Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 09:31 pm BST

PDB ID	:	7PX0 / pdb_00007px0
Title	:	Drosophila melanogaster Aldehyde Oxidase 1
Authors	:	Vilela-Alves, G.; Mota, C.; Romao, M.J.
Deposited on	:	2021-10-07
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

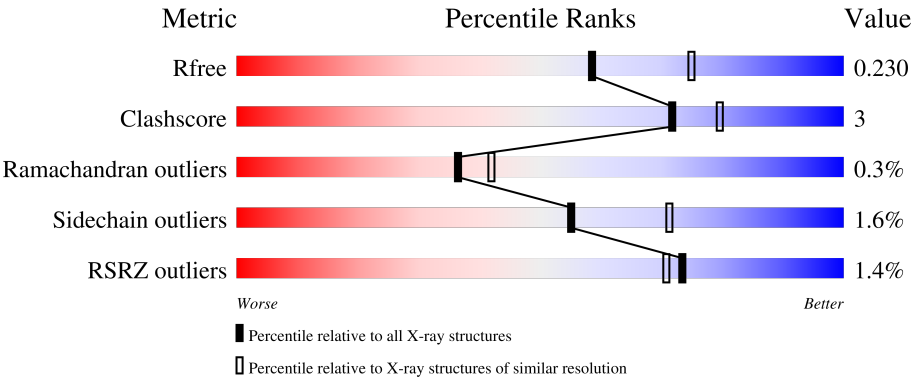
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1273	90% 7%
1	B	1273	89% 9%
1	C	1273	89% 9%
1	D	1273	3% 86% 10%

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
4	GOL	A	1310	-	-	X	-
5	PEG	A	1309	-	-	X	-

2 Entry composition

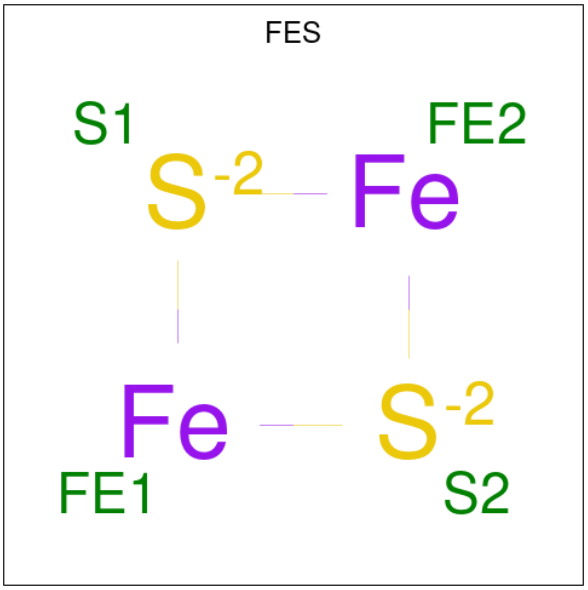
There are 8 unique types of molecules in this entry. The entry contains 41321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1249	Total	C	N	O	S	0	2	0
			9615	6082	1651	1823	59			
1	B	1253	Total	C	N	O	S	0	2	0
			9643	6097	1659	1829	58			
1	C	1252	Total	C	N	O	S	0	2	0
			9639	6096	1656	1830	57			
1	D	1236	Total	C	N	O	S	0	1	0
			9513	6019	1638	1800	56			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

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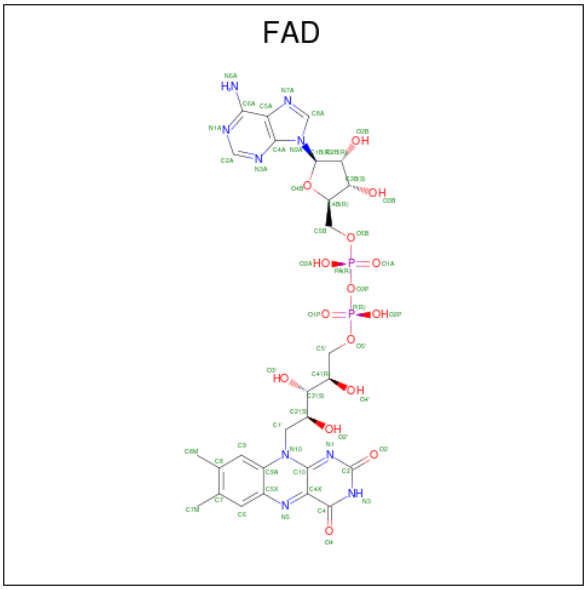
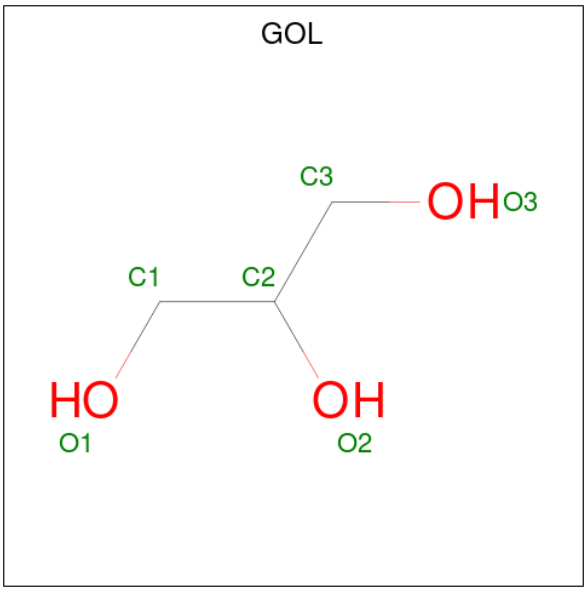
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



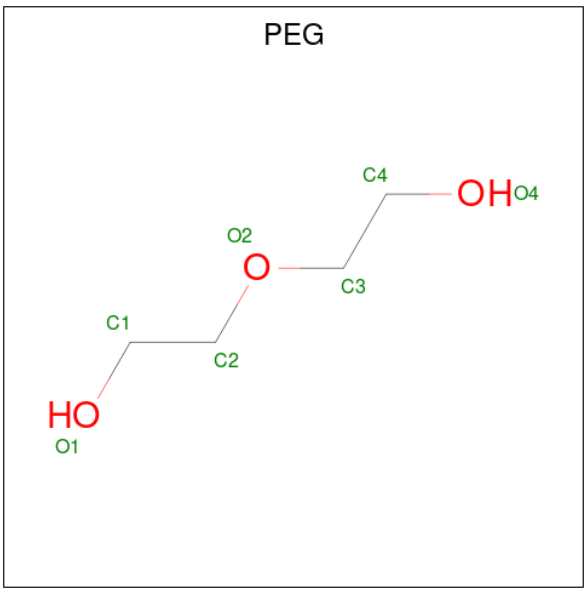
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



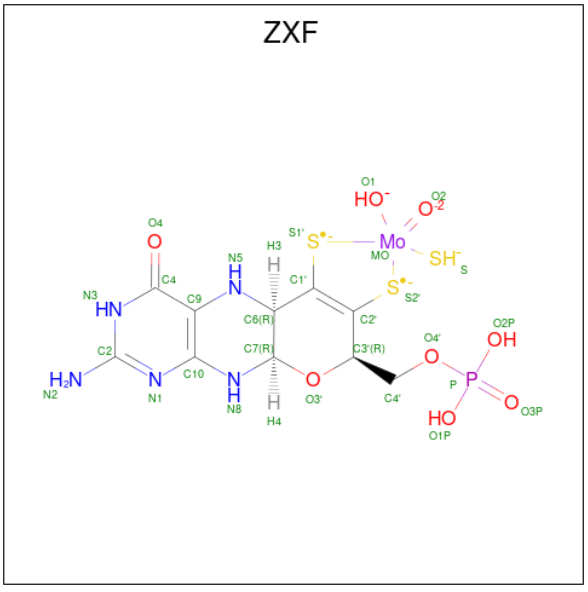
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0

- Molecule 6 is Molybdopterin hydoxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $C_{10}H_{14}MoN_5O_8PS_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Mo	N	O	P	S		
6	A	1	28	10	1	5	8	1	3	0	0

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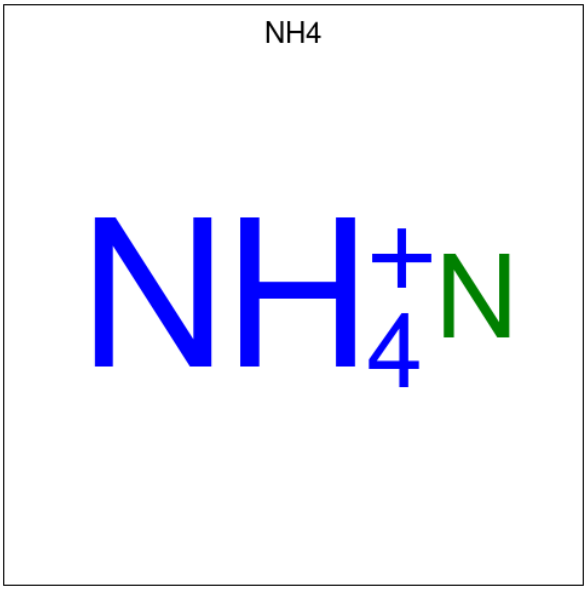
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
6	C	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
6	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 7 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	N	0	0
			1	1		

- Molecule 8 is water.

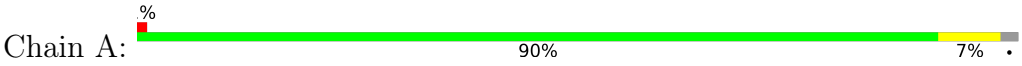
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	776	Total	O	0	0
			776	776		
8	B	619	Total	O	0	0
			619	619		
8	C	607	Total	O	0	0
			607	607		
8	D	461	Total	O	0	0
			461	461		

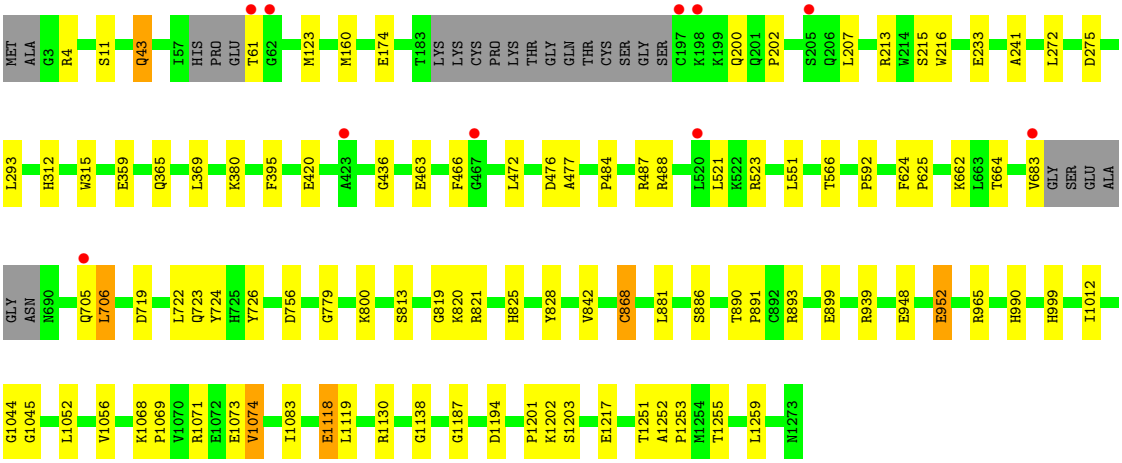
3 Residue-property plots (i)

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: Aldehyde oxidase 1

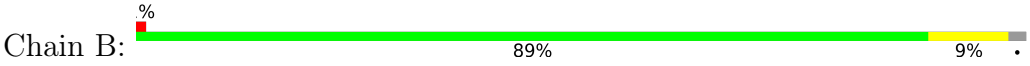
Chain A:

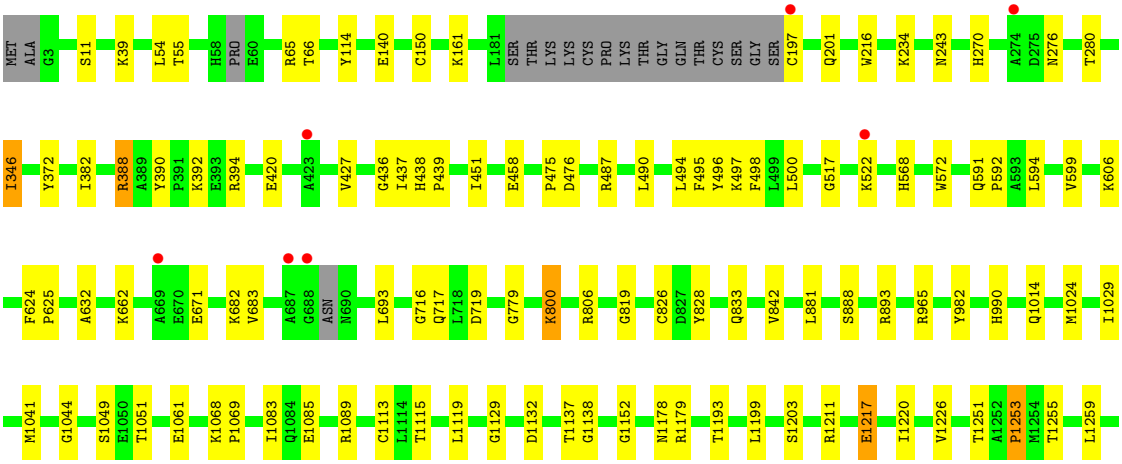


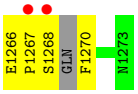


• Molecule 1: Aldehyde oxidase 1

Chain B:

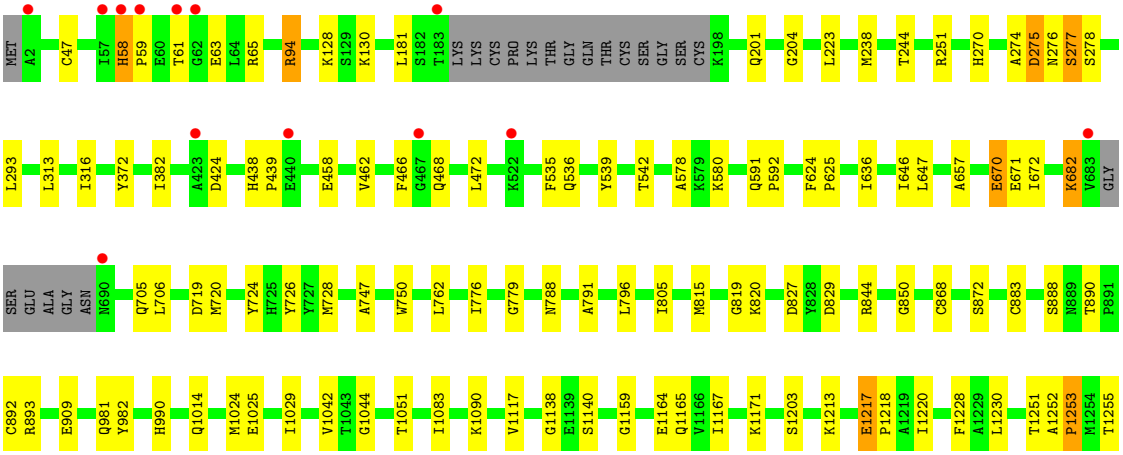


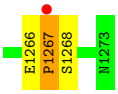




• Molecule 1: Aldehyde oxidase 1

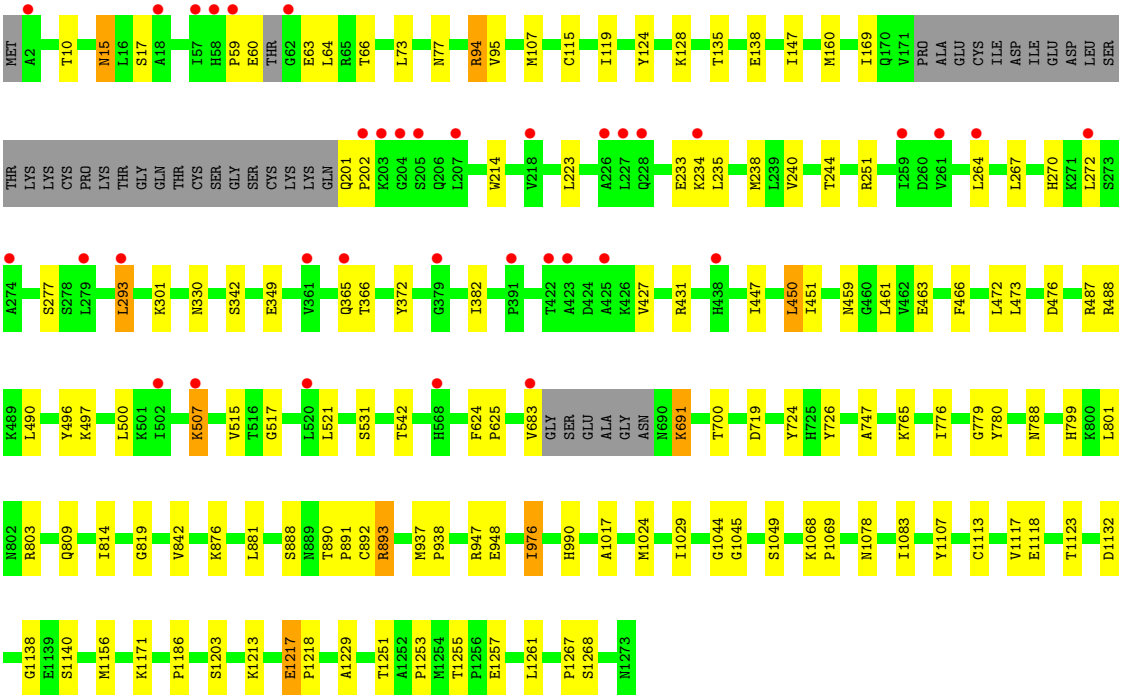
Chain C:





• Molecule 1: Aldehyde oxidase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.66Å 127.91Å 152.55Å 90.00° 110.63° 90.00°	Depositor
Resolution (Å)	48.66 – 2.20 48.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.66-2.20) 97.8 (48.66-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.175 , 0.220 0.184 , 0.230	Depositor DCC
R_{free} test set	12900 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41321	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, FAD, PEG, GOL, ZXF, FES

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	1.03	0/9816	1.35	6/13297 (0.0%)
1	B	1.03	0/9844	1.34	1/13333 (0.0%)
1	C	1.04	0/9842	1.37	10/13335 (0.1%)
1	D	1.03	0/9711	1.39	9/13156 (0.1%)
All	All	1.03	0/39213	1.36	26/53121 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	868	CYS	CB-CA-C	-7.71	98.53	111.02
1	C	59	PRO	N-CA-CB	6.31	110.45	103.26
1	C	275	ASP	CB-CA-C	-6.25	101.07	110.88
1	D	976	ILE	CA-C-N	6.15	126.87	121.58
1	D	976	ILE	C-N-CA	6.15	126.87	121.58
1	C	274	ALA	CA-C-N	6.08	128.35	120.44
1	C	274	ALA	C-N-CA	6.08	128.35	120.44
1	D	1078	ASN	CA-C-N	6.00	128.60	120.38
1	D	1078	ASN	C-N-CA	6.00	128.60	120.38
1	C	424	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	788	ASN	CA-CB-CG	-5.52	107.08	112.60
1	C	535	PHE	CA-C-N	5.46	128.35	120.38
1	C	535	PHE	C-N-CA	5.46	128.35	120.38
1	B	632	ALA	CA-C-O	-5.43	115.22	121.19
1	A	1187	GLY	CA-C-N	5.31	127.65	120.38
1	A	1187	GLY	C-N-CA	5.31	127.65	120.38
1	A	756	ASP	N-CA-C	-5.30	105.20	110.97
1	D	1186	PRO	CA-C-N	5.21	128.10	122.16
1	D	1186	PRO	C-N-CA	5.21	128.10	122.16
1	C	868	CYS	CB-CA-C	-5.16	102.71	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	58	HIS	CA-C-N	5.13	125.17	119.32
1	C	58	HIS	C-N-CA	5.13	125.17	119.32
1	D	124	TYR	CA-C-N	5.11	125.77	119.99
1	D	124	TYR	C-N-CA	5.11	125.77	119.99
1	A	551	LEU	CA-C-O	-5.06	115.49	120.70
1	A	1118	GLU	CB-CG-CD	5.02	121.14	112.60

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	9615	0	9569	64	0
1	B	9643	0	9587	61	0
1	C	9639	0	9581	59	0
1	D	9513	0	9463	76	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	0	0
3	C	53	0	31	1	0
3	D	53	0	31	0	0
4	A	30	0	40	11	0
4	B	30	0	40	1	0
4	C	12	0	16	0	0
4	D	12	0	16	1	0
5	A	7	0	10	4	0
6	A	28	0	0	2	0
6	B	28	0	0	2	0
6	C	28	0	0	1	0
6	D	28	0	0	3	0
7	D	1	0	0	0	0
8	A	776	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	619	0	0	3	1
8	C	607	0	0	3	0
8	D	461	0	0	3	0
All	All	41321	0	38446	257	1

