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

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 07:52 pm BST

PDB ID	:	6UNZ
Title	:	Crystal structure of cytosolic fumarate hydratase from Leishmania major
Authors	:	Feliciano, P.R.; Drennan, C.L.
Deposited on	:	2019-10-14
Resolution	:	3.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

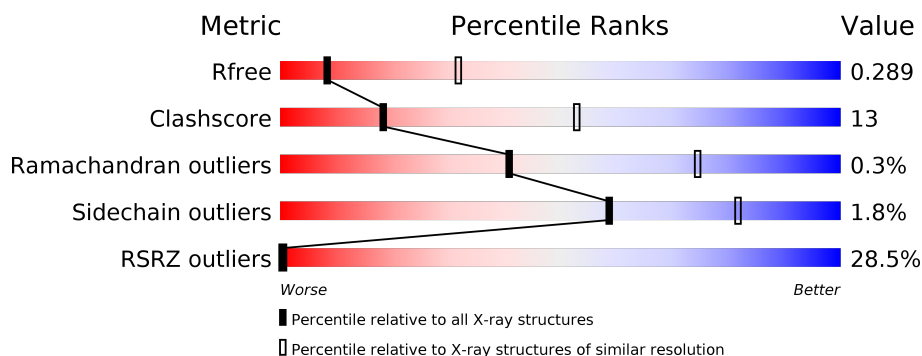|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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		0.289
Clashscore		13
Ramachandran outliers		0.3%
Sidechain outliers		1.8%
RSRZ outliers		28.5%

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	604	22% / 68% 20% 11%
1	B	604	20% / 67% 21% • 12%
1	C	604	29% / 62% 25% • 12%
1	D	604	28% / 66% 21% • 12%
1	E	604	29% / 66% 21% • 12%
1	F	604	20% / 64% 24% • 12%

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Mol	Chain	Length	Quality of chain
1	G	604	29% / 66% / 22% / 12%
1	H	604	25% / 62% / 25% / 12%

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
2	SF4	B	601	-	-	X	-
2	SF4	C	601	-	-	X	-
2	SF4	F	601	-	-	X	-

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called fumarate hydratase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total 3933	C 2469	N 688	O 758	S 18	0	0	0
1	B	534	Total 3933	C 2480	N 681	O 755	S 17	0	0	0
1	C	532	Total 3822	C 2387	N 678	O 737	S 20	0	0	0
1	D	530	Total 3874	C 2440	N 677	O 738	S 19	0	0	0
1	E	531	Total 3863	C 2429	N 677	O 736	S 21	0	0	0
1	F	531	Total 3981	C 2512	N 690	O 759	S 20	0	1	0
1	G	532	Total 3873	C 2430	N 684	O 742	S 17	0	0	0
1	H	531	Total 3888	C 2448	N 673	O 749	S 18	0	0	0

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP E9AE57
A	-34	GLY	-	expression tag	UNP E9AE57
A	-33	SER	-	expression tag	UNP E9AE57
A	-32	SER	-	expression tag	UNP E9AE57
A	-31	HIS	-	expression tag	UNP E9AE57
A	-30	HIS	-	expression tag	UNP E9AE57
A	-29	HIS	-	expression tag	UNP E9AE57
A	-28	HIS	-	expression tag	UNP E9AE57
A	-27	HIS	-	expression tag	UNP E9AE57
A	-26	HIS	-	expression tag	UNP E9AE57
A	-25	SER	-	expression tag	UNP E9AE57
A	-24	SER	-	expression tag	UNP E9AE57
A	-23	GLY	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	LEU	-	expression tag	UNP E9AE57
A	-21	VAL	-	expression tag	UNP E9AE57
A	-20	PRO	-	expression tag	UNP E9AE57
A	-19	ARG	-	expression tag	UNP E9AE57
A	-18	GLY	-	expression tag	UNP E9AE57
A	-17	SER	-	expression tag	UNP E9AE57
A	-16	HIS	-	expression tag	UNP E9AE57
A	-15	MET	-	expression tag	UNP E9AE57
A	-14	ALA	-	expression tag	UNP E9AE57
A	-13	SER	-	expression tag	UNP E9AE57
A	-12	MET	-	expression tag	UNP E9AE57
A	-11	THR	-	expression tag	UNP E9AE57
A	-10	GLY	-	expression tag	UNP E9AE57
A	-9	GLY	-	expression tag	UNP E9AE57
A	-8	GLN	-	expression tag	UNP E9AE57
A	-7	GLN	-	expression tag	UNP E9AE57
A	-6	MET	-	expression tag	UNP E9AE57
A	-5	GLY	-	expression tag	UNP E9AE57
A	-4	ARG	-	expression tag	UNP E9AE57
A	-3	GLY	-	expression tag	UNP E9AE57
A	-2	SER	-	expression tag	UNP E9AE57
A	-1	GLU	-	expression tag	UNP E9AE57
A	0	PHE	-	expression tag	UNP E9AE57
B	-35	MET	-	expression tag	UNP E9AE57
B	-34	GLY	-	expression tag	UNP E9AE57
B	-33	SER	-	expression tag	UNP E9AE57
B	-32	SER	-	expression tag	UNP E9AE57
B	-31	HIS	-	expression tag	UNP E9AE57
B	-30	HIS	-	expression tag	UNP E9AE57
B	-29	HIS	-	expression tag	UNP E9AE57
B	-28	HIS	-	expression tag	UNP E9AE57
B	-27	HIS	-	expression tag	UNP E9AE57
B	-26	HIS	-	expression tag	UNP E9AE57
B	-25	SER	-	expression tag	UNP E9AE57
B	-24	SER	-	expression tag	UNP E9AE57
B	-23	GLY	-	expression tag	UNP E9AE57
B	-22	LEU	-	expression tag	UNP E9AE57
B	-21	VAL	-	expression tag	UNP E9AE57
B	-20	PRO	-	expression tag	UNP E9AE57
B	-19	ARG	-	expression tag	UNP E9AE57
B	-18	GLY	-	expression tag	UNP E9AE57
B	-17	SER	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP E9AE57
B	-15	MET	-	expression tag	UNP E9AE57
B	-14	ALA	-	expression tag	UNP E9AE57
B	-13	SER	-	expression tag	UNP E9AE57
B	-12	MET	-	expression tag	UNP E9AE57
B	-11	THR	-	expression tag	UNP E9AE57
B	-10	GLY	-	expression tag	UNP E9AE57
B	-9	GLY	-	expression tag	UNP E9AE57
B	-8	GLN	-	expression tag	UNP E9AE57
B	-7	GLN	-	expression tag	UNP E9AE57
B	-6	MET	-	expression tag	UNP E9AE57
B	-5	GLY	-	expression tag	UNP E9AE57
B	-4	ARG	-	expression tag	UNP E9AE57
B	-3	GLY	-	expression tag	UNP E9AE57
B	-2	SER	-	expression tag	UNP E9AE57
B	-1	GLU	-	expression tag	UNP E9AE57
B	0	PHE	-	expression tag	UNP E9AE57
C	-35	MET	-	expression tag	UNP E9AE57
C	-34	GLY	-	expression tag	UNP E9AE57
C	-33	SER	-	expression tag	UNP E9AE57
C	-32	SER	-	expression tag	UNP E9AE57
C	-31	HIS	-	expression tag	UNP E9AE57
C	-30	HIS	-	expression tag	UNP E9AE57
C	-29	HIS	-	expression tag	UNP E9AE57
C	-28	HIS	-	expression tag	UNP E9AE57
C	-27	HIS	-	expression tag	UNP E9AE57
C	-26	HIS	-	expression tag	UNP E9AE57
C	-25	SER	-	expression tag	UNP E9AE57
C	-24	SER	-	expression tag	UNP E9AE57
C	-23	GLY	-	expression tag	UNP E9AE57
C	-22	LEU	-	expression tag	UNP E9AE57
C	-21	VAL	-	expression tag	UNP E9AE57
C	-20	PRO	-	expression tag	UNP E9AE57
C	-19	ARG	-	expression tag	UNP E9AE57
C	-18	GLY	-	expression tag	UNP E9AE57
C	-17	SER	-	expression tag	UNP E9AE57
C	-16	HIS	-	expression tag	UNP E9AE57
C	-15	MET	-	expression tag	UNP E9AE57
C	-14	ALA	-	expression tag	UNP E9AE57
C	-13	SER	-	expression tag	UNP E9AE57
C	-12	MET	-	expression tag	UNP E9AE57
C	-11	THR	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP E9AE57
C	-9	GLY	-	expression tag	UNP E9AE57
C	-8	GLN	-	expression tag	UNP E9AE57
C	-7	GLN	-	expression tag	UNP E9AE57
C	-6	MET	-	expression tag	UNP E9AE57
C	-5	GLY	-	expression tag	UNP E9AE57
C	-4	ARG	-	expression tag	UNP E9AE57
C	-3	GLY	-	expression tag	UNP E9AE57
C	-2	SER	-	expression tag	UNP E9AE57
C	-1	GLU	-	expression tag	UNP E9AE57
C	0	PHE	-	expression tag	UNP E9AE57
D	-35	MET	-	expression tag	UNP E9AE57
D	-34	GLY	-	expression tag	UNP E9AE57
D	-33	SER	-	expression tag	UNP E9AE57
D	-32	SER	-	expression tag	UNP E9AE57
D	-31	HIS	-	expression tag	UNP E9AE57
D	-30	HIS	-	expression tag	UNP E9AE57
D	-29	HIS	-	expression tag	UNP E9AE57
D	-28	HIS	-	expression tag	UNP E9AE57
D	-27	HIS	-	expression tag	UNP E9AE57
D	-26	HIS	-	expression tag	UNP E9AE57
D	-25	SER	-	expression tag	UNP E9AE57
D	-24	SER	-	expression tag	UNP E9AE57
D	-23	GLY	-	expression tag	UNP E9AE57
D	-22	LEU	-	expression tag	UNP E9AE57
D	-21	VAL	-	expression tag	UNP E9AE57
D	-20	PRO	-	expression tag	UNP E9AE57
D	-19	ARG	-	expression tag	UNP E9AE57
D	-18	GLY	-	expression tag	UNP E9AE57
D	-17	SER	-	expression tag	UNP E9AE57
D	-16	HIS	-	expression tag	UNP E9AE57
D	-15	MET	-	expression tag	UNP E9AE57
D	-14	ALA	-	expression tag	UNP E9AE57
D	-13	SER	-	expression tag	UNP E9AE57
D	-12	MET	-	expression tag	UNP E9AE57
D	-11	THR	-	expression tag	UNP E9AE57
D	-10	GLY	-	expression tag	UNP E9AE57
D	-9	GLY	-	expression tag	UNP E9AE57
D	-8	GLN	-	expression tag	UNP E9AE57
D	-7	GLN	-	expression tag	UNP E9AE57
D	-6	MET	-	expression tag	UNP E9AE57
D	-5	GLY	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ARG	-	expression tag	UNP E9AE57
D	-3	GLY	-	expression tag	UNP E9AE57
D	-2	SER	-	expression tag	UNP E9AE57
D	-1	GLU	-	expression tag	UNP E9AE57
D	0	PHE	-	expression tag	UNP E9AE57
E	-35	MET	-	expression tag	UNP E9AE57
E	-34	GLY	-	expression tag	UNP E9AE57
E	-33	SER	-	expression tag	UNP E9AE57
E	-32	SER	-	expression tag	UNP E9AE57
E	-31	HIS	-	expression tag	UNP E9AE57
E	-30	HIS	-	expression tag	UNP E9AE57
E	-29	HIS	-	expression tag	UNP E9AE57
E	-28	HIS	-	expression tag	UNP E9AE57
E	-27	HIS	-	expression tag	UNP E9AE57
E	-26	HIS	-	expression tag	UNP E9AE57
E	-25	SER	-	expression tag	UNP E9AE57
E	-24	SER	-	expression tag	UNP E9AE57
E	-23	GLY	-	expression tag	UNP E9AE57
E	-22	LEU	-	expression tag	UNP E9AE57
E	-21	VAL	-	expression tag	UNP E9AE57
E	-20	PRO	-	expression tag	UNP E9AE57
E	-19	ARG	-	expression tag	UNP E9AE57
E	-18	GLY	-	expression tag	UNP E9AE57
E	-17	SER	-	expression tag	UNP E9AE57
E	-16	HIS	-	expression tag	UNP E9AE57
E	-15	MET	-	expression tag	UNP E9AE57
E	-14	ALA	-	expression tag	UNP E9AE57
E	-13	SER	-	expression tag	UNP E9AE57
E	-12	MET	-	expression tag	UNP E9AE57
E	-11	THR	-	expression tag	UNP E9AE57
E	-10	GLY	-	expression tag	UNP E9AE57
E	-9	GLY	-	expression tag	UNP E9AE57
E	-8	GLN	-	expression tag	UNP E9AE57
E	-7	GLN	-	expression tag	UNP E9AE57
E	-6	MET	-	expression tag	UNP E9AE57
E	-5	GLY	-	expression tag	UNP E9AE57
E	-4	ARG	-	expression tag	UNP E9AE57
E	-3	GLY	-	expression tag	UNP E9AE57
E	-2	SER	-	expression tag	UNP E9AE57
E	-1	GLU	-	expression tag	UNP E9AE57
E	0	PHE	-	expression tag	UNP E9AE57
F	-35	MET	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	GLY	-	expression tag	UNP E9AE57
F	-33	SER	-	expression tag	UNP E9AE57
F	-32	SER	-	expression tag	UNP E9AE57
F	-31	HIS	-	expression tag	UNP E9AE57
F	-30	HIS	-	expression tag	UNP E9AE57
F	-29	HIS	-	expression tag	UNP E9AE57
F	-28	HIS	-	expression tag	UNP E9AE57
F	-27	HIS	-	expression tag	UNP E9AE57
F	-26	HIS	-	expression tag	UNP E9AE57
F	-25	SER	-	expression tag	UNP E9AE57
F	-24	SER	-	expression tag	UNP E9AE57
F	-23	GLY	-	expression tag	UNP E9AE57
F	-22	LEU	-	expression tag	UNP E9AE57
F	-21	VAL	-	expression tag	UNP E9AE57
F	-20	PRO	-	expression tag	UNP E9AE57
F	-19	ARG	-	expression tag	UNP E9AE57
F	-18	GLY	-	expression tag	UNP E9AE57
F	-17	SER	-	expression tag	UNP E9AE57
F	-16	HIS	-	expression tag	UNP E9AE57
F	-15	MET	-	expression tag	UNP E9AE57
F	-14	ALA	-	expression tag	UNP E9AE57
F	-13	SER	-	expression tag	UNP E9AE57
F	-12	MET	-	expression tag	UNP E9AE57
F	-11	THR	-	expression tag	UNP E9AE57
F	-10	GLY	-	expression tag	UNP E9AE57
F	-9	GLY	-	expression tag	UNP E9AE57
F	-8	GLN	-	expression tag	UNP E9AE57
F	-7	GLN	-	expression tag	UNP E9AE57
F	-6	MET	-	expression tag	UNP E9AE57
F	-5	GLY	-	expression tag	UNP E9AE57
F	-4	ARG	-	expression tag	UNP E9AE57
F	-3	GLY	-	expression tag	UNP E9AE57
F	-2	SER	-	expression tag	UNP E9AE57
F	-1	GLU	-	expression tag	UNP E9AE57
F	0	PHE	-	expression tag	UNP E9AE57
G	-35	MET	-	expression tag	UNP E9AE57
G	-34	GLY	-	expression tag	UNP E9AE57
G	-33	SER	-	expression tag	UNP E9AE57
G	-32	SER	-	expression tag	UNP E9AE57
G	-31	HIS	-	expression tag	UNP E9AE57
G	-30	HIS	-	expression tag	UNP E9AE57
G	-29	HIS	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-28	HIS	-	expression tag	UNP E9AE57
G	-27	HIS	-	expression tag	UNP E9AE57
G	-26	HIS	-	expression tag	UNP E9AE57
G	-25	SER	-	expression tag	UNP E9AE57
G	-24	SER	-	expression tag	UNP E9AE57
G	-23	GLY	-	expression tag	UNP E9AE57
G	-22	LEU	-	expression tag	UNP E9AE57
G	-21	VAL	-	expression tag	UNP E9AE57
G	-20	PRO	-	expression tag	UNP E9AE57
G	-19	ARG	-	expression tag	UNP E9AE57
G	-18	GLY	-	expression tag	UNP E9AE57
G	-17	SER	-	expression tag	UNP E9AE57
G	-16	HIS	-	expression tag	UNP E9AE57
G	-15	MET	-	expression tag	UNP E9AE57
G	-14	ALA	-	expression tag	UNP E9AE57
G	-13	SER	-	expression tag	UNP E9AE57
G	-12	MET	-	expression tag	UNP E9AE57
G	-11	THR	-	expression tag	UNP E9AE57
G	-10	GLY	-	expression tag	UNP E9AE57
G	-9	GLY	-	expression tag	UNP E9AE57
G	-8	GLN	-	expression tag	UNP E9AE57
G	-7	GLN	-	expression tag	UNP E9AE57
G	-6	MET	-	expression tag	UNP E9AE57
G	-5	GLY	-	expression tag	UNP E9AE57
G	-4	ARG	-	expression tag	UNP E9AE57
G	-3	GLY	-	expression tag	UNP E9AE57
G	-2	SER	-	expression tag	UNP E9AE57
G	-1	GLU	-	expression tag	UNP E9AE57
G	0	PHE	-	expression tag	UNP E9AE57
H	-35	MET	-	expression tag	UNP E9AE57
H	-34	GLY	-	expression tag	UNP E9AE57
H	-33	SER	-	expression tag	UNP E9AE57
H	-32	SER	-	expression tag	UNP E9AE57
H	-31	HIS	-	expression tag	UNP E9AE57
H	-30	HIS	-	expression tag	UNP E9AE57
H	-29	HIS	-	expression tag	UNP E9AE57
H	-28	HIS	-	expression tag	UNP E9AE57
H	-27	HIS	-	expression tag	UNP E9AE57
H	-26	HIS	-	expression tag	UNP E9AE57
H	-25	SER	-	expression tag	UNP E9AE57
H	-24	SER	-	expression tag	UNP E9AE57
H	-23	GLY	-	expression tag	UNP E9AE57

