
4	B	604	TDK	CMB-CMA-PC-OM4
4	B	604	TDK	C4'-C5'-C7'-N3
4	C	603	TDK	PA-O3A-PB-O2B
4	C	603	TDK	C4-C5-C6-C7
4	C	603	TDK	C2-CMA-PC-OM2
4	C	603	TDK	C2-CMA-PC-OM4
4	C	603	TDK	OM1-CMA-PC-OM3
4	C	603	TDK	OM1-CMA-PC-OM2
4	C	603	TDK	OM1-CMA-PC-OM4
4	C	603	TDK	CMB-CMA-PC-OM3

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Mol	Chain	Res	Type	Atoms
4	C	603	TDK	CMB-CMA-PC-OM2
4	C	603	TDK	CMB-CMA-PC-OM4
4	C	603	TDK	CMC-OM2-PC-CMA
4	C	603	TDK	C4'-C5'-C7'-N3
4	D	603	TDK	C2-CMA-PC-OM2
4	D	603	TDK	C2-CMA-PC-OM4
4	D	603	TDK	OM1-CMA-PC-OM2
4	D	603	TDK	CMB-CMA-PC-OM3
4	D	603	TDK	CMB-CMA-PC-OM2
4	D	603	TDK	CMB-CMA-PC-OM4
4	D	603	TDK	C4'-C5'-C7'-N3
4	E	603	TDK	PA-O3A-PB-O2B
4	E	603	TDK	C4-C5-C6-C7
4	E	603	TDK	C2-CMA-PC-OM2
4	E	603	TDK	C4'-C5'-C7'-N3
4	F	604	TDK	C4-C5-C6-C7
4	F	604	TDK	C2-CMA-PC-OM2
4	F	604	TDK	C2-CMA-PC-OM4
4	F	604	TDK	OM1-CMA-PC-OM3
4	F	604	TDK	OM1-CMA-PC-OM2
4	F	604	TDK	OM1-CMA-PC-OM4
4	F	604	TDK	CMB-CMA-PC-OM3
4	F	604	TDK	CMB-CMA-PC-OM2
4	F	604	TDK	CMB-CMA-PC-OM4
4	F	604	TDK	C4'-C5'-C7'-N3
5	B	605	ALU	C5-O3-P1-C2
8	A	609	DTT	O2-C2-C3-C4
8	A	609	DTT	C2-C3-C4-S4
8	A	610	DTT	S1-C1-C2-O2
8	A	610	DTT	S1-C1-C2-C3
8	A	610	DTT	C1-C2-C3-O3
8	A	610	DTT	O2-C2-C3-O3
8	A	610	DTT	O2-C2-C3-C4
8	B	607	DTT	S1-C1-C2-O2
8	B	607	DTT	S1-C1-C2-C3
8	B	607	DTT	C2-C3-C4-S4
8	B	607	DTT	O3-C3-C4-S4
7	A	607	PEG	C4-C3-O2-C2
7	A	621[A]	PEG	O1-C1-C2-O2
7	F	606	PEG	O2-C3-C4-O4
4	E	603	TDK	CMC-OM2-PC-OM4
5	B	605	ALU	C5-O3-P1-O2

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Mol	Chain	Res	Type	Atoms
7	C	607	PEG	O1-C1-C2-O2
10	A	613	PGE	O1-C1-C2-O2
4	B	604	TDK	CMC-OM2-PC-OM4
7	A	614	PEG	O1-C1-C2-O2
10	A	613	PGE	O3-C5-C6-O4
4	D	603	TDK	OM1-CMA-PC-OM3
4	A	604	TDK	CMC-OM2-PC-OM4
4	C	603	TDK	CMC-OM2-PC-OM4
7	A	621[A]	PEG	C1-C2-O2-C3
7	A	621[B]	PEG	C1-C2-O2-C3
4	A	604	TDK	PA-O3A-PB-O2B
4	D	603	TDK	PA-O3A-PB-O2B
10	A	613	PGE	C4-C3-O2-C2
3	E	602	FAD	C5B-O5B-PA-O3P
3	F	603	FAD	C5'-O5'-P-O3P
4	A	604	TDK	OM1-CMA-PC-OM2
4	E	603	TDK	OM1-CMA-PC-OM2
7	F	606	PEG	C4-C3-O2-C2
3	B	603	FAD	P-O3P-PA-O1A
3	D	602	FAD	P-O3P-PA-O1A
3	F	603	FAD	P-O3P-PA-O1A
10	A	613	PGE	C6-C5-O3-C4
3	A	603	FAD	C5B-O5B-PA-O2A
3	B	603	FAD	C5B-O5B-PA-O2A
3	D	602	FAD	C5B-O5B-PA-O2A
3	F	603	FAD	C5B-O5B-PA-O2A
8	A	610	DTT	C1-C2-C3-C4
6	B	606	UQ0	C4-C3-O3-CM3
8	A	609	DTT	O3-C3-C4-S4
8	A	610	DTT	O3-C3-C4-S4
4	B	604	TDK	CMB-CMA-PC-OM2
6	A	606[A]	UQ0	C1-C2-O2-CM2
12	E	605	DTU	O2-C2-C3-O3
5	A	605	ALU	C5-O3-P1-O2
7	F	606	PEG	O1-C1-C2-O2
3	A	603	FAD	P-O3P-PA-O1A
3	C	602	FAD	P-O3P-PA-O1A
7	A	621[A]	PEG	C4-C3-O2-C2
7	A	621[B]	PEG	C4-C3-O2-C2
7	B	610	PEG	C1-C2-O2-C3
10	A	613	PGE	O2-C3-C4-O3
8	A	609	DTT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
12	E	605	DTU	C1-C2-C3-O3
4	A	604	TDK	OM1-CMA-PC-OM4
4	D	603	TDK	OM1-CMA-PC-OM4
4	E	603	TDK	OM1-CMA-PC-OM4
6	A	606[A]	UQ0	C3-C2-O2-CM2
8	A	610	DTT	C2-C3-C4-S4
6	C	604	UQ0	C1-C2-O2-CM2
10	A	613	PGE	C3-C4-O3-C5
4	A	604	TDK	C2-CMA-PC-OM4
4	E	603	TDK	C2-CMA-PC-OM4
8	A	609	DTT	O2-C2-C3-O3
8	B	607	DTT	O2-C2-C3-O3
4	F	604	TDK	PA-O3A-PB-O2B
4	B	604	TDK	OM1-CMA-PC-OM3
3	E	602	FAD	P-O3P-PA-O1A
3	F	603	FAD	P-O3P-PA-O2A
3	A	603	FAD	C3'-C4'-C5'-O5'
3	C	602	FAD	C5B-O5B-PA-O2A
3	C	602	FAD	C5'-O5'-P-O1P
3	F	603	FAD	C5'-O5'-P-O1P
4	A	604	TDK	C6'-C5'-C7'-N3
4	B	604	TDK	C6'-C5'-C7'-N3
4	C	603	TDK	C6'-C5'-C7'-N3
4	D	603	TDK	C6'-C5'-C7'-N3
4	E	603	TDK	C6'-C5'-C7'-N3
7	A	608	PEG	O2-C3-C4-O4
5	D	605	ALU	C5-O3-P1-O2

There are no ring outliers.

30 monomers are involved in 99 short contacts:

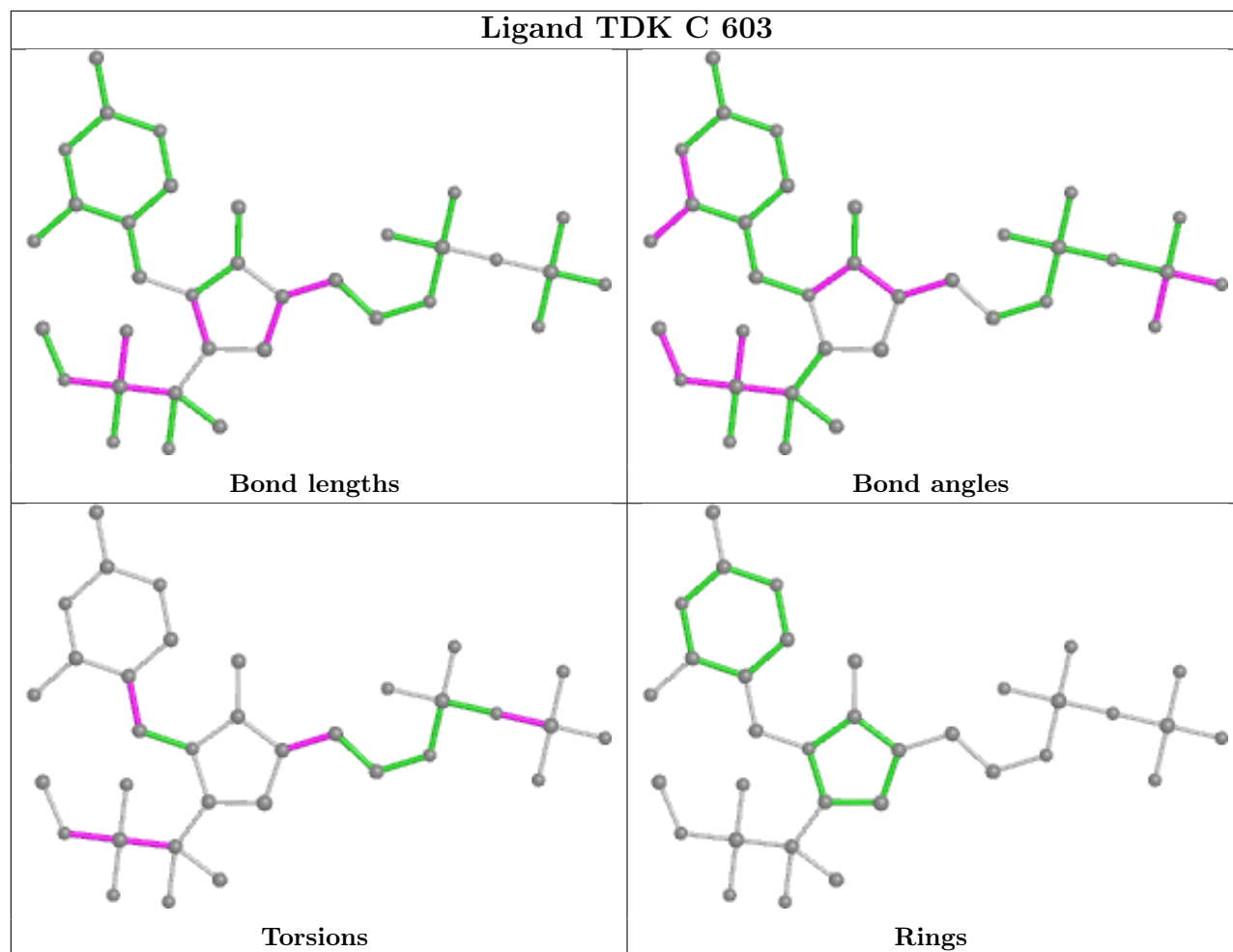
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	TDK	4	0
5	C	606	ALU	1	0
9	B	612	FMT	1	0
3	D	602	FAD	3	0
4	F	604	TDK	7	0
3	F	603	FAD	3	0
5	D	605	ALU	6	0
9	A	623	FMT	1	0
9	D	607	FMT	1	0
7	B	610	PEG	1	0