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 3.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HD11	5:A:1309:PEG:H21	1.49	0.94
1:A:723:GLN:HE21	1:A:821:ARG:HE	1.33	0.73
1:B:833:GLN:NE2	8:B:1402:HOH:O	2.20	0.73
1:D:1268:SER:HB3	8:D:1631:HOH:O	1.89	0.71
1:A:952:GLU:HA	4:A:1310:GOL:H2	1.73	0.71
1:D:447:ILE:CD1	1:D:472:LEU:HD21	2.21	0.71
1:A:592:PRO:HG2	1:A:662:LYS:HE2	1.72	0.69
1:B:1268:SER:C	1:B:1270:PHE:N	2.51	0.69
1:A:521:LEU:HD22	1:A:1118:GLU:HG2	1.75	0.68
1:B:427:VAL:HG21	1:B:451:ILE:HD12	1.79	0.65
1:A:722:LEU:CD1	5:A:1309:PEG:H21	2.25	0.64
1:C:204:GLY:O	8:C:1401:HOH:O	2.15	0.64
1:D:366:THR:N	8:D:1401:HOH:O	2.30	0.64
1:D:1044:GLY:HA2	6:D:1309:ZXF:S2'	2.38	0.63
1:C:458:GLU:O	1:C:462:VAL:HG23	1.98	0.63
1:B:1115:THR:HG21	1:B:1226:VAL:HG22	1.80	0.63
1:D:447:ILE:HD11	1:D:472:LEU:HD21	1.80	0.63
1:D:521:LEU:HD22	1:D:1118:GLU:HG2	1.82	0.62
1:A:213:ARG:NH2	1:A:233:GLU:OE1	2.33	0.61
1:C:1025:GLU:OE2	1:D:765:LYS:HE2	2.00	0.61
1:A:1253:PRO:HG2	1:A:1255:THR:HG23	1.82	0.60
1:A:813:SER:HA	4:A:1308:GOL:H12	1.84	0.60
1:A:1044:GLY:HA2	6:A:1312:ZXF:S2'	2.41	0.59
1:D:890:THR:OG1	1:D:891:PRO:HD2	2.02	0.59
1:B:1068:LYS:HB3	1:B:1069:PRO:HD3	1.85	0.58
1:D:990:HIS:HA	1:D:1083:ILE:HG22	1.84	0.58
4:A:1306:GOL:H32	8:A:1832:HOH:O	2.04	0.57
1:D:349:GLU:O	1:D:431:ARG:NH1	2.37	0.57
1:D:1045:GLY:N	6:D:1309:ZXF:S2'	2.78	0.56
1:A:899:GLU:CD	8:A:1404:HOH:O	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:LEU:HD12	1:D:267:LEU:HD12	1.88	0.56
1:B:476:ASP:O	1:B:487:ARG:NH2	2.39	0.56
1:C:275:ASP:HB2	1:C:277:SER:H	1.72	0.55
1:B:990:HIS:HA	1:B:1083:ILE:HG22	1.87	0.55
1:C:1138:GLY:HA2	1:C:1203:SER:O	2.06	0.55
1:A:476:ASP:O	1:A:487:ARG:NH2	2.40	0.54
1:D:1117:VAL:HG22	1:D:1229:ALA:HB1	1.87	0.54
1:C:647:LEU:HD22	1:C:805:ILE:HD12	1.88	0.54
1:B:1061:GLU:OE1	8:B:1401:HOH:O	2.18	0.54
1:C:1165:GLN:OE1	1:C:1167:ILE:HD11	2.07	0.54
1:A:948:GLU:OE2	8:A:1401:HOH:O	2.19	0.54
1:C:990:HIS:HA	1:C:1083:ILE:HG22	1.90	0.53
1:D:135:THR:OG1	1:D:138:GLU:HG3	2.08	0.53
1:D:842:VAL:HG13	1:D:876:LYS:HD3	1.90	0.53
1:D:201:GLN:HB3	1:D:202:PRO:HD2	1.89	0.53
1:B:436:GLY:O	1:B:487:ARG:HD2	2.09	0.52
1:D:270:HIS:CG	1:D:293:LEU:HD21	2.44	0.52
1:C:1253:PRO:HG2	1:C:1255:THR:HG23	1.91	0.52
1:A:624:PHE:N	1:A:625:PRO:CD	2.73	0.52
1:D:801:LEU:O	1:D:803:ARG:HG3	2.10	0.52
1:A:463:GLU:O	1:A:466:PHE:O	2.28	0.51
1:D:233:GLU:HB2	1:D:235:LEU:HG	1.91	0.51
1:B:800:LYS:HE2	8:B:1991:HOH:O	2.09	0.51
1:B:1129:GLY:HA2	1:B:1193:THR:HG22	1.92	0.51
1:B:1268:SER:O	1:B:1270:PHE:N	2.44	0.51
1:C:238:MET:SD	1:C:251:ARG:HD2	2.51	0.51
1:A:436:GLY:O	1:A:487:ARG:HD2	2.11	0.51
1:D:447:ILE:HD12	1:D:472:LEU:HD21	1.91	0.51
1:A:952:GLU:OE2	4:A:1310:GOL:H31	2.11	0.50
1:C:670:GLU:N	1:C:670:GLU:CD	2.68	0.50
1:A:4:ARG:CZ	1:A:11:SER:OG	2.59	0.50
1:A:722:LEU:HD11	5:A:1309:PEG:C2	2.32	0.50
1:C:536:GLN:HA	1:C:539:TYR:CD1	2.46	0.50
1:A:719:ASP:O	1:A:1251:THR:HA	2.11	0.50
1:C:670:GLU:CD	1:C:670:GLU:H	2.20	0.50
1:D:115:CYS:O	1:D:119:ILE:HG12	2.12	0.50
1:D:490:LEU:CD1	1:D:1123:THR:HA	2.42	0.50
1:B:1178:ASN:OD1	1:B:1179:ARG:HG3	2.12	0.50
1:C:788:ASN:HA	1:C:791:ALA:HB3	1.92	0.50
1:D:947:ARG:HH21	4:D:1307:GOL:H12	1.77	0.49
1:D:223:LEU:C	1:D:223:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:SER:HB2	4:A:1308:GOL:H31	1.92	0.49
1:A:1138:GLY:HA2	1:A:1203:SER:O	2.12	0.49
1:D:66:THR:HB	1:D:128:LYS:HB3	1.95	0.49
1:C:94:ARG:HD2	1:D:799:HIS:O	2.12	0.49
1:A:948:GLU:O	4:A:1310:GOL:H32	2.12	0.49
1:B:671:GLU:OE1	1:B:682:LYS:HE2	2.12	0.49
1:B:881:LEU:C	1:B:881:LEU:HD23	2.38	0.49
1:A:723:GLN:NE2	1:A:821:ARG:HE	2.08	0.49
1:A:241:ALA:HB3	3:A:1305:FAD:O2P	2.13	0.48
1:D:1253:PRO:HG2	1:D:1255:THR:HG23	1.94	0.48
1:A:359:GLU:HB3	1:A:380:LYS:HG2	1.94	0.48
1:B:624:PHE:N	1:B:625:PRO:CD	2.76	0.48
1:B:1044:GLY:HA2	6:B:1311:ZXF:S2'	2.53	0.48
1:B:1253:PRO:HG2	1:B:1255:THR:HG23	1.95	0.48
1:C:313:LEU:HD23	1:C:316:ILE:HD12	1.95	0.48
1:A:1068:LYS:HB3	1:A:1069:PRO:HD3	1.95	0.48
1:B:150:CYS:O	1:B:1152:GLY:HA3	2.14	0.48
1:B:438[B]:HIS:ND1	1:B:439:PRO:HD2	2.29	0.48
1:D:1113:CYS:HA	1:D:1132:ASP:O	2.13	0.48
1:A:952:GLU:N	4:A:1310:GOL:H32	2.29	0.48
1:D:59:PRO:O	1:D:60:GLU:HB2	2.14	0.47
1:D:496:TYR:CZ	1:D:500:LEU:HD11	2.48	0.47
1:D:238:MET:SD	1:D:251:ARG:HD3	2.54	0.47
1:D:94:ARG:HG3	1:D:95:VAL:N	2.29	0.47
1:B:606:LYS:NZ	4:B:1310:GOL:O1	2.47	0.47
1:C:819:GLY:HA3	1:C:888:SER:O	2.15	0.47
1:C:1217:GLU:H	1:C:1218:PRO:CD	2.27	0.47
1:A:200:GLN:HG2	1:A:202:PRO:HD3	1.97	0.47
1:D:892:CYS:O	1:D:893:ARG:C	2.58	0.47
1:C:671:GLU:OE1	1:C:682:LYS:HE2	2.15	0.47
1:D:15:ASN:ND2	1:D:17:SER:OG	2.48	0.47
1:A:207:LEU:HD21	1:A:213:ARG:HH11	1.80	0.47
1:C:909:GLU:HG3	1:C:1228:PHE:CD1	2.50	0.47
1:B:1138:GLY:HA2	1:B:1203:SER:O	2.15	0.46
1:D:1029:ILE:N	1:D:1029:ILE:HD12	2.30	0.46
1:C:646:ILE:HG21	1:C:657:ALA:HB3	1.97	0.46
1:C:58:HIS:HB3	1:C:61:THR:HG22	1.98	0.46
1:C:819:GLY:C	1:C:820:LYS:HG3	2.40	0.46
1:C:1014:GLN:HG3	1:C:1024:MET:HE3	1.98	0.46
1:A:705:GLN:C	1:A:706:LEU:HD23	2.40	0.46
1:B:1085:GLU:OE1	1:B:1089:ARG:NH1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:LYS:H	1:D:691:LYS:HD3	1.81	0.46
1:A:813:SER:HB2	4:A:1308:GOL:C3	2.46	0.45
1:B:140:GLU:OE2	1:B:161:LYS:NZ	2.43	0.45
1:D:809:GLN:HB3	1:D:814:ILE:HG13	1.98	0.45
1:A:488:ARG:HD2	8:A:1921:HOH:O	2.16	0.45
1:C:47:CYS:HB2	1:C:728:MET:HE1	1.98	0.45
1:C:724:TYR:CE2	1:C:726:TYR:HA	2.51	0.45
1:D:747:ALA:HA	1:D:776:ILE:HG22	1.97	0.45
1:C:827:ASP:OD2	1:C:844:ARG:NH1	2.49	0.45
1:A:43:GLN:HA	1:A:43:GLN:HE21	1.81	0.45
1:A:886:SER:CB	5:A:1309:PEG:H12	2.47	0.45
1:D:94:ARG:HB2	1:D:94:ARG:HH11	1.82	0.45
1:D:473:LEU:O	1:D:488:ARG:NH1	2.50	0.45
1:C:850:GLY:O	1:C:883:CYS:HA	2.17	0.45
1:D:1257:GLU:O	1:D:1261:LEU:HG	2.16	0.45
1:C:128:LYS:HD3	1:C:181:LEU:HD22	1.99	0.45
1:C:624:PHE:N	1:C:625:PRO:CD	2.80	0.45
1:A:123:MET:HG2	1:A:160:MET:SD	2.57	0.45
1:A:890:THR:OG1	1:A:891:PRO:HD2	2.17	0.45
1:D:719:ASP:O	1:D:1251:THR:HA	2.17	0.45
1:B:437:ILE:O	1:B:475:PRO:HA	2.18	0.44
1:B:819:GLY:HA3	1:B:888:SER:O	2.17	0.44
1:B:346:ILE:HD12	1:B:346:ILE:HA	1.83	0.44
1:B:394:ARG:NH2	1:B:420:GLU:OE2	2.49	0.44
1:A:1045:GLY:N	6:A:1312:ZXF:S2'	2.91	0.44
1:B:490:LEU:O	1:B:494:LEU:HG	2.18	0.44
1:B:1266:GLU:C	1:B:1268:SER:H	2.25	0.44
1:C:591:GLN:N	1:C:592:PRO:CD	2.80	0.44
1:D:223:LEU:HD23	1:D:223:LEU:O	2.17	0.44
1:B:201:GLN:HG3	1:B:216:TRP:HB3	2.00	0.44
1:C:275:ASP:O	1:C:276:ASN:HB2	2.18	0.44
1:A:523:ARG:HD2	8:A:1810:HOH:O	2.17	0.44
1:C:270:HIS:HB3	1:C:293:LEU:HD21	2.00	0.44
1:D:330:ASN:OD1	1:D:342:SER:OG	2.26	0.44
1:D:1049:SER:N	6:D:1309:ZXF:O2P	2.50	0.44
1:C:982:TYR:CD1	1:C:1051:THR:HG21	2.53	0.44
1:D:77:ASN:HD22	1:D:214:TRP:CD1	2.35	0.44
1:B:55:THR:HA	1:B:65:ARG:O	2.17	0.43
1:D:819:GLY:HA3	1:D:888:SER:O	2.18	0.43
1:D:1068:LYS:HB3	1:D:1069:PRO:HD3	1.99	0.43
1:A:952:GLU:HG3	4:A:1310:GOL:H31	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:PRO:HB2	1:A:1202:LYS:HE3	2.00	0.43
1:B:496:TYR:CE1	1:B:1270:PHE:HB3	2.53	0.43
1:B:1119:LEU:HD13	1:B:1259:LEU:HD13	2.01	0.43
1:C:981:GLN:NE2	8:C:1443:HOH:O	2.50	0.43
1:C:719:ASP:C	1:C:720:MET:HG3	2.43	0.43
1:C:578:ALA:HB1	1:C:636:ILE:HG13	2.01	0.43
1:A:990:HIS:HA	1:A:1083:ILE:HG22	1.99	0.43
1:B:591:GLN:N	1:B:592:PRO:CD	2.82	0.43
1:C:1252:ALA:HA	1:C:1253:PRO:HA	1.81	0.43
1:D:201:GLN:HB3	1:D:202:PRO:CD	2.48	0.43
1:D:881:LEU:HD23	1:D:881:LEU:C	2.43	0.43
1:D:1213:LYS:HE3	8:D:1421:HOH:O	2.18	0.43
1:D:372:TYR:CZ	1:D:382:ILE:HD11	2.53	0.43
1:D:497:LYS:HG2	1:D:517:GLY:O	2.19	0.43
1:B:572:TRP:HA	1:B:806:ARG:O	2.19	0.43
1:C:1217:GLU:O	1:C:1220:ILE:HG22	2.19	0.43
1:B:1049:SER:N	6:B:1311:ZXF:O2P	2.51	0.43
1:B:1137:THR:HG21	1:B:1199:LEU:HD22	2.01	0.43
1:C:275:ASP:HB2	1:C:277:SER:HB3	2.00	0.43
1:C:747:ALA:HA	1:C:776:ILE:HG22	2.00	0.43
1:A:881:LEU:C	1:A:881:LEU:HD23	2.44	0.43
1:D:160:MET:HE2	1:D:160:MET:N	2.33	0.43
1:D:459:ASN:O	1:D:463:GLU:HG3	2.18	0.43
1:B:828:TYR:HA	1:B:842:VAL:O	2.19	0.42
1:B:1217:GLU:O	1:B:1220:ILE:HG22	2.19	0.42
1:D:160:MET:HE2	1:D:160:MET:HA	2.00	0.42
1:C:705:GLN:O	1:C:706:LEU:HB2	2.19	0.42
1:C:1044:GLY:HA2	6:C:1308:ZXF:S2'	2.60	0.42
1:D:937:MET:HB3	1:D:938:PRO:HD3	2.01	0.42
1:A:952:GLU:HG3	4:A:1310:GOL:C3	2.48	0.42
1:C:892:CYS:O	1:C:893:ARG:C	2.62	0.42
1:A:566:THR:OG1	1:B:568:HIS:HE1	2.02	0.42
1:B:495:PHE:O	1:B:498:PHE:HB3	2.20	0.42
1:D:976:ILE:HG21	1:D:1107:TYR:CZ	2.54	0.42
1:D:1217:GLU:H	1:D:1218:PRO:CD	2.32	0.42
1:A:207:LEU:HD21	1:A:213:ARG:NH1	2.34	0.42
1:B:717:GLN:HA	1:B:826:CYS:O	2.19	0.42
1:C:815:MET:O	1:C:820:LYS:NZ	2.49	0.42
1:D:107:MET:HE1	1:D:169:ILE:HG21	2.00	0.42
1:A:1252:ALA:HA	1:A:1253:PRO:HA	1.86	0.42
1:C:1117:VAL:HG21	1:C:1230:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LEU:HD13	1:D:244:THR:HA	2.02	0.42
1:D:427:VAL:HG22	1:D:451:ILE:O	2.20	0.42
1:B:594:LEU:HD23	1:B:599:VAL:HG12	2.02	0.42
1:B:1029:ILE:N	1:B:1029:ILE:HD12	2.34	0.42
1:C:466:PHE:HB3	1:C:1267:PRO:HB3	2.02	0.42
1:A:828:TYR:HA	1:A:842:VAL:O	2.20	0.42
1:C:372:TYR:CZ	1:C:382:ILE:HD11	2.54	0.42
1:D:1138:GLY:HA2	1:D:1203:SER:O	2.19	0.42
1:A:312:HIS:HA	1:A:315:TRP:CE3	2.54	0.42
1:A:999:HIS:HB2	1:A:1052:LEU:HD12	2.02	0.42
1:B:39:LYS:HB3	1:B:114:TYR:CE2	2.55	0.42
1:B:372:TYR:CZ	1:B:382:ILE:HD11	2.55	0.41
1:C:1159:GLY:HA3	1:C:1164:GLU:OE2	2.20	0.41
1:D:724:TYR:CE2	1:D:726:TYR:HA	2.55	0.41
1:A:395:PHE:CE1	1:A:420:GLU:HB2	2.55	0.41
1:B:388:ARG:HD2	1:B:390:TYR:CE1	2.55	0.41
1:B:1129:GLY:C	1:B:1193:THR:HG22	2.45	0.41
1:C:438:HIS:CG	1:C:439:PRO:HD2	2.56	0.41
1:D:466:PHE:CZ	1:D:496:TYR:HB2	2.55	0.41
1:A:1073:GLU:HG3	1:A:1074:VAL:HG13	2.01	0.41
1:A:1119:LEU:HD13	1:A:1259:LEU:HD13	2.03	0.41
1:C:672:ILE:HD12	1:C:1171:LYS:O	2.20	0.41
1:C:1213:LYS:HE3	8:C:1422:HOH:O	2.20	0.41
1:D:780:TYR:CD1	1:D:1156:MET:HE1	2.55	0.41
1:A:1130:ARG:HA	1:A:1194:ASP:HB3	2.03	0.41
1:B:1113:CYS:HA	1:B:1132:ASP:O	2.21	0.41
1:D:542:THR:HA	1:D:1140:SER:O	2.20	0.41
1:B:1014:GLN:HG3	1:B:1024:MET:HE3	2.02	0.41
1:B:1211[A]:ARG:NH2	1:C:872:SER:OG	2.53	0.41
1:C:719:ASP:O	1:C:1251:THR:HA	2.19	0.41
1:C:750:TRP:CD2	1:C:1042:VAL:HB	2.55	0.41
1:D:1017:ALA:HB2	1:D:1024:MET:HA	2.03	0.41
1:B:497:LYS:HG2	1:B:517:GLY:O	2.21	0.41
1:C:542:THR:HA	1:C:1140:SER:O	2.20	0.41
1:A:1012:ILE:HG23	1:A:1056:VAL:HG21	2.03	0.41
1:B:496:TYR:CZ	1:B:500:LEU:HD11	2.55	0.41
1:A:477:ALA:HB2	1:A:484:PRO:HG3	2.03	0.41
1:C:762:LEU:HD21	1:C:796:LEU:HA	2.03	0.41
1:D:450:LEU:HD22	1:D:461:LEU:HD11	2.02	0.41
1:D:476:ASP:O	1:D:487:ARG:NH2	2.54	0.41
1:D:624:PHE:N	1:D:625:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HG2	1:A:216:TRP:CE3	2.56	0.41
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.83	0.41
1:A:719:ASP:OD1	1:A:825:HIS:ND1	2.44	0.41
1:B:243:ASN:CG	1:B:243:ASN:O	2.64	0.41
1:B:719:ASP:O	1:B:1251:THR:HA	2.20	0.41
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.81	0.41
1:A:724:TYR:CE2	1:A:726:TYR:HA	2.56	0.41
1:A:819:GLY:C	1:A:820:LYS:HG3	2.46	0.41
1:A:1071:ARG:NH2	8:A:1477:HOH:O	2.54	0.41
1:B:716:GLY:HA3	1:B:828:TYR:CZ	2.56	0.41
1:B:982:TYR:CD1	1:B:1051:THR:HG21	2.56	0.41
1:C:1029:ILE:HD12	1:C:1029:ILE:N	2.36	0.41
1:D:160:MET:HE2	1:D:160:MET:CA	2.51	0.41
1:B:270:HIS:HA	1:B:280:THR:O	2.20	0.40
1:C:244:THR:OG1	3:C:1305:FAD:H4'	2.21	0.40
1:D:64:LEU:HD23	1:D:64:LEU:HA	1.93	0.40
1:D:147:ILE:HG21	1:D:726:TYR:CE1	2.56	0.40
1:A:275:ASP:OD1	1:A:275:ASP:N	2.52	0.40
1:B:54:LEU:O	1:B:66:THR:HA	2.22	0.40
1:D:1171:LYS:HE3	1:D:1171:LYS:HB3	1.97	0.40
1:A:952:GLU:CA	4:A:1310:GOL:H2	2.48	0.40
1:B:982:TYR:CZ	1:B:1041:MET:HB3	2.55	0.40

All (1) 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)
8:A:1527:HOH:O	8:B:1934:HOH:O[2_746]	2.03	0.17

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	1243/1273 (98%)	1200 (96%)	39 (3%)	4 (0%)	36	42
1	B	1245/1273 (98%)	1200 (96%)	41 (3%)	4 (0%)	36	42
1	C	1248/1273 (98%)	1206 (97%)	40 (3%)	2 (0%)	43	51
1	D	1229/1273 (96%)	1185 (96%)	38 (3%)	6 (0%)	24	27
All	All	4965/5092 (98%)	4791 (96%)	158 (3%)	16 (0%)	36	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	893	ARG
1	A	706	LEU
1	A	893	ARG
1	B	893	ARG
1	B	1267	PRO
1	D	234	LYS
1	A	779	GLY
1	B	779	GLY
1	C	779	GLY
1	D	507	LYS
1	B	1217	GLU
1	C	1217	GLU
1	D	779	GLY
1	D	1217	GLU
1	A	1217	GLU
1	D	1267	PRO

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	1037/1053 (98%)	1021 (98%)	16 (2%)	57	73
1	B	1038/1053 (99%)	1023 (99%)	15 (1%)	59	75
1	C	1038/1053 (99%)	1018 (98%)	20 (2%)	50	66
1	D	1023/1053 (97%)	1006 (98%)	17 (2%)	53	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4136/4212 (98%)	4068 (98%)	68 (2%)	55 71

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	61	THR
1	A	174	GLU
1	A	215	SER
1	A	293	LEU
1	A	365	GLN
1	A	369	LEU
1	A	472	LEU
1	A	664	THR
1	A	683	VAL
1	A	800	LYS
1	A	868	CYS
1	A	939	ARG
1	A	952	GLU
1	A	965	ARG
1	A	1074	VAL
1	B	11	SER
1	B	197	CYS
1	B	234	LYS
1	B	276	ASN
1	B	346	ILE
1	B	388	ARG
1	B	392	LYS
1	B	458	GLU
1	B	522	LYS
1	B	662	LYS
1	B	683	VAL
1	B	693	LEU
1	B	800	LYS
1	B	965	ARG
1	B	1253	PRO
1	C	63	GLU
1	C	65	ARG
1	C	94	ARG
1	C	130	LYS
1	C	201	GLN
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	277	SER
1	C	278	SER
1	C	468	GLN
1	C	472	LEU
1	C	580	LYS
1	C	670	GLU
1	C	682	LYS
1	C	829	ASP
1	C	890	THR
1	C	1090	LYS
1	C	1253	PRO
1	C	1266	GLU
1	C	1267	PRO
1	C	1268	SER
1	D	10	THR
1	D	15	ASN
1	D	63	GLU
1	D	94	ARG
1	D	240	VAL
1	D	277	SER
1	D	293	LEU
1	D	301	LYS
1	D	365	GLN
1	D	450	LEU
1	D	507	LYS
1	D	515	VAL
1	D	531	SER
1	D	683	VAL
1	D	691	LYS
1	D	700	THR
1	D	948	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	228	GLN
1	A	296	GLN
1	A	410	HIS
1	A	474	GLN
1	A	567	GLN
1	A	723	GLN