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-22	LEU	-	expression tag	UNP E9AE57
H	-21	VAL	-	expression tag	UNP E9AE57
H	-20	PRO	-	expression tag	UNP E9AE57
H	-19	ARG	-	expression tag	UNP E9AE57
H	-18	GLY	-	expression tag	UNP E9AE57
H	-17	SER	-	expression tag	UNP E9AE57
H	-16	HIS	-	expression tag	UNP E9AE57
H	-15	MET	-	expression tag	UNP E9AE57
H	-14	ALA	-	expression tag	UNP E9AE57
H	-13	SER	-	expression tag	UNP E9AE57
H	-12	MET	-	expression tag	UNP E9AE57
H	-11	THR	-	expression tag	UNP E9AE57
H	-10	GLY	-	expression tag	UNP E9AE57
H	-9	GLY	-	expression tag	UNP E9AE57
H	-8	GLN	-	expression tag	UNP E9AE57
H	-7	GLN	-	expression tag	UNP E9AE57
H	-6	MET	-	expression tag	UNP E9AE57
H	-5	GLY	-	expression tag	UNP E9AE57
H	-4	ARG	-	expression tag	UNP E9AE57
H	-3	GLY	-	expression tag	UNP E9AE57
H	-2	SER	-	expression tag	UNP E9AE57
H	-1	GLU	-	expression tag	UNP E9AE57
H	0	PHE	-	expression tag	UNP E9AE57