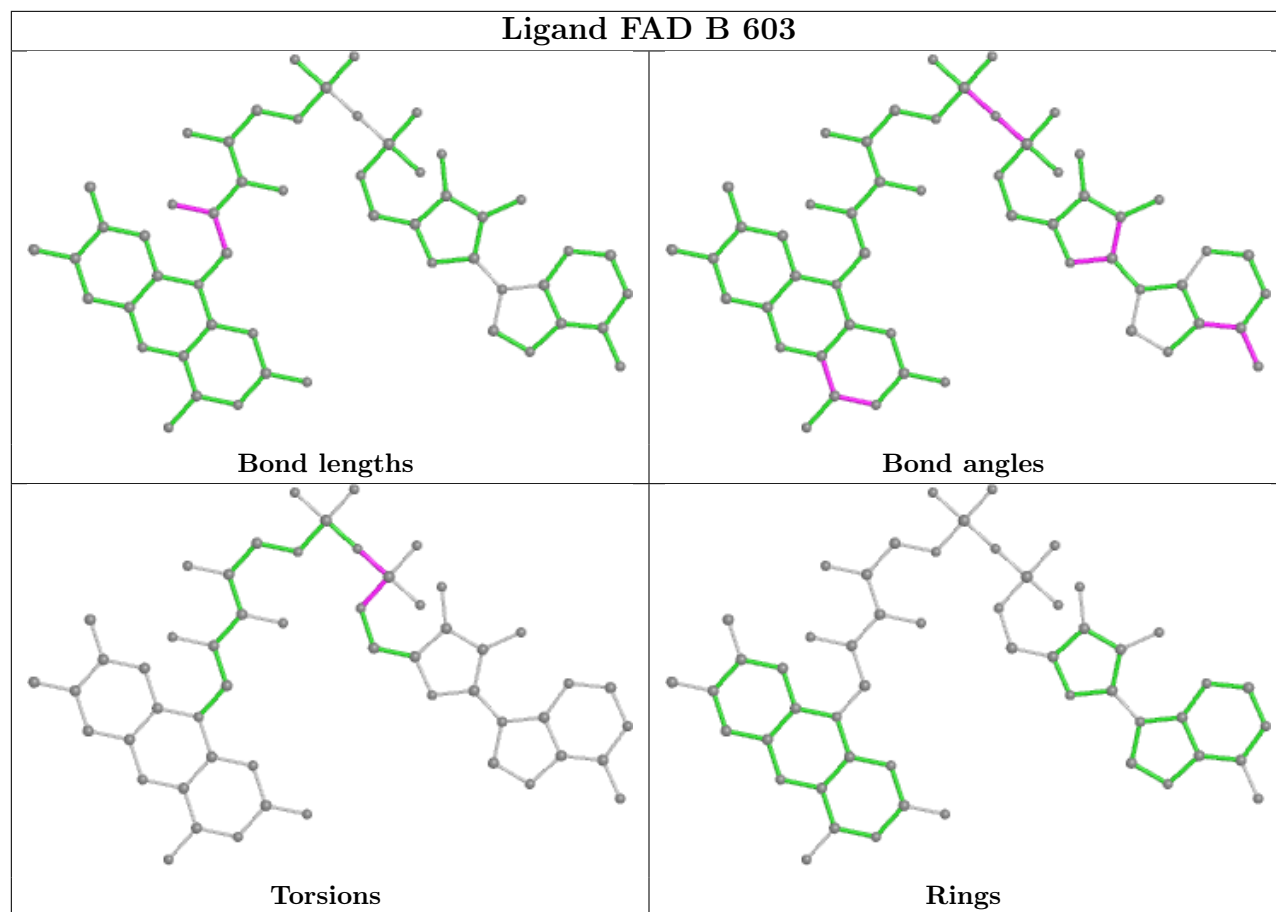
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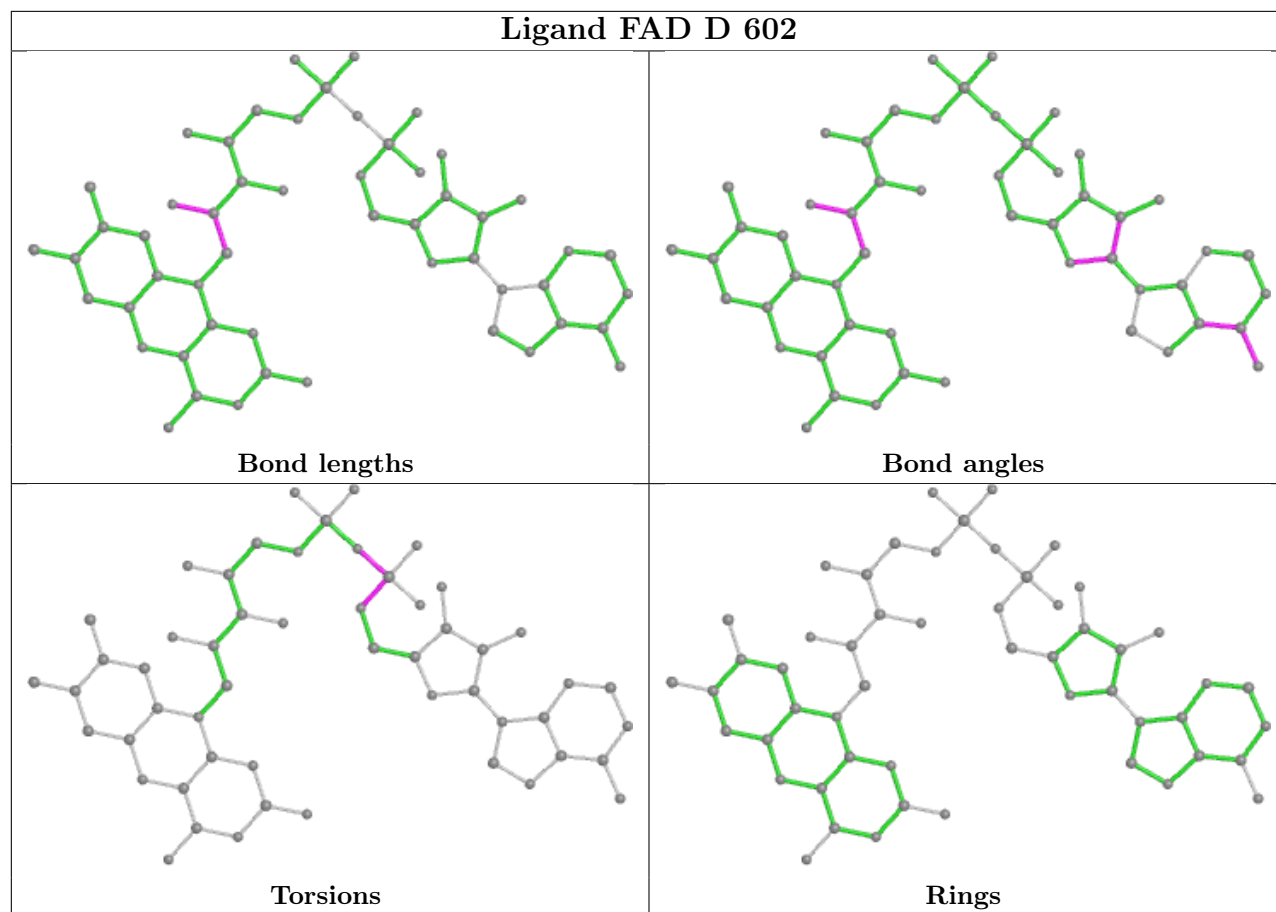
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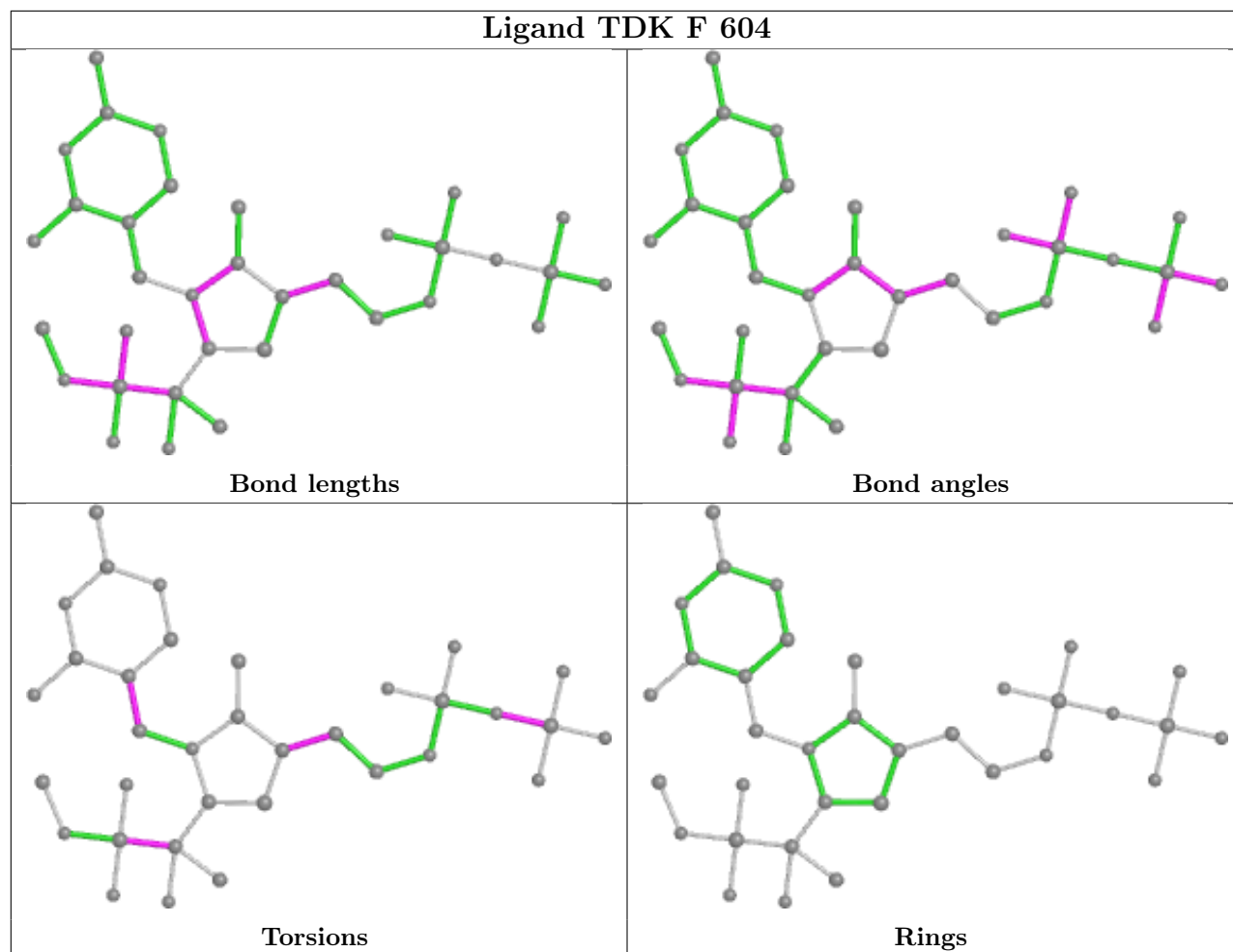
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	608	PEG	7	0
3	C	602	FAD	3	0
4	B	604	TDK	8	0
7	A	607	PEG	3	0
4	D	603	TDK	4	0
4	E	603	TDK	8	0
7	C	607	PEG	2	0
8	B	607	DTT	4	0
4	A	604	TDK	6	0
6	E	604	UQ0	1	0
12	E	605	DTU	9	0
5	A	605	ALU	1	0
8	A	609	DTT	7	0
7	A	621[A]	PEG	3	0
6	A	606[A]	UQ0	2	0
10	A	613	PGE	1	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

