



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2021 – 12:30 PM EST

PDB ID : 6VJR
Title : Oxygen tolerant Archeal 4hydroxybutyrylCoA dehydratase (4HBD) from N. maritimus
Authors : DeMirci, H.
Deposited on : 2020-01-17
Resolution : 1.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

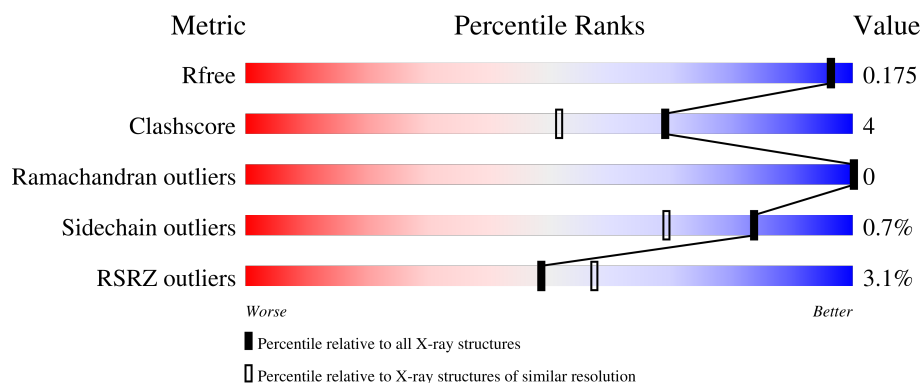
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	502	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
1	B	502	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	C	502	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	D	502	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>

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	A	601	-	-	X	-
2	SF4	B	601	-	-	X	X
2	SF4	C	601	-	-	X	-
2	SF4	D	601	-	-	X	-

2 Entry composition [i](#)

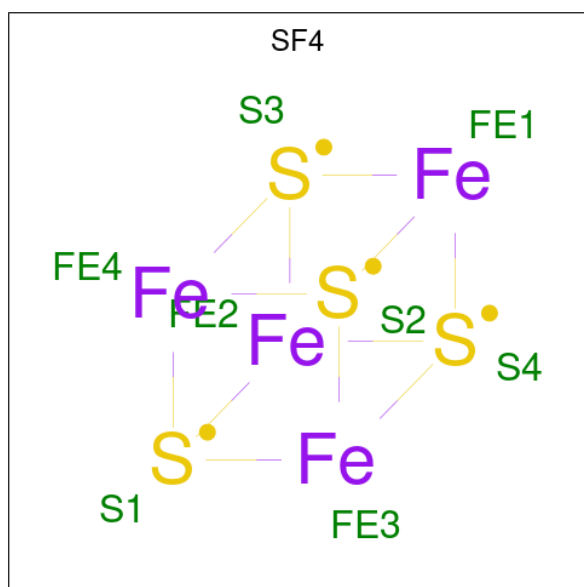
There are 7 unique types of molecules in this entry. The entry contains 18155 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Vinylacetyl-CoA Delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	19	0
			4074	2547	716	783	28			
1	B	501	Total	C	N	O	S	8	14	0
			4029	2522	708	774	25			
1	C	500	Total	C	N	O	S	0	15	0
			4024	2517	707	773	27			
1	D	500	Total	C	N	O	S	0	14	0
			4021	2513	706	775	27			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



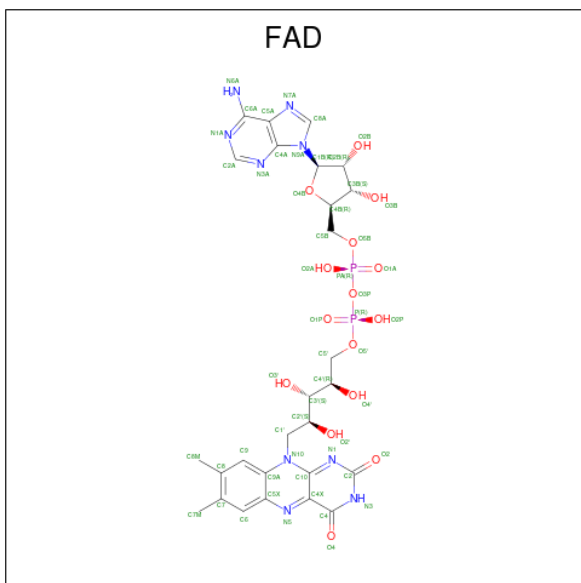
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



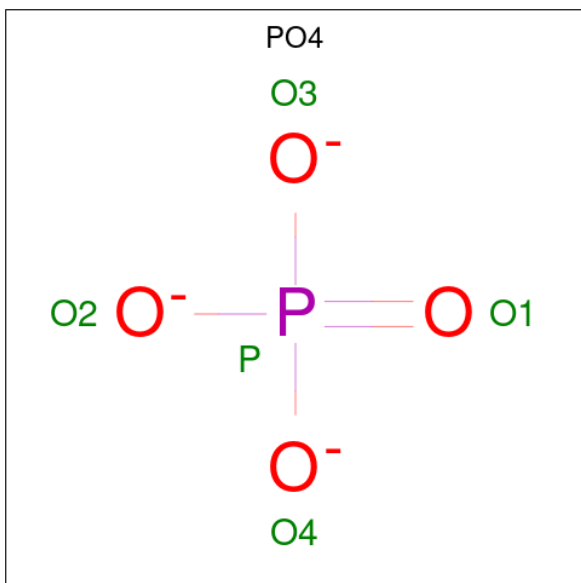
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

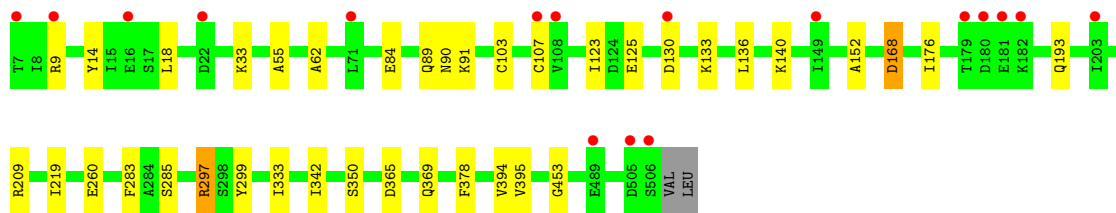
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		
6	A	1	Total	Fe	0	0
			1	1		
6	D	1	Total	Fe	0	0
			1	1		
6	C	1	Total	Fe	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	434	Total	O	0	10
			444	444		
7	B	430	Total	O	0	4
			435	435		
7	C	420	Total	O	0	4
			424	424		
7	D	416	Total	O	0	14
			431	431		

- Molecule 1: Vinylacetyl-CoA Delta-isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.53Å 72.95Å 180.52Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	34.86 – 1.55 34.86 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.86-1.55) 97.8 (34.86-1.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.55Å)	Xtrriage
Refinement program	PHENIX phenix-dev-3318	Depositor
R, R_{free}	0.158 , 0.175 0.158 , 0.175	Depositor DCC
R_{free} test set	1998 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtrriage
Anisotropy	0.681	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18155	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 31.72 % 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 1.0562e-03. 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: PO4, SF4, SO4, FAD, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/4144	0.47	0/5584
1	B	0.27	0/4102	0.49	2/5528 (0.0%)
1	C	0.26	0/4106	0.45	0/5529
1	D	0.26	0/4094	0.45	0/5515
All	All	0.26	0/16446	0.46	2/22156 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	B	466	ARG	NE-CZ-NH1	-7.52	116.54	120.30