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Mol	Chain	Res	Type
1	A	743	GLN
1	A	906	ASN
1	A	981	GLN
1	A	1026	GLN
1	A	1098	GLN
1	A	1101	GLN
1	A	1165	GLN
1	B	102	GLN
1	B	170	GLN
1	B	206	GLN
1	B	276	ASN
1	B	337	HIS
1	B	365	GLN
1	B	468	GLN
1	B	474	GLN
1	B	505	GLN
1	B	568	HIS
1	B	809	GLN
1	B	1101	GLN
1	C	146	ASN
1	C	201	GLN
1	C	311	GLN
1	C	354	GLN
1	C	717	GLN
1	C	802	ASN
1	C	833	GLN
1	C	860	HIS
1	C	963	HIS
1	C	1036	ASN
1	C	1125	ASN
1	C	1273	ASN
1	D	15	ASN
1	D	206	GLN
1	D	228	GLN
1	D	365	GLN
1	D	407	GLN
1	D	529	GLN
1	D	981	GLN
1	D	1026	GLN
1	D	1036	ASN
1	D	1098	GLN
1	D	1125	ASN

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Mol	Chain	Res	Type
1	D	1273	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 1 is modelled with single atom - leaving 31 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	$\#\|Z\| > 2$
5	PEG	A	1309	-	6,6,6	0.76	0	5,5,5	0.70	0
4	GOL	B	1310	-	5,5,5	0.18	0	5,5,5	0.45	0
3	FAD	D	1305	-	56,58,58	0.55	0	81,89,89	0.66	0
2	FES	B	1302	1	0,4,4	-	-	-		
3	FAD	B	1305	-	56,58,58	0.64	1 (1%)	81,89,89	0.68	0
2	FES	D	1301	1	0,4,4	-	-	-		
2	FES	A	1302	1	0,4,4	-	-	-		
2	FES	B	1301	1	0,4,4	-	-	-		
6	ZXF	B	1311	-	23,31,31	4.14	3 (13%)	20,52,52	1.63	4 (20%)
4	GOL	B	1309	-	5,5,5	0.08	0	5,5,5	0.21	0
3	FAD	C	1305	-	56,58,58	0.54	0	81,89,89	0.73	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	1306	-	5,5,5	0.14	0	5,5,5	0.62	0
4	GOL	B	1308	-	5,5,5	0.14	0	5,5,5	0.56	0
4	GOL	A	1308	-	5,5,5	0.38	0	5,5,5	0.58	0
2	FES	C	1302	1	0,4,4	-	-	-		
4	GOL	A	1310	-	5,5,5	0.36	0	5,5,5	0.75	0
6	ZXF	C	1308	-	23,31,31	3.25	3 (13%)	20,52,52	1.67	4 (20%)
2	FES	C	1301	1	0,4,4	-	-	-		
4	GOL	A	1307	-	5,5,5	0.06	0	5,5,5	0.29	0
4	GOL	C	1306	-	5,5,5	0.17	0	5,5,5	0.35	0
4	GOL	D	1307	-	5,5,5	0.13	0	5,5,5	0.43	0
6	ZXF	D	1309	-	23,31,31	2.84	3 (13%)	20,52,52	1.33	2 (10%)
4	GOL	B	1307	-	5,5,5	0.11	0	5,5,5	0.29	0
3	FAD	A	1305	-	56,58,58	0.54	0	81,89,89	0.70	1 (1%)
4	GOL	C	1307	-	5,5,5	0.12	0	5,5,5	0.39	0
4	GOL	D	1306	-	5,5,5	0.11	0	5,5,5	0.29	0
4	GOL	A	1311	-	5,5,5	0.22	0	5,5,5	0.44	0
4	GOL	B	1306	-	5,5,5	0.06	0	5,5,5	0.32	0
2	FES	A	1301	1	0,4,4	-	-	-		
2	FES	D	1302	1	0,4,4	-	-	-		
6	ZXF	A	1312	-	23,31,31	2.25	3 (13%)	20,52,52	1.82	4 (20%)

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
5	PEG	A	1309	-	-	2/4/4/4	-
4	GOL	B	1310	-	-	2/4/4/4	-
3	FAD	D	1305	-	-	0/34/50/50	0/6/6/6
3	FAD	B	1305	-	-	0/34/50/50	0/6/6/6
2	FES	B	1302	1	-	-	0/1/1/1
2	FES	D	1301	1	-	-	0/1/1/1
2	FES	A	1302	1	-	-	0/1/1/1
2	FES	B	1301	1	-	-	0/1/1/1
6	ZXF	B	1311	-	-	3/6/46/46	0/4/4/4
4	GOL	B	1309	-	-	0/4/4/4	-
3	FAD	C	1305	-	-	0/34/50/50	0/6/6/6
4	GOL	A	1306	-	-	2/4/4/4	-
4	GOL	B	1308	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1308	-	-	2/4/4/4	-
2	FES	C	1302	1	-	-	0/1/1/1
4	GOL	A	1310	-	-	4/4/4/4	-
6	ZXF	C	1308	-	-	4/6/46/46	0/4/4/4
2	FES	C	1301	1	-	-	0/1/1/1
4	GOL	A	1307	-	-	3/4/4/4	-
4	GOL	C	1306	-	-	0/4/4/4	-
4	GOL	D	1307	-	-	0/4/4/4	-
6	ZXF	D	1309	-	-	3/6/46/46	0/4/4/4
4	GOL	B	1307	-	-	0/4/4/4	-
3	FAD	A	1305	-	-	0/34/50/50	0/6/6/6
4	GOL	C	1307	-	-	0/4/4/4	-
4	GOL	D	1306	-	-	0/4/4/4	-
4	GOL	A	1311	-	-	2/4/4/4	-
4	GOL	B	1306	-	-	4/4/4/4	-
2	FES	A	1301	1	-	-	0/1/1/1
2	FES	D	1302	1	-	-	0/1/1/1
6	ZXF	A	1312	-	-	3/6/46/46	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1311	ZXF	MO-S2'	16.55	2.62	2.39
6	C	1308	ZXF	MO-S2'	11.30	2.55	2.39
6	D	1309	ZXF	MO-S2'	9.16	2.52	2.39
6	B	1311	ZXF	MO-S1'	-8.17	2.27	2.39
6	D	1309	ZXF	O2-MO	8.14	1.90	1.69
6	C	1308	ZXF	O2-MO	8.12	1.90	1.69
6	C	1308	ZXF	MO-S1'	-6.61	2.30	2.39
6	B	1311	ZXF	O2-MO	6.56	1.86	1.69
6	A	1312	ZXF	MO-S2'	6.44	2.48	2.39
6	A	1312	ZXF	O2-MO	6.36	1.85	1.69
6	A	1312	ZXF	MO-S1'	-5.34	2.31	2.39
6	D	1309	ZXF	MO-S1'	-5.01	2.32	2.39
3	B	1305	FAD	C1'-C2'	-2.96	1.48	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1312	ZXF	O3'-C7-C6	4.25	111.80	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1312	ZXF	C1'-C2'-S2'	3.97	122.40	120.15
6	B	1311	ZXF	O3'-C7-C6	3.59	111.36	108.96
6	C	1308	ZXF	C2'-C1'-S1'	3.56	122.17	120.15
6	D	1309	ZXF	O3'-C7-C6	3.20	111.10	108.96
6	B	1311	ZXF	C2'-C1'-S1'	3.18	121.95	120.15
6	A	1312	ZXF	C2-N1-C10	2.96	118.78	113.43
6	C	1308	ZXF	C2-N1-C10	2.88	118.62	113.43
6	D	1309	ZXF	C2-N1-C10	2.83	118.54	113.43
6	C	1308	ZXF	C1'-C2'-S2'	2.73	121.70	120.15
6	B	1311	ZXF	C2-N1-C10	2.54	118.01	113.43
6	C	1308	ZXF	O3'-C7-C6	2.49	110.62	108.96
3	C	1305	FAD	P-O3P-PA	-2.25	125.12	132.83
6	B	1311	ZXF	O3'-C7-N8	-2.18	106.33	108.57
6	A	1312	ZXF	C4-C9-N5	2.16	122.55	116.76
3	A	1305	FAD	C4-N3-C2	-2.03	121.90	125.64

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1306	GOL	O1-C1-C2-C3
4	A	1308	GOL	C1-C2-C3-O3
4	A	1310	GOL	O1-C1-C2-C3
4	A	1311	GOL	C1-C2-C3-O3
4	B	1306	GOL	O1-C1-C2-C3
4	B	1306	GOL	C1-C2-C3-O3
6	A	1312	ZXF	C3'-C4'-O4'-P
6	A	1312	ZXF	C4'-O4'-P-O3P
6	B	1311	ZXF	C3'-C4'-O4'-P
6	B	1311	ZXF	C4'-O4'-P-O2P
6	B	1311	ZXF	C4'-O4'-P-O1P
6	C	1308	ZXF	C4'-O4'-P-O2P
6	C	1308	ZXF	C4'-O4'-P-O1P
6	D	1309	ZXF	C3'-C4'-O4'-P
6	D	1309	ZXF	C4'-O4'-P-O2P
6	C	1308	ZXF	C3'-C4'-O4'-P
4	A	1310	GOL	O1-C1-C2-O2
4	B	1306	GOL	O1-C1-C2-O2
4	A	1310	GOL	C1-C2-C3-O3
4	B	1308	GOL	O1-C1-C2-C3
4	B	1310	GOL	C1-C2-C3-O3
4	A	1308	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1311	GOL	O2-C2-C3-O3
4	A	1306	GOL	O1-C1-C2-O2
4	A	1310	GOL	O2-C2-C3-O3
6	C	1308	ZXF	C4'-O4'-P-O3P
6	A	1312	ZXF	C4'-O4'-P-O1P
6	D	1309	ZXF	C4'-O4'-P-O1P
4	A	1307	GOL	O2-C2-C3-O3
4	B	1306	GOL	O2-C2-C3-O3
5	A	1309	PEG	C4-C3-O2-C2
4	B	1308	GOL	O1-C1-C2-O2
4	A	1307	GOL	O1-C1-C2-C3
4	A	1307	GOL	C1-C2-C3-O3
4	B	1310	GOL	O2-C2-C3-O3
5	A	1309	PEG	C1-C2-O2-C3

There are no ring outliers.

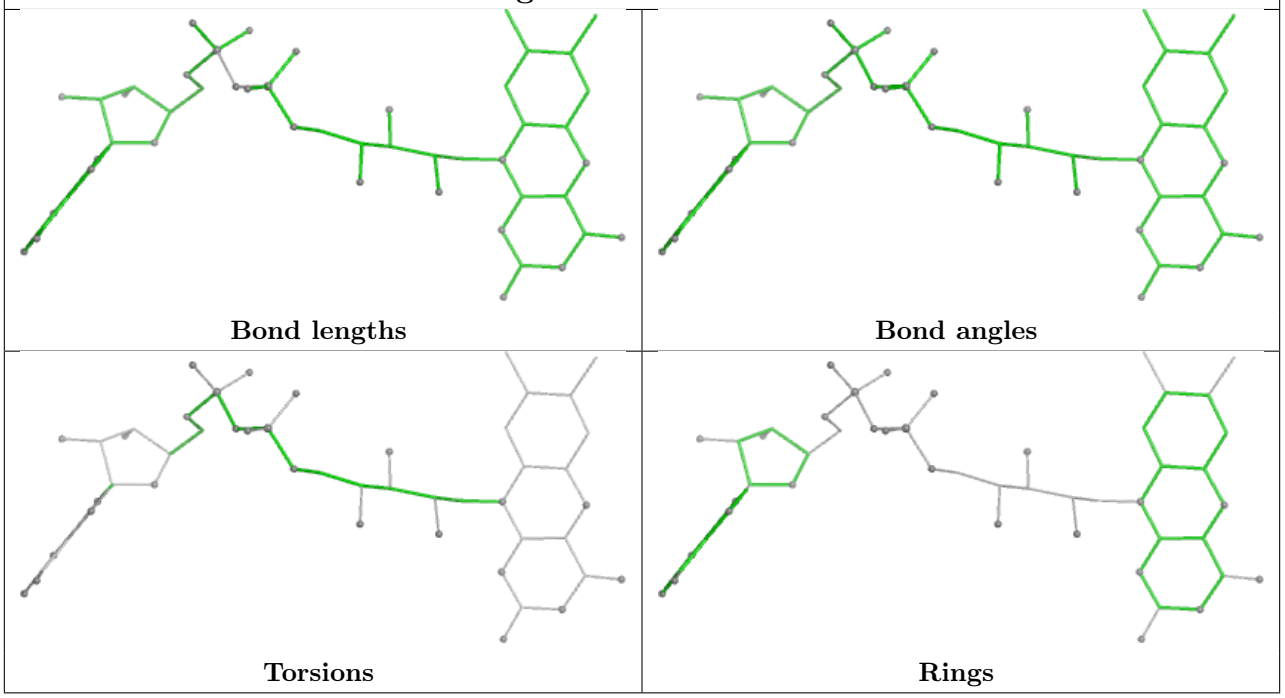
12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1309	PEG	4	0
4	B	1310	GOL	1	0
6	B	1311	ZXF	2	0
3	C	1305	FAD	1	0
4	A	1306	GOL	1	0
4	A	1308	GOL	3	0
4	A	1310	GOL	7	0
6	C	1308	ZXF	1	0
4	D	1307	GOL	1	0
6	D	1309	ZXF	3	0
3	A	1305	FAD	1	0
6	A	1312	ZXF	2	0

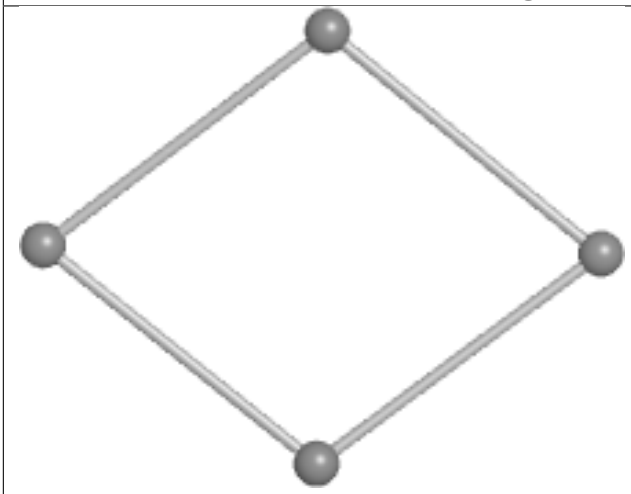
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