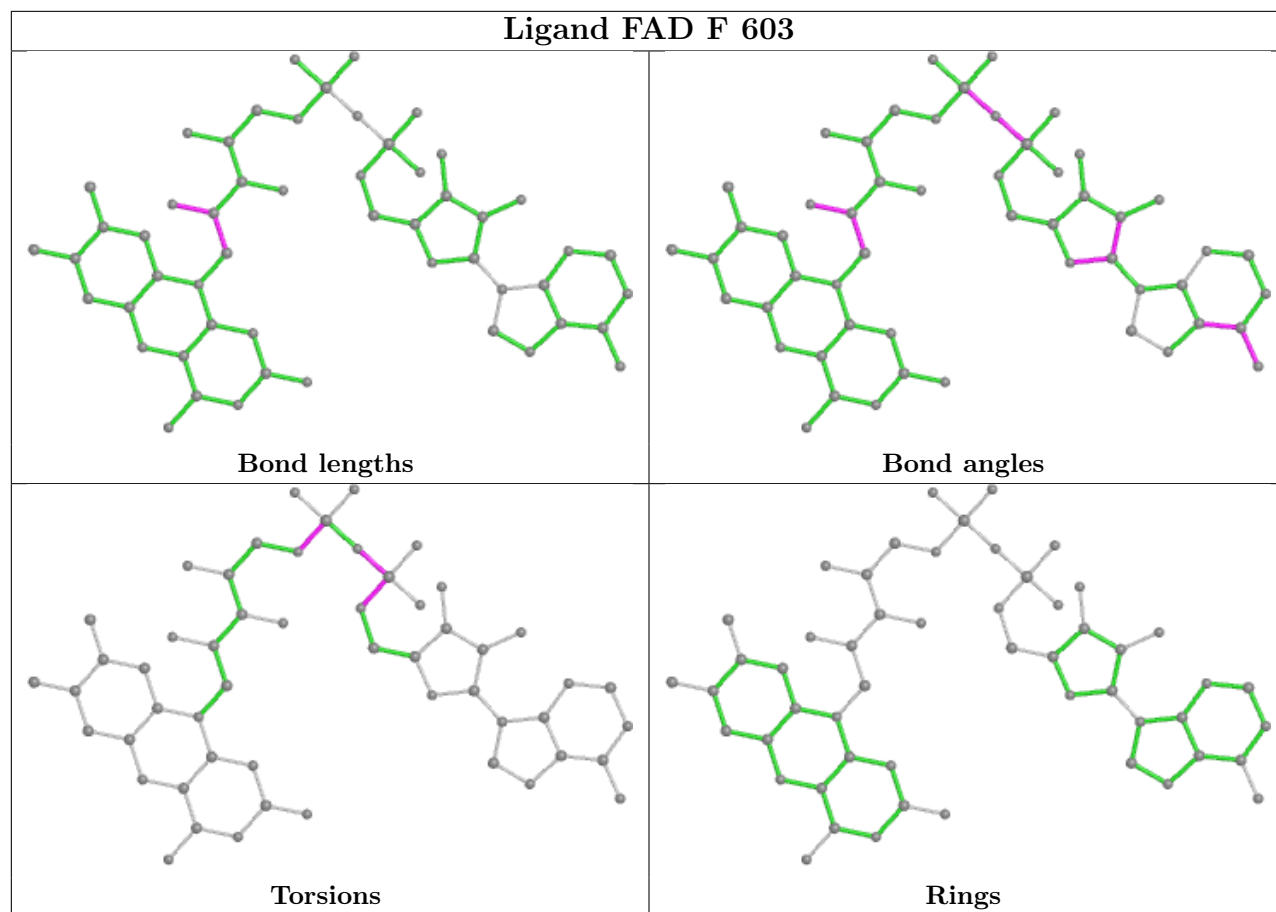
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