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	4074	0	4030	31	0
1	B	4029	0	3994	31	0
1	C	4024	0	3991	26	0
1	D	4021	0	3973	28	0
2	A	8	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	0	9	0
2	C	8	0	0	4	0
2	D	8	0	0	3	0
3	A	53	0	29	0	0
3	B	53	0	29	1	0
3	C	53	0	29	1	0
3	D	53	0	29	1	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	444	0	0	7	0
7	B	435	0	0	4	0
7	C	424	0	0	4	0
7	D	431	0	0	6	0
All	All	18155	0	16104	122	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 4.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:NH1	1:B:350:SER:OG	1.61	1.28
2:A:601:SF4:S3	7:A:761:HOH:O	2.09	1.11
2:B:601:SF4:S2	2:B:601:SF4:FE3	1.47	1.06
1:D:89:GLN:OE1	1:D:297:ARG:NH1	1.95	0.98
2:D:601:SF4:S2	7:D:849:HOH:O	2.23	0.96
2:C:601:SF4:S3	7:C:731:HOH:O	2.22	0.95
1:B:89:GLN:OE1	1:B:297:ARG:NH2	2.01	0.94
2:B:601:SF4:S4	7:B:904:HOH:O	2.30	0.89
2:D:601:SF4:FE2	2:D:601:SF4:S4	1.66	0.86
2:D:601:SF4:S3	2:D:601:SF4:FE3	1.68	0.85
2:B:601:SF4:FE1	2:B:601:SF4:S4	1.70	0.84
2:B:601:SF4:S2	2:B:601:SF4:S1	2.77	0.82
1:C:208:ILE:HD13	1:C:209:ARG:O	1.88	0.74
1:D:84:GLU:OE1	7:D:701:HOH:O	2.06	0.73
1:D:297:ARG:NH2	1:D:350:SER:OG	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLU:OE1	2:B:601:SF4:S4	2.49	0.71
2:B:601:SF4:S1	2:B:601:SF4:FE2	1.83	0.71
1:D:33:LYS:NZ	7:D:704:HOH:O	2.24	0.70
1:A:449:GLU:OE1	2:A:601:SF4:S4	2.50	0.70
1:A:215:LYS:NZ	7:A:703:HOH:O	2.25	0.69
1:C:207:THR:HG23	1:C:208:ILE:HG23	1.73	0.69
1:C:449[A]:GLU:OE2	2:C:601:SF4:S4	2.51	0.69
1:A:301[C]:CYS:SG	7:A:1042:HOH:O	2.51	0.69
1:C:212:GLU:O	1:C:215:LYS:HG3	1.97	0.65
1:C:423:ASP:OD1	7:C:701:HOH:O	2.12	0.65
2:B:601:SF4:S1	2:B:601:SF4:FE4	1.89	0.65
1:D:130:ASP:OD1	7:D:702[A]:HOH:O	2.14	0.65
1:C:129:THR:O	7:C:702[A]:HOH:O	2.15	0.64
1:D:209:ARG:HG3	1:D:285:SER:HB3	1.81	0.63
1:B:69:THR:HG21	1:B:140:LYS:HA	1.80	0.63
2:B:601:SF4:S2	2:B:601:SF4:FE4	1.90	0.62
1:D:103[B]:CYS:SG	7:D:1039[B]:HOH:O	2.56	0.62
1:A:507:VAL:HG13	1:A:508:LEU:HD13	1.82	0.61
1:D:107:CYS:SG	7:D:849:HOH:O	2.57	0.60
1:C:208:ILE:O	1:C:208:ILE:HD12	2.01	0.60
1:B:488:GLU:OE1	7:B:701:HOH:O	2.18	0.57
1:C:208:ILE:C	1:C:208:ILE:HD12	2.26	0.56
1:A:59:GLU:OE2	7:A:702:HOH:O	2.18	0.56
1:A:59:GLU:OE1	7:A:701:HOH:O	2.18	0.56
1:A:468:MET:HE1	1:D:333:ILE:HG12	1.89	0.55
1:D:136:LEU:O	1:D:140:LYS:HG3	2.08	0.53
1:A:468:MET:HE1	1:D:333:ILE:HA	1.91	0.53
1:D:130:ASP:HA	1:D:133:LYS:HE2	1.89	0.53
1:C:449[B]:GLU:OE1	2:C:601:SF4:S4	2.68	0.52
1:A:7:THR:N	7:A:723:HOH:O	2.42	0.51
1:D:394:VAL:HG13	1:D:395:VAL:HG13	1.93	0.49
1:D:365:ASP:O	1:D:369:GLN:HG2	2.13	0.48
1:B:228:LYS:HE2	1:B:228:LYS:HA	1.95	0.48
1:C:365:ASP:O	1:C:369:GLN:HG2	2.12	0.48
1:B:301:CYS:SG	2:B:601:SF4:S3	3.12	0.48
1:A:372[B]:LYS:O	1:A:375[B]:VAL:HG12	2.14	0.48
1:A:397:LEU:HD11	1:A:428:MET:HG2	1.95	0.48
1:B:365:ASP:O	1:B:369:GLN:HG2	2.15	0.47
1:A:168:ASP:OD1	1:C:420:LYS:HD2	2.14	0.47
1:A:394:VAL:HG13	1:A:395:VAL:HG13	1.97	0.47
1:A:365:ASP:O	1:A:369:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:HD11	1:B:428:MET:HG2	1.97	0.46
1:D:297:ARG:HH21	1:D:350:SER:HG	1.62	0.46
1:D:55:ALA:HA	1:D:62:ALA:HB3	1.96	0.46
1:C:210:LEU:HD22	1:C:214:ASP:HB3	1.97	0.45
1:C:301:CYS:SG	2:C:601:SF4:S3	3.13	0.45
1:D:176:ILE:HD11	1:D:219:ILE:HD13	1.97	0.45
1:A:103[A]:CYS:HA	2:A:601:SF4:S1	2.56	0.45
1:C:208:ILE:C	1:C:208:ILE:CD1	2.84	0.45
1:C:55:ALA:HA	1:C:62:ALA:HB3	1.99	0.45
1:A:103[B]:CYS:HA	2:A:601:SF4:S1	2.56	0.45
1:A:162:LYS:HB3	1:A:166:GLU:HB2	1.98	0.45
1:D:90:ASN:ND2	1:D:297:ARG:NH2	2.65	0.45
1:B:179[B]:THR:HG22	1:B:184:VAL:HG12	1.97	0.45
1:C:294:TYR:HD1	1:C:297:ARG:HH21	1.65	0.44
1:D:9:ARG:HB2	1:D:9:ARG:CZ	2.47	0.44
1:A:302:LYS:NZ	7:A:724[A]:HOH:O	2.42	0.44
1:B:181:GLU:H	1:B:181:GLU:CD	2.19	0.44
1:D:14:TYR:CZ	1:D:18:LEU:HD11	2.52	0.44
1:B:69:THR:CG2	1:B:140:LYS:HA	2.47	0.44
1:B:76:PHE:CD1	1:B:106:ARG:HB3	2.53	0.44
1:A:299:TYR:OH	1:A:453:GLY:HA3	2.18	0.44
1:D:299:TYR:OH	1:D:453:GLY:HA3	2.18	0.44
1:B:152:ALA:HA	1:B:193:GLN:OE1	2.19	0.43
1:B:452:HIS:O	3:B:602:FAD:H4'	2.19	0.43
1:A:76:PHE:CD1	1:A:106:ARG:HB3	2.54	0.43
1:A:27:LEU:HD13	1:A:234:TYR:HB3	2.01	0.43
1:B:420:LYS:HD2	1:D:168:ASP:OD1	2.19	0.43
1:C:182:LYS:HB2	1:C:182:LYS:HE3	1.76	0.43
1:A:181:GLU:HG2	1:A:182:LYS:HG2	2.01	0.43
1:C:152:ALA:HA	1:C:193:GLN:OE1	2.19	0.43
1:C:302:LYS:NZ	7:C:717:HOH:O	2.43	0.43
1:C:400:GLU:O	1:C:404:ARG:HG2	2.19	0.43
1:D:342:ILE:HD11	1:D:378:PHE:HB2	2.01	0.43
1:B:55:ALA:HA	1:B:62:ALA:HB3	2.00	0.43
1:C:257:GLY:HA2	1:C:442:ASN:HD21	1.84	0.43
1:A:152:ALA:HA	1:A:193:GLN:OE1	2.19	0.42
1:B:342:ILE:HD11	1:B:378:PHE:HB2	2.02	0.42
1:D:260[A]:GLU:HG2	3:D:602:FAD:HM72	2.01	0.42
1:B:90:ASN:OD1	1:B:297:ARG:NH1	2.53	0.42
1:B:69:THR:O	1:B:71:LEU:N	2.52	0.42
1:B:394:VAL:HG13	1:B:395:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LYS:O	1:B:375[B]:VAL:HG12	2.19	0.42
1:A:55:ALA:HA	1:A:62:ALA:HB3	2.01	0.41
1:B:400:GLU:O	1:B:404:ARG:HG2	2.20	0.41
1:A:468:MET:HG3	1:A:470:VAL:HG23	2.01	0.41
1:C:394:VAL:HG13	1:C:395:VAL:HG13	2.02	0.41
1:B:90:ASN:HD21	1:B:297:ARG:HD2	1.86	0.41
1:B:468:MET:HG3	1:B:470:VAL:HG23	2.02	0.41
1:A:342:ILE:HD11	1:A:378:PHE:HB2	2.03	0.41
1:A:449:GLU:CD	2:A:601:SF4:S4	2.98	0.41
1:D:123:ILE:HG12	1:D:283:PHE:CG	2.55	0.41
1:C:342:ILE:HD11	1:C:378:PHE:HB2	2.03	0.41
1:B:302:LYS:NZ	7:B:714:HOH:O	2.39	0.41
1:D:152:ALA:HA	1:D:193:GLN:OE1	2.21	0.41
1:C:452:HIS:O	3:C:602:FAD:H4'	2.20	0.41
1:B:345:ALA:HA	1:C:344:ALA:HB1	2.03	0.41
1:B:103[A]:CYS:SG	7:B:985:HOH:O	2.63	0.41
1:A:72:LYS:HA	1:A:72:LYS:HD2	1.90	0.40
1:B:175:ARG:HB3	1:B:217:TRP:CD1	2.55	0.40
1:B:502:LYS:HB3	1:B:502:LYS:HE3	1.81	0.40
1:D:90:ASN:CG	1:D:297:ARG:NH2	2.75	0.40
1:A:44:SER:HA	1:A:257:GLY:O	2.22	0.40
1:A:257:GLY:HA2	1:A:442:ASN:HD21	1.87	0.40
1:A:502:LYS:O	1:D:91:LYS:NZ	2.40	0.40
1:B:299:TYR:OH	1:B:453:GLY:HA3	2.21	0.40
1:C:14:TYR:CZ	1:C:18:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	520/502 (104%)	514 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	514/502 (102%)	508 (99%)	6 (1%)	0	100	100
1	C	514/502 (102%)	510 (99%)	4 (1%)	0	100	100
1	D	513/502 (102%)	508 (99%)	5 (1%)	0	100	100
All	All	2061/2008 (103%)	2040 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/425 (105%)	441 (99%)	4 (1%)	78	61
1	B	439/425 (103%)	436 (99%)	3 (1%)	84	69
1	C	439/425 (103%)	436 (99%)	3 (1%)	84	69
1	D	438/425 (103%)	435 (99%)	3 (1%)	84	69
All	All	1761/1700 (104%)	1748 (99%)	13 (1%)	84	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
1	A	179[A]	THR
1	A	179[B]	THR
1	A	297	ARG
1	B	106	ARG
1	B	215	LYS
1	B	297	ARG
1	C	251	ASP
1	C	297	ARG
1	C	504	LYS
1	D	125	GLU
1	D	168	ASP
1	D	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	442	ASN
1	B	436	ASN
1	B	442	ASN
1	C	436	ASN
1	C	442	ASN
1	D	436	ASN
1	D	442	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SF4	C	601	1,7	0,12,12	0.00	-	-		
2	SF4	D	601	1,7	0,12,12	0.00	-	-		
4	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	602	-	51,58,58	3.04	14 (27%)	60,89,89	2.60	14 (23%)
3	FAD	C	602	-	51,58,58	3.04	14 (27%)	60,89,89	2.64	15 (25%)
4	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.05	0
3	FAD	D	602	-	51,58,58	3.05	14 (27%)	60,89,89	2.59	15 (25%)
4	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.06	0
3	FAD	B	602	-	51,58,58	3.05	15 (29%)	60,89,89	2.61	16 (26%)
5	PO4	A	606	-	4,4,4	0.92	0	6,6,6	0.41	0
2	SF4	A	601	1,7	0,12,12	0.00	-	-	-	-
2	SF4	B	601	1,7	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
2	SF4	C	601	1,7	-	-	0/6/5/5
2	SF4	D	601	1,7	-	-	1/6/5/5
3	FAD	A	602	-	-	6/30/50/50	0/6/6/6
3	FAD	C	602	-	-	6/30/50/50	0/6/6/6
3	FAD	D	602	-	-	6/30/50/50	0/6/6/6
3	FAD	B	602	-	-	6/30/50/50	0/6/6/6
2	SF4	A	601	1,7	-	-	0/6/5/5
2	SF4	B	601	1,7	-	-	0/6/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	FAD	O2'-C2'	-11.02	1.20	1.43
3	A	602	FAD	O2'-C2'	-11.01	1.20	1.43
3	B	602	FAD	O2'-C2'	-10.96	1.20	1.43
3	C	602	FAD	O2'-C2'	-10.88	1.20	1.43
3	A	602	FAD	C2B-C3B	-9.84	1.26	1.53
3	B	602	FAD	C2B-C3B	-9.83	1.26	1.53
3	D	602	FAD	C2B-C3B	-9.82	1.26	1.53
3	C	602	FAD	C2B-C3B	-9.79	1.26	1.53
3	C	602	FAD	O4B-C1B	7.23	1.51	1.41
3	A	602	FAD	O4B-C1B	7.22	1.51	1.41
3	B	602	FAD	O4B-C1B	7.13	1.51	1.41
3	D	602	FAD	O4B-C1B	7.01	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	FAD	O4B-C4B	-6.05	1.31	1.45
3	D	602	FAD	O4-C4	6.02	1.39	1.24
3	C	602	FAD	O4B-C4B	-6.02	1.31	1.45
3	D	602	FAD	O4B-C4B	-6.00	1.31	1.45
3	C	602	FAD	O4-C4	5.99	1.39	1.24
3	A	602	FAD	O4B-C4B	-5.93	1.31	1.45
3	B	602	FAD	O4-C4	5.91	1.39	1.24
3	A	602	FAD	O4-C4	5.91	1.39	1.24
3	C	602	FAD	C3B-C4B	5.34	1.66	1.53
3	B	602	FAD	C3B-C4B	5.30	1.66	1.53
3	A	602	FAD	C3B-C4B	5.28	1.66	1.53
3	D	602	FAD	C3B-C4B	5.25	1.66	1.53
3	B	602	FAD	C2B-C1B	4.49	1.60	1.53
3	C	602	FAD	C2B-C1B	4.46	1.60	1.53
3	D	602	FAD	C2B-C1B	4.44	1.60	1.53
3	A	602	FAD	C2B-C1B	4.42	1.60	1.53
3	B	602	FAD	C6A-N6A	3.46	1.46	1.34
3	D	602	FAD	C6A-N6A	3.45	1.46	1.34
3	A	602	FAD	C6A-N6A	3.43	1.46	1.34
3	C	602	FAD	C6A-N6A	3.42	1.46	1.34
3	C	602	FAD	O2B-C2B	3.08	1.50	1.43
3	B	602	FAD	O2B-C2B	3.05	1.50	1.43
3	D	602	FAD	O2B-C2B	3.03	1.50	1.43
3	A	602	FAD	O2B-C2B	2.95	1.49	1.43
3	A	602	FAD	C2-N3	-2.59	1.33	1.38
3	D	602	FAD	O3B-C3B	2.57	1.49	1.43
3	C	602	FAD	C2-N3	-2.57	1.33	1.38
3	B	602	FAD	C2-N3	-2.55	1.33	1.38
3	D	602	FAD	C2-N3	-2.54	1.33	1.38
3	B	602	FAD	O3B-C3B	2.46	1.48	1.43
3	A	602	FAD	O3B-C3B	2.44	1.48	1.43
3	C	602	FAD	O3B-C3B	2.43	1.48	1.43
3	B	602	FAD	C2-N1	-2.39	1.33	1.38
3	D	602	FAD	C2-N1	-2.36	1.33	1.38
3	C	602	FAD	C2-N1	-2.33	1.33	1.38
3	A	602	FAD	C2-N1	-2.33	1.33	1.38
3	B	602	FAD	C9A-C5X	-2.19	1.38	1.42
3	C	602	FAD	C9A-C5X	-2.16	1.38	1.42
3	D	602	FAD	C9A-C5X	-2.13	1.38	1.42
3	A	602	FAD	C9A-C5X	-2.08	1.38	1.42
3	D	602	FAD	C7M-C7	2.08	1.55	1.51
3	B	602	FAD	C5'-C4'	2.08	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	FAD	C7M-C7	2.07	1.55	1.51
3	A	602	FAD	C7M-C7	2.07	1.55	1.51
3	B	602	FAD	C7M-C7	2.05	1.55	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	FAD	C1'-N10-C10	-9.31	110.07	118.41
3	B	602	FAD	C1'-N10-C10	-8.67	110.64	118.41
3	A	602	FAD	C1'-N10-C10	-8.65	110.67	118.41
3	D	602	FAD	C1'-N10-C10	-8.61	110.70	118.41
3	B	602	FAD	C1'-N10-C9A	-8.50	111.60	118.29
3	A	602	FAD	C1'-N10-C9A	-8.32	111.75	118.29
3	C	602	FAD	C4-N3-C2	8.29	122.14	115.14
3	D	602	FAD	C1'-N10-C9A	-8.17	111.86	118.29
3	C	602	FAD	C1'-N10-C9A	-8.16	111.87	118.29
3	A	602	FAD	C4-N3-C2	7.88	121.80	115.14
3	B	602	FAD	C4-N3-C2	7.78	121.71	115.14
3	D	602	FAD	C4-N3-C2	7.70	121.64	115.14
3	D	602	FAD	C9A-N10-C10	-7.04	112.68	121.91
3	B	602	FAD	C9A-N10-C10	-7.00	112.74	121.91
3	C	602	FAD	C9A-N10-C10	-6.97	112.78	121.91
3	A	602	FAD	C9A-N10-C10	-6.73	113.10	121.91
3	A	602	FAD	N3A-C2A-N1A	-4.28	121.98	128.68
3	D	602	FAD	N3A-C2A-N1A	-4.17	122.16	128.68
3	B	602	FAD	N3A-C2A-N1A	-4.13	122.23	128.68
3	D	602	FAD	C4X-C4-N3	-4.04	117.91	123.43
3	C	602	FAD	O2'-C2'-C1'	4.02	119.27	109.59
3	C	602	FAD	N3A-C2A-N1A	-4.01	122.41	128.68
3	A	602	FAD	O2'-C2'-C1'	3.98	119.19	109.59
3	B	602	FAD	O2'-C2'-C1'	3.91	119.01	109.59
3	C	602	FAD	O2'-C2'-C3'	3.89	118.57	109.10
3	B	602	FAD	O2'-C2'-C3'	3.89	118.55	109.10
3	D	602	FAD	O2'-C2'-C1'	3.85	118.87	109.59
3	A	602	FAD	O2'-C2'-C3'	3.82	118.39	109.10
3	B	602	FAD	C4X-C4-N3	-3.72	118.35	123.43
3	C	602	FAD	C4X-C4-N3	-3.70	118.37	123.43
3	D	602	FAD	O2'-C2'-C3'	3.66	118.01	109.10
3	A	602	FAD	C4X-C4-N3	-3.66	118.43	123.43
3	A	602	FAD	C10-C4X-N5	-3.51	118.83	121.26
3	D	602	FAD	C10-C4X-N5	-3.31	118.97	121.26
3	B	602	FAD	O4B-C1B-C2B	-3.21	102.23	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	FAD	O4B-C1B-C2B	-3.15	102.32	106.93
3	B	602	FAD	C10-C4X-N5	-3.12	119.10	121.26
3	C	602	FAD	C4-C4X-N5	2.99	122.01	118.60
3	A	602	FAD	C4-C4X-N5	2.98	122.01	118.60
3	C	602	FAD	C10-C4X-N5	-2.94	119.23	121.26
3	B	602	FAD	C4-C4X-N5	2.87	121.87	118.60
3	A	602	FAD	P-O3P-PA	-2.83	123.12	132.83
3	D	602	FAD	P-O3P-PA	-2.82	123.13	132.83
3	C	602	FAD	C4A-C5A-N7A	-2.81	106.47	109.40
3	B	602	FAD	C4A-C5A-N7A	-2.81	106.47	109.40
3	D	602	FAD	C4A-C5A-N7A	-2.78	106.50	109.40
3	A	602	FAD	C4A-C5A-N7A	-2.74	106.54	109.40
3	C	602	FAD	P-O3P-PA	-2.74	123.43	132.83
3	B	602	FAD	P-O3P-PA	-2.73	123.45	132.83
3	D	602	FAD	C4-C4X-N5	2.73	121.71	118.60
3	D	602	FAD	C4-C4X-C10	-2.71	118.16	119.95
3	D	602	FAD	O4B-C1B-C2B	-2.69	103.00	106.93
3	C	602	FAD	O4B-C1B-C2B	-2.67	103.02	106.93
3	B	602	FAD	C4-C4X-C10	-2.51	118.29	119.95
3	C	602	FAD	C4-C4X-C10	-2.47	118.32	119.95
3	B	602	FAD	C3B-C2B-C1B	2.45	104.67	100.98
3	A	602	FAD	C3B-C2B-C1B	2.37	104.54	100.98
3	D	602	FAD	C3B-C2B-C1B	2.24	104.35	100.98
3	C	602	FAD	C3B-C2B-C1B	2.14	104.20	100.98
3	B	602	FAD	C1'-C2'-C3'	2.01	115.39	109.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	FAD	C5B-O5B-PA-O2A
3	A	602	FAD	C2'-C1'-N10-C10
3	C	602	FAD	C5B-O5B-PA-O2A
3	C	602	FAD	C2'-C1'-N10-C10
3	D	602	FAD	C5B-O5B-PA-O2A
3	D	602	FAD	C2'-C1'-N10-C10
3	B	602	FAD	C5B-O5B-PA-O2A
3	B	602	FAD	C2'-C1'-N10-C10
3	C	602	FAD	O2'-C2'-C3'-O3'
3	D	602	FAD	O2'-C2'-C3'-O3'
3	B	602	FAD	O2'-C2'-C3'-O3'
3	A	602	FAD	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	C	602	FAD	O2'-C2'-C3'-C4'
3	D	602	FAD	O2'-C2'-C3'-C4'
3	B	602	FAD	O2'-C2'-C3'-C4'
3	A	602	FAD	O2'-C2'-C3'-O3'
3	A	602	FAD	C5B-O5B-PA-O3P
3	C	602	FAD	C5B-O5B-PA-O3P
3	D	602	FAD	C5B-O5B-PA-O3P
3	B	602	FAD	C5B-O5B-PA-O3P
3	A	602	FAD	C5B-O5B-PA-O1A
3	C	602	FAD	C5B-O5B-PA-O1A
3	D	602	FAD	C5B-O5B-PA-O1A
3	B	602	FAD	C5B-O5B-PA-O1A