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by author).
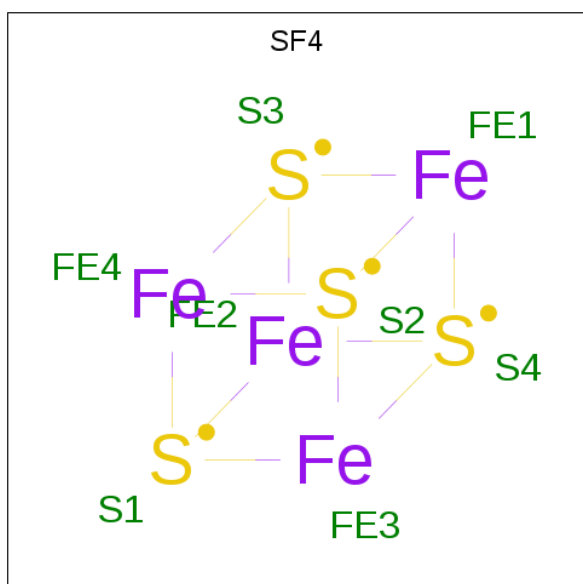
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
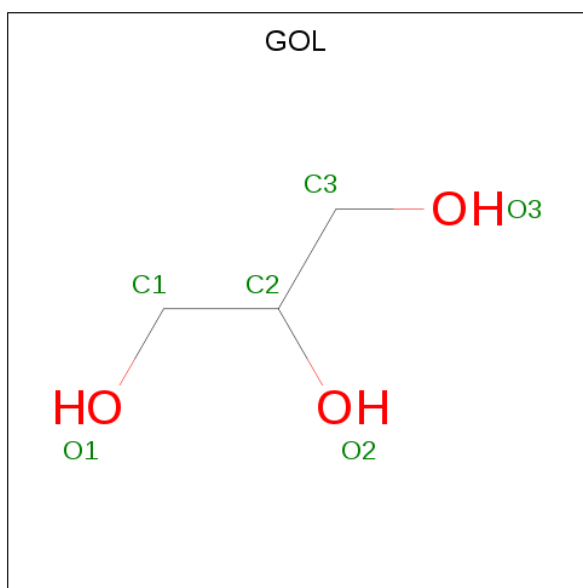
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: fumarate hydratase 2
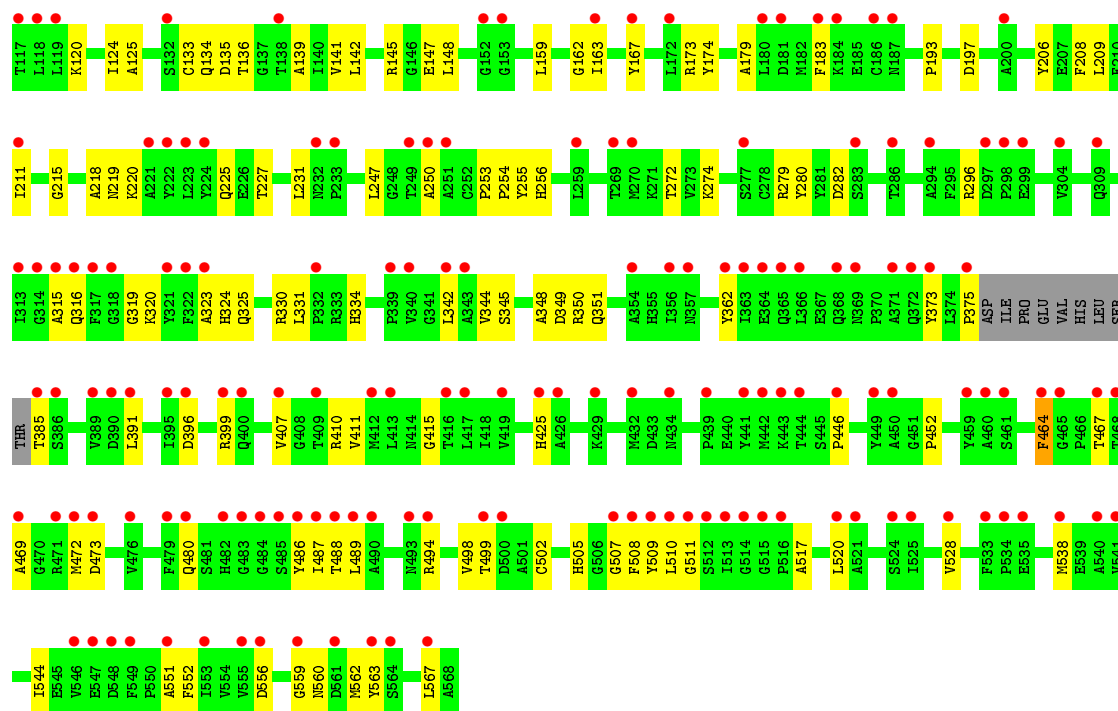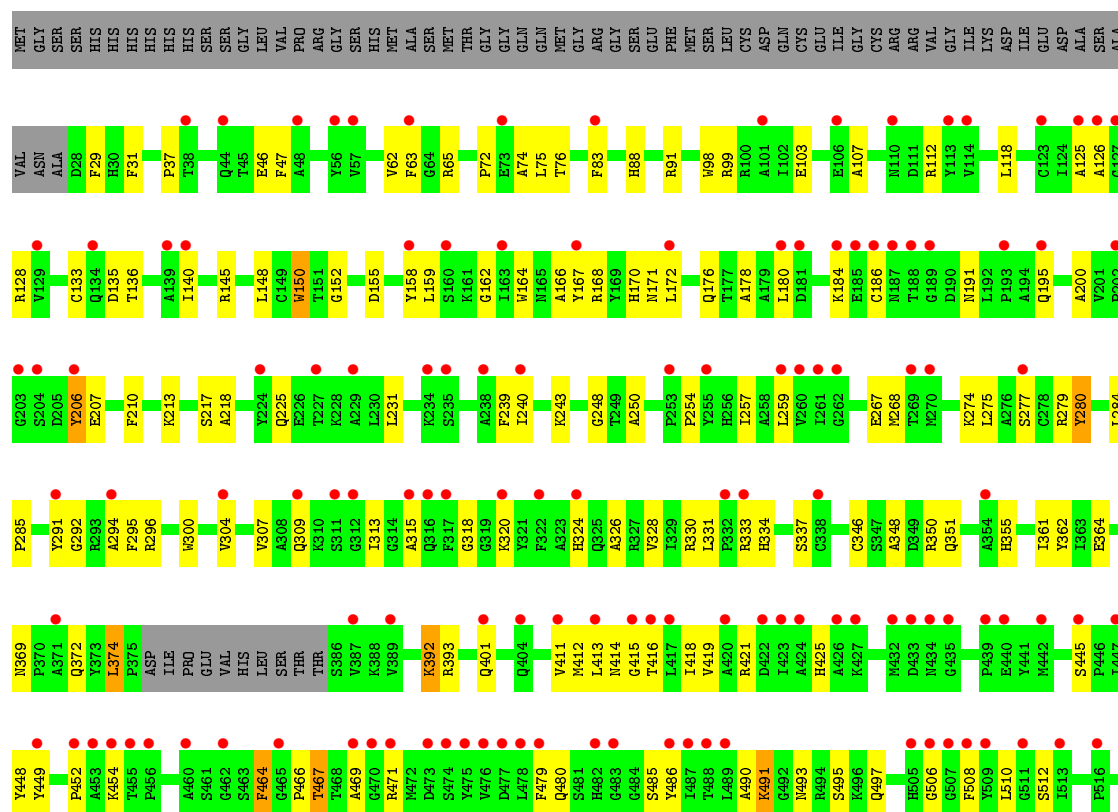

- Molecule 1: fumarate hydratase 2

• Molecule 1: fumarate hydratase 2

• Molecule 1: fumarate hydratase 2

Chain D:

• Molecule 1: fumarate hydratase 2

Chain E:

L391 K392 R393 P394 I395 D396 K397 V398 K397 R399 Q400 Q401 L402 S403 Q404 Y405 P406 V407 G408 T409 R410 V411 M412 L413 N414 G415 T416 L417 I418 V419 A420 R421 D422 K429 E430 M431 M432 L438 P439 E440 Y441 M442 K443 T444 S445 P446 I447 Y448 Y449 A450 G451 P452 A453 P456 A460 S463

F464 G465 P466 T467 T468 A469 G470 R471 M472 D473 S474 Y475 F479 Q480 S481 G484 S485 T488 L489 A490 R494 S495 K496 Q497 V498 T499 D500 K503 G506 G507 F508 Y509 L510 G511 S512 I513 G514 G515 P516 A517 A518 I519 L520 D523 S524 I525 K526 Q527 V528 T529 C530 L531 A532

F533 P534 E535 L536 G537 M538 E539 A540 V541 W542 K543 I544 E545 V546 E547 D548 F552 I553 V554 V555 D556 D557 G558 G559 N560 M562 Y563 S564 K565 T566 L567 A568

• Molecule 1: fumarate hydratase 2

Chain F:

Chain G:

T117 L118 L119 K120 I124 A125 S132 C133 Q134 D135 T136 G137 T138 A139 I140 V141 L142 R145 G146 E447 L148 G152 G153 L159 G162 I163 Y167 L172 R173 Y174 A179 L180 D181 M182 F183 K184 E185 C186 N187 P193 D197 A200 Y206 E207 F208 L209 F210

I211 G215 A218 N219 K220 A221 Y222 L223 Y224 Q225 E226 T227 L231 N232 P233 L247 Q248 T249 A250 A251 C252 P253 P254 Y255 H256 L259 T269 M270 K271 T272 V273 K274 S277 C278 R279 Y280 Y281 D282 S283 T286 A294 F295 R296 D297 P298 E299 V304 Q309

I313 G314 A315 Q316 F317 G318 G319 K320 Y321 F322 A323 H324 Q325 R330 L331 P332 R333 H334 F339 V340 G341 L342 A343 V344 S345 A348 D349 R350 Q351 A354 H355 I356 N357 Y362 I363 E364 Q365 L366 E367 Q368 N369 P370 A371 Q372 Y373 L374 P375 ASP ILE PRO GLU VAL HIS LEU SER

THR T385 S386 V389 D390 L391 I395 D396 R399 Q400 V407 G408 T409 R410 V411 M412 L413 N414 G415 T416 L417 I418 V419 H425 A426 K429 M432 D433 N434 P439 E440 Y441 M442 K443 T444 S445 P446 Y449 A450 G451 P452 Y459 A460 S461 F464 G465 P466 T467 T468

A469 G470 R471 M472 D473 V476 F479 Q480 S481 H482 G483 G484 S485 Y486 I487 T488 L489 A490 N493 R494 V498 T499 D500 A501 C502 H505 G506 G507 F508 Y509 L510 G511 S512 I513 G514 G515 P516 A517 L520 A521 S524 I525 V528 F533 P534 E535 M538 E539 A540 V541

I544 E545 V546 E547 D548 F549 P550 A551 F552 I553 V554 V555 D556 G559 N560 D561 M562 Y563 S564 L567 A568

• Molecule 1: fumarate hydratase 2

Chain H:

25%

62%   25% • 12%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN MET GLY ARG GLY SER GLU PHE MET SER LEU CYS ASP GLN CYS GLU ILE GLY CYS ARG ARG VAL GLY ILE LYS ASP ILE GLU ASP ALA SER ALA

VAL ASN ALA D28 F29 H30 F31 P37 T38 Q44 T45 E46 F47 A48 Y56 V57 V62 F63 G64 R65 P72 E73 A74 L75 T76 F83 H88 R91 W98 R99 R100 A101 I102 E103 E106 A107 N110 D111 R112 Y113 V114 L118 C123 I124 A125 A126 G127

R128 V129 C133 Q134 D135 T136 A139 I140 R145 L148 C149 W150 T151 G152 D155 Y158 L159 S160 K161 G162 I163 M164 N165 A166 Y167 R168 Y169 H170 N171 L172 Q176 T177 A178 A179 L180 D181 K184 E185 C186 N187 T188 G189 D190 M191 L192 P193 A194 Q195 A200 V201 P202

G203 S204 D205 Y206 E207 F210 K213 S217 A218 Y224 Q225 E226 T227 K228 A229 L230 L231 K234 S235 A238 P239 I240 K243 Q248 T249 A250 P253 P254 Y255 H256 I257 A258 L259 V260 I261 C262 E267 M268 T269 M270 K274 L275 A276 S277 C278 R279 Y280 L284

P285 Y291 G292 R293 A294 F295 R296 W300 V304 V307 A308 Q309 K310 S311 G312 I313 G314 A315 Q316 F317 G318 G319 K320 Y321 F322 A323 H324 Q325 A326 R327 V328 I329 L331 P332 R333 H334 S337 C338 C346 S347 A348 D349 R350 Q351 A354 H355 I361 Y362 I363 E364

N369 P370 A371 Q372 Y373 L374 P375 ASP ILE PRO GLU VAL HIS LEU SER THR S386 V387 K388 V389 K392 R393 Q401 Q404 V411 M412 L413 N414 G415 T416 L417 I418 V419 A420 R421 D422 I423 A424 H425 A426 K427 M432 D433 N434 G435 P439 E440 Y441 M442 S445 P446 I447

Y448 Y449 P452 A453 K454 T455 P456 A460 S461 G462 S463 F464 G465 P466 T467 T468 A469 G470 R471 M472 D473 S474 Y475 V476 D477 L478 F479 Q480 S481 H482 G483 G484 S485 Y486 I487 T488 L489 A490 K491 Q492 N493 R494 S495 K496 Q497 H505 G506 G507 F508 Y509 L510 G511 S512 I513 P516

L520 V528 T529 C530 F533 P534 E535 M538 E539 A540 V541 W542 K543 I544 E545 V546 E547 D548 F549 P550 A551 F552 I553 D556 D557 K558 G559 N560 D561 S564 A568

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	159.09Å 66.07Å 238.09Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.71 – 3.19 49.71 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.71-3.19) 90.2 (49.71-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	714.55 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.245 , 0.289 0.246 , 0.289	Depositor DCC
R_{free} test set	3752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.398 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 75107 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	31246	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: GOL, SF4