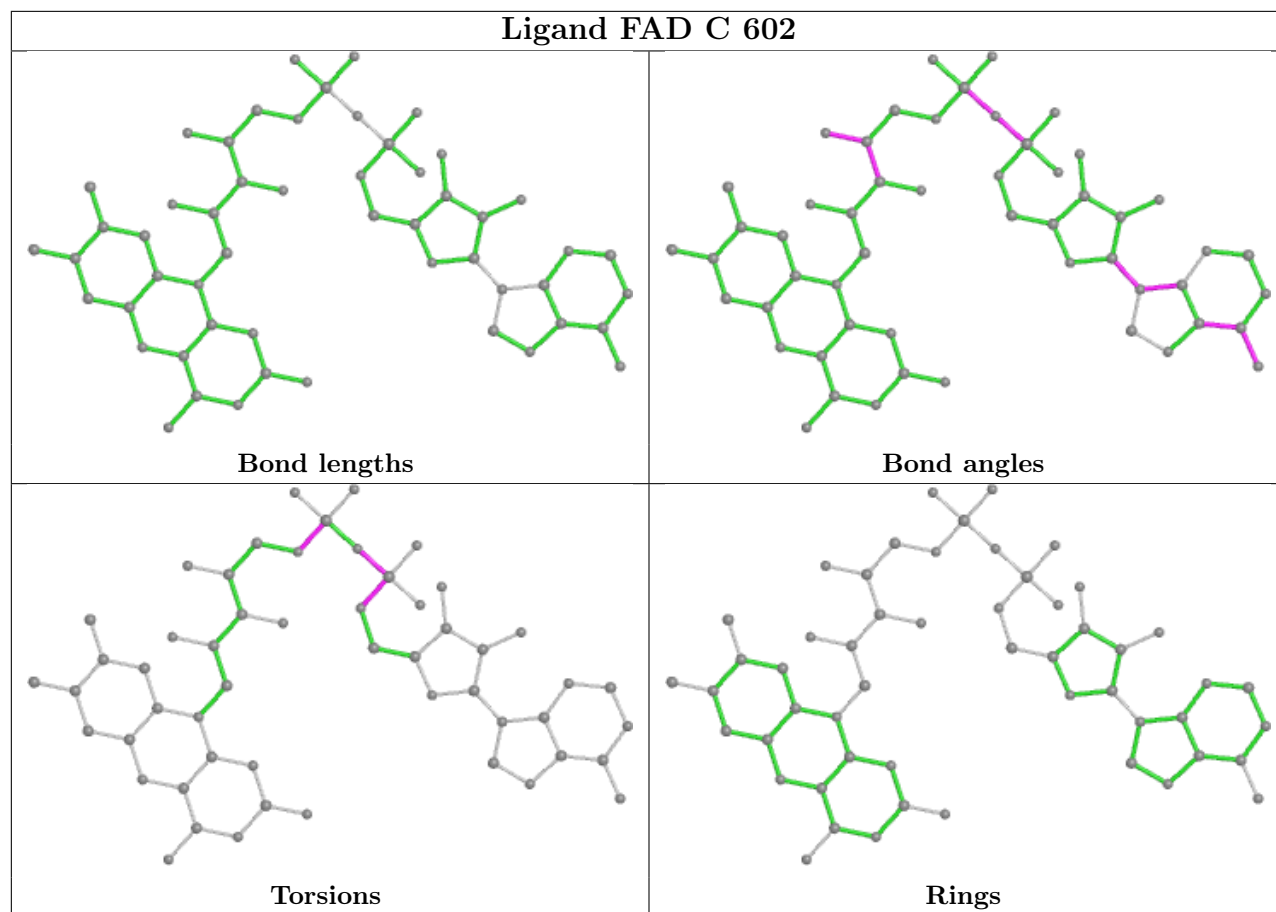


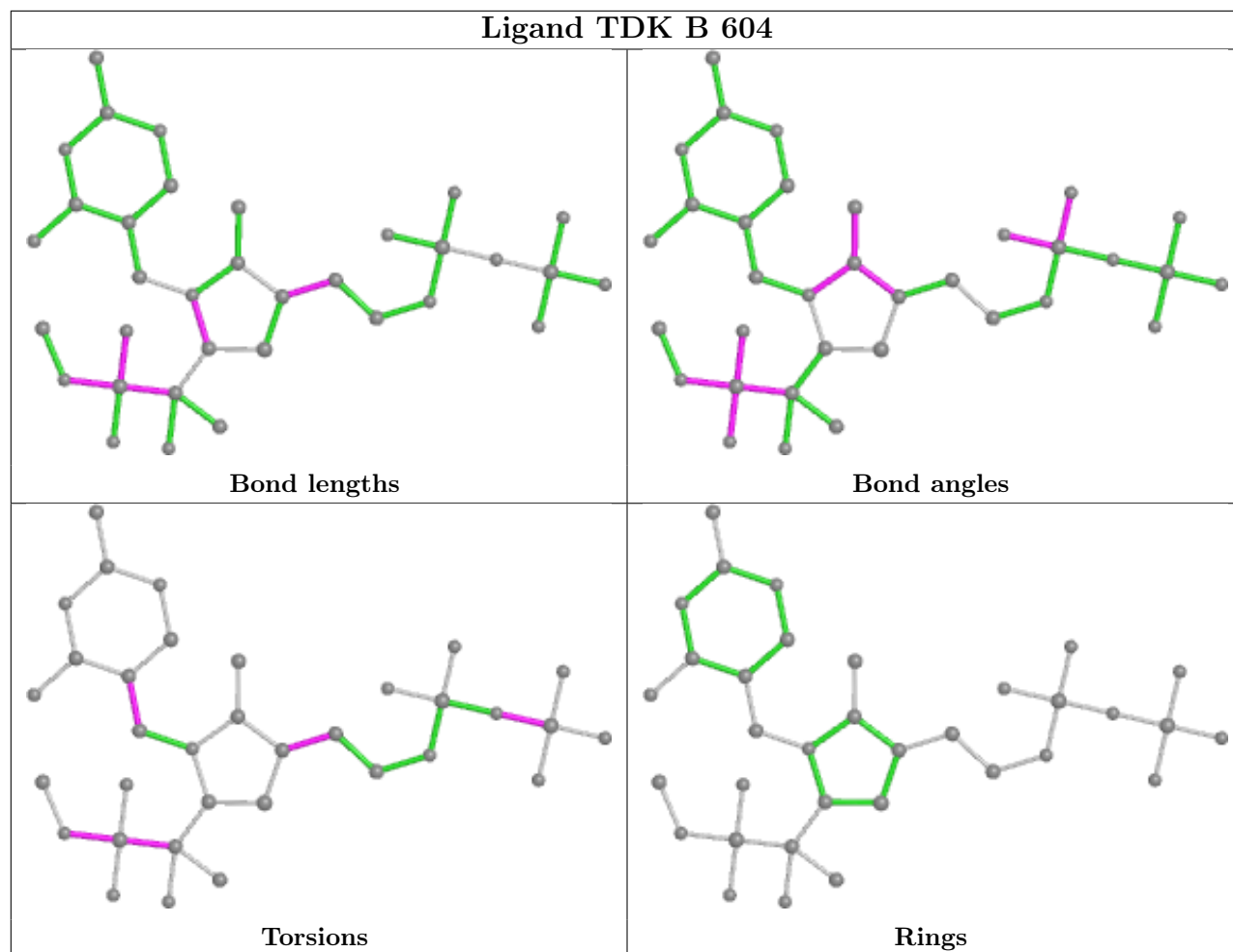


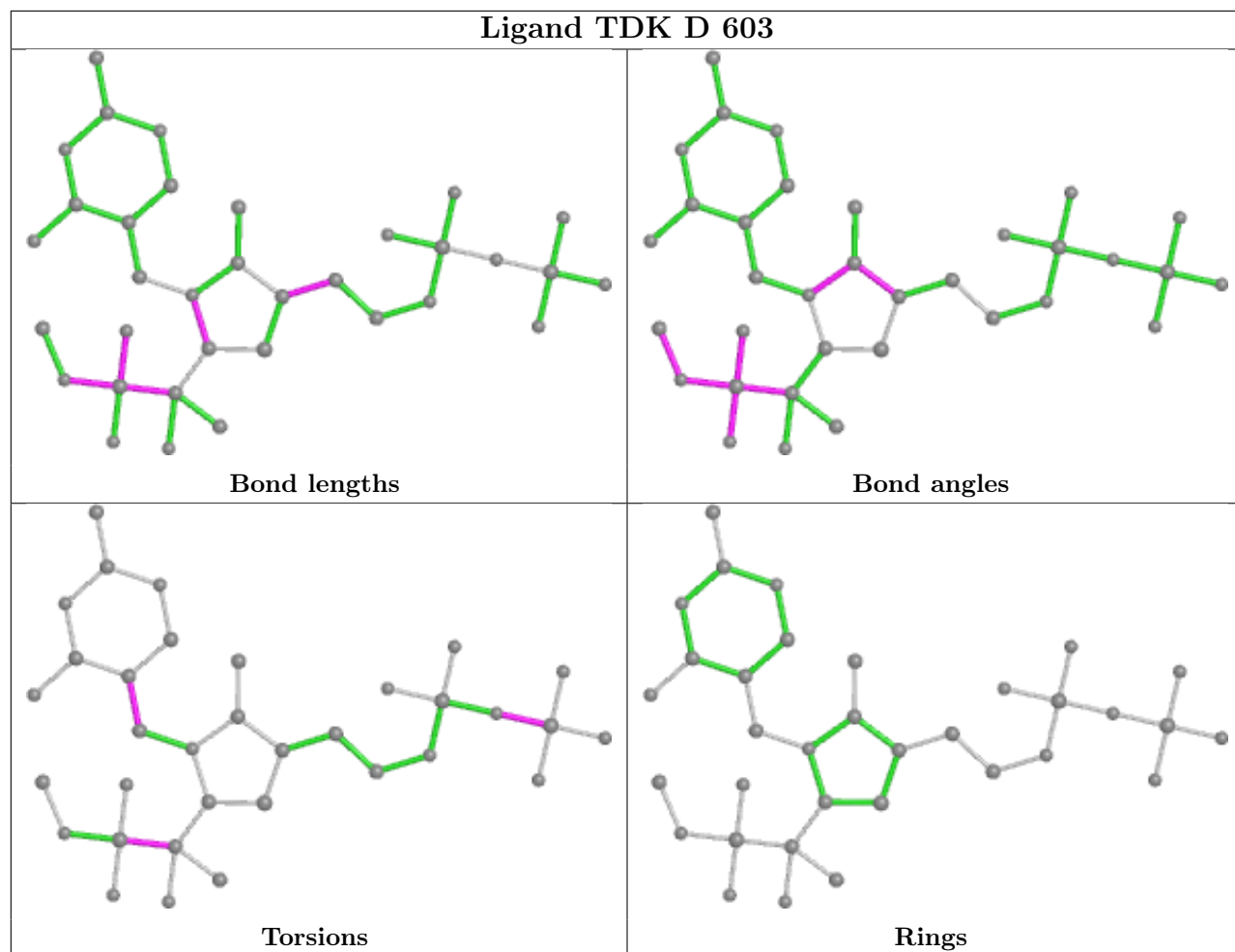


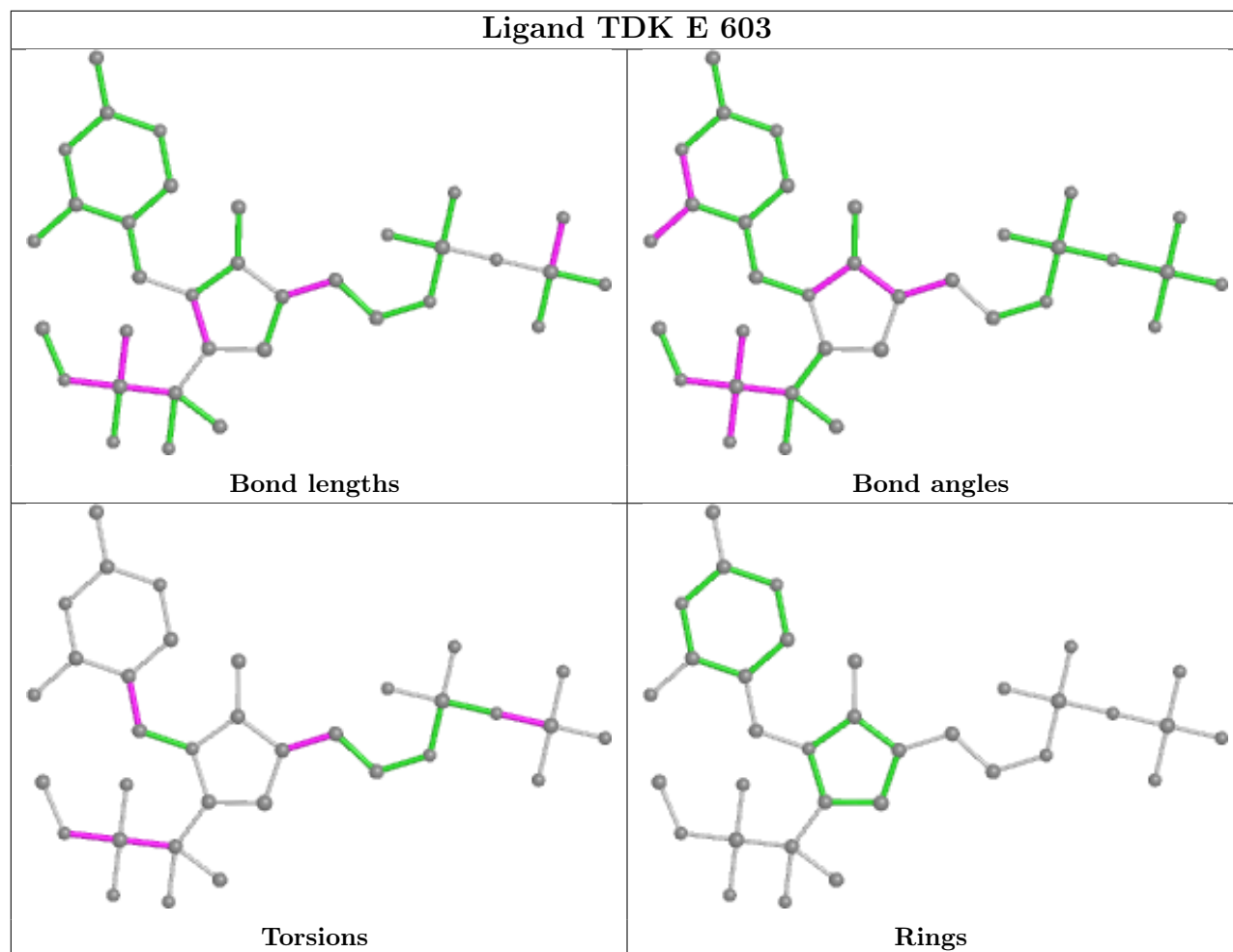


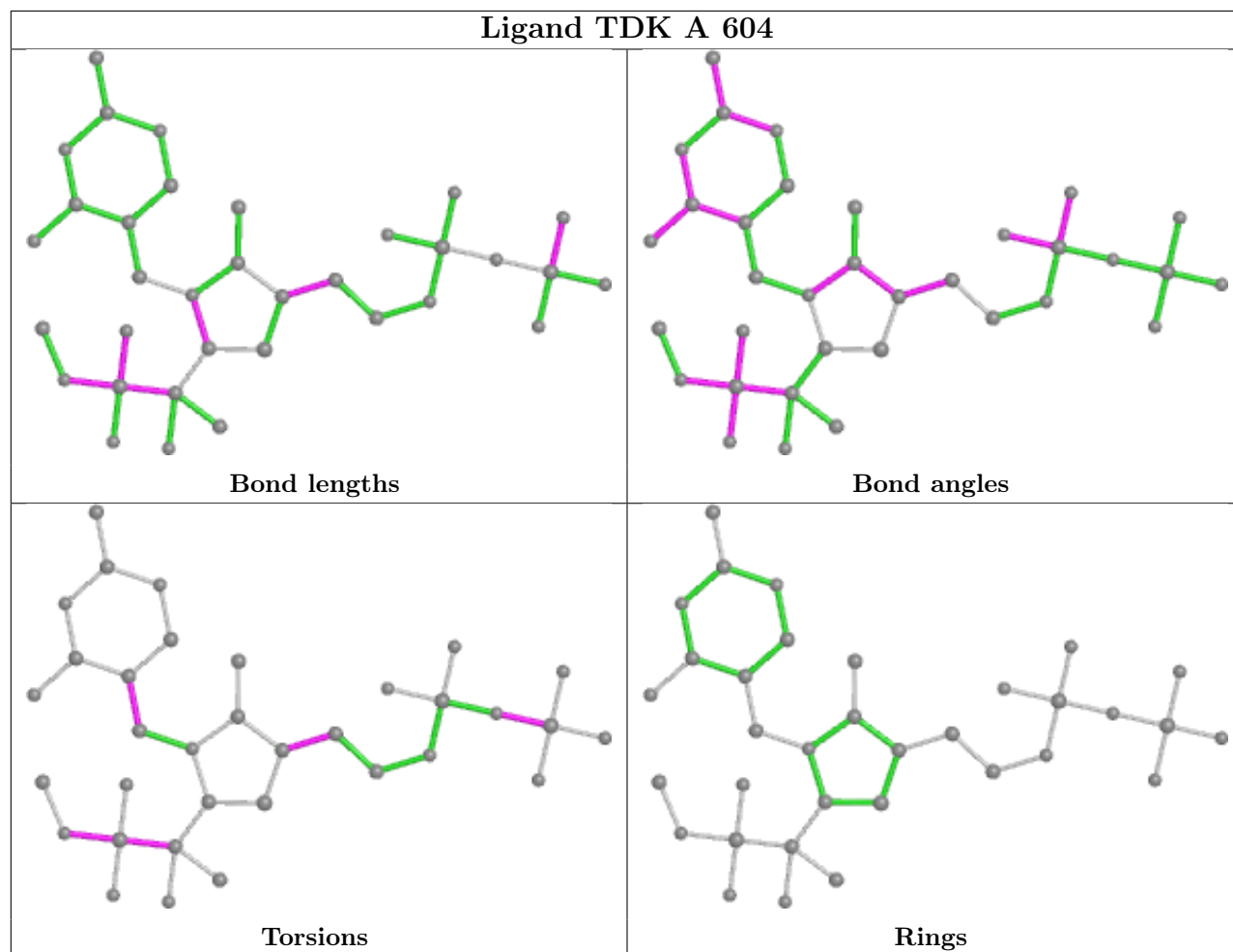