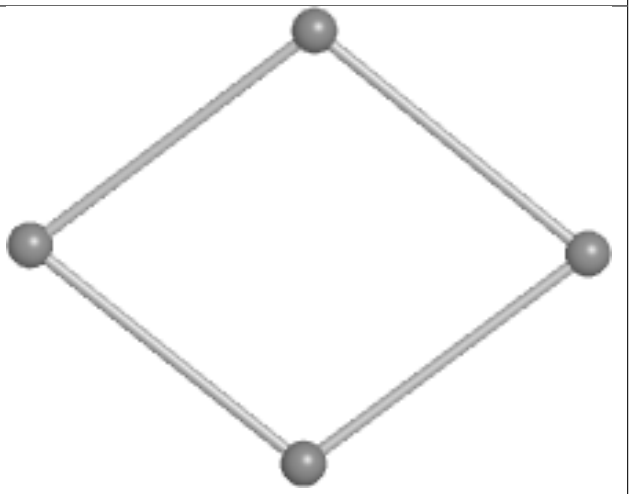
Ligand FAD D 1305



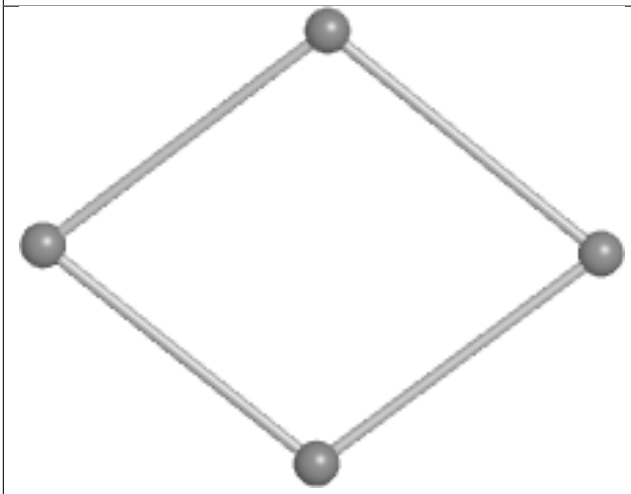
Ligand FES B 1302



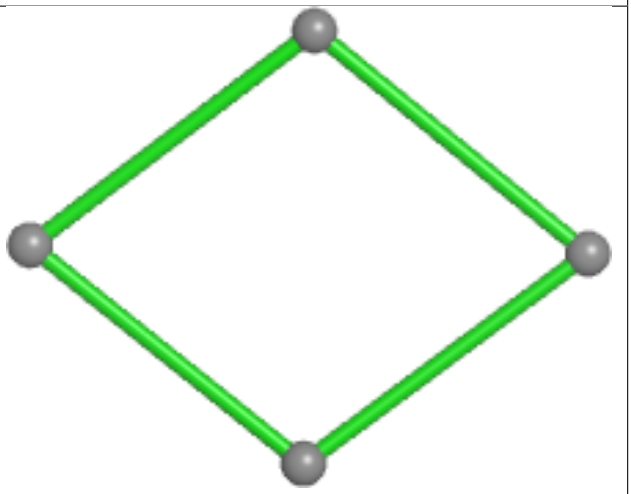
Bond lengths



Bond angles

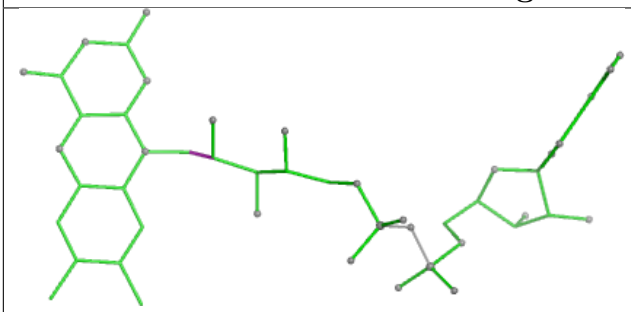


Torsions

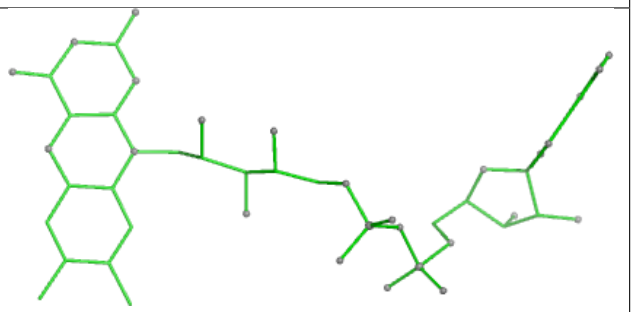


Rings

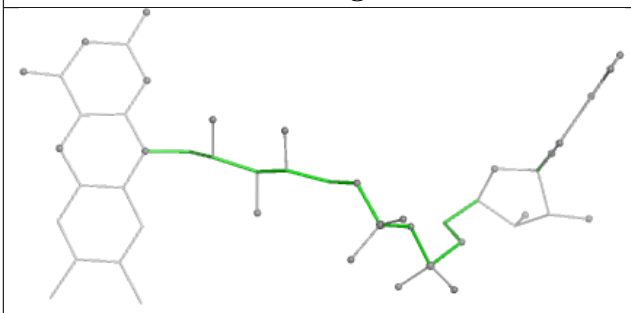
Ligand FAD B 1305



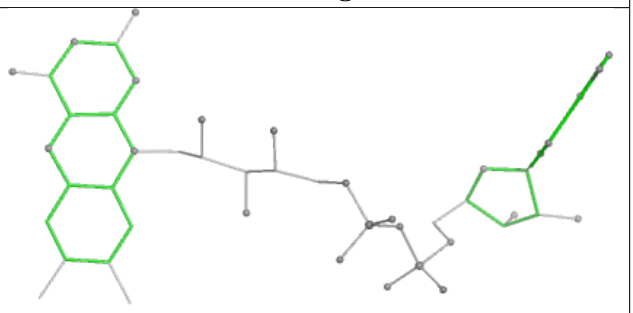
Bond lengths



Bond angles

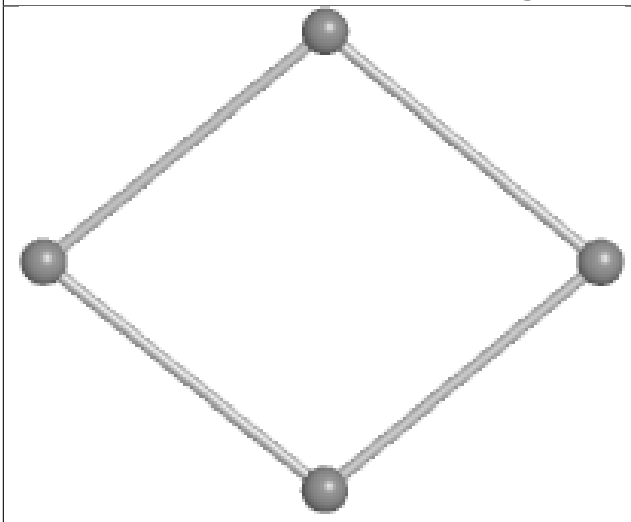


Torsions

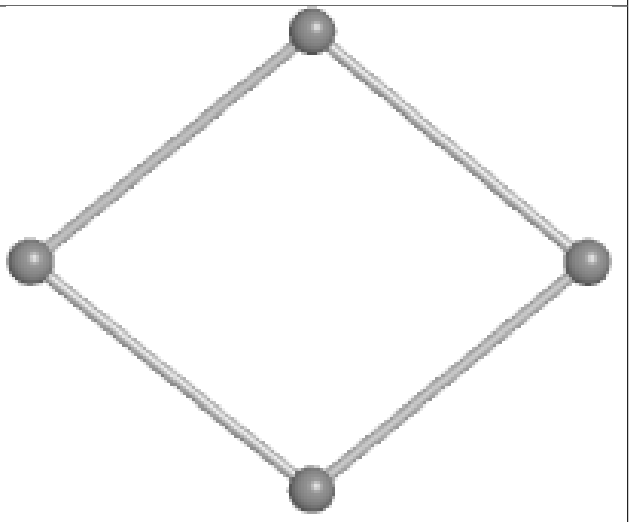


Rings

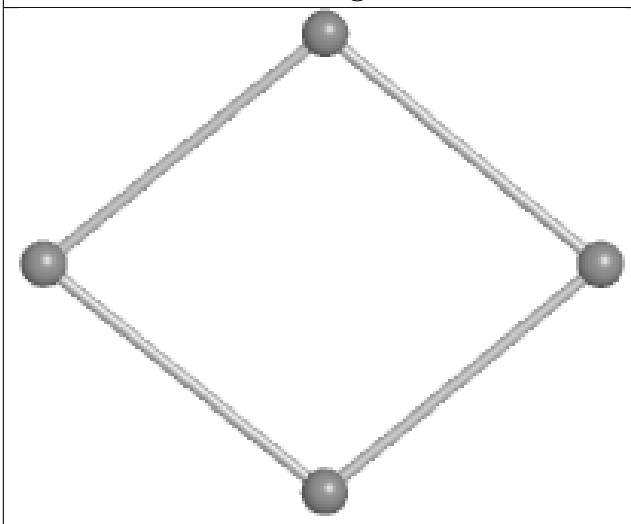
Ligand FES D 1301



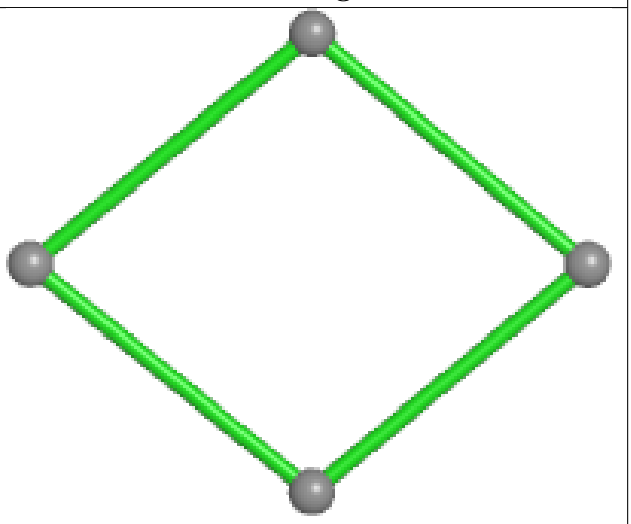
Bond lengths



Bond angles

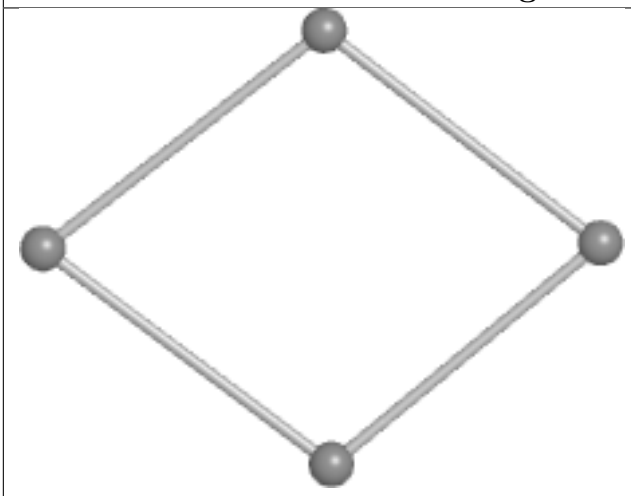


Torsions



Rings

Ligand FES A 1302



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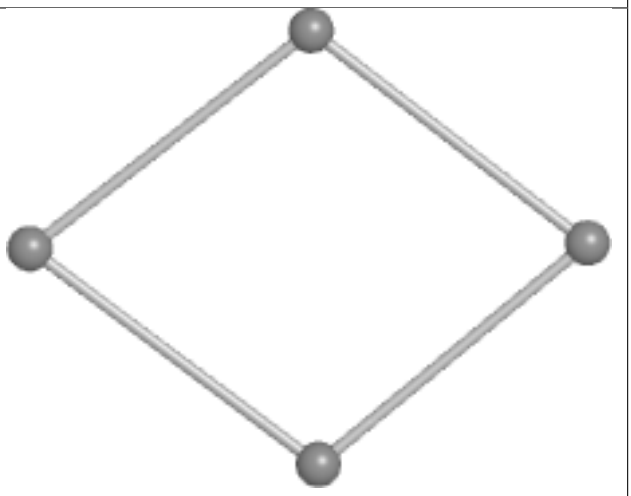

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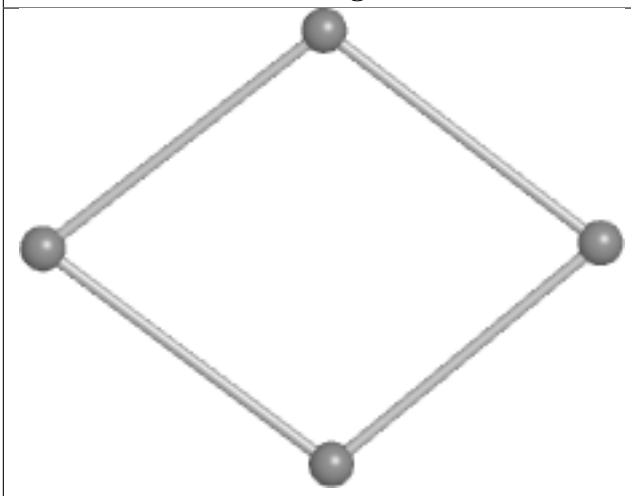

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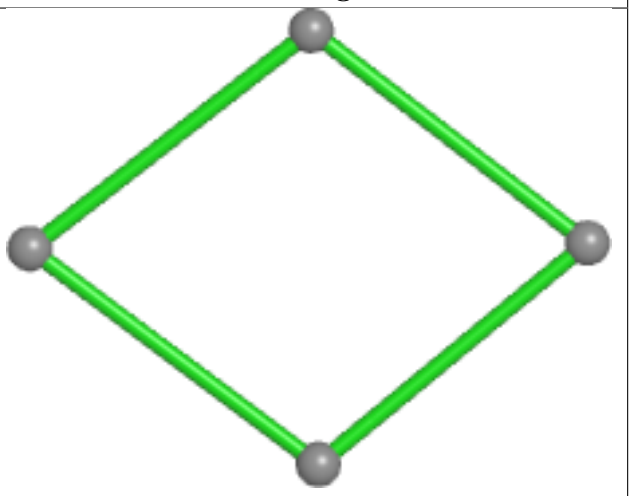
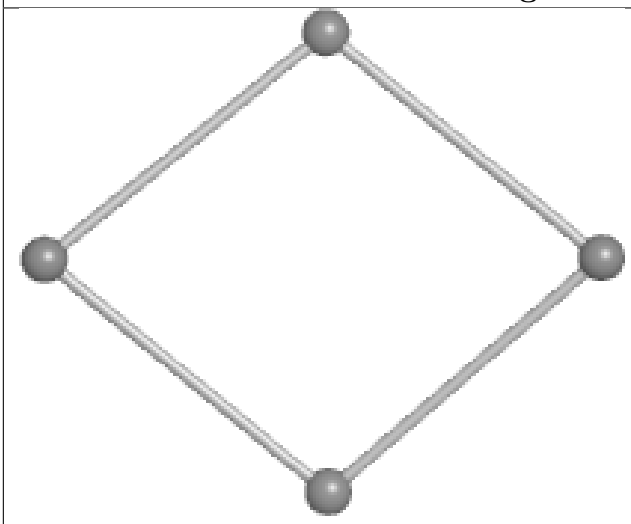


Rings

Ligand FES B 1301



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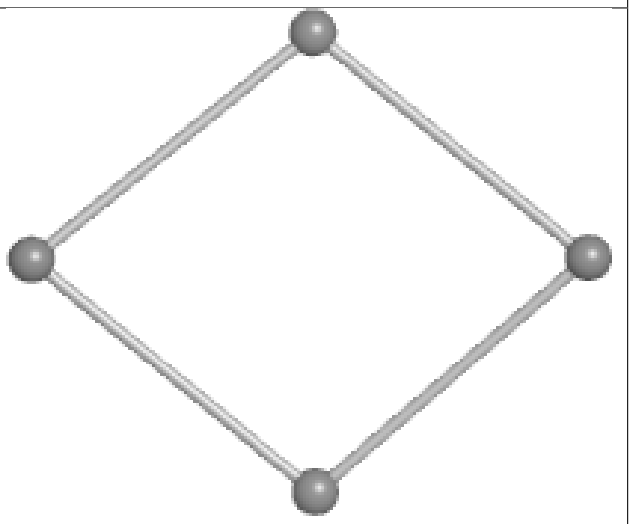
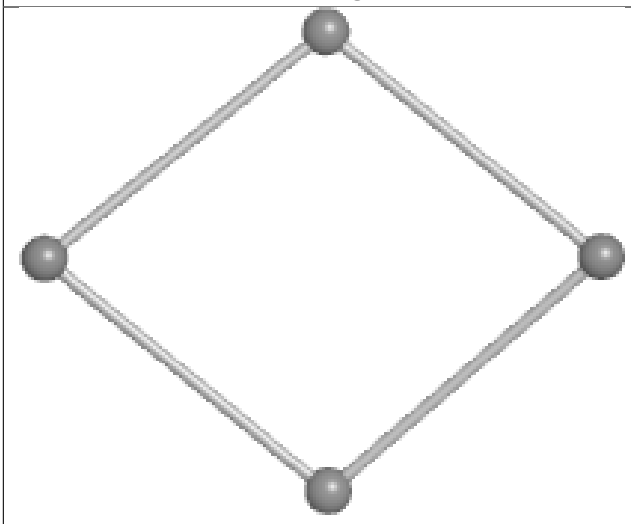