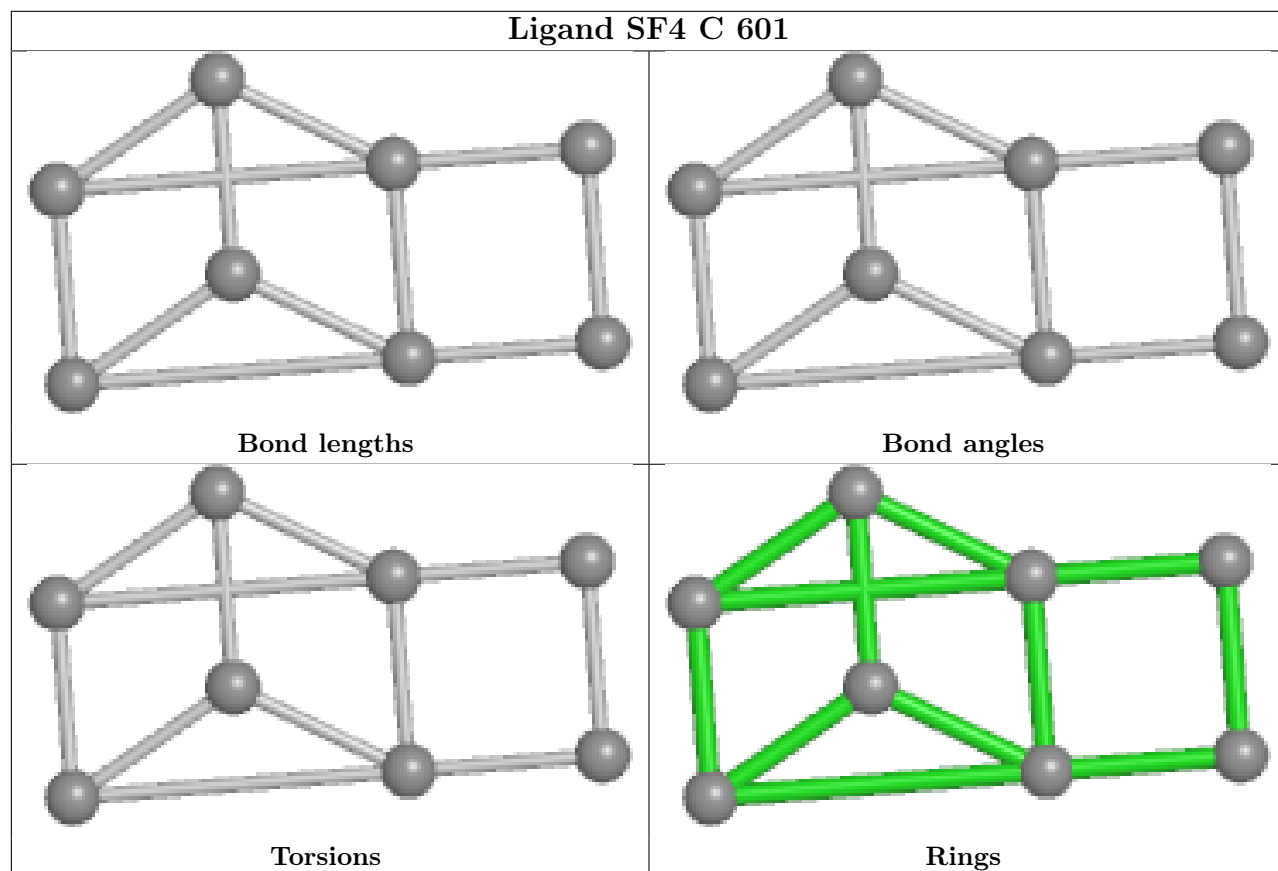
All (1) ring outliers are listed below:

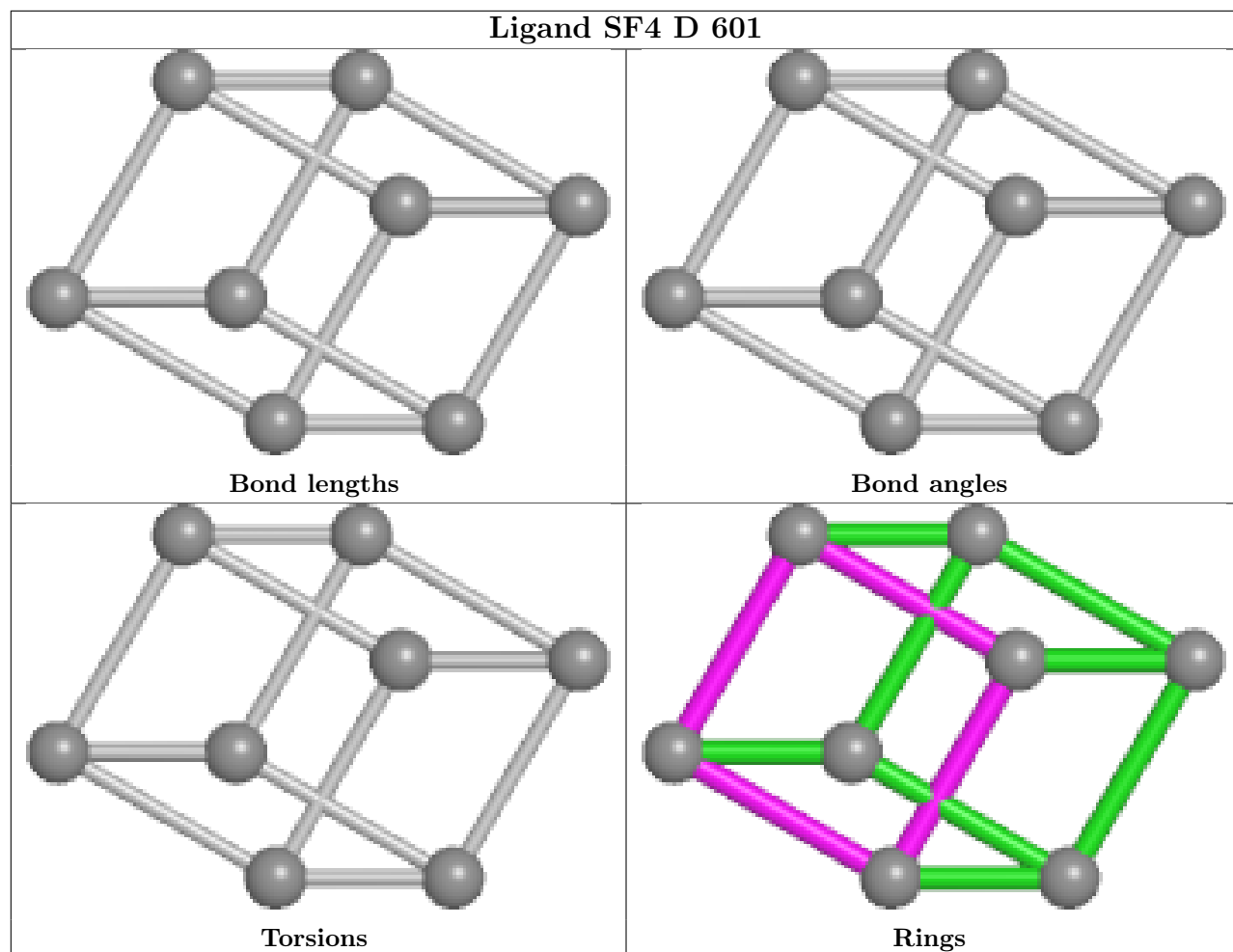
Mol	Chain	Res	Type	Atoms
2	D	601	SF4	FE2-FE4-S1-S3

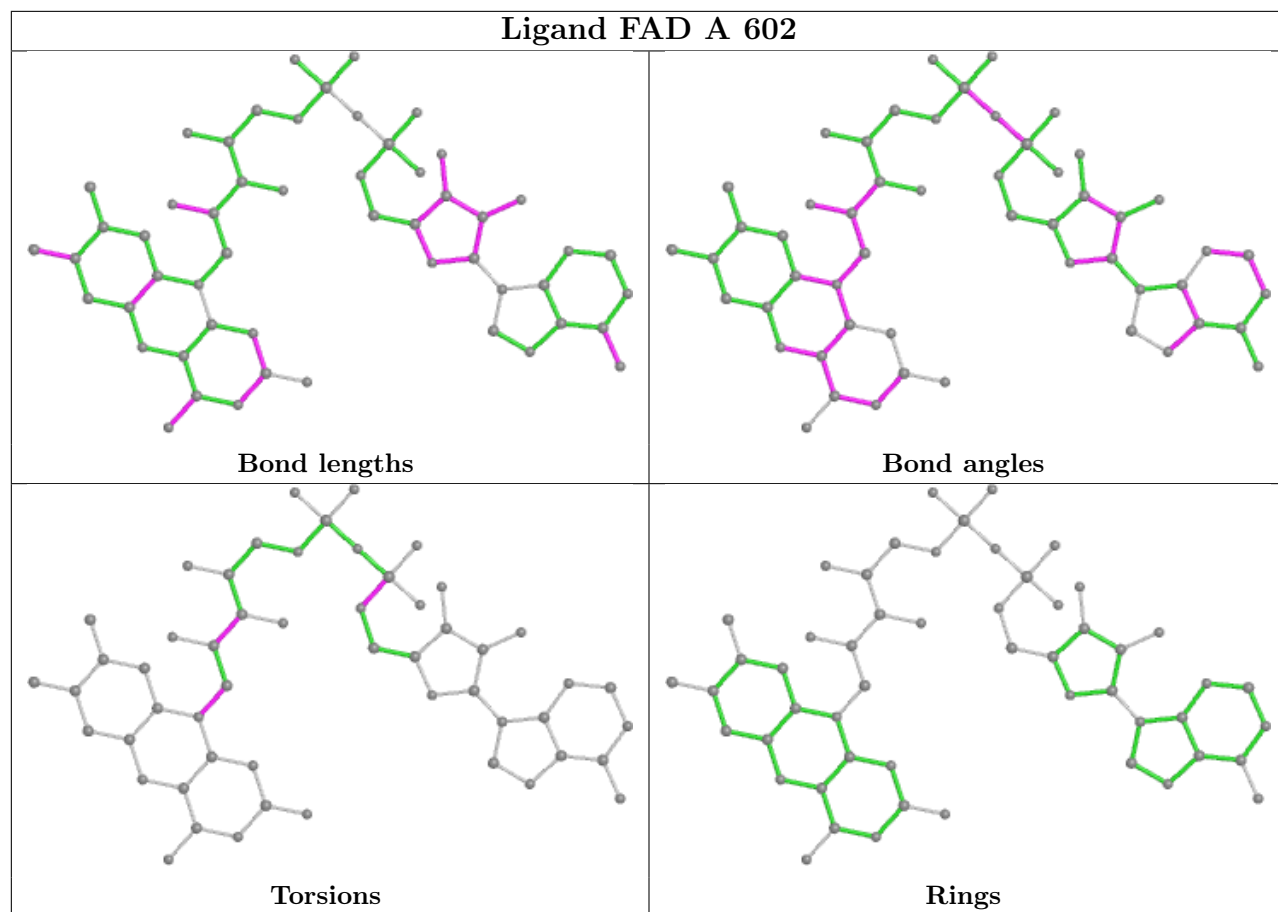
7 monomers are involved in 24 short contacts:

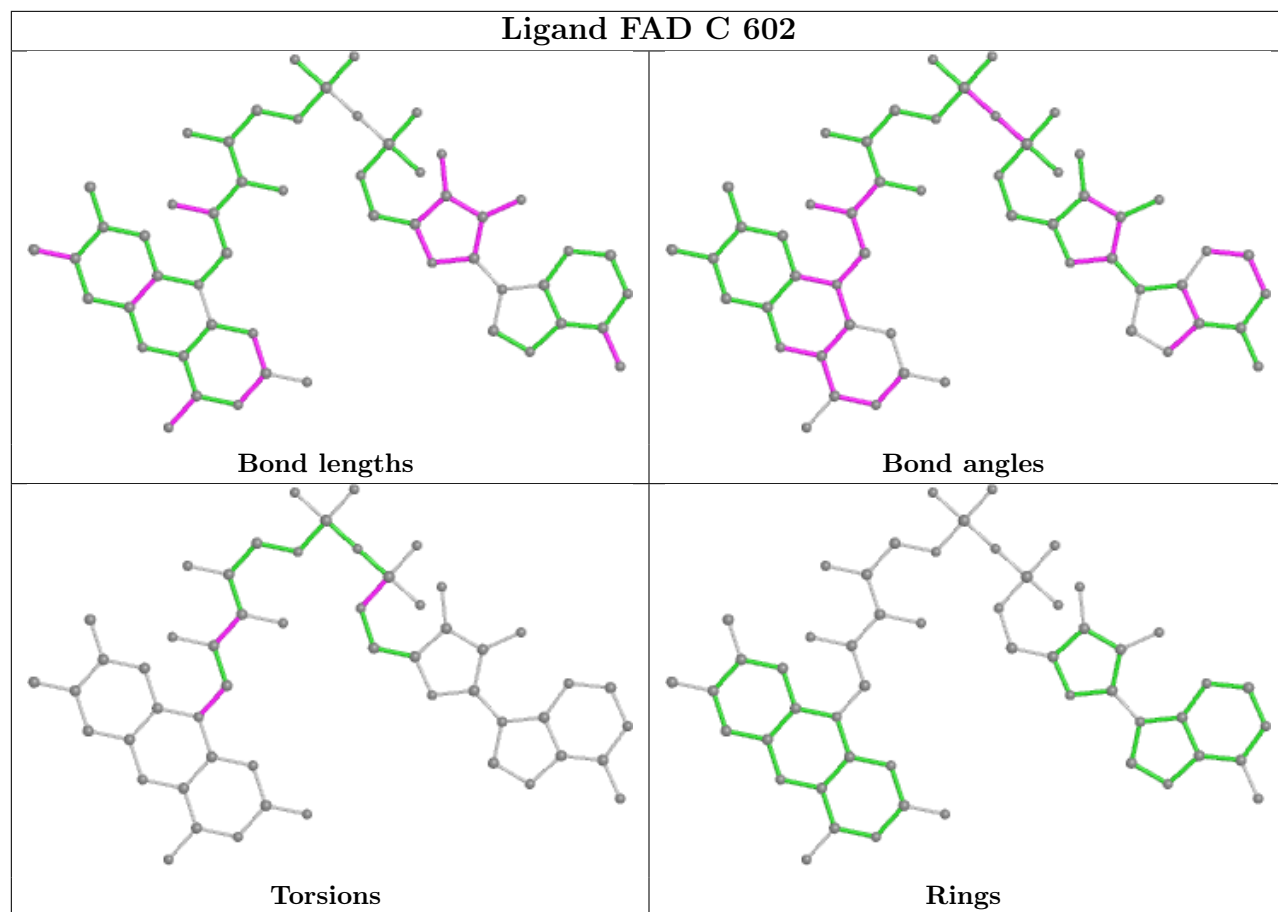
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	SF4	4	0
2	D	601	SF4	3	0
3	C	602	FAD	1	0
3	D	602	FAD	1	0
3	B	602	FAD	1	0
2	A	601	SF4	5	0
2	B	601	SF4	9	0

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.