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	0.36	0/4024	0.67	1/5476 (0.0%)
1	B	0.39	0/4029	0.69	0/5489
1	C	0.34	0/3911	0.64	0/5329
1	D	0.35	0/3966	0.62	0/5399
1	E	0.36	0/3952	0.63	0/5380
1	F	0.36	0/4076	0.62	0/5542
1	G	0.36	0/3965	0.65	0/5401
1	H	0.38	1/3984 (0.0%)	0.65	0/5432
All	All	0.36	1/31907 (0.0%)	0.65	1/43448 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	150	TRP	CB-CG	-5.38	1.40	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3933	0	3563	90	0
1	B	3933	0	3571	97	0
1	C	3822	0	3400	123	0
1	D	3874	0	3531	91	0
1	E	3863	0	3537	102	0
1	F	3981	0	3721	115	0
1	G	3873	0	3489	107	0
1	H	3888	0	3506	124	0
2	A	8	0	0	1	0
2	B	8	0	0	2	0
2	C	8	0	0	5	0
2	D	8	0	0	0	0
2	E	8	0	0	1	0
2	F	8	0	0	3	0
2	G	8	0	0	0	0
2	H	8	0	0	0	0
3	B	6	0	8	2	0
3	E	6	0	8	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
All	All	31246	0	28334	792	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 792 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:ARG:HD2	1:G:509:TYR:CD1	2.00	0.96
1:B:421:ARG:HH11	1:B:451:GLY:HA3	1.32	0.95
1:G:494:ARG:HD2	1:G:509:TYR:CE1	2.07	0.89
1:E:399:ARG:HD2	1:E:506:GLY:O	1.73	0.89
1:C:134:GLN:NE2	2:C:601:SF4:S4	2.48	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/604 (89%)	513 (96%)	20 (4%)	2 (0%)	34	69
1	B	530/604 (88%)	511 (96%)	17 (3%)	2 (0%)	34	69
1	C	528/604 (87%)	512 (97%)	16 (3%)	0	100	100
1	D	526/604 (87%)	508 (97%)	17 (3%)	1 (0%)	47	79
1	E	527/604 (87%)	506 (96%)	17 (3%)	4 (1%)	19	58
1	F	528/604 (87%)	510 (97%)	16 (3%)	2 (0%)	34	69
1	G	528/604 (87%)	513 (97%)	15 (3%)	0	100	100
1	H	527/604 (87%)	510 (97%)	16 (3%)	1 (0%)	47	79
All	All	4229/4832 (88%)	4083 (96%)	134 (3%)	12 (0%)	41	74

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	VAL
1	B	438	LEU
1	E	386	SER
1	E	395	ILE
1	H	374	LEU

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	363/492 (74%)	355 (98%)	8 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	369/492 (75%)	363 (98%)	6 (2%)	62	84
1	C	347/492 (70%)	342 (99%)	5 (1%)	67	86
1	D	362/492 (74%)	353 (98%)	9 (2%)	47	77
1	E	363/492 (74%)	357 (98%)	6 (2%)	60	83
1	F	391/492 (80%)	383 (98%)	8 (2%)	55	80
1	G	357/492 (73%)	353 (99%)	4 (1%)	73	88
1	H	365/492 (74%)	358 (98%)	7 (2%)	57	81
All	All	2917/3936 (74%)	2864 (98%)	53 (2%)	59	82

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	358	LYS
1	E	206	TYR
1	H	374	LEU
1	D	374	LEU
1	D	491	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	F	170	HIS
1	F	324	HIS
1	H	480	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	B	602	-	5,5,5	0.98	0	5,5,5	0.94	0
2	SF4	F	601	1	0,12,12	0.00	-	-		
2	SF4	E	601	1	0,12,12	0.00	-	-		
2	SF4	G	601	1	0,12,12	0.00	-	-		
2	SF4	B	601	1	0,12,12	0.00	-	-		
2	SF4	A	601	1	0,12,12	0.00	-	-		
2	SF4	D	601	1	0,12,12	0.00	-	-		
2	SF4	C	601	1	0,12,12	0.00	-	-		
3	GOL	E	602	-	5,5,5	0.94	0	5,5,5	1.16	1 (20%)
2	SF4	H	601	1	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	602	-	-	2/4/4/4	-
2	SF4	F	601	1	-	-	0/6/5/5
2	SF4	E	601	1	-	-	0/6/5/5
2	SF4	G	601	1	-	-	0/6/5/5
2	SF4	B	601	1	-	-	0/6/5/5
2	SF4	A	601	1	-	-	0/6/5/5
2	SF4	D	601	1	-	-	0/6/5/5
2	SF4	C	601	1	-	-	0/6/5/5
3	GOL	E	602	-	-	2/4/4/4	-
2	SF4	H	601	1	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	602	GOL	C3-C2-C1	-2.01	103.91	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	E	602	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	2	0
2	F	601	SF4	3	0
2	E	601	SF4	1	0
2	B	601	SF4	2	0
2	A	601	SF4	1	0
2	C	601	SF4	5	0
3	E	602	GOL	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 SF4 F 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 H 601