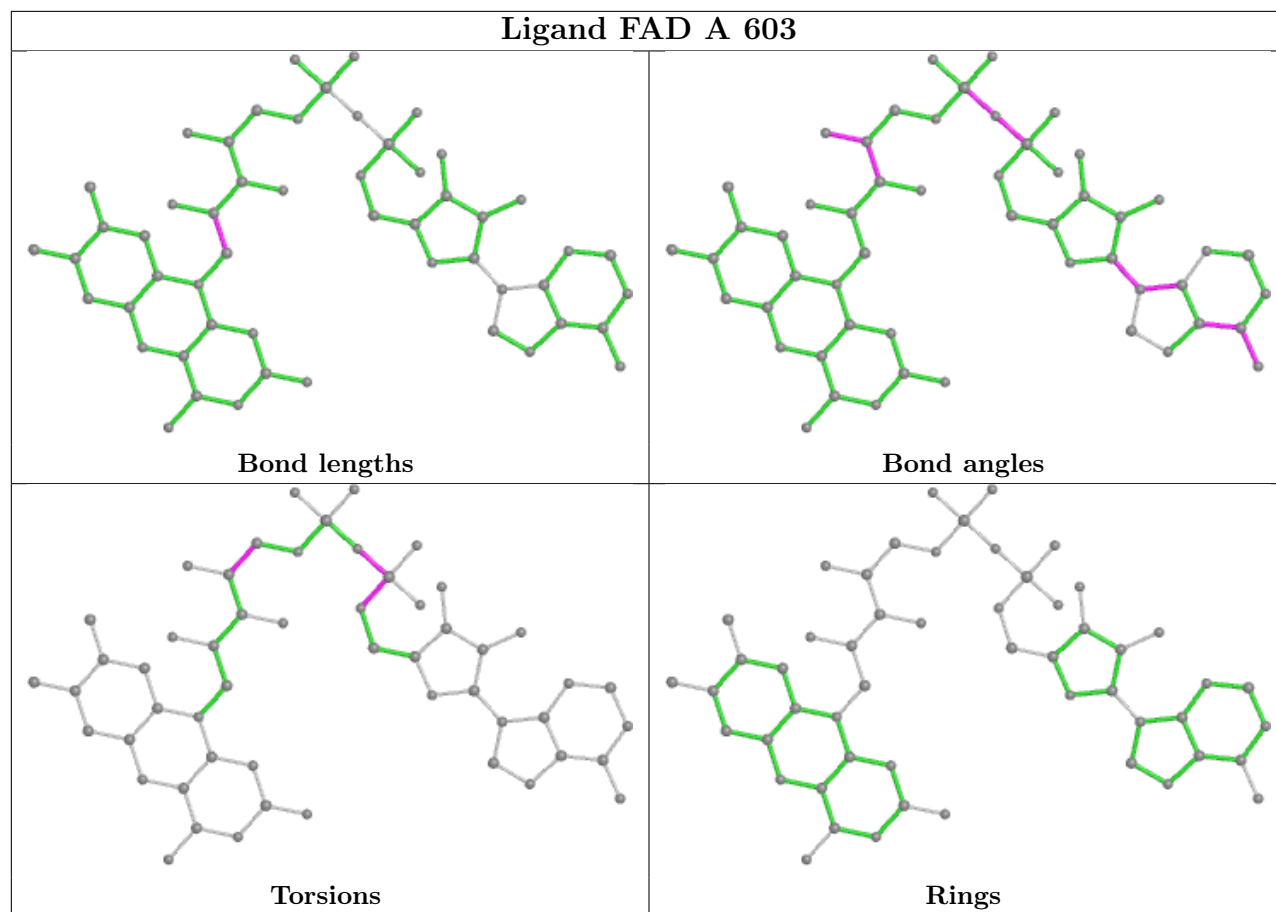


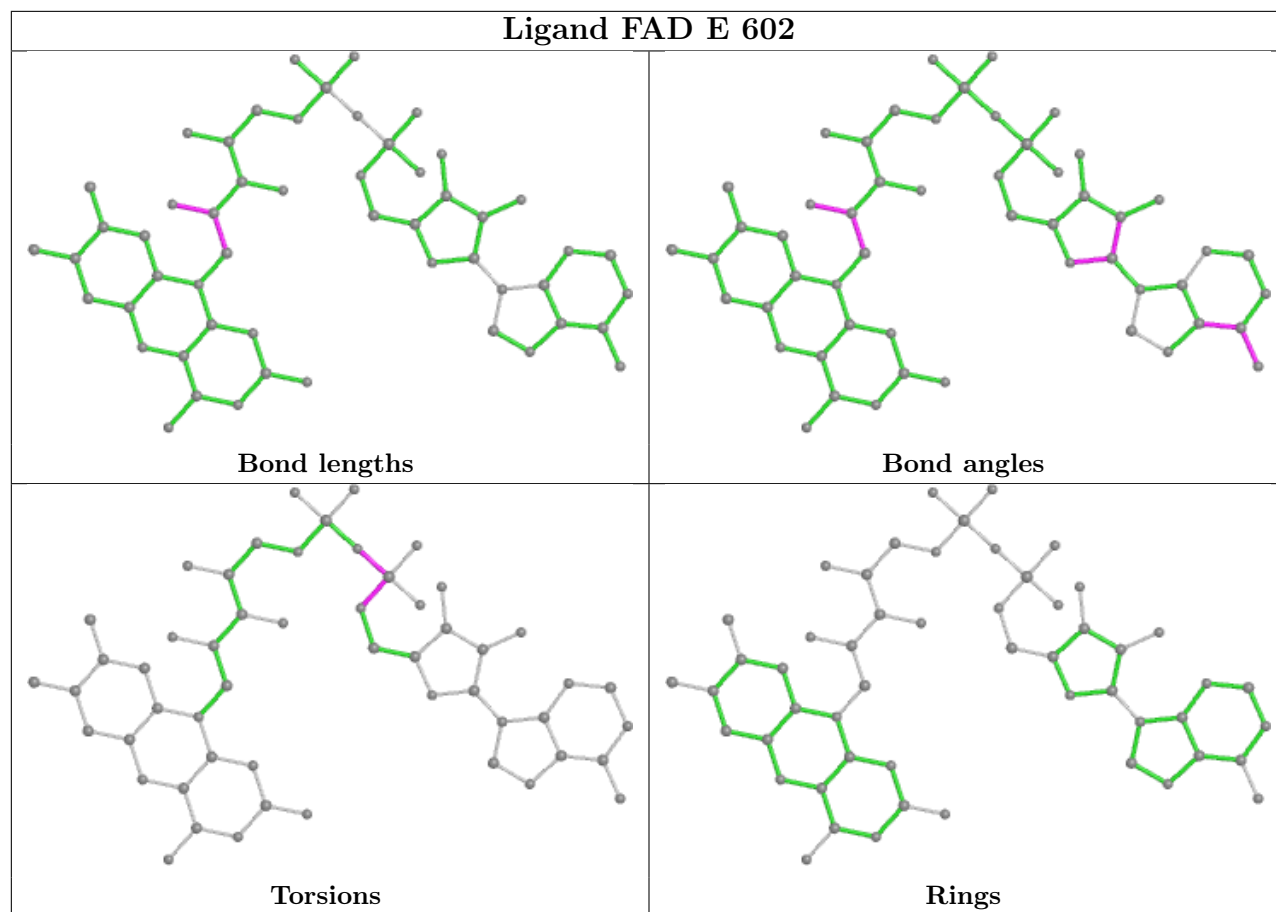












5.7 Other polymers [i](#)

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	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