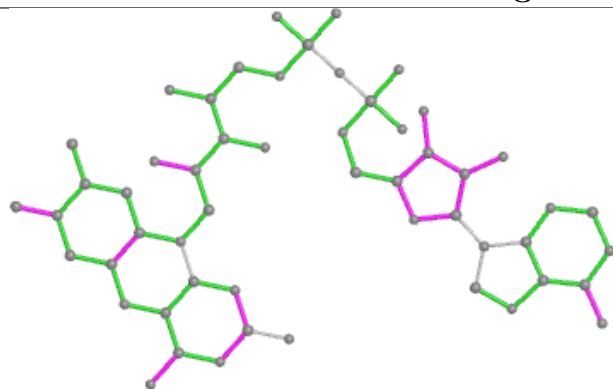




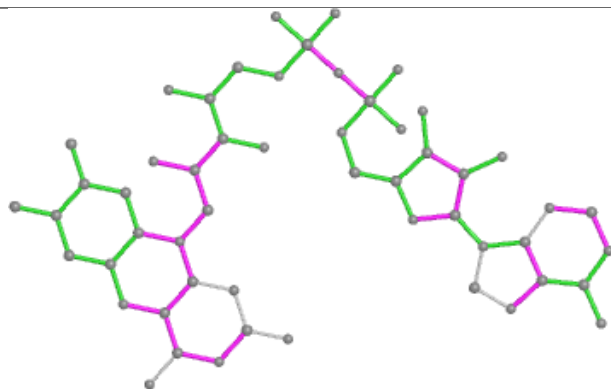




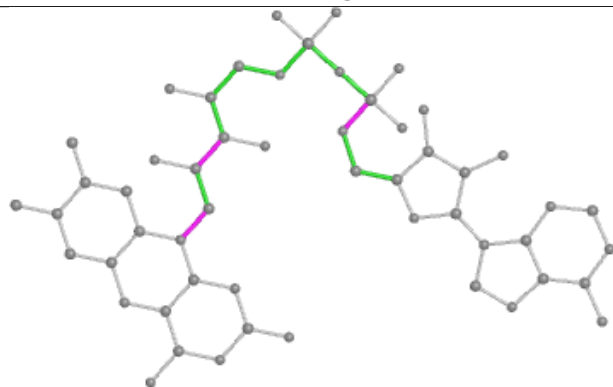
Ligand FAD D 602



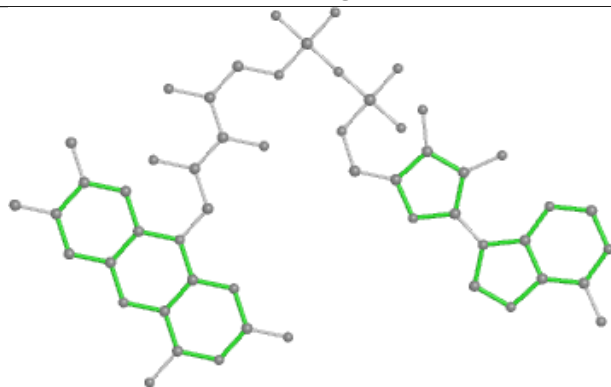
Bond lengths



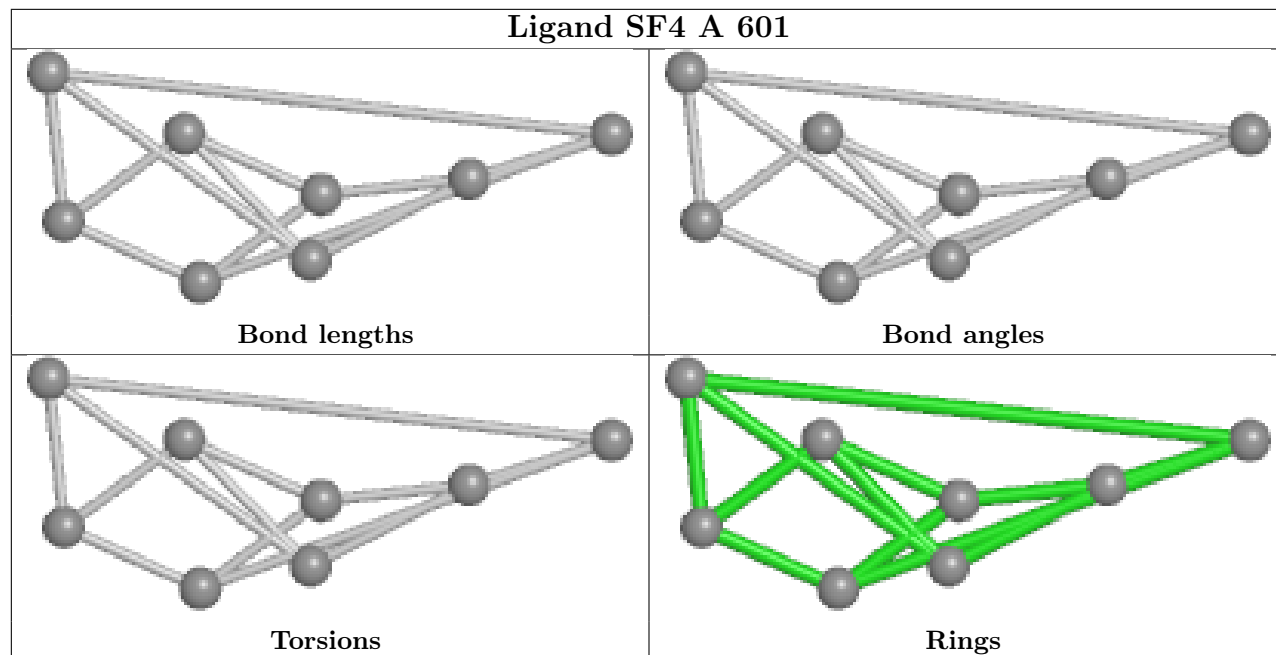
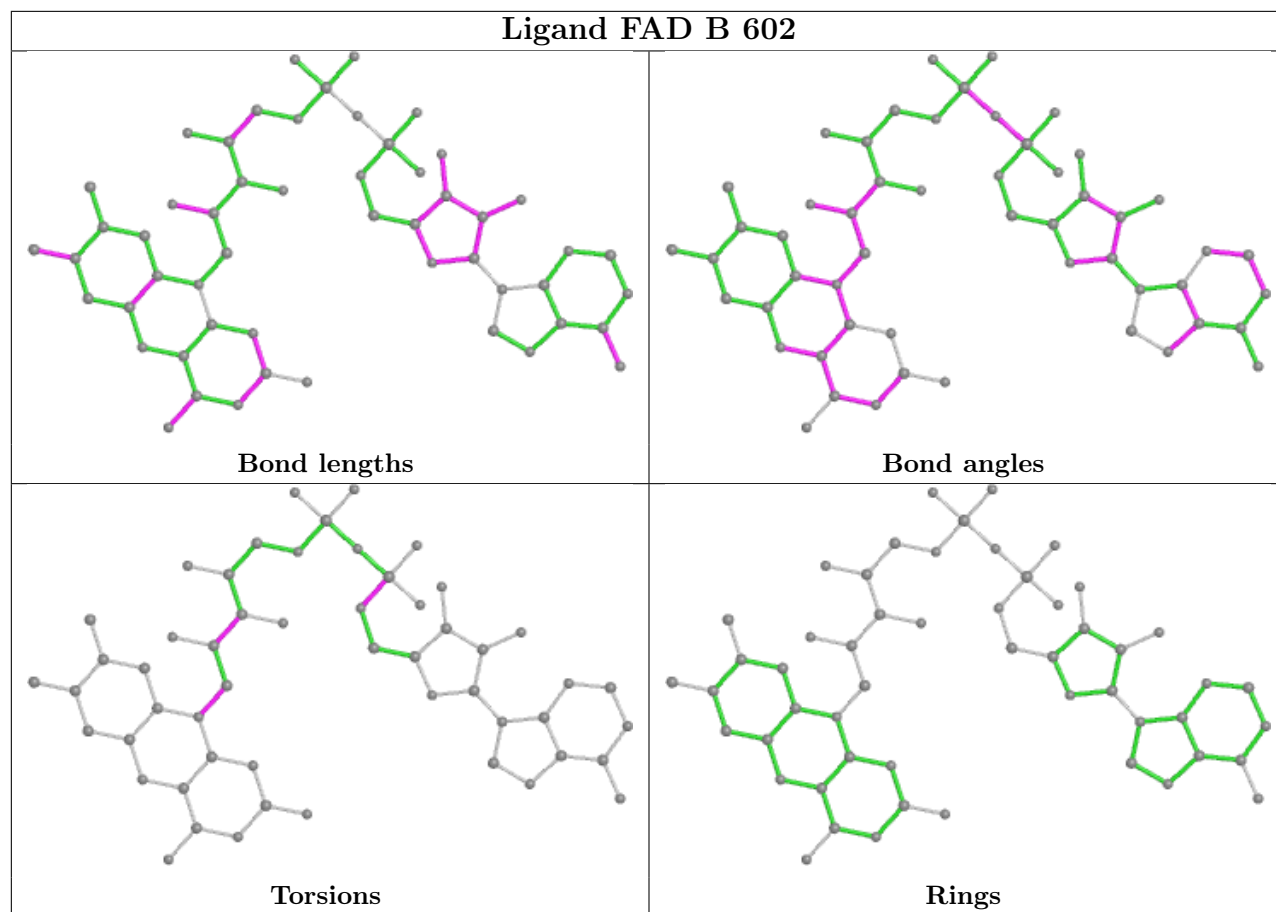
Bond angles

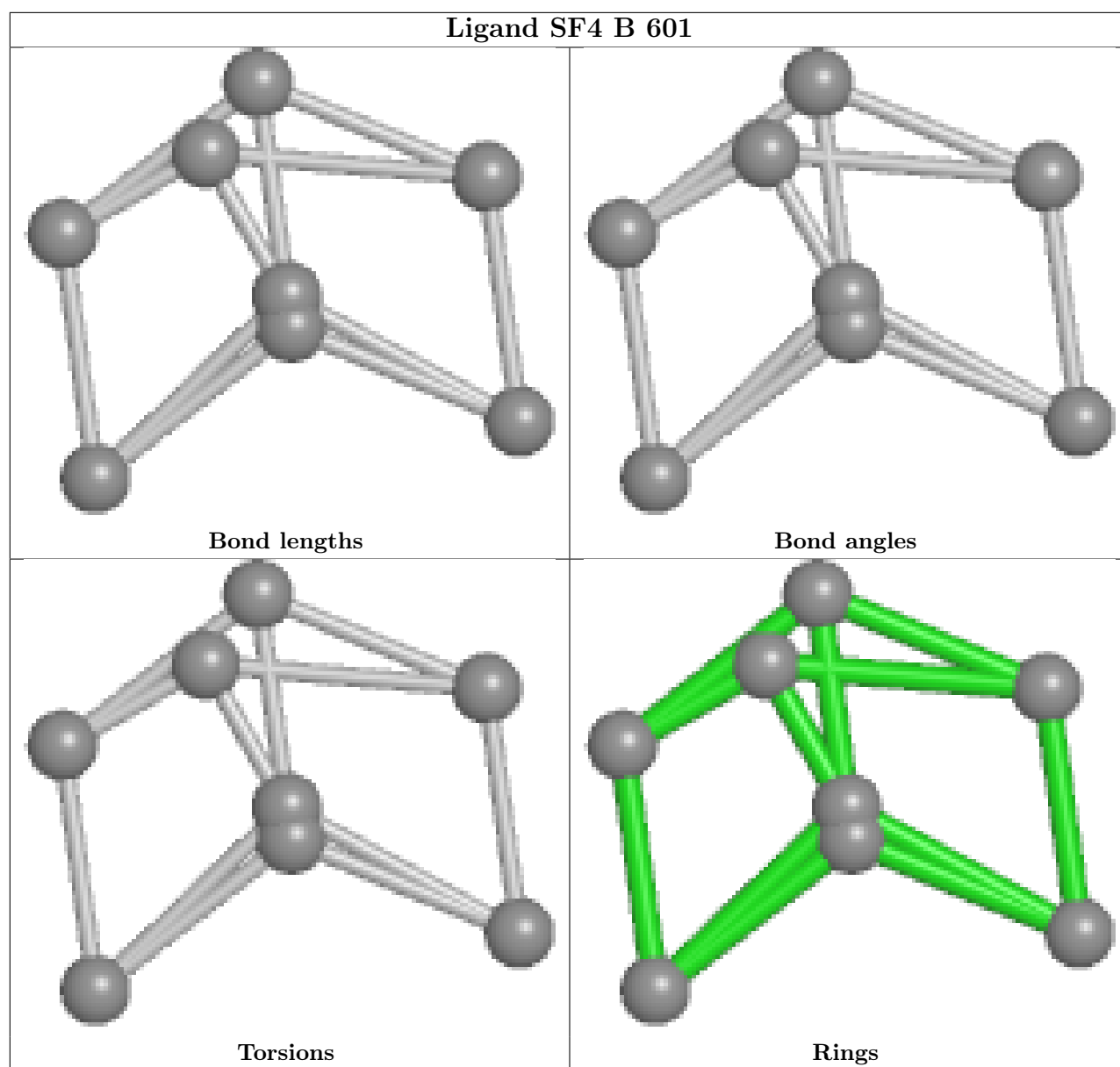


Torsions



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	502/502 (100%)	0.04	10 (1%) 65 71	12, 18, 35, 59	0
1	B	501/502 (99%)	0.07	18 (3%) 42 50	12, 19, 37, 67	0
1	C	500/502 (99%)	0.09	17 (3%) 45 52	11, 19, 37, 63	0
1	D	500/502 (99%)	0.10	17 (3%) 45 52	11, 20, 39, 60	0
All	All	2003/2008 (99%)	0.07	62 (3%) 49 57	11, 19, 37, 67	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	LEU	7.8
1	A	507	VAL	4.6
1	B	507	VAL	4.3
1	A	108	VAL	4.2
1	B	69	THR	4.2
1	C	180	ASP	4.0
1	B	22	ASP	3.9
1	B	108	VAL	3.8
1	C	181	GLU	3.6
1	D	506	SER	3.6
1	D	9	ARG	3.4
1	C	108	VAL	3.4
1	D	7	THR	3.3
1	C	505	ASP	3.2
1	D	108	VAL	3.2
1	B	489	GLU	3.0
1	D	181	GLU	3.0
1	C	7	THR	3.0
1	D	505	ASP	3.0
1	A	505	ASP	2.9
1	D	489	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	181	GLU	2.9
1	A	22	ASP	2.9
1	D	182	LYS	2.9
1	C	504	LYS	2.8
1	D	130	ASP	2.7
1	B	505	ASP	2.7
1	D	22	ASP	2.7
1	D	180	ASP	2.7
1	C	489	GLU	2.7
1	A	7	THR	2.7
1	B	297	ARG	2.6
1	C	125	GLU	2.6
1	C	56	LEU	2.6
1	D	149	ILE	2.6
1	A	181	GLU	2.6
1	D	71	LEU	2.5
1	B	180	ASP	2.5
1	B	447	LEU	2.5
1	C	246	GLU	2.4
1	D	107	CYS	2.4
1	C	179	THR	2.4
1	C	22	ASP	2.3
1	C	212	GLU	2.3
1	A	299	TYR	2.3
1	B	16	GLU	2.2
1	B	246	GLU	2.2
1	A	489	GLU	2.2
1	B	272	TRP	2.2
1	B	128	GLY	2.2
1	D	16[A]	GLU	2.1
1	C	299	TYR	2.1
1	C	202	ILE	2.1
1	B	291	PHE	2.1
1	D	179	THR	2.1
1	B	7	THR	2.1
1	B	125	GLU	2.0
1	B	292	THR	2.0
1	C	76	PHE	2.0
1	A	48	VAL	2.0
1	D	203	ILE	2.0
1	C	211	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