Bond lengths

Bond angles

Torsions

Rings
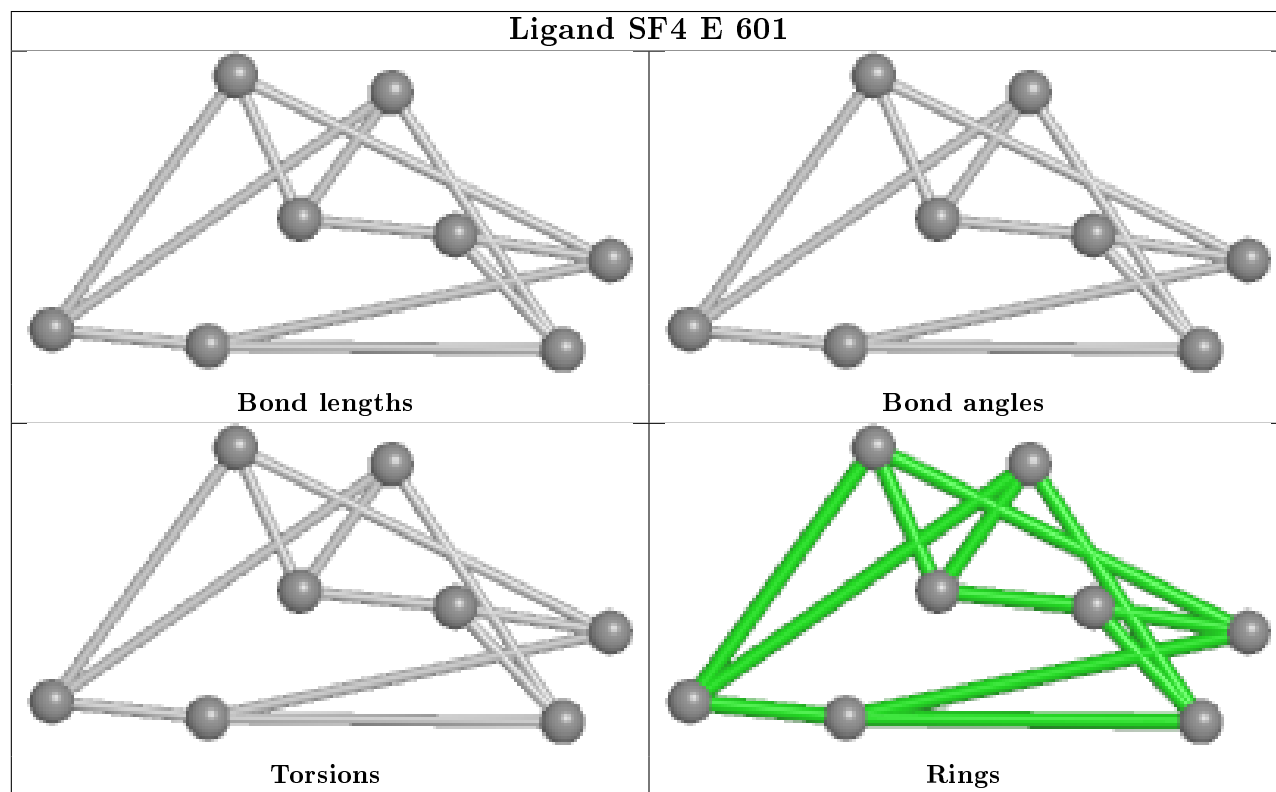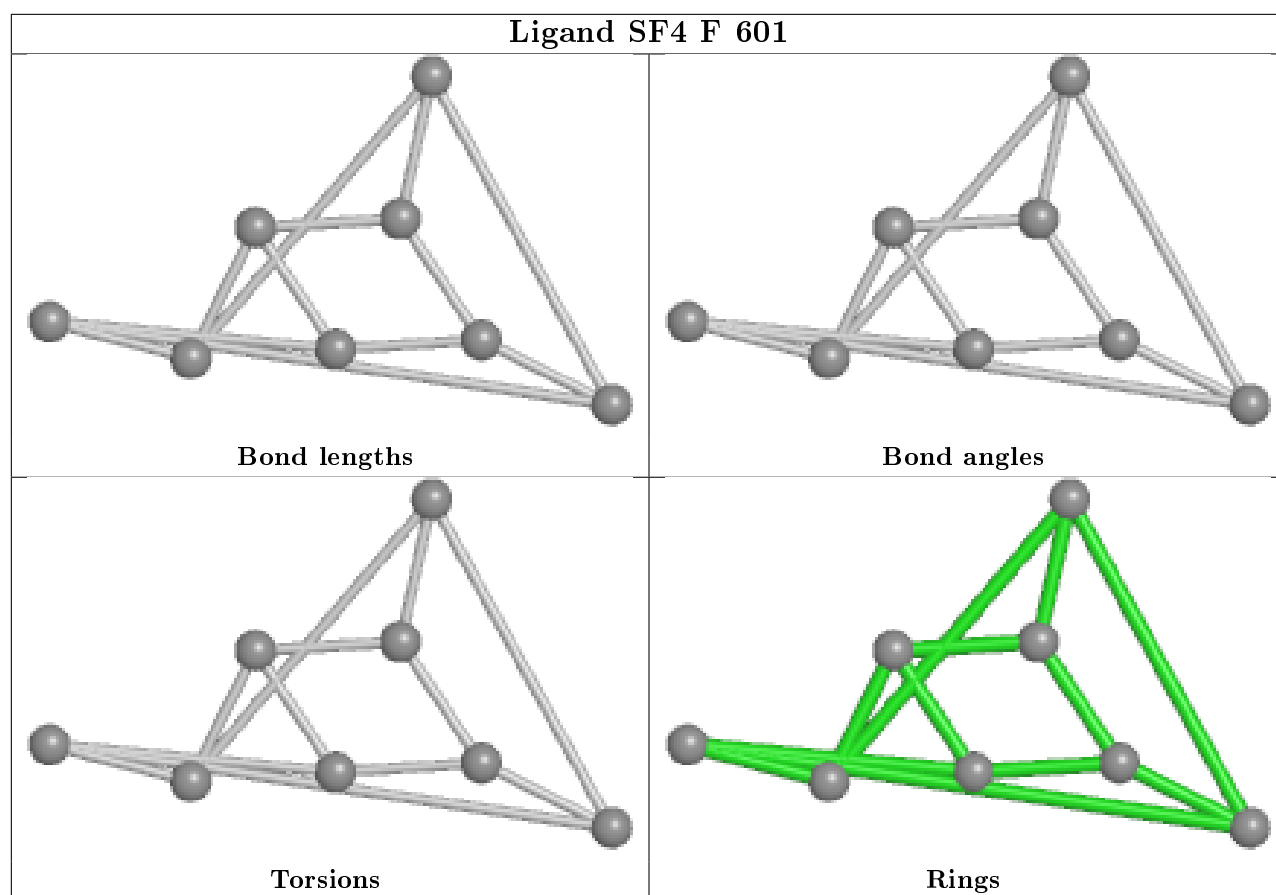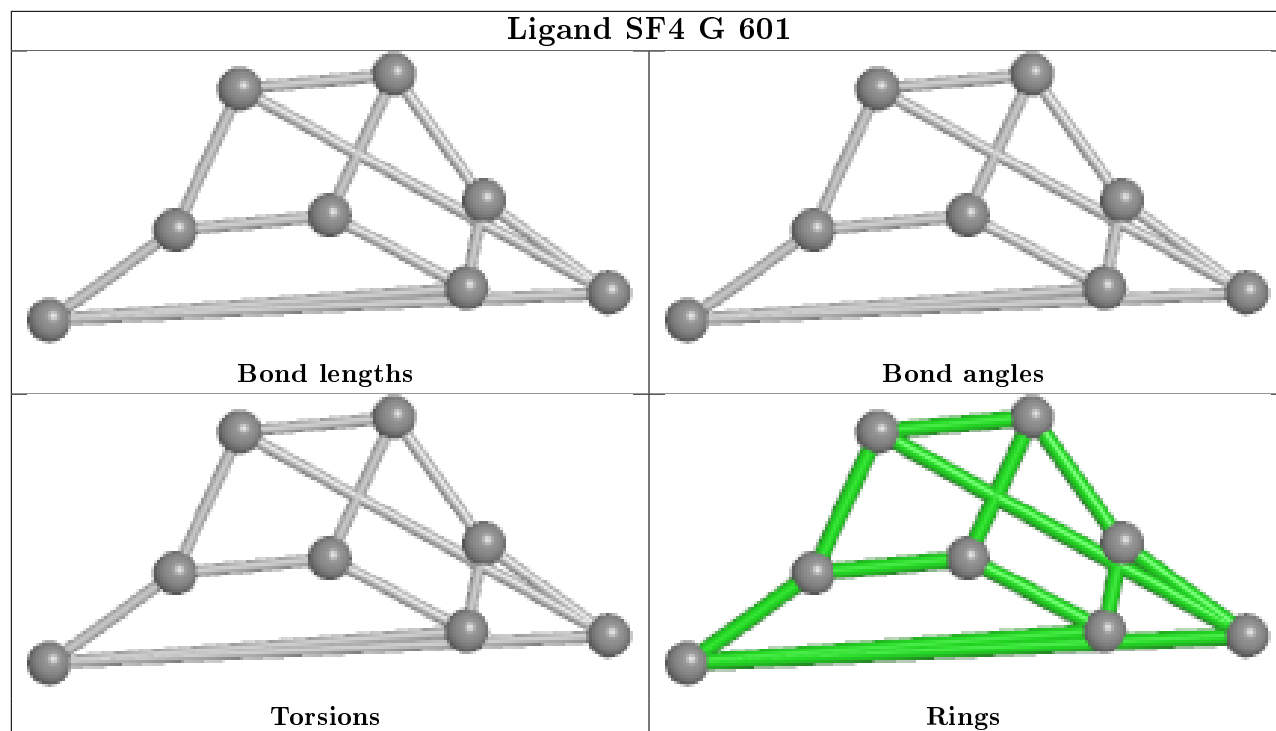