All (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
1	D	338	LYS	3.8
1	D	2	ALA	3.6
1	E	338	LYS	3.6
1	B	338	LYS	3.5
1	D	339	ALA	3.5
1	F	172	GLU	3.5
1	B	2	ALA	3.5
1	F	81	THR	3.5
1	F	117	VAL	3.4
1	E	202	GLN	3.3
1	E	339	ALA	3.3
1	F	122	ILE	3.3
1	F	338	LYS	3.3
1	C	172	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	191	MET	3.3
1	F	119	ILE	3.3
1	E	197	VAL	3.2
1	C	336	MET	3.2
1	E	201	ILE	3.2
1	F	84	ILE	3.2
1	F	109	LEU	3.1
1	D	173	PHE	3.1
1	E	487	ASP	3.1
1	E	270	ALA	3.0
1	F	173	PHE	3.0
1	F	86	ALA	3.0
1	D	12	TYR	2.9
1	F	177	MET	2.9
1	C	593	GLU	2.9
1	D	172	GLU	2.9
1	F	339	ALA	2.9
1	A	338	LYS	2.9
1	D	487	ASP	2.9
1	E	340	GLY	2.9
1	C	333	ALA	2.9
1	F	51	VAL	2.8
1	F	78	PRO	2.8
1	F	175	PRO	2.8
1	D	341	ARG	2.8
1	C	175	PRO	2.8
1	D	3	LYS	2.8
1	C	332	VAL	2.8
1	C	176	ASP	2.8
1	F	452	LEU	2.8
1	E	2	ALA	2.8
1	F	41	GLY	2.7
1	D	340	GLY	2.7
1	F	121	ALA	2.7
1	F	176	ASP	2.7
1	E	198	GLU	2.7
1	B	81	THR	2.7
1	F	85	THR	2.7
1	D	85	THR	2.7
1	F	341	ARG	2.6
1	E	199	MET	2.6
1	D	176	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	593	GLU	2.6
1	E	341	ARG	2.6
1	E	176	ASP	2.6
1	F	202	GLN	2.6
1	F	123	ALA	2.6
1	D	81	THR	2.6
1	D	88	TYR	2.5
1	D	421	LEU	2.5
1	C	339	ALA	2.5
1	E	333	ALA	2.5
1	F	12	TYR	2.5
1	D	125	PRO	2.4
1	F	333	ALA	2.4
1	A	593	GLU	2.4
1	D	593	GLU	2.4
1	B	85	THR	2.4
1	E	175	PRO	2.4
1	F	336	MET	2.4
1	D	451	PHE	2.4
1	D	485	ALA	2.4
1	F	79	ALA	2.4
1	C	341	ARG	2.4
1	F	82	ASP	2.4
1	C	340	GLY	2.4
1	D	419	GLY	2.4
1	F	368	VAL	2.4
1	E	297	LYS	2.4
1	E	593	GLU	2.4
1	F	4	MET	2.4
1	C	202	GLN	2.3
1	C	342	LEU	2.3
1	F	130	ALA	2.3
1	B	593	GLU	2.3
1	D	415	CYS	2.3
1	C	191	MET	2.3
1	F	191	MET	2.3
1	D	418	ALA	2.3
1	F	540	ALA	2.3
1	C	328	LEU	2.3
1	F	110	HIS	2.3
1	C	337	GLN	2.2
1	E	332	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	332	VAL	2.2
1	E	336	MET	2.2
1	E	343	PRO	2.2
1	B	339	ALA	2.2
1	F	83	MET	2.2
1	B	3	LYS	2.2
1	D	202	GLN	2.2
1	F	88	TYR	2.2
1	A	339	ALA	2.2
1	C	313	CYS	2.2
1	C	335	GLU	2.2
1	D	452	LEU	2.2
1	E	328	LEU	2.2
1	D	336	MET	2.2
1	B	88	TYR	2.2
1	D	422	GLY	2.2
1	B	84	ILE	2.1
1	F	487	ASP	2.1
1	F	125	PRO	2.1
1	D	177	MET	2.1
1	D	337	GLN	2.1
1	D	368	VAL	2.1
1	F	77	GLY	2.1
1	D	201	ILE	2.1
1	E	204	GLU	2.1
1	C	198	GLU	2.1
1	C	36	ALA	2.1
1	D	198	GLU	2.1
1	E	337	GLN	2.0
1	F	76	SER	2.0
1	B	125	PRO	2.0
1	F	558	VAL	2.0
1	B	122	ILE	2.0
1	E	195	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(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
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 [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(Å ²)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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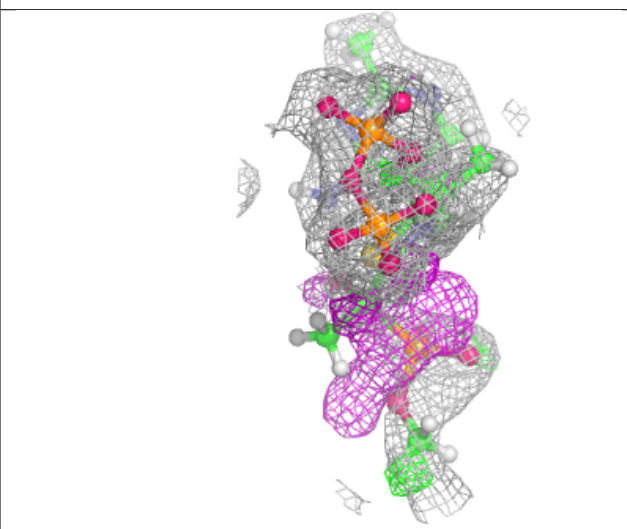
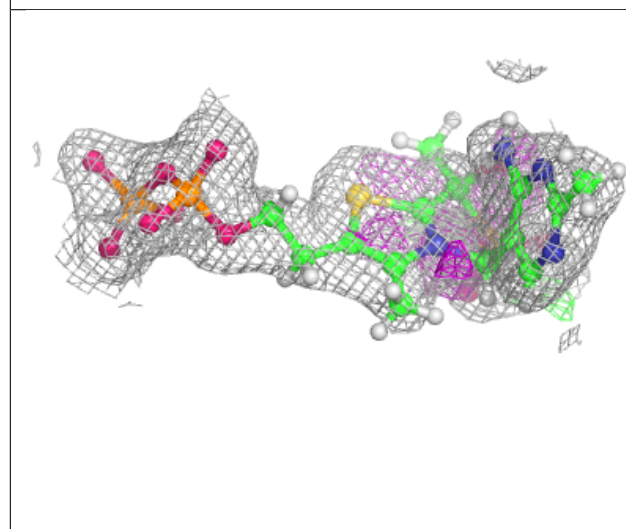
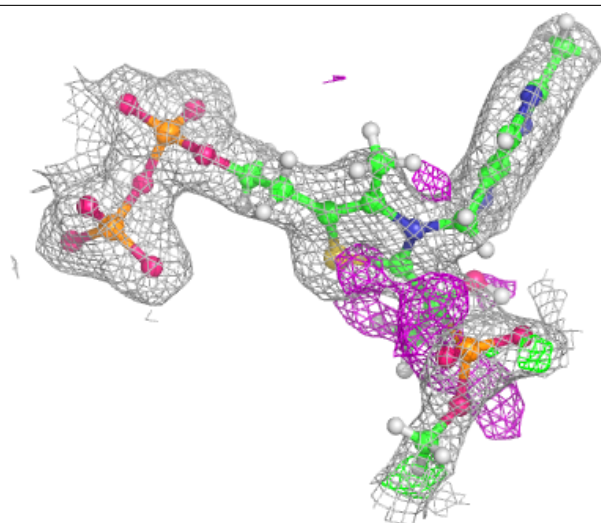
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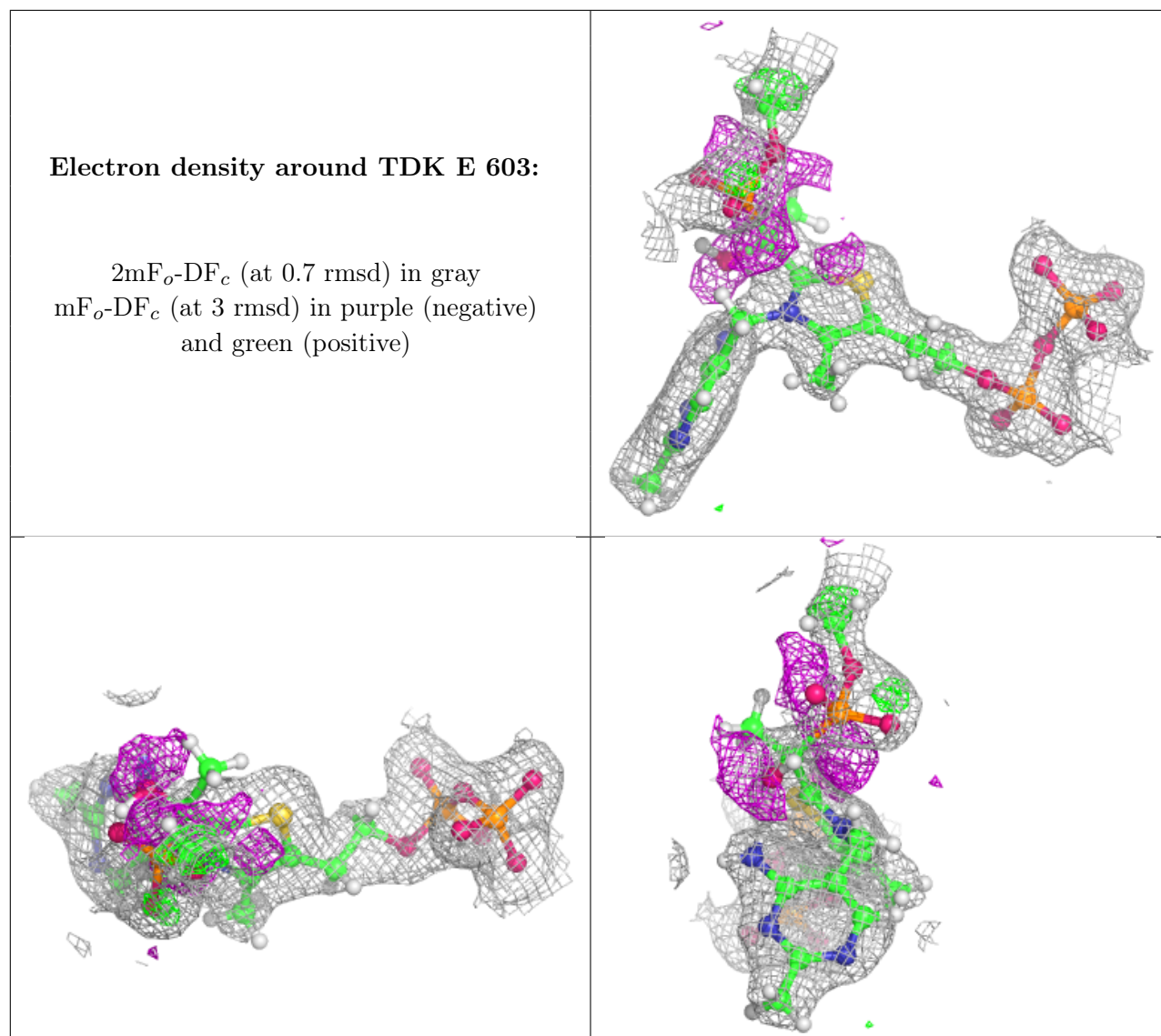
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CL	E	610	1/1	0.94	0.35	73,73,73,73	0
9	FMT	B	613	3/3	0.95	0.09	50,52,55,56	1
4	TDK	F	604	34/34	0.95	0.14	26,39,81,93	3
6	UQ0	D	604	13/13	0.95	0.12	48,57,62,63	0
11	NA	E	615	1/1	0.96	0.12	50,50,50,50	0
4	TDK	E	603	34/34	0.96	0.13	30,41,91,93	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:

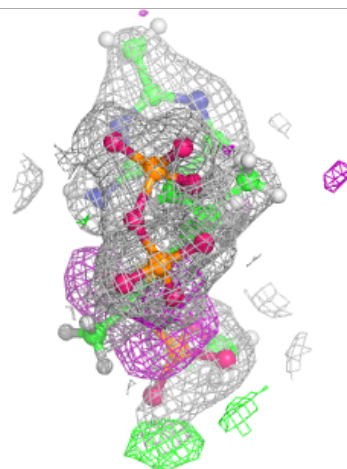
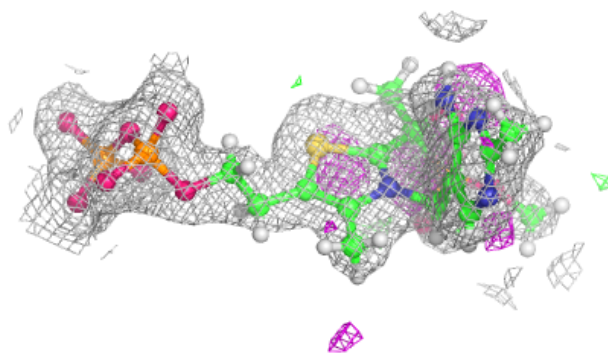
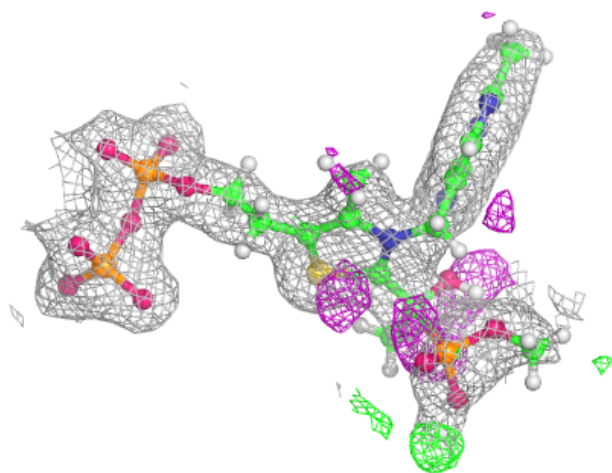
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





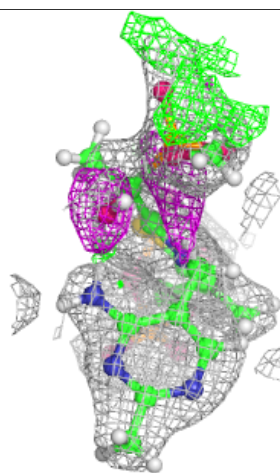
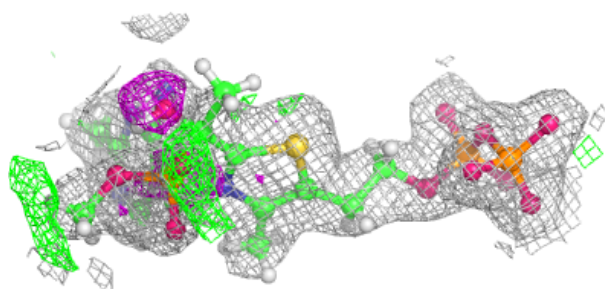
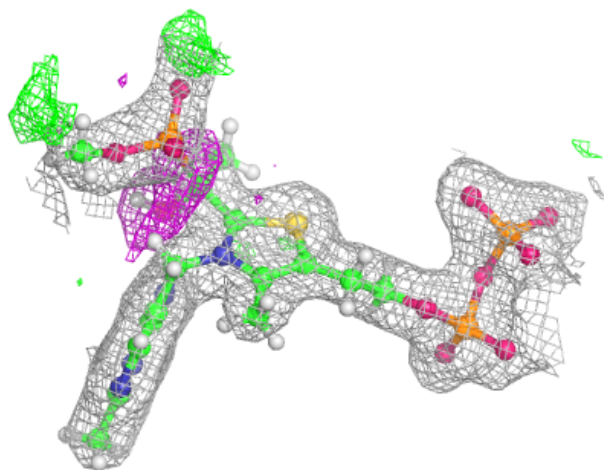
Electron density around TDK D 603:

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



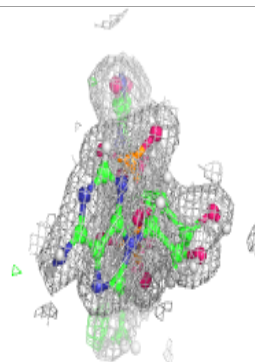
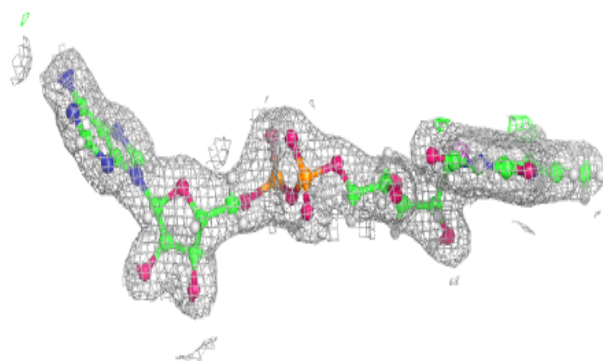
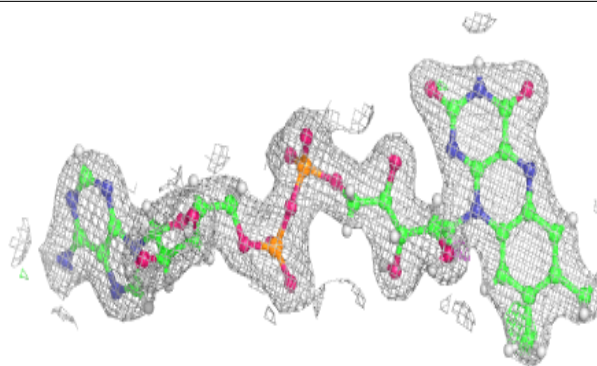
Electron density around TDK C 603:

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



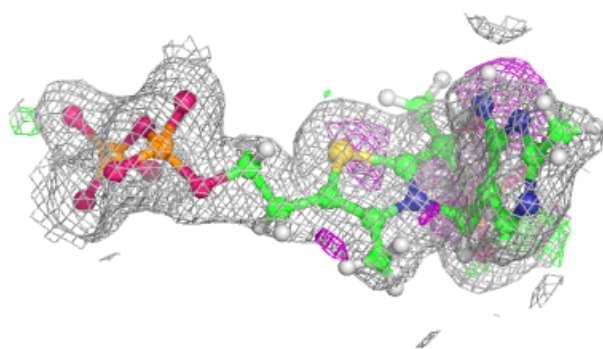
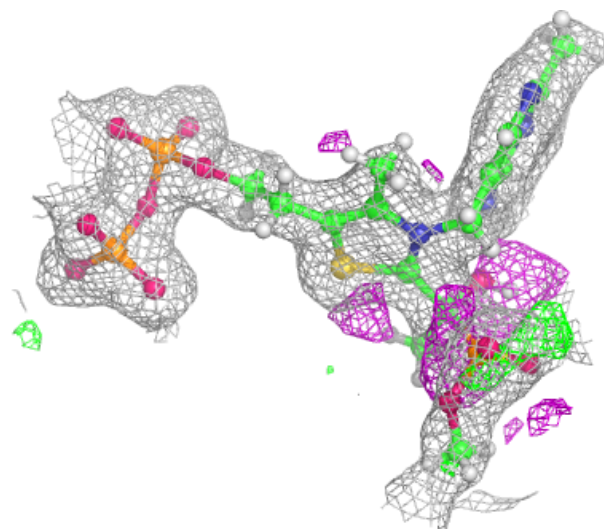
Electron density around FAD E 602:

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



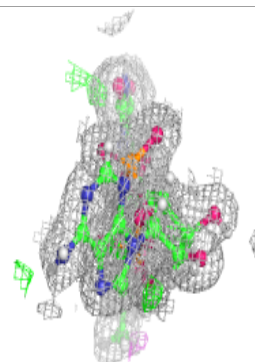
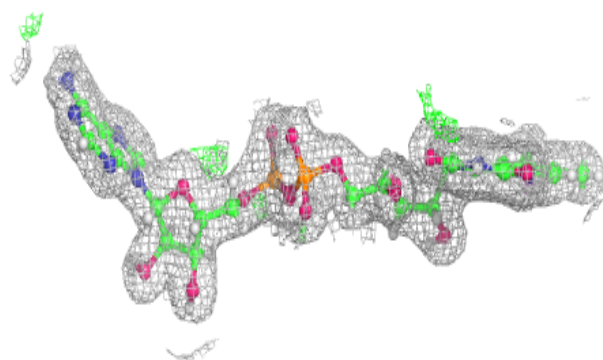
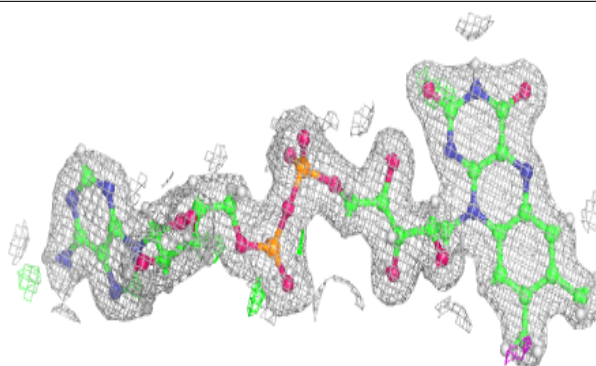
Electron density around TDK B 604:

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

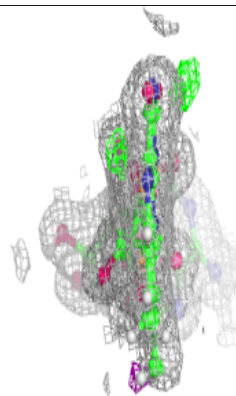
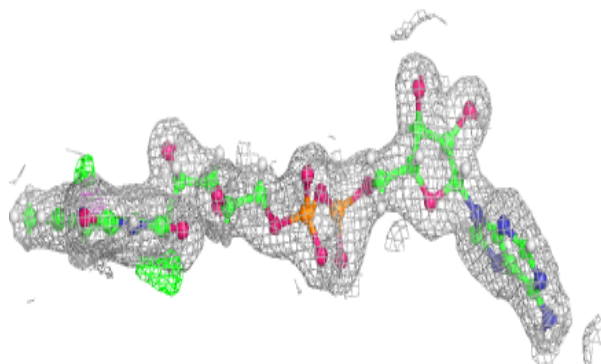
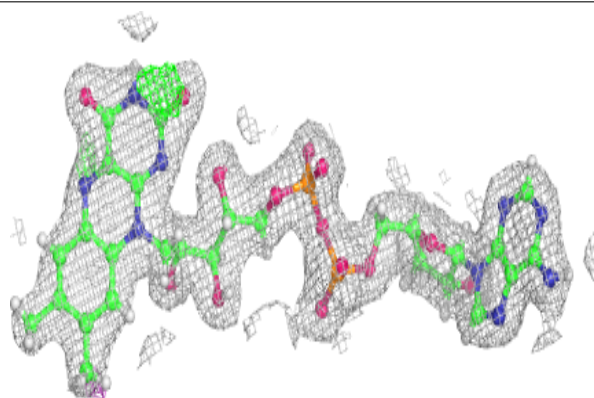


Electron density around FAD A 603:

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

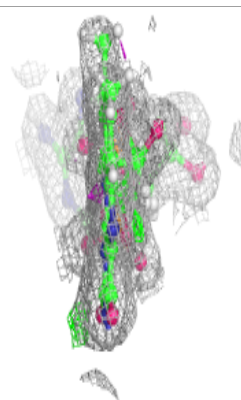
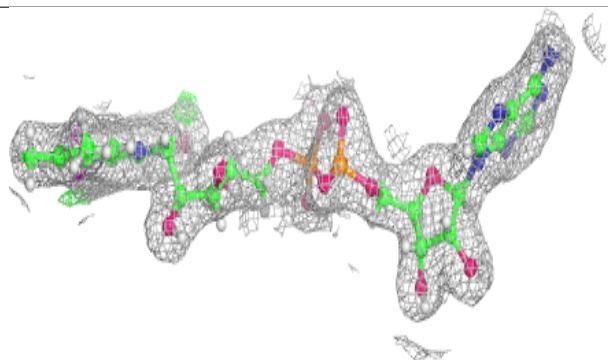
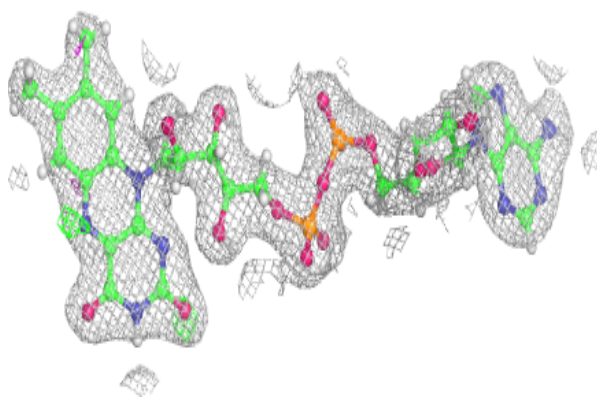
**Electron density around FAD C 602:**

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

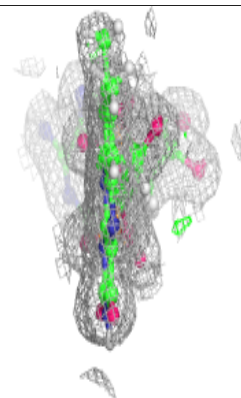
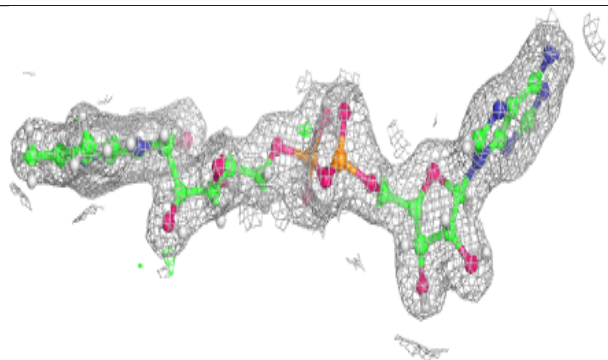
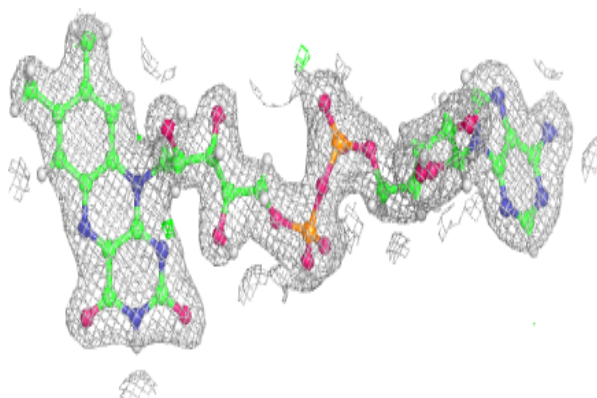


Electron density around FAD D 602:

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

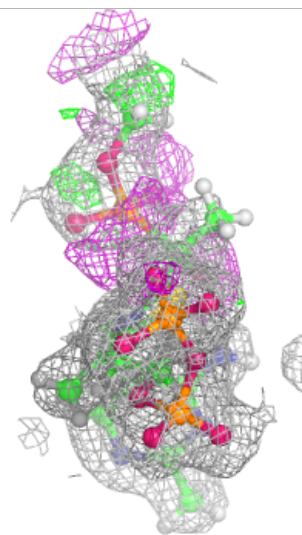
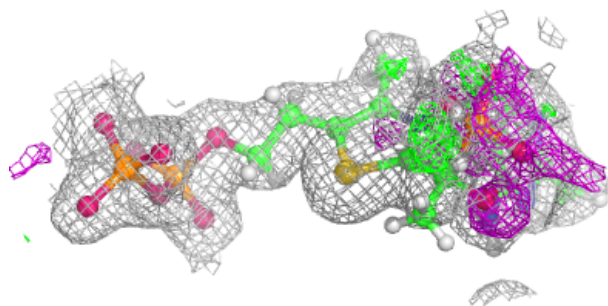
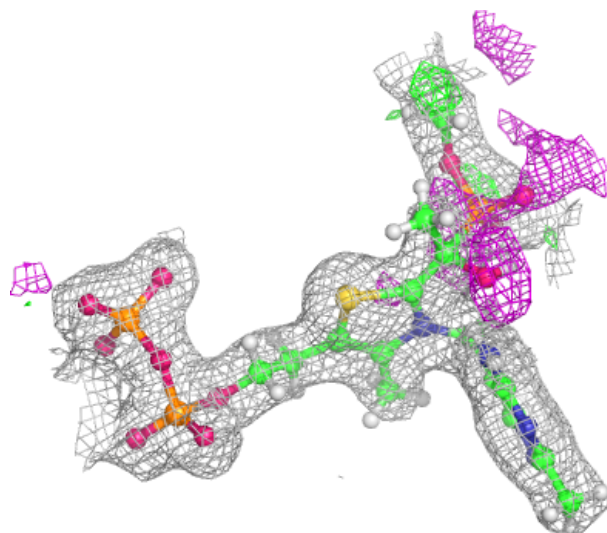
**Electron density around FAD F 603:**

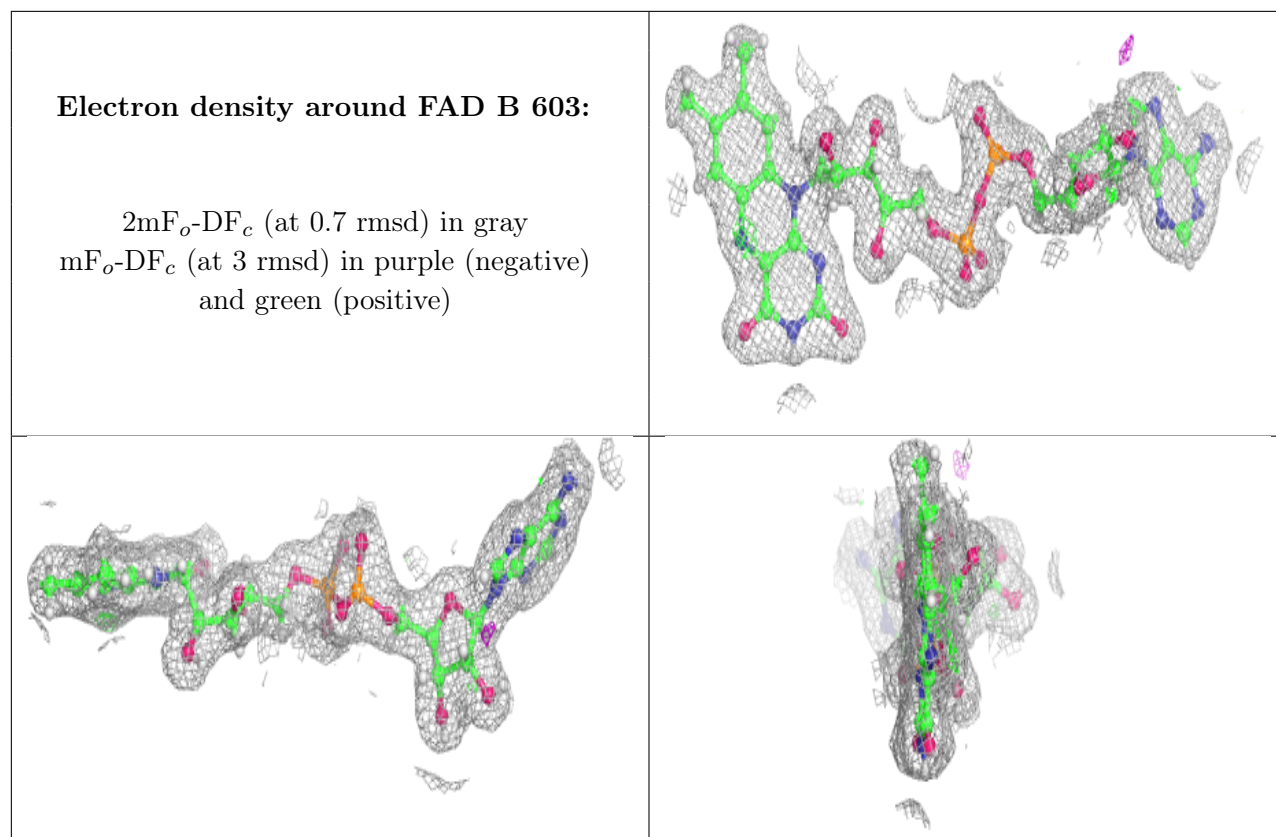
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TDK A 604:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.