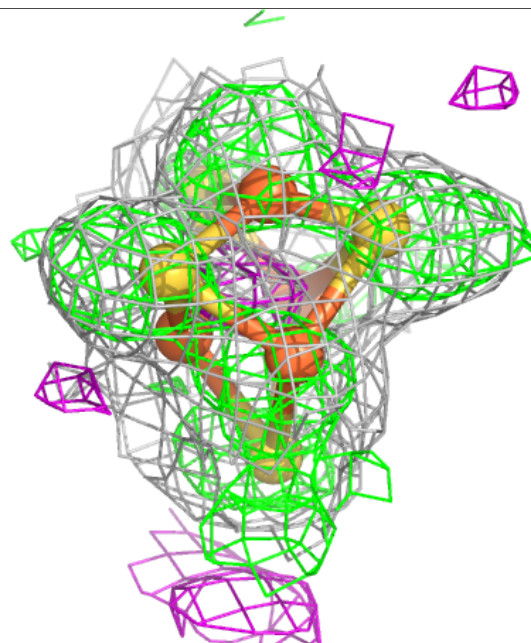
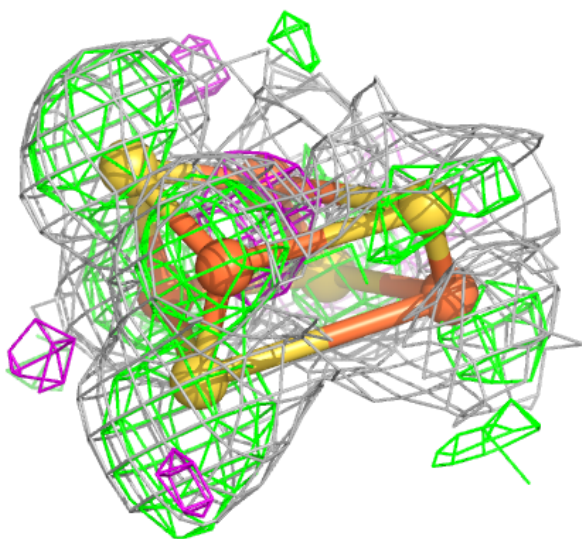
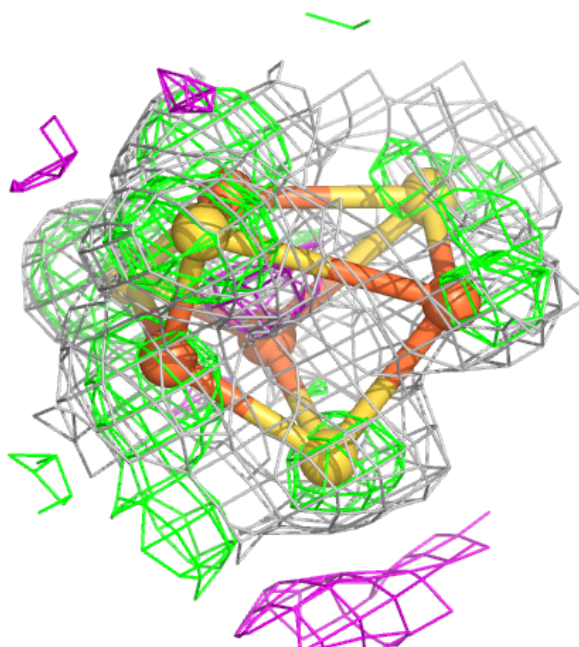
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SF4	B	601	8/8	-0.07	0.43	142,223,225,227	2
2	SF4	C	601	8/8	0.17	0.33	20,162,205,205	3
2	SF4	D	601	8/8	0.32	0.40	59,194,196,196	2
2	SF4	A	601	8/8	0.59	0.36	25,123,130,132	5
4	SO4	A	605	5/5	0.73	0.22	101,102,102,105	0
4	SO4	B	603	5/5	0.74	0.18	114,114,115,116	0
4	SO4	A	604	5/5	0.76	0.22	96,99,100,101	0
5	PO4	A	606	5/5	0.78	0.18	102,103,104,105	0
4	SO4	A	603	5/5	0.87	0.16	69,70,75,81	0
3	FAD	D	602	53/53	0.93	0.10	11,15,18,19	0
3	FAD	A	602	53/53	0.93	0.11	11,13,17,18	0
3	FAD	B	602	53/53	0.94	0.11	11,13,16,19	0
3	FAD	C	602	53/53	0.94	0.10	11,14,17,20	0
6	FE	A	607	1/1	0.97	0.12	19,19,19,19	1
6	FE	B	604	1/1	0.98	0.07	18,18,18,18	1
6	FE	D	603	1/1	0.99	0.10	19,19,19,19	1
6	FE	C	603	1/1	0.99	0.08	19,19,19,19	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.

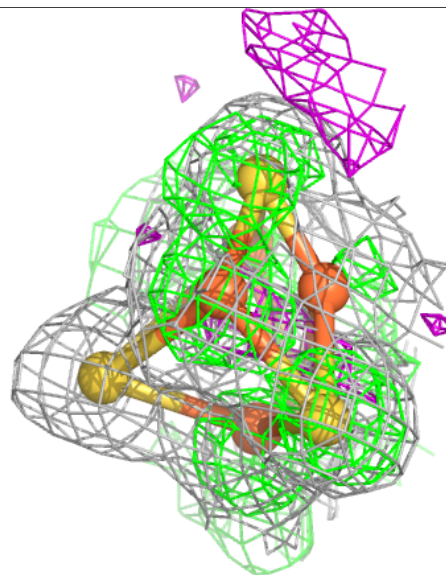
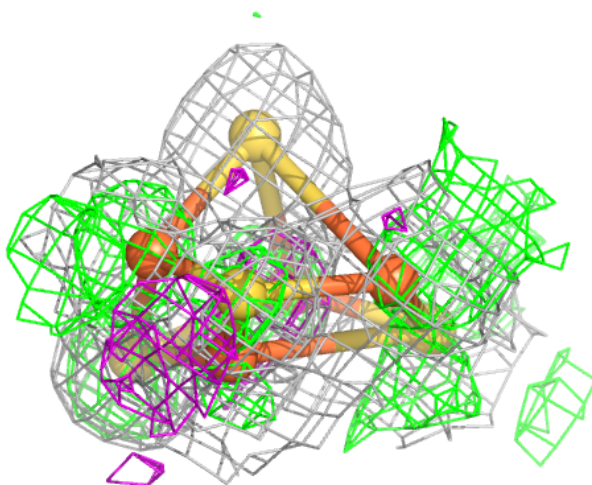
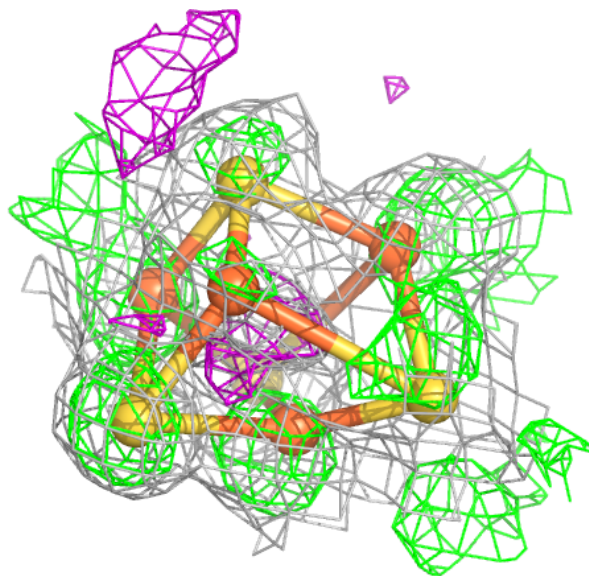
Electron density around SF4 B 601:

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



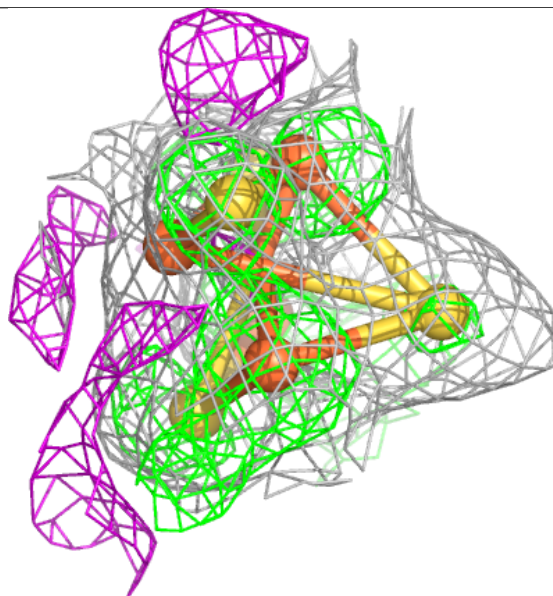
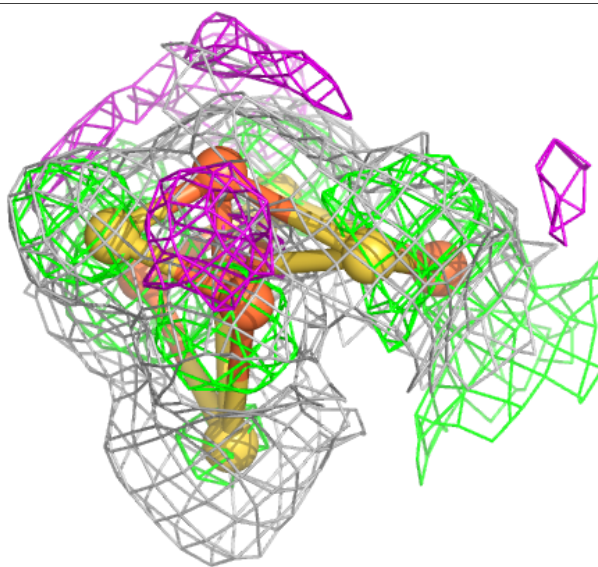
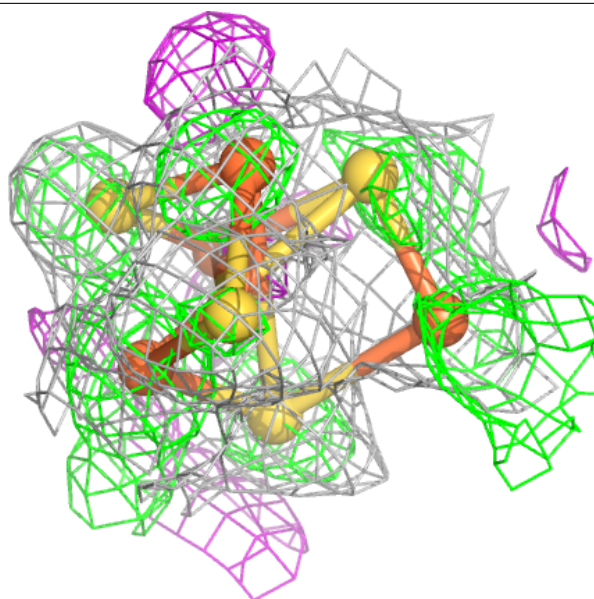
Electron density around SF4 C 601:

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



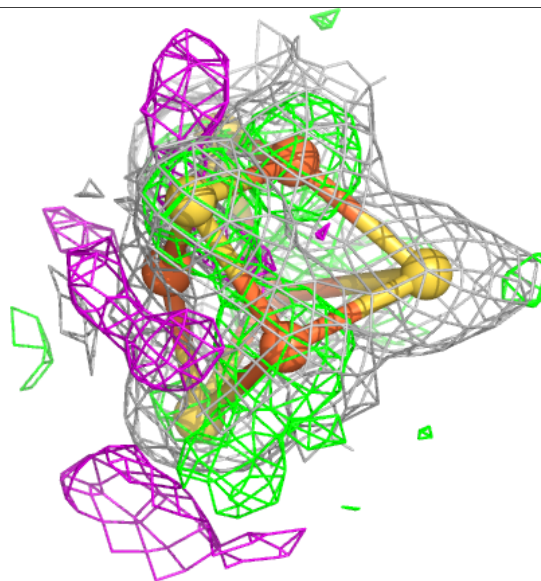
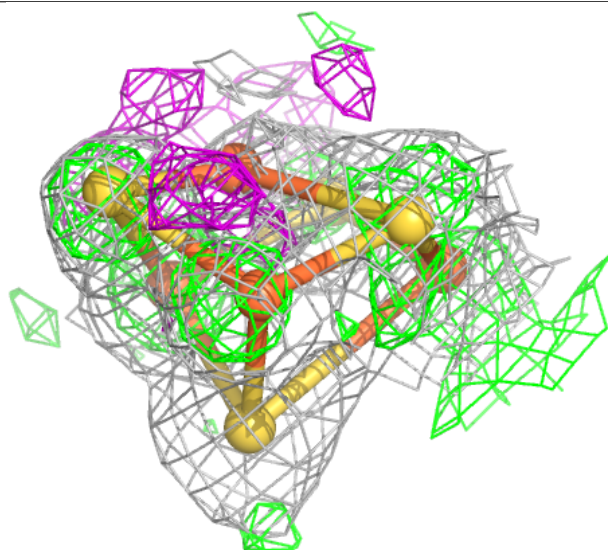
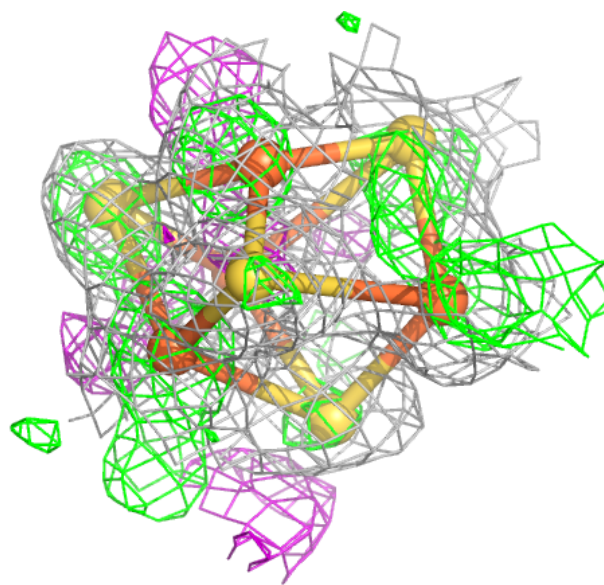
Electron density around SF4 D 601:

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



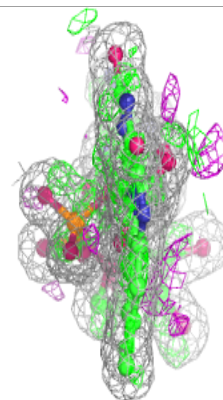
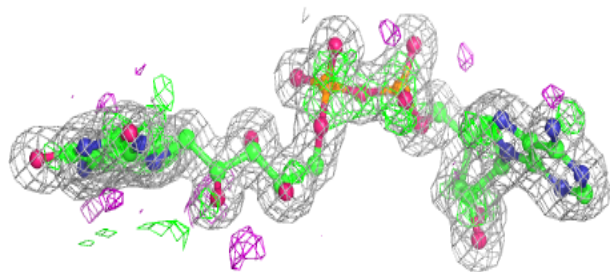
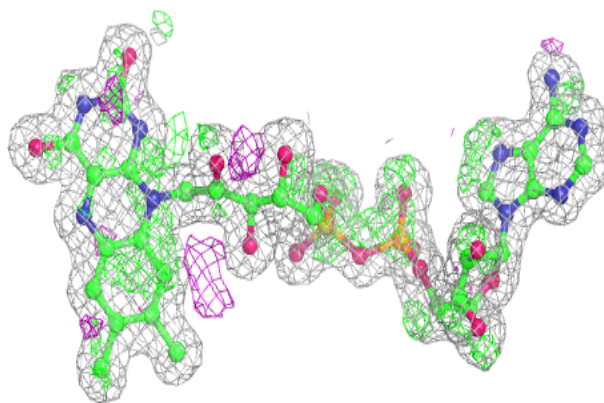
Electron density around SF4 A 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

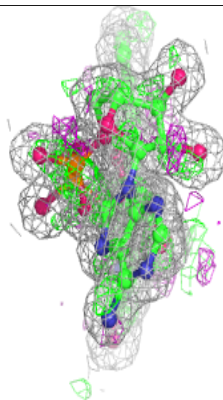
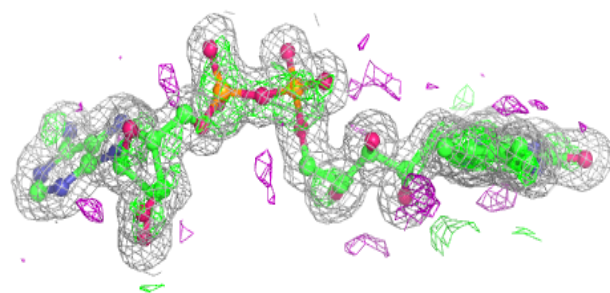
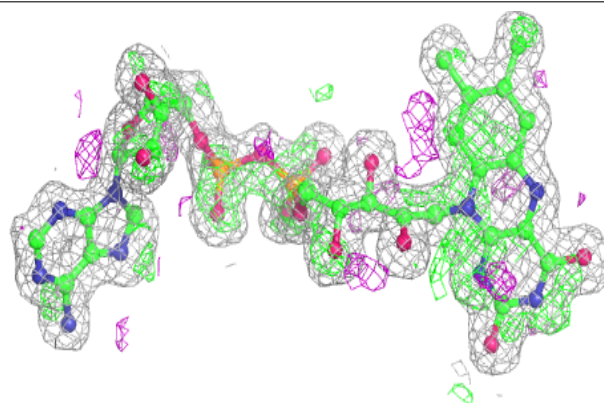


Electron density around FAD D 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

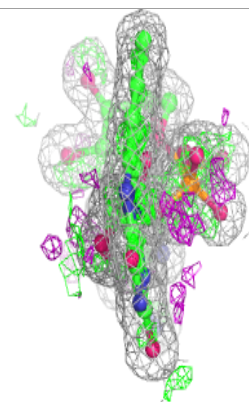
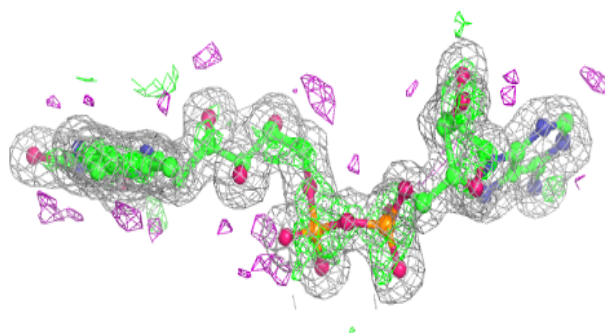
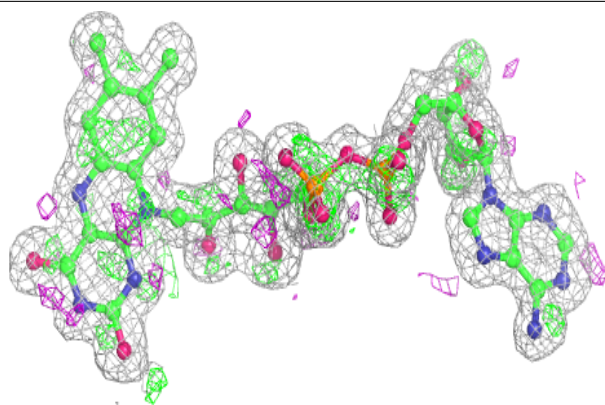
**Electron density around FAD A 602:**

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

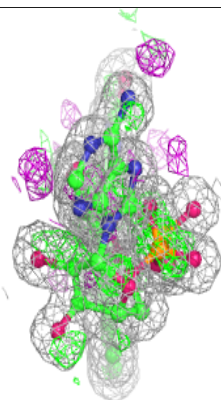
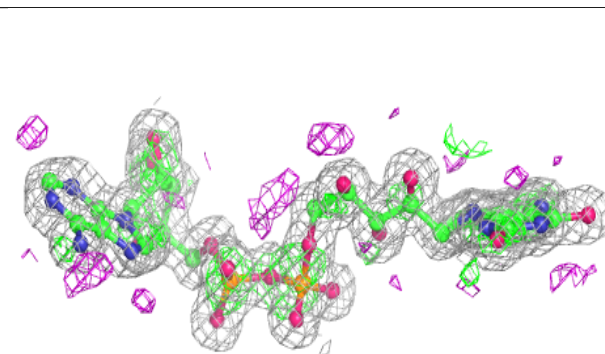
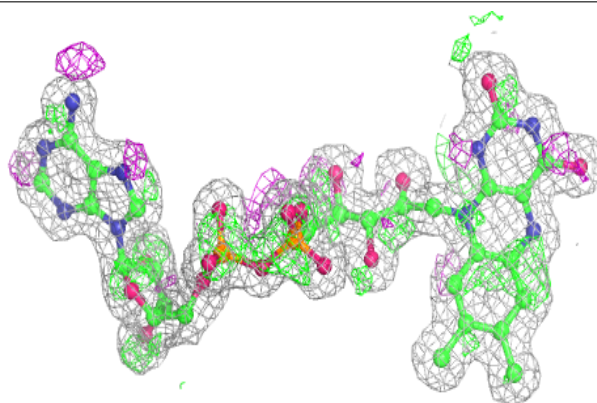


Electron density around FAD B 602:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.