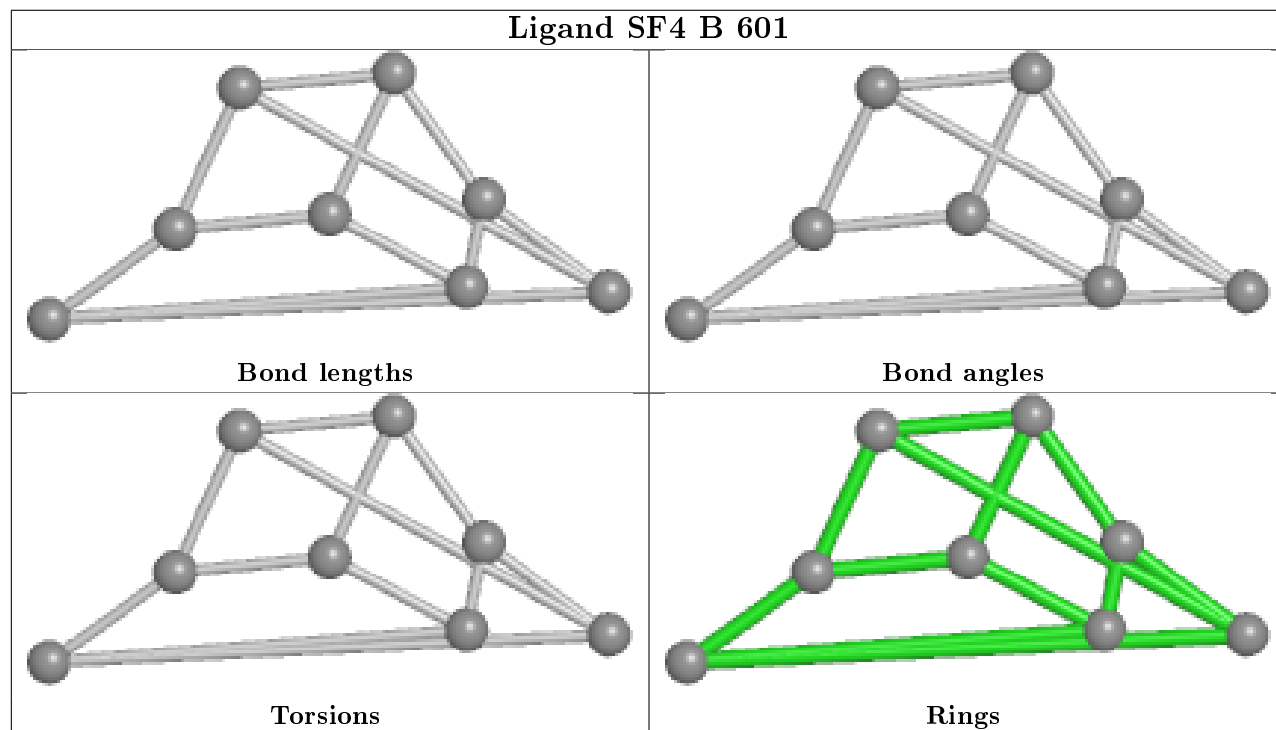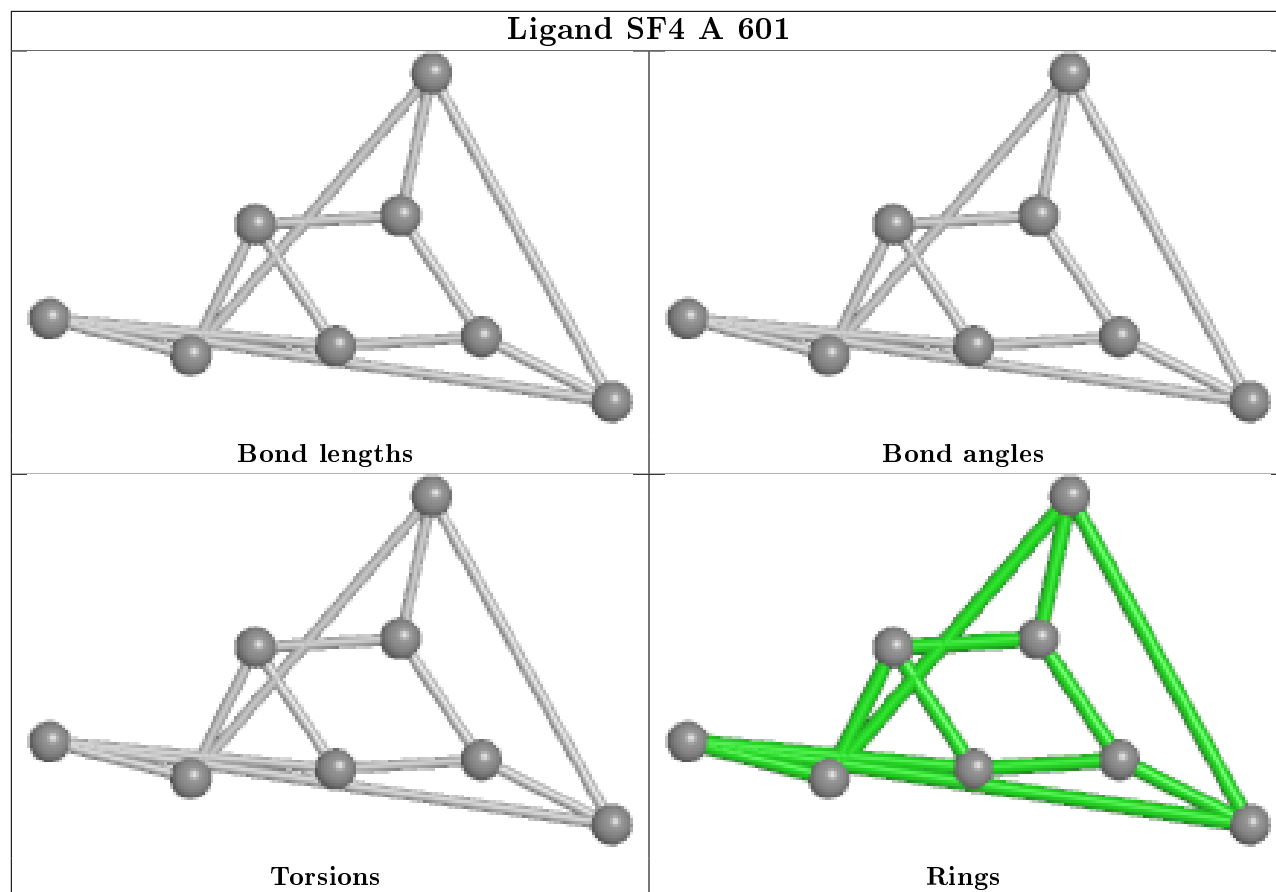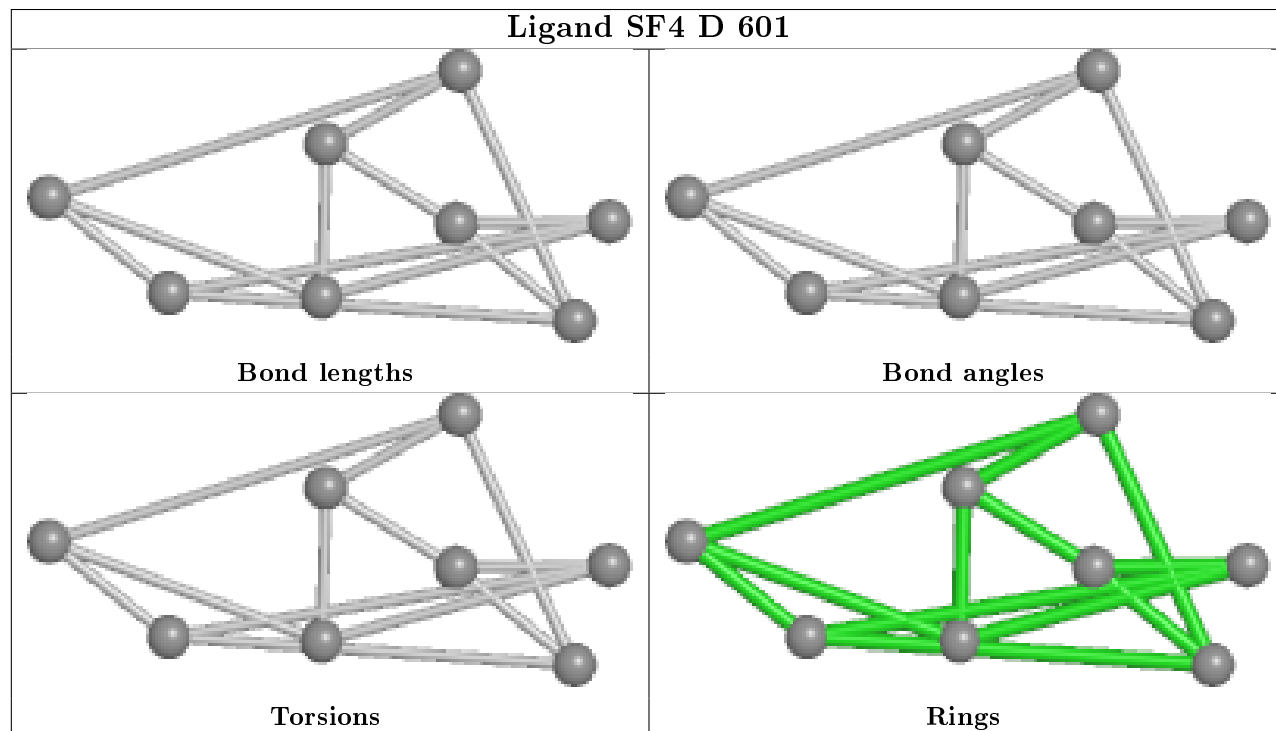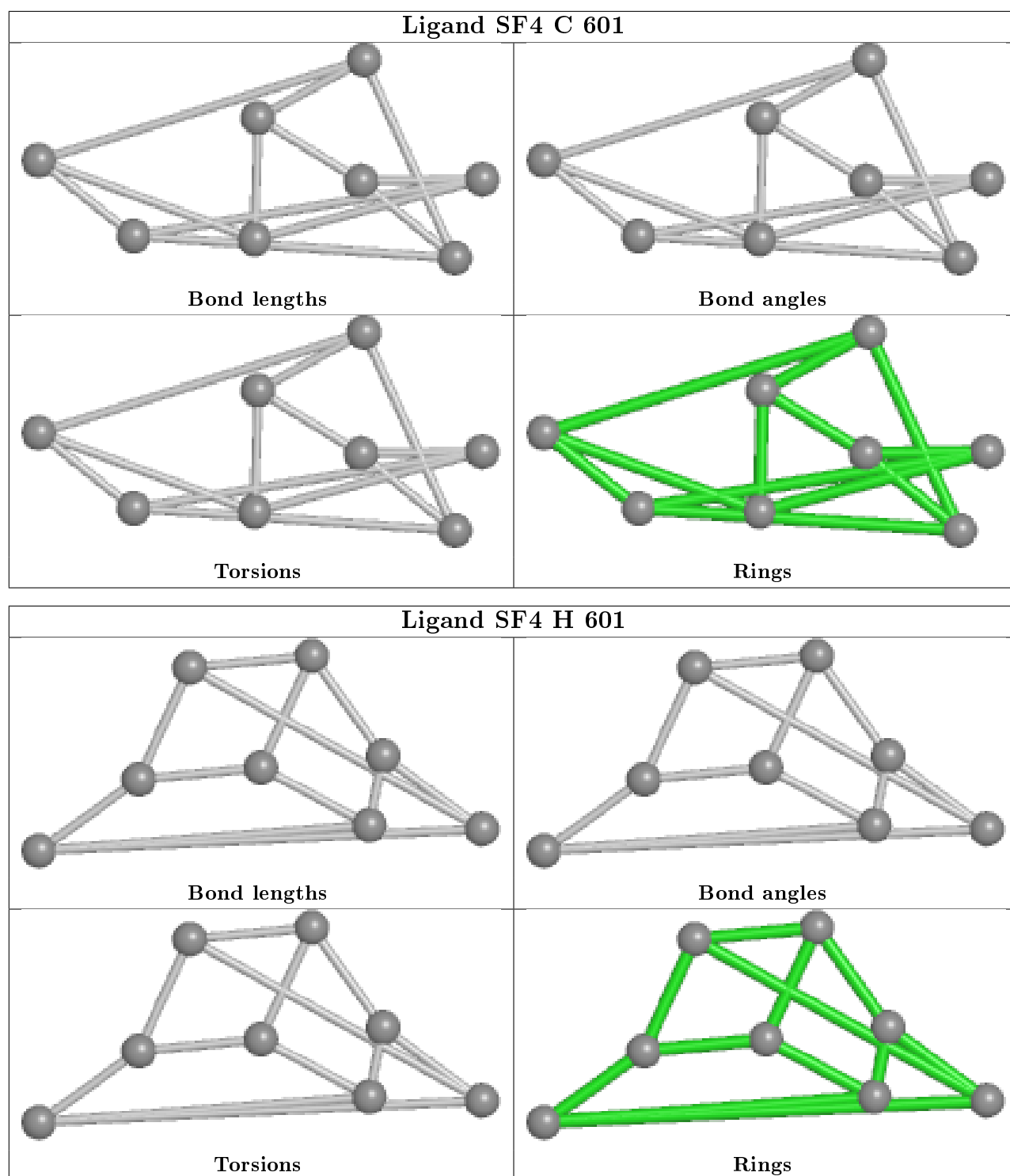
5.7 Other polymers (i)