Bond angles



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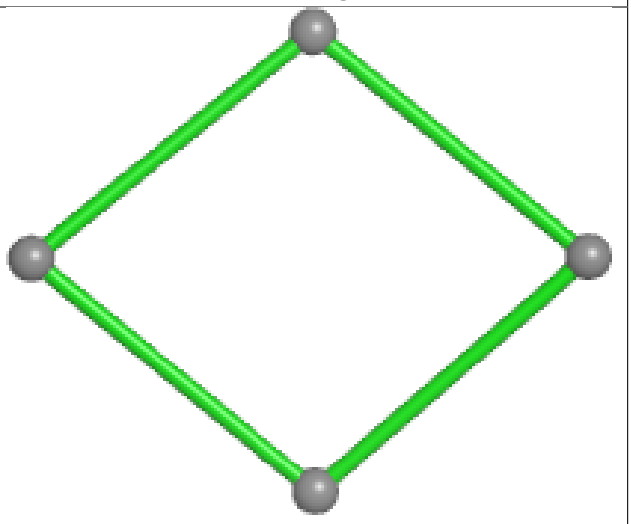
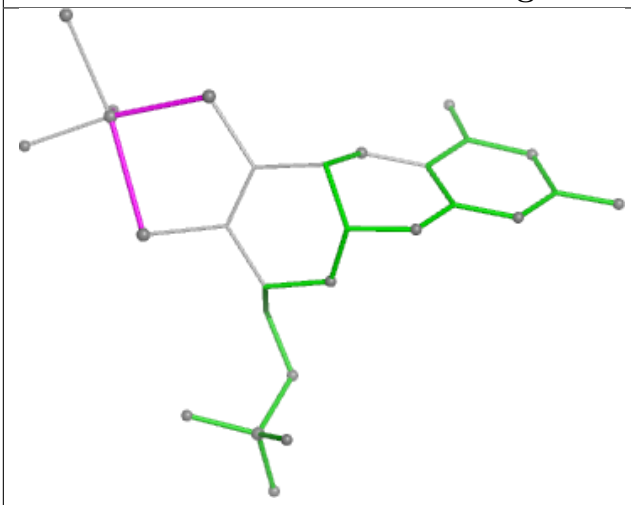
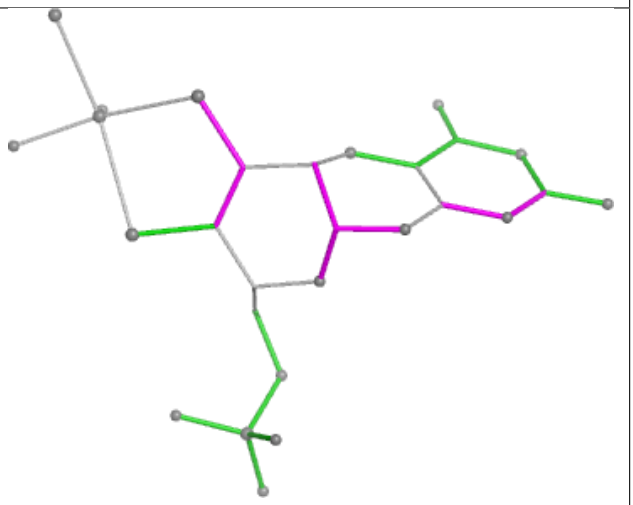


Rings

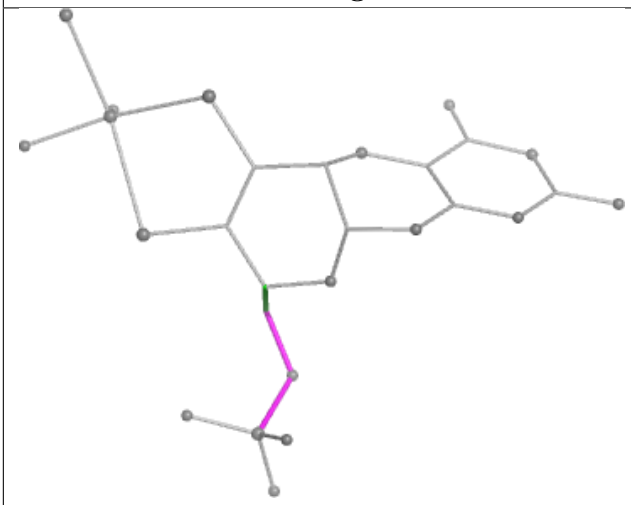
Ligand ZXF B 1311



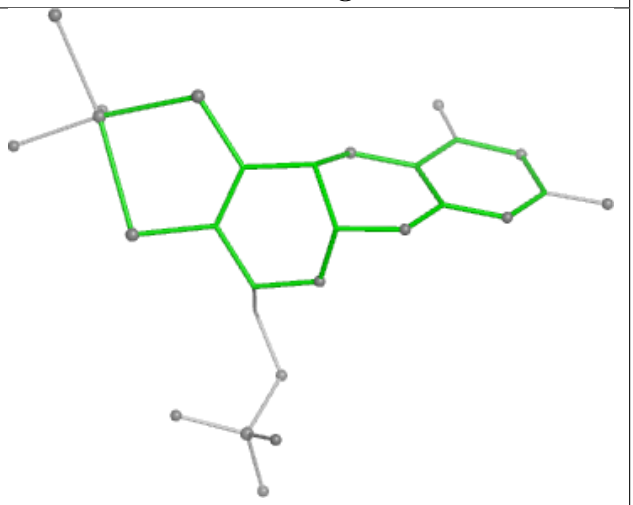
Bond lengths



Bond angles

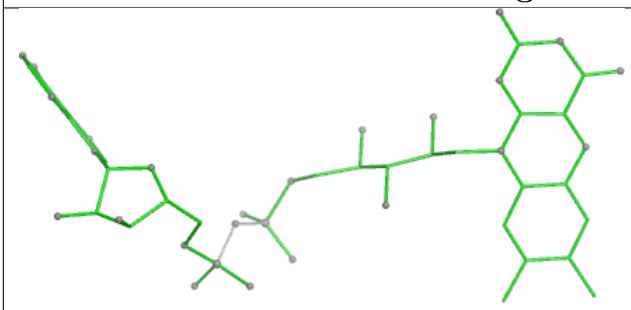


Torsions



Rings

Ligand FAD C 1305



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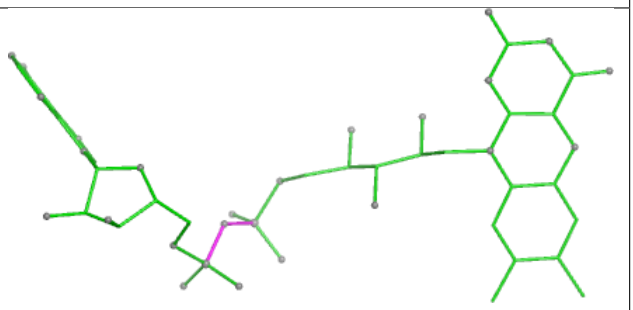
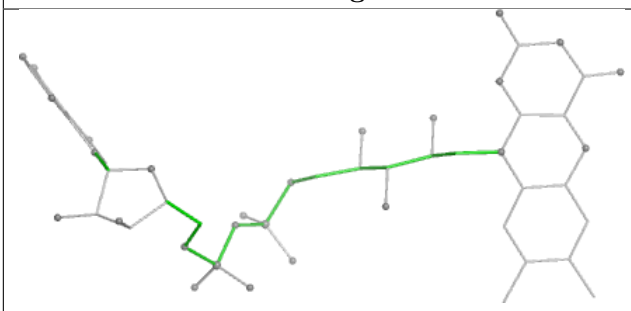
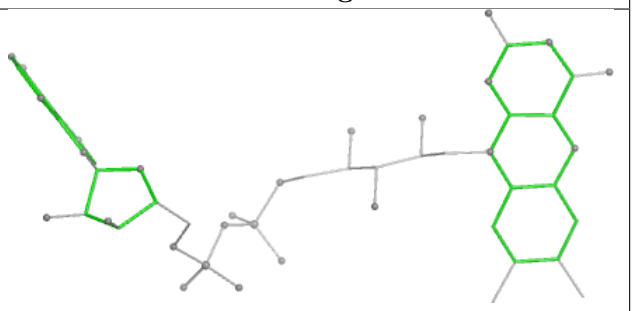


Bond angles

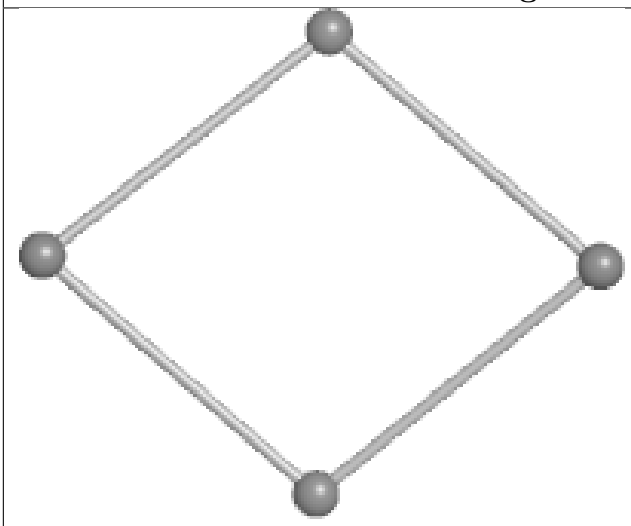


Torsions



Rings

Ligand FES C 1302



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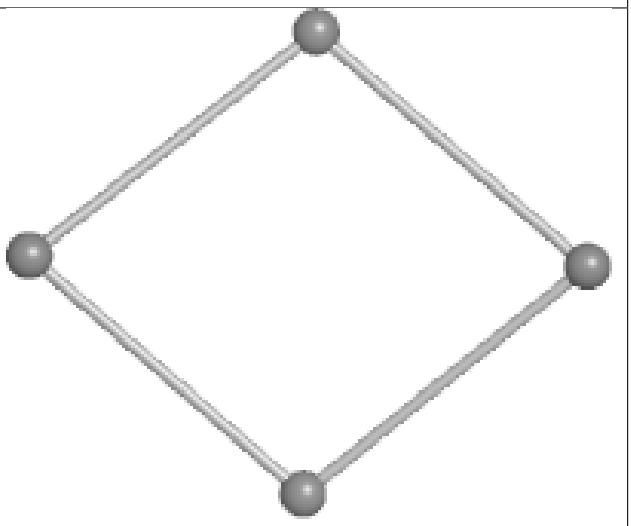
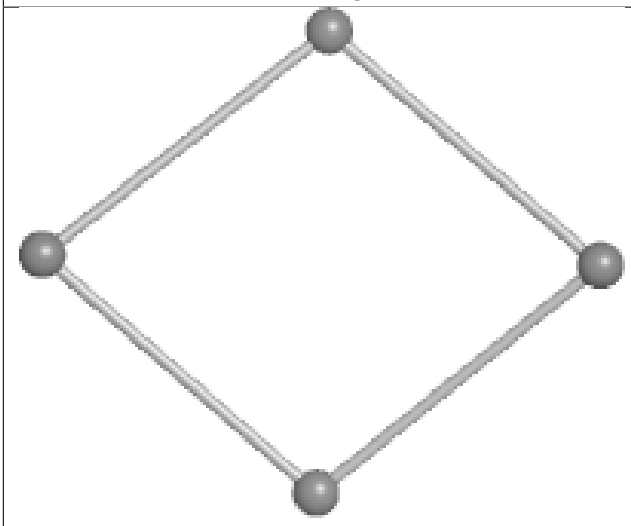


Bond angles



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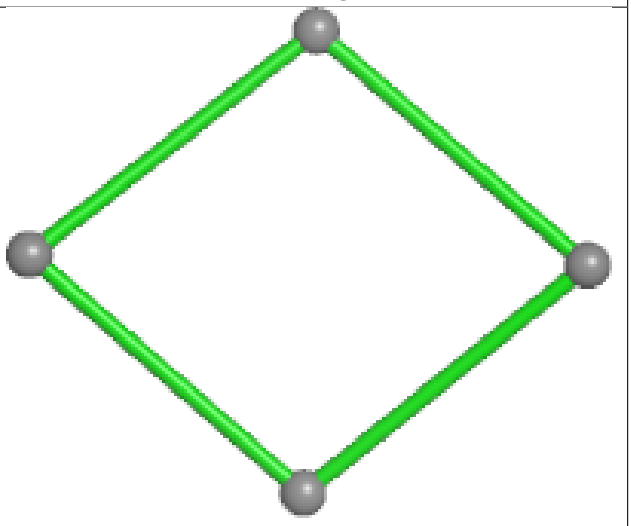
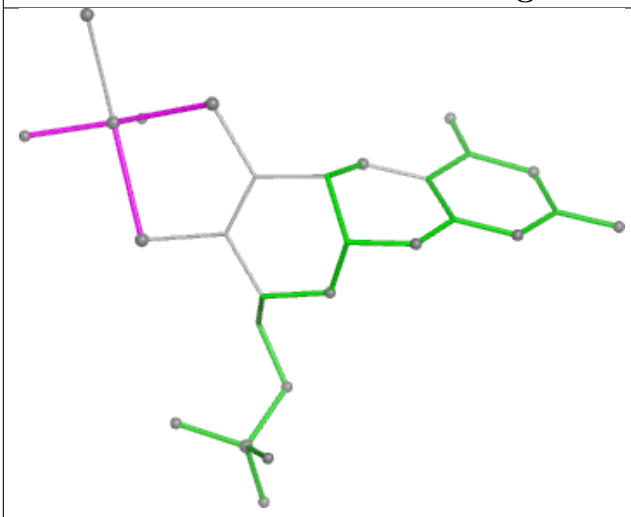


Rings

Ligand ZXF C 1308



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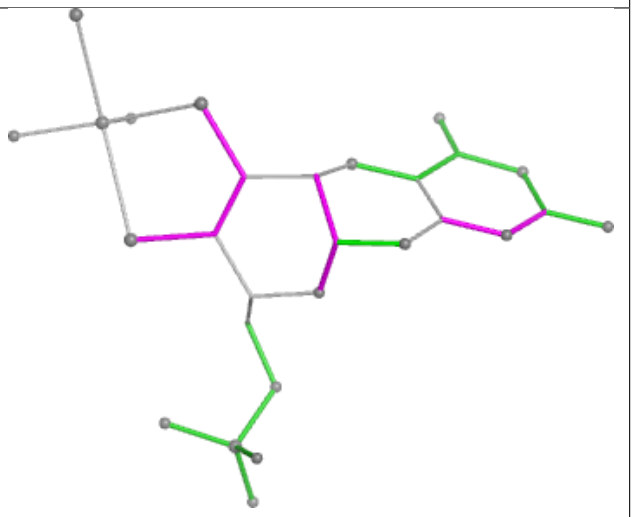
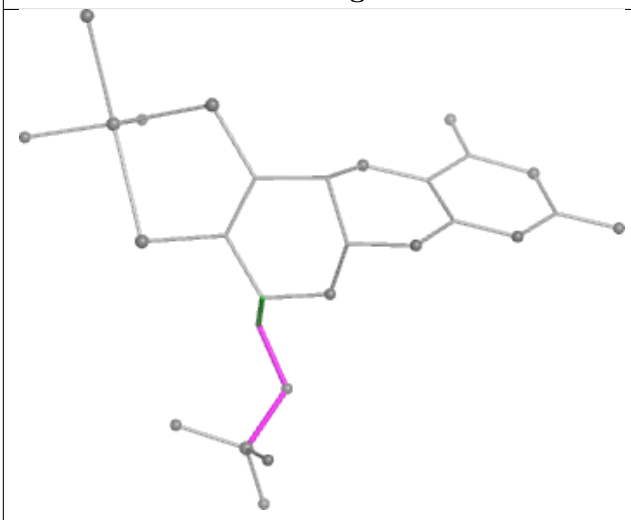


Bond angles



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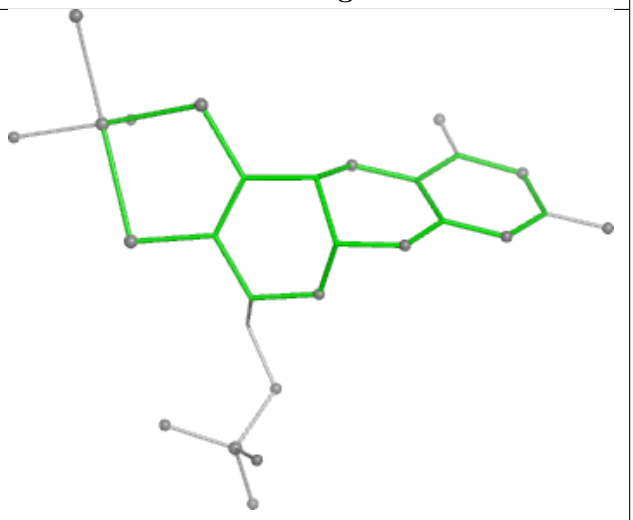
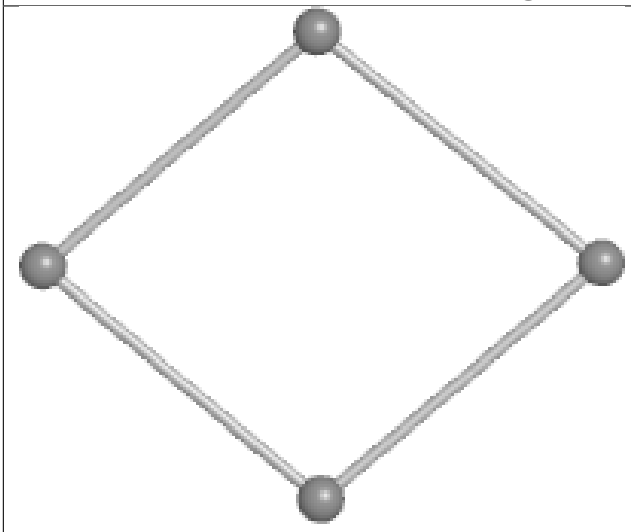


Rings

Ligand FES C 1301



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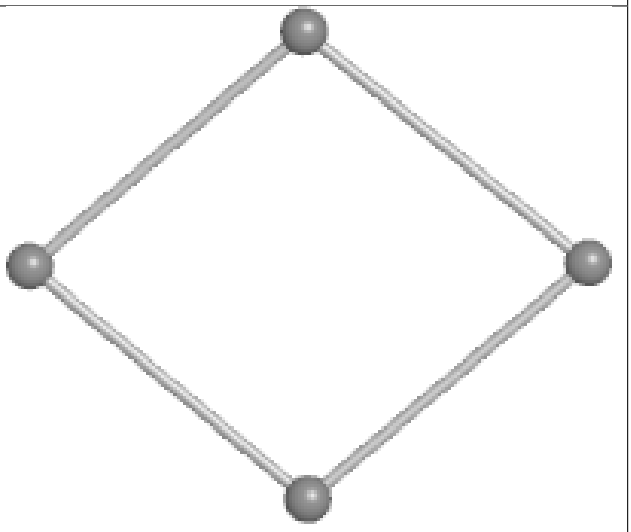
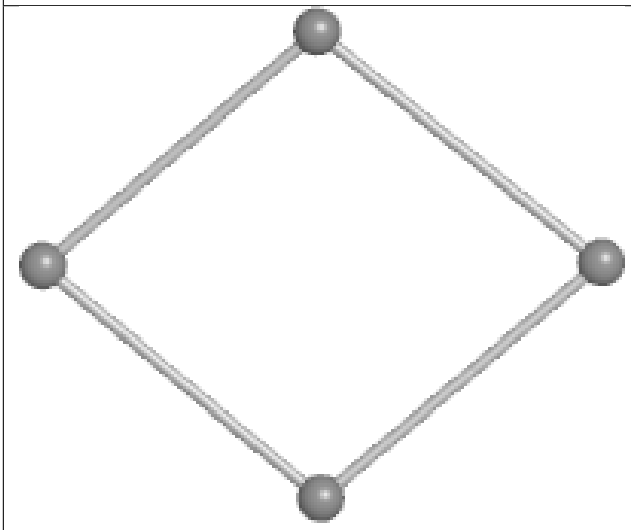


Bond angles



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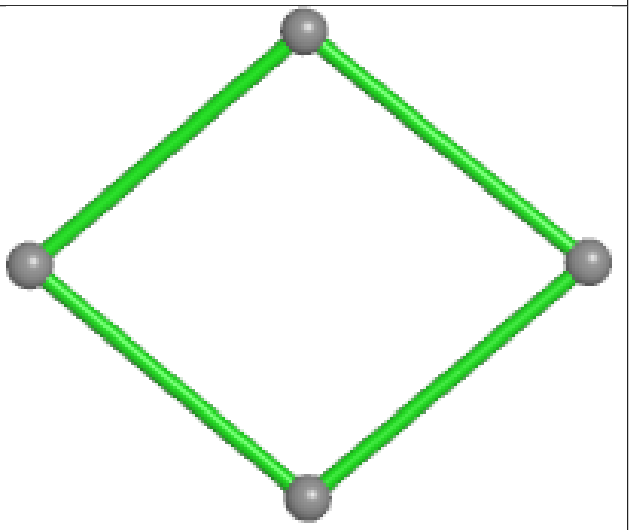
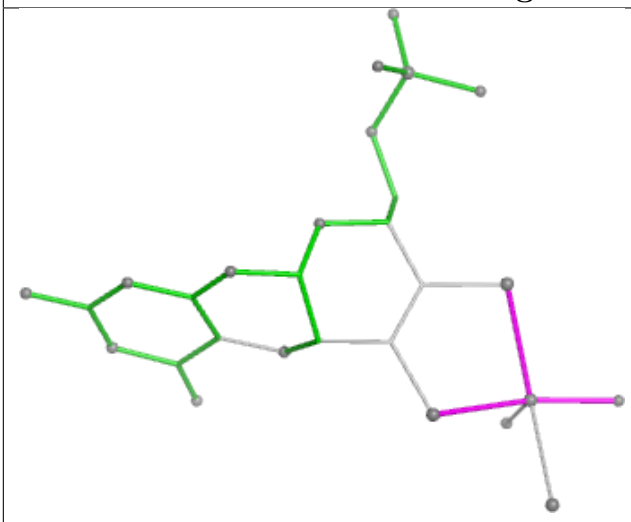


Rings

Ligand ZXF D 1309



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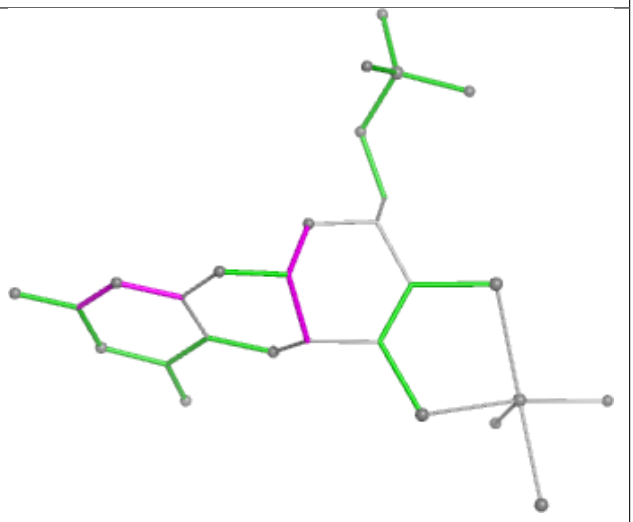

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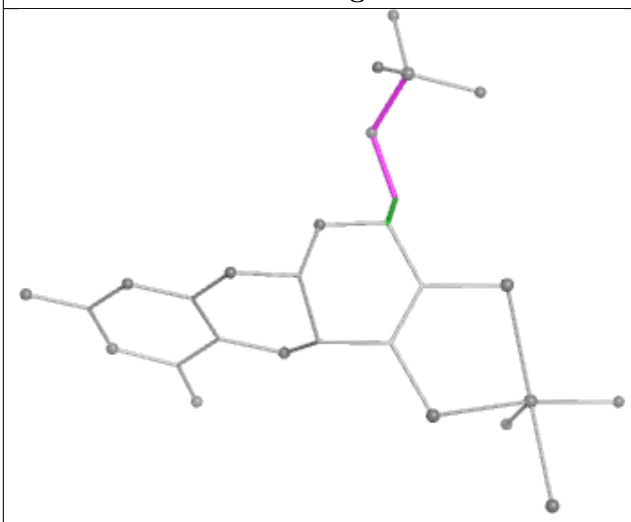
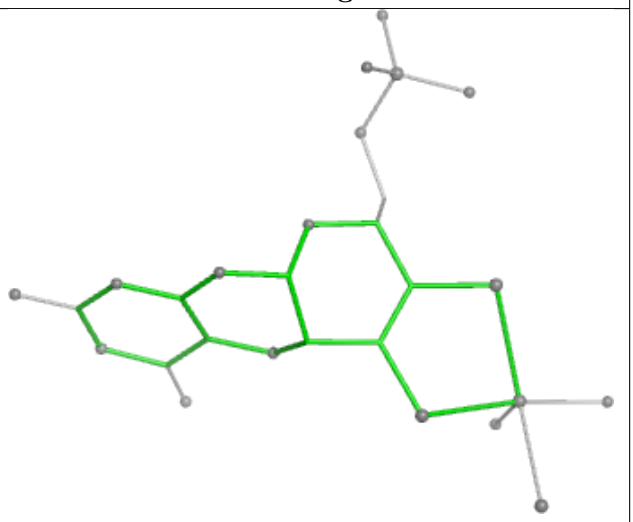
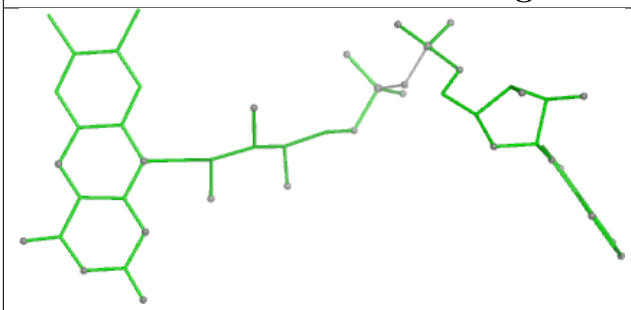


Torsions

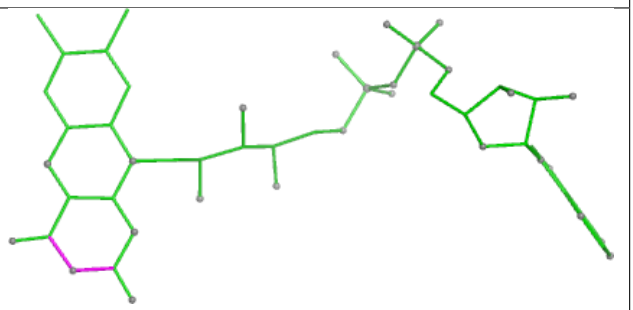


Rings

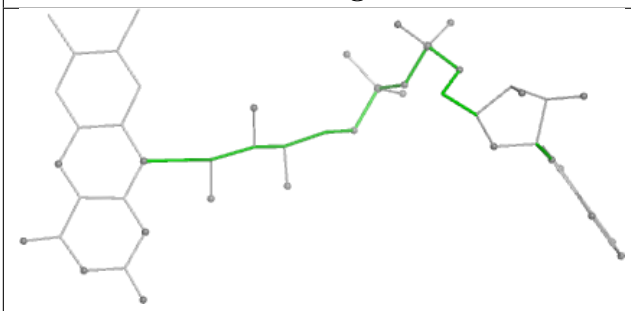
Ligand FAD A 1305



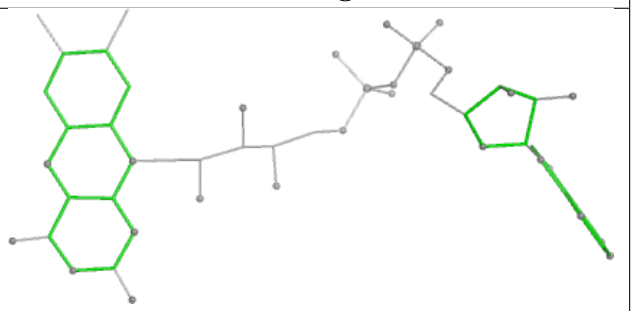
Bond lengths



Bond angles

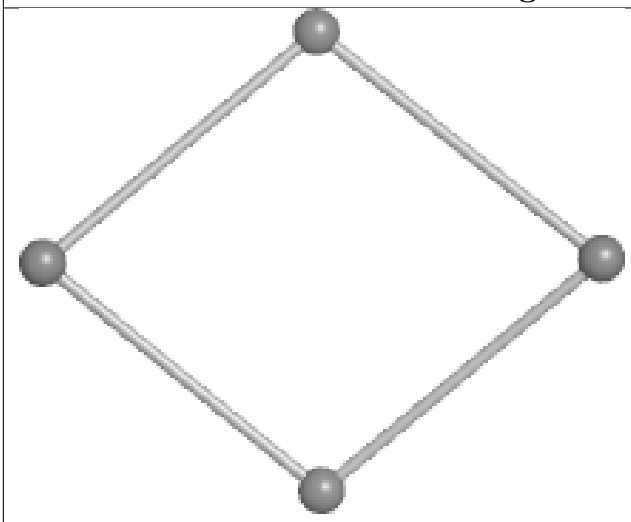


Torsions



Rings

Ligand FES A 1301



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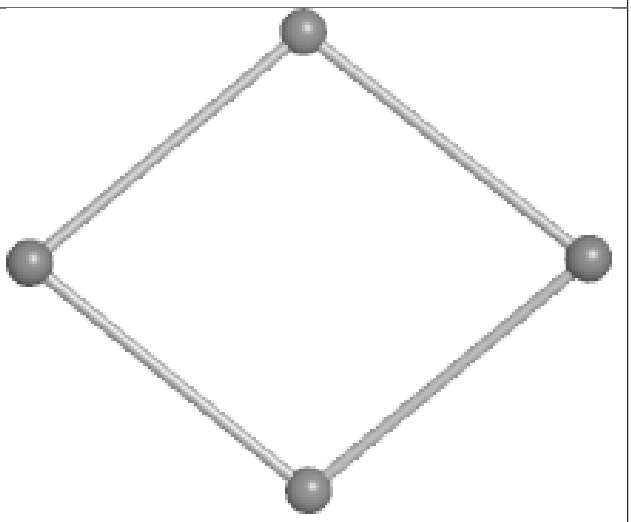
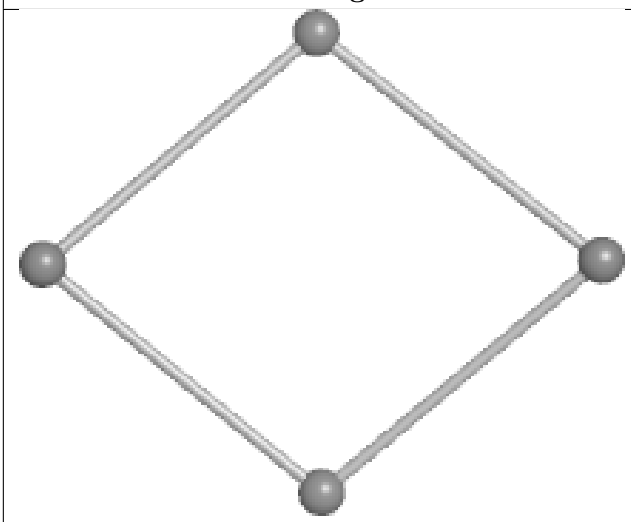