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	539/604 (89%)	1.50	133 (24%)	0	0	23, 58, 89, 106	0
1	B	534/604 (88%)	1.39	121 (22%)	0	0	24, 50, 79, 89	0
1	C	532/604 (88%)	1.68	173 (32%)	0	0	37, 80, 91, 100	0
1	D	530/604 (87%)	1.66	168 (31%)	0	0	29, 72, 89, 102	0
1	E	531/604 (87%)	1.76	177 (33%)	0	0	34, 65, 92, 103	0
1	F	531/604 (87%)	1.28	118 (22%)	0	0	34, 57, 71, 81	0
1	G	532/604 (88%)	1.71	173 (32%)	0	0	28, 66, 91, 102	0
1	H	531/604 (87%)	1.52	153 (28%)	0	0	22, 65, 88, 111	0
All	All	4260/4832 (88%)	1.56	1216 (28%)	0	0	22, 64, 89, 111	0

The worst 5 of 1216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	13.7
1	C	437	PRO	12.8
1	E	489	LEU	12.8
1	E	547	GLU	12.7
1	A	480	GLN	12.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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
3	GOL	E	602	6/6	0.65	0.26	58,59,65,65	0
3	GOL	B	602	6/6	0.66	0.36	35,37,41,41	0
2	SF4	C	601	8/8	0.88	0.14	80,84,105,116	0
2	SF4	F	601	8/8	0.89	0.13	51,77,94,94	0
2	SF4	E	601	8/8	0.90	0.13	55,69,89,96	0
2	SF4	G	601	8/8	0.90	0.16	48,80,92,96	0
2	SF4	H	601	8/8	0.91	0.12	65,70,94,94	0
2	SF4	A	601	8/8	0.93	0.13	53,65,77,81	0
2	SF4	B	601	8/8	0.93	0.18	29,40,52,74	0
2	SF4	D	601	8/8	0.95	0.16	52,59,78,85	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
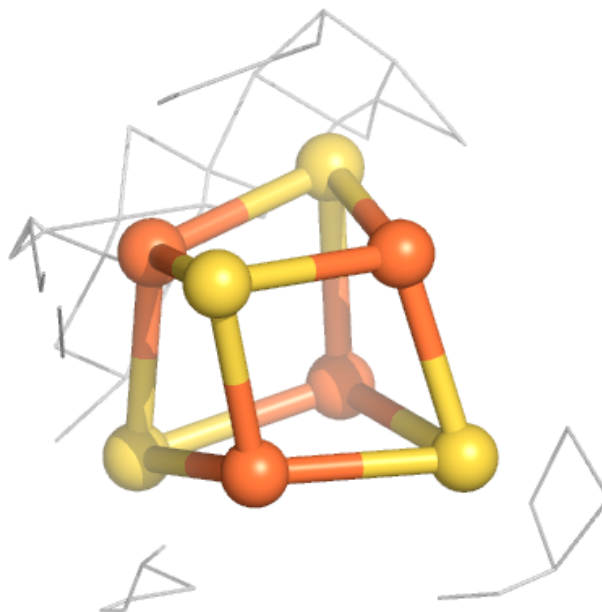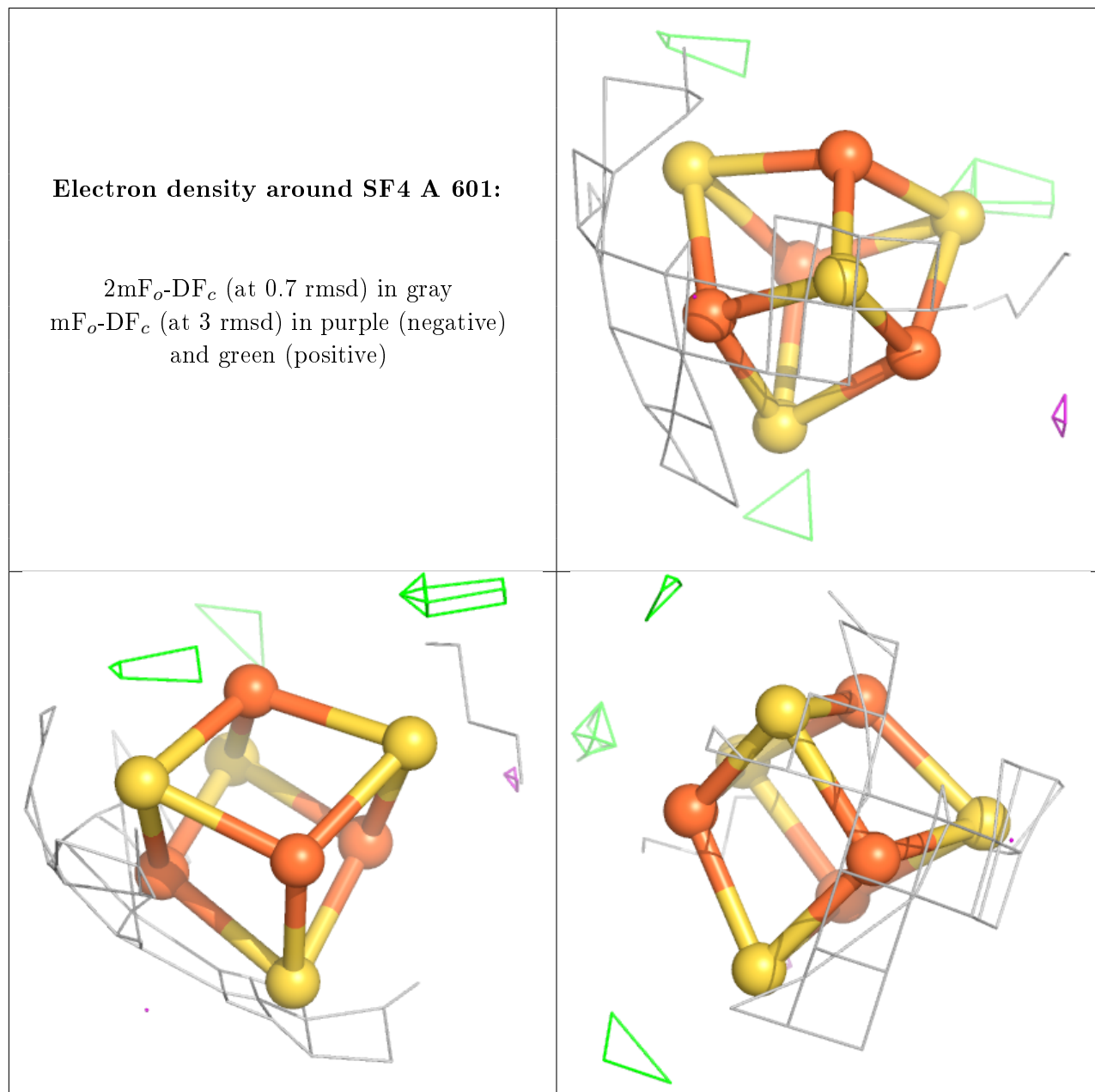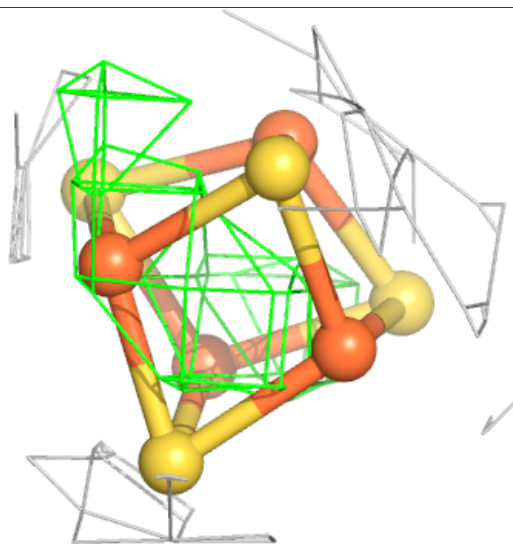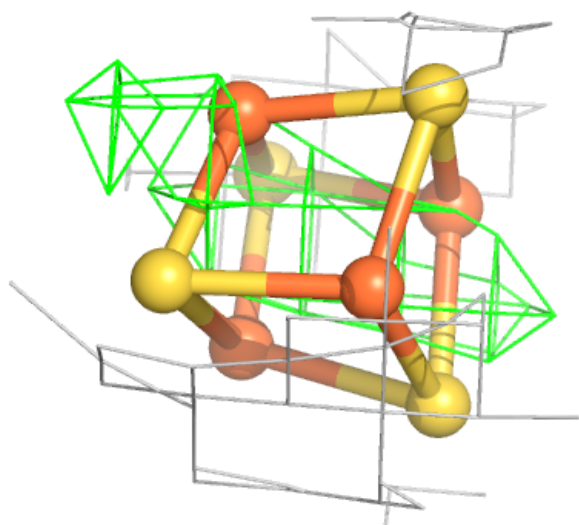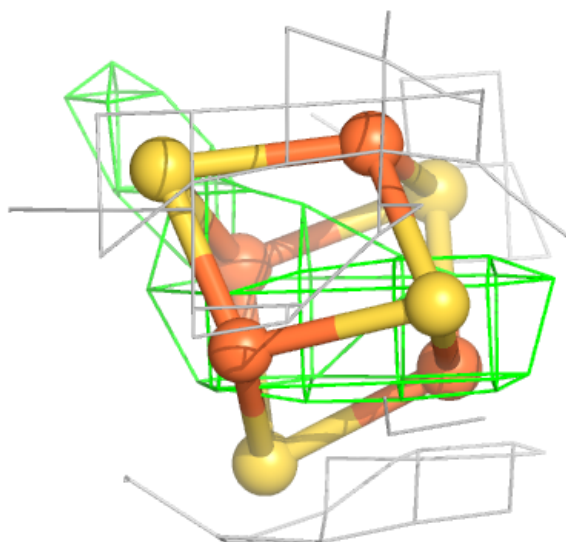
Electron density around SF4 C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
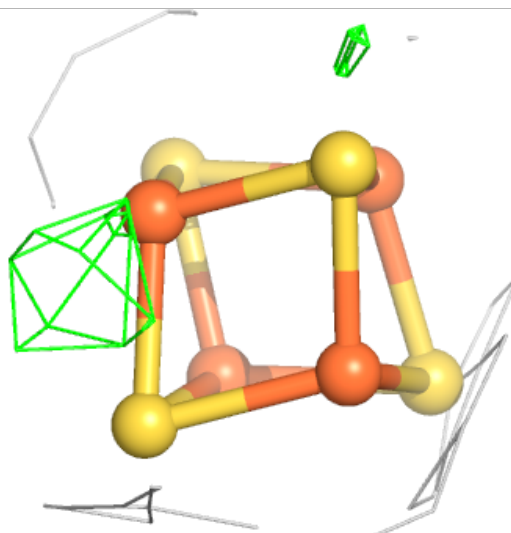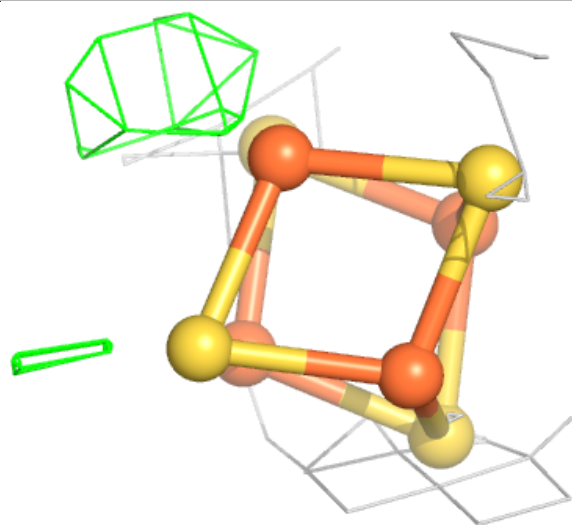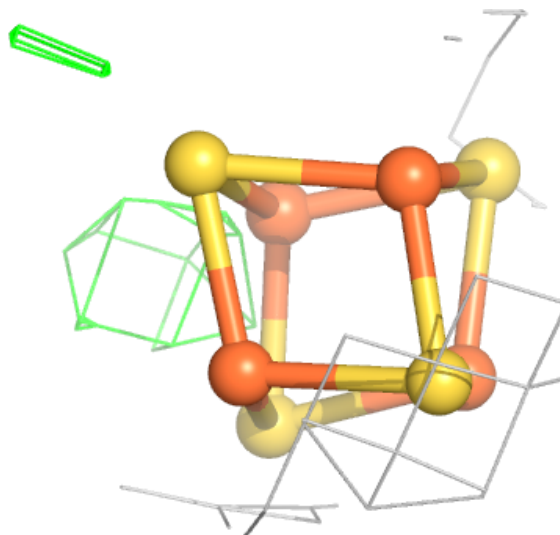
Electron density around SF4 F 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
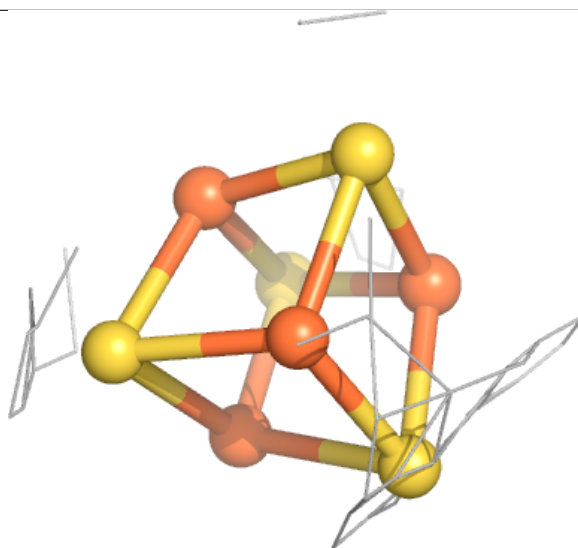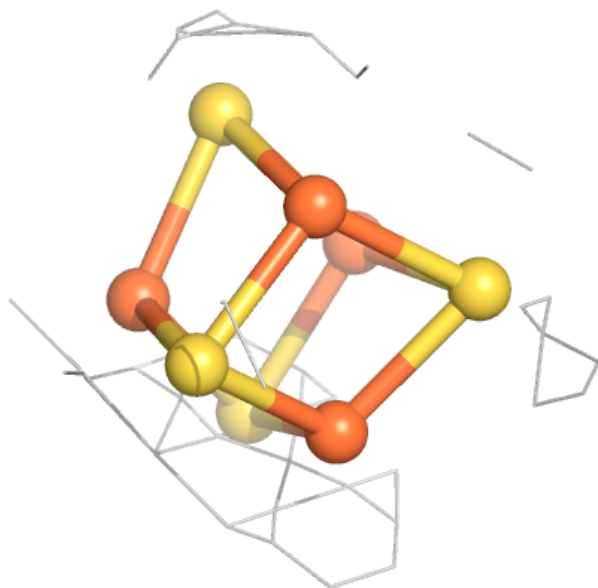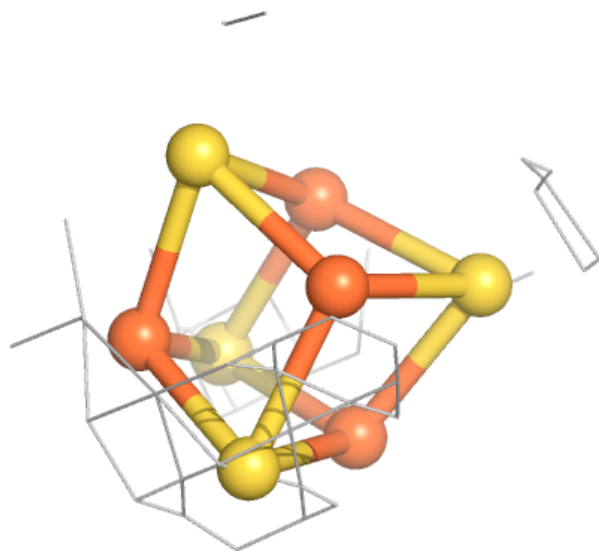
Electron density around SF4 E 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
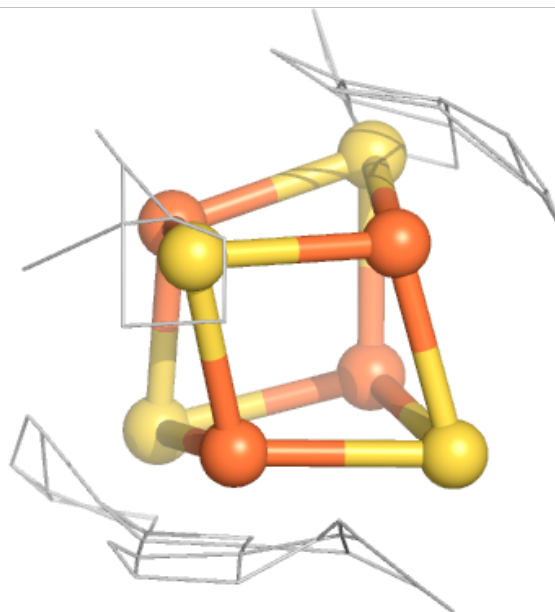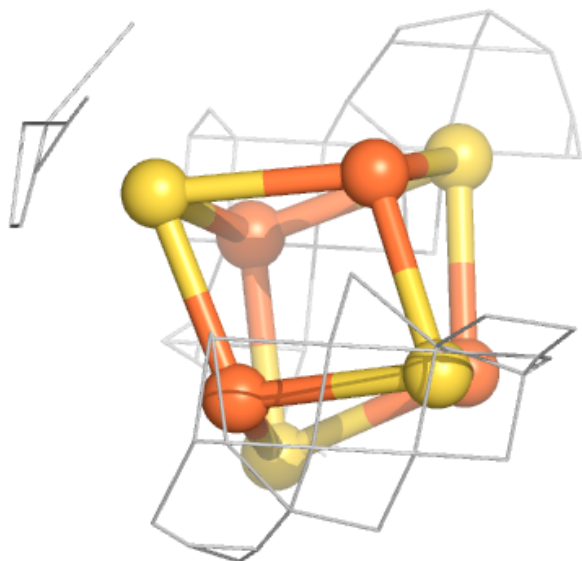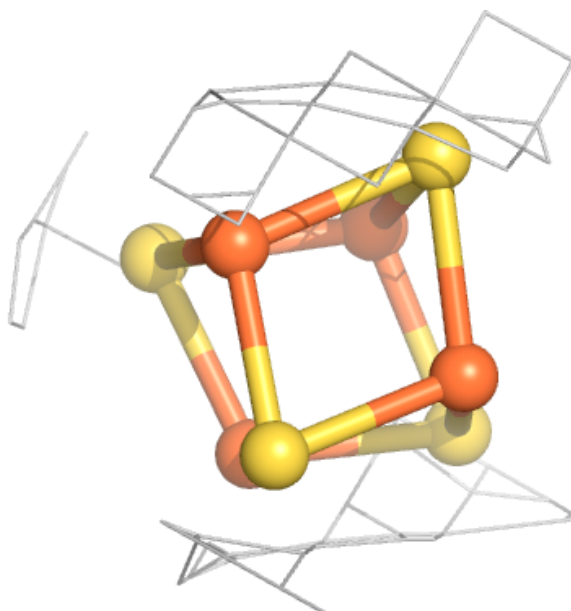
Electron density around SF4 G 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
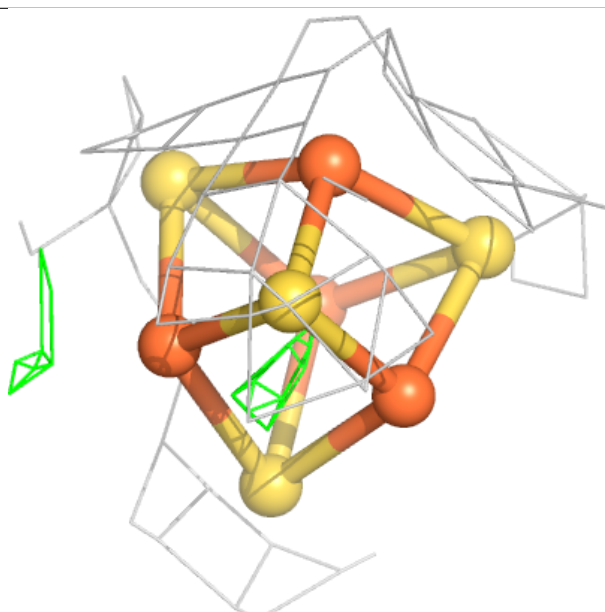and green (positive)
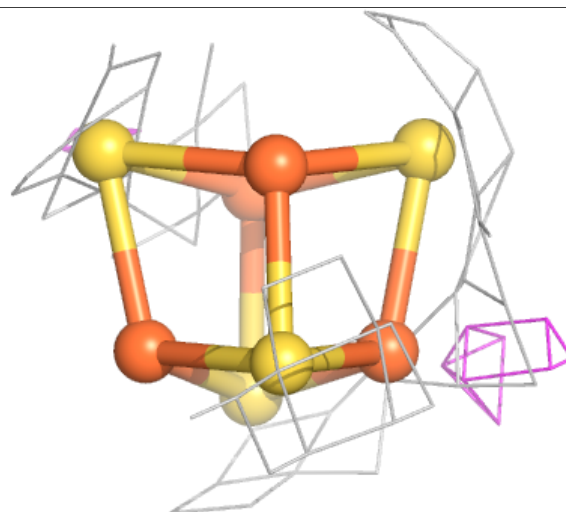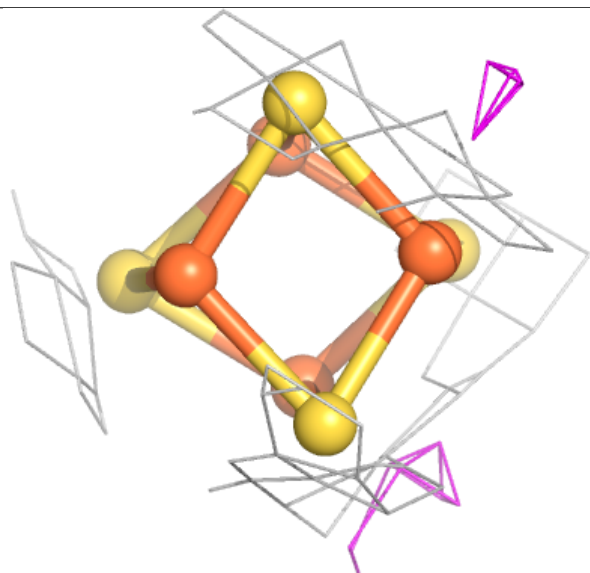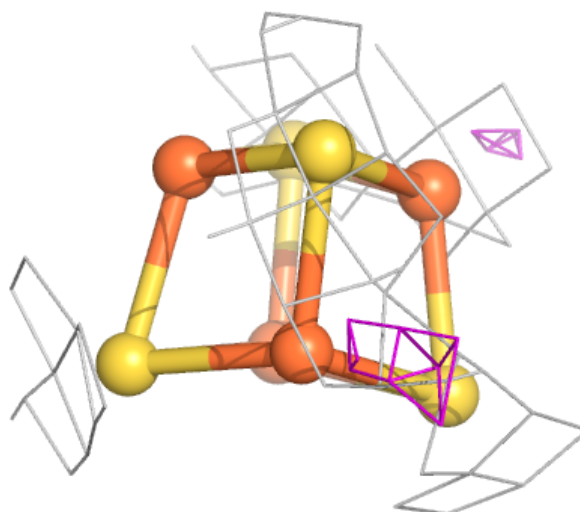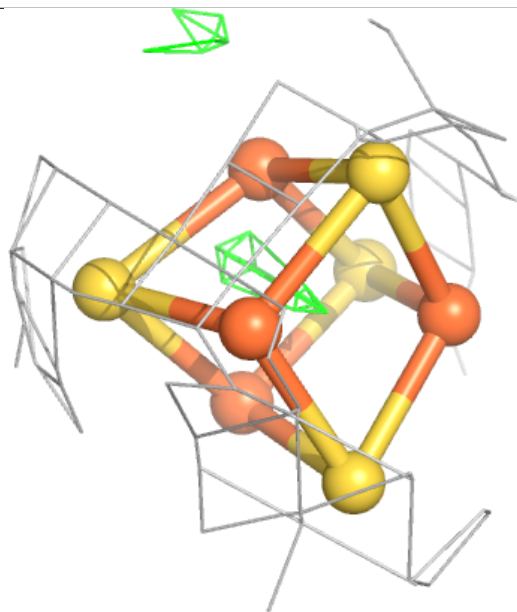
Electron density around SF4 H 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
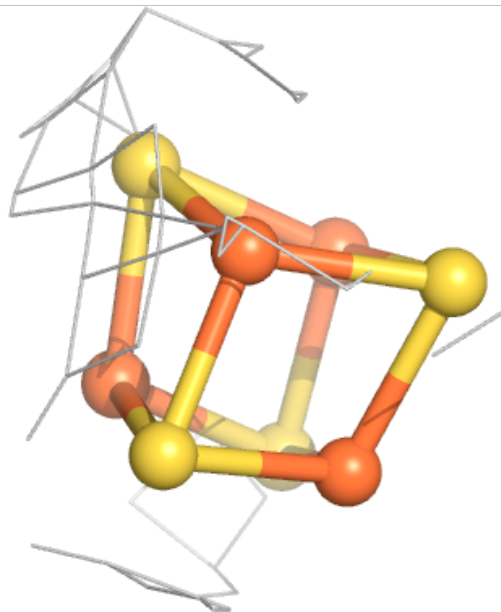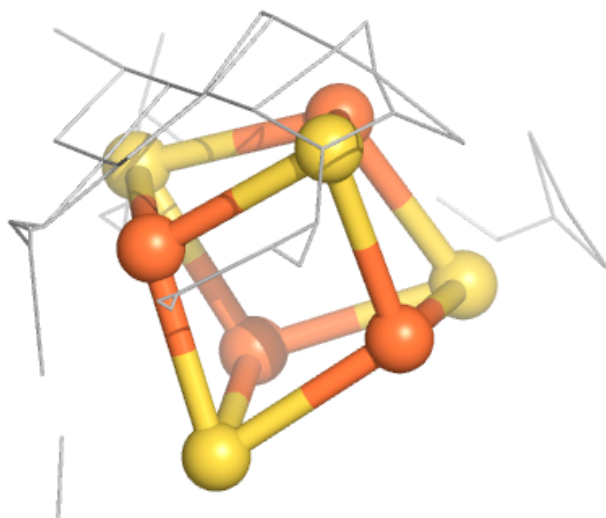
Electron density around SF4 A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
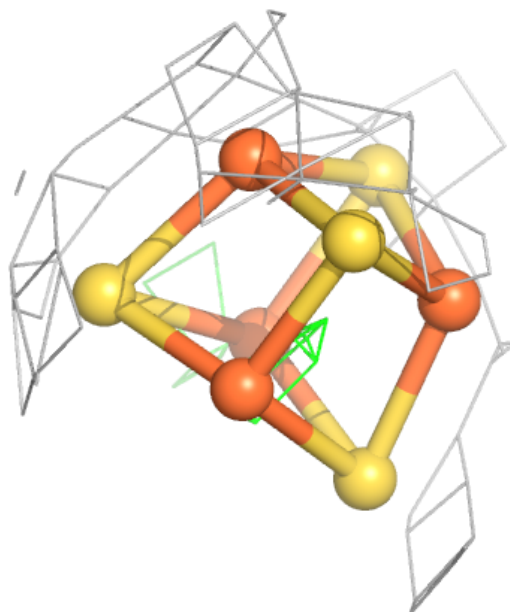
Electron density around SF4 B 601:

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

Electron density around SF4 D 601:

$2mF_o\text{-}DF_c$ (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.