Bond angles



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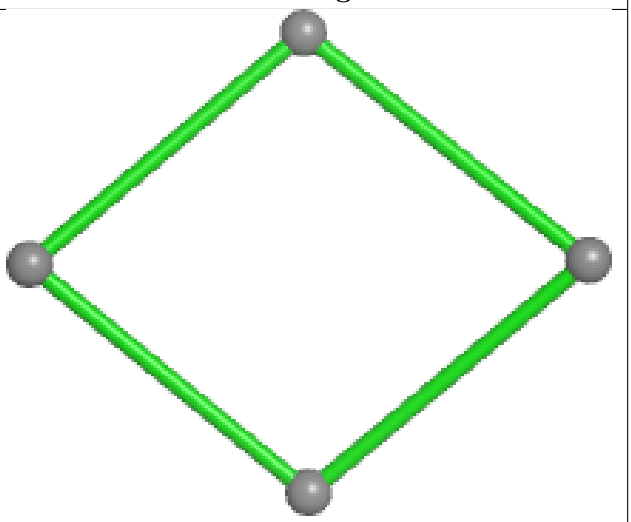
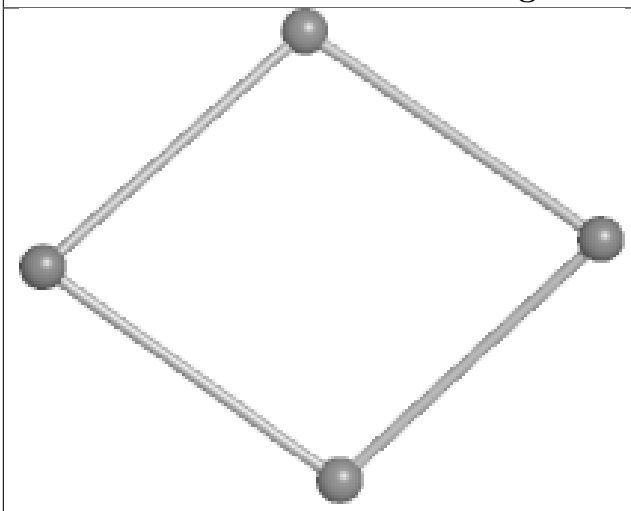
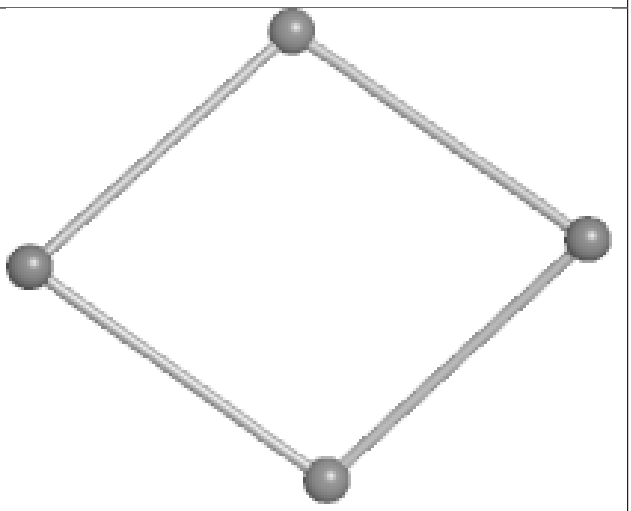


Rings

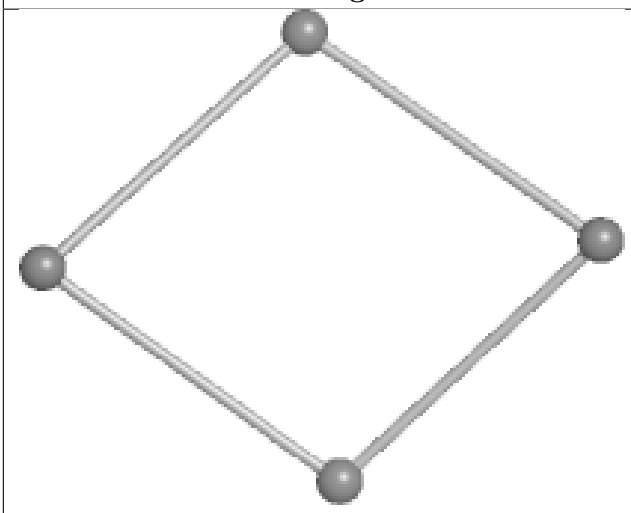
Ligand FES D 1302



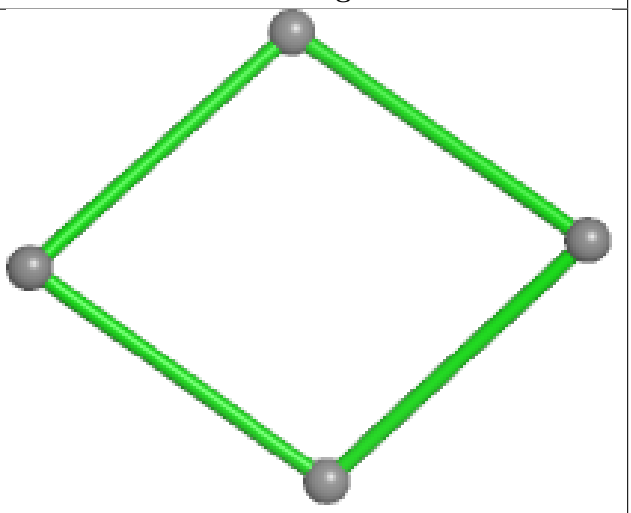
Bond lengths



Bond angles

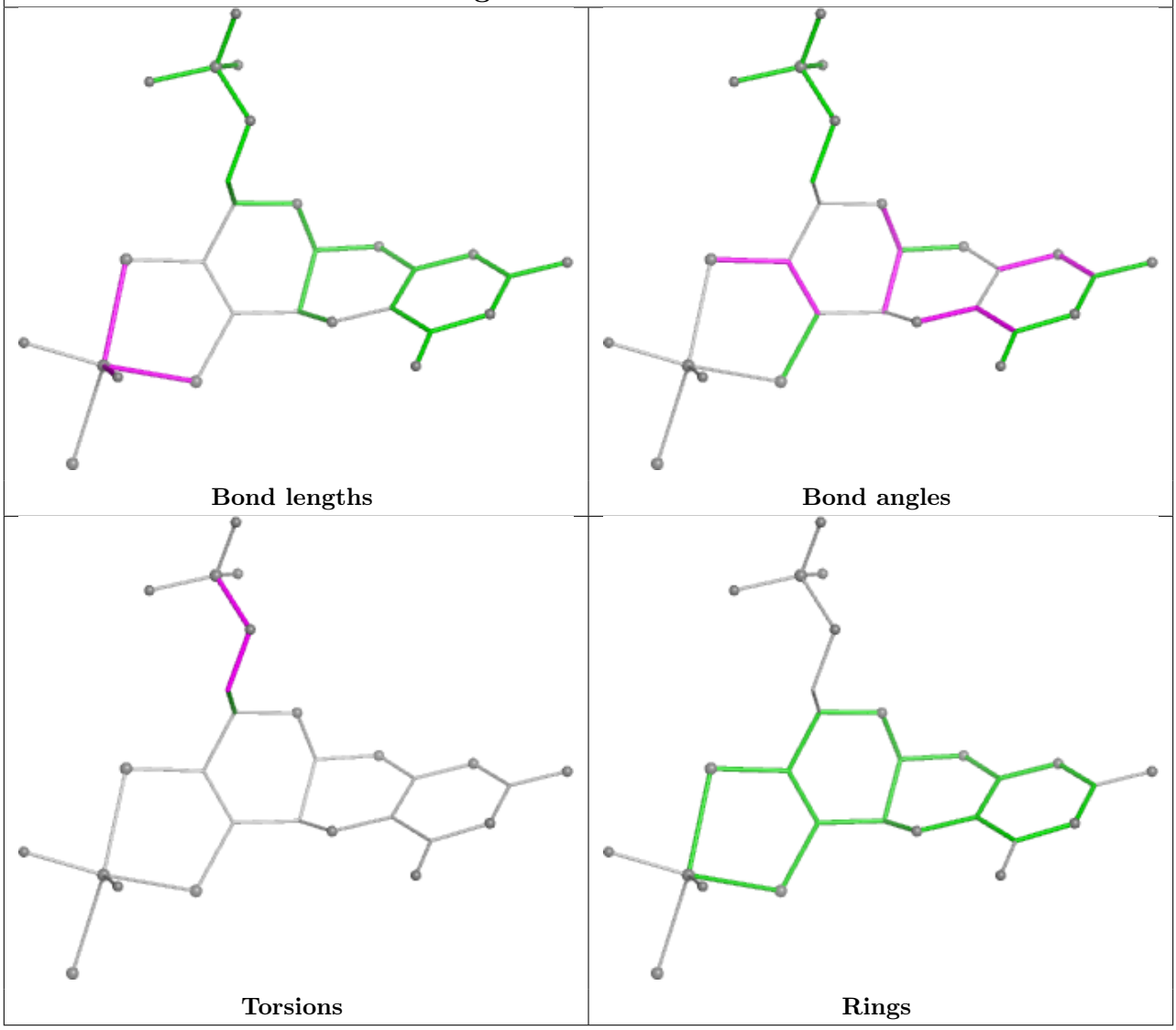


Torsions



Rings

Ligand ZXF A 1312



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, 95^{th} 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	1249/1273 (98%)	-0.41	10 (0%)	82	80	12, 23, 49, 85	2 (0%)
1	B	1253/1273 (98%)	-0.23	9 (0%)	84	82	13, 28, 61, 89	2 (0%)
1	C	1252/1273 (98%)	-0.16	14 (1%)	78	76	16, 30, 58, 105	2 (0%)
1	D	1236/1273 (97%)	0.09	36 (2%)	53	50	15, 36, 72, 102	1 (0%)
All	All	4990/5092 (97%)	-0.18	69 (1%)	73	71	12, 29, 62, 105	7 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	GLY	4.5
1	B	274	ALA	4.3
1	C	58	HIS	3.8
1	A	197	CYS	3.8
1	D	57	ILE	3.8
1	D	683	VAL	3.6
1	B	688	GLY	3.6
1	C	690	ASN	3.5
1	B	687	ALA	3.5
1	B	197	CYS	3.3
1	C	62	GLY	3.2
1	D	204	GLY	3.1
1	D	59	PRO	3.0
1	D	2	ALA	3.0
1	D	438	HIS	2.9
1	C	183	THR	2.9
1	D	202	PRO	2.9
1	A	198	LYS	2.9
1	D	58	HIS	2.8
1	C	467	GLY	2.8
1	B	1267	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	683	VAL	2.8
1	D	274	ALA	2.8
1	C	59	PRO	2.7
1	C	522	LYS	2.7
1	D	228	GLN	2.7
1	D	520	LEU	2.7
1	D	218	VAL	2.5
1	B	522	LYS	2.5
1	B	669	ALA	2.5
1	C	440	GLU	2.5
1	D	207	LEU	2.5
1	D	272	LEU	2.4
1	A	205	SER	2.4
1	D	293	LEU	2.4
1	A	467	GLY	2.3
1	A	423	ALA	2.3
1	B	423	ALA	2.3
1	C	1267	PRO	2.3
1	D	502	ILE	2.3
1	D	227	LEU	2.3
1	D	264	LEU	2.3
1	A	62	GLY	2.3
1	C	61	THR	2.3
1	D	422	THR	2.3
1	C	57	ILE	2.3
1	D	205	SER	2.3
1	D	568	HIS	2.3
1	A	705	GLN	2.3
1	D	361	VAL	2.3
1	D	379	GLY	2.2
1	C	423	ALA	2.2
1	D	365	GLN	2.2
1	D	259	ILE	2.2
1	D	423	ALA	2.2
1	D	391	PRO	2.1
1	C	2	ALA	2.1
1	D	279	LEU	2.1
1	D	226	ALA	2.1
1	D	425	ALA	2.1
1	A	520	LEU	2.1
1	D	261	VAL	2.1
1	B	1268	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	18	ALA	2.1
1	A	683	VAL	2.1
1	D	234	LYS	2.0
1	A	61	THR	2.0
1	D	203	LYS	2.0
1	D	507	LYS	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 oligosaccharides 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, 95^{th} 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
4	GOL	D	1307	6/6	0.74	0.15	45,49,50,51	6
4	GOL	A	1308	6/6	0.78	0.18	35,42,44,46	0
4	GOL	B	1310	6/6	0.80	0.18	54,60,62,62	0
5	PEG	A	1309	7/7	0.84	0.18	32,32,38,39	0
4	GOL	C	1307	6/6	0.85	0.12	52,55,56,56	0
4	GOL	A	1307	6/6	0.86	0.12	45,50,50,52	0
4	GOL	A	1311	6/6	0.86	0.12	43,46,49,51	0
4	GOL	B	1308	6/6	0.88	0.13	39,42,44,52	0
4	GOL	B	1309	6/6	0.88	0.12	29,42,46,52	0
4	GOL	A	1310	6/6	0.89	0.16	34,41,43,48	0
4	GOL	D	1306	6/6	0.89	0.11	31,33,35,40	0
6	ZXF	B	1311	28/28	0.92	0.10	30,42,52,56	4
6	ZXF	D	1309	28/28	0.92	0.11	32,46,49,66	4
3	FAD	D	1305	53/53	0.94	0.08	37,45,51,56	0
6	ZXF	A	1312	28/28	0.94	0.10	22,40,50,52	4
4	GOL	A	1306	6/6	0.94	0.07	25,30,32,33	0
4	GOL	B	1306	6/6	0.94	0.08	29,32,34,36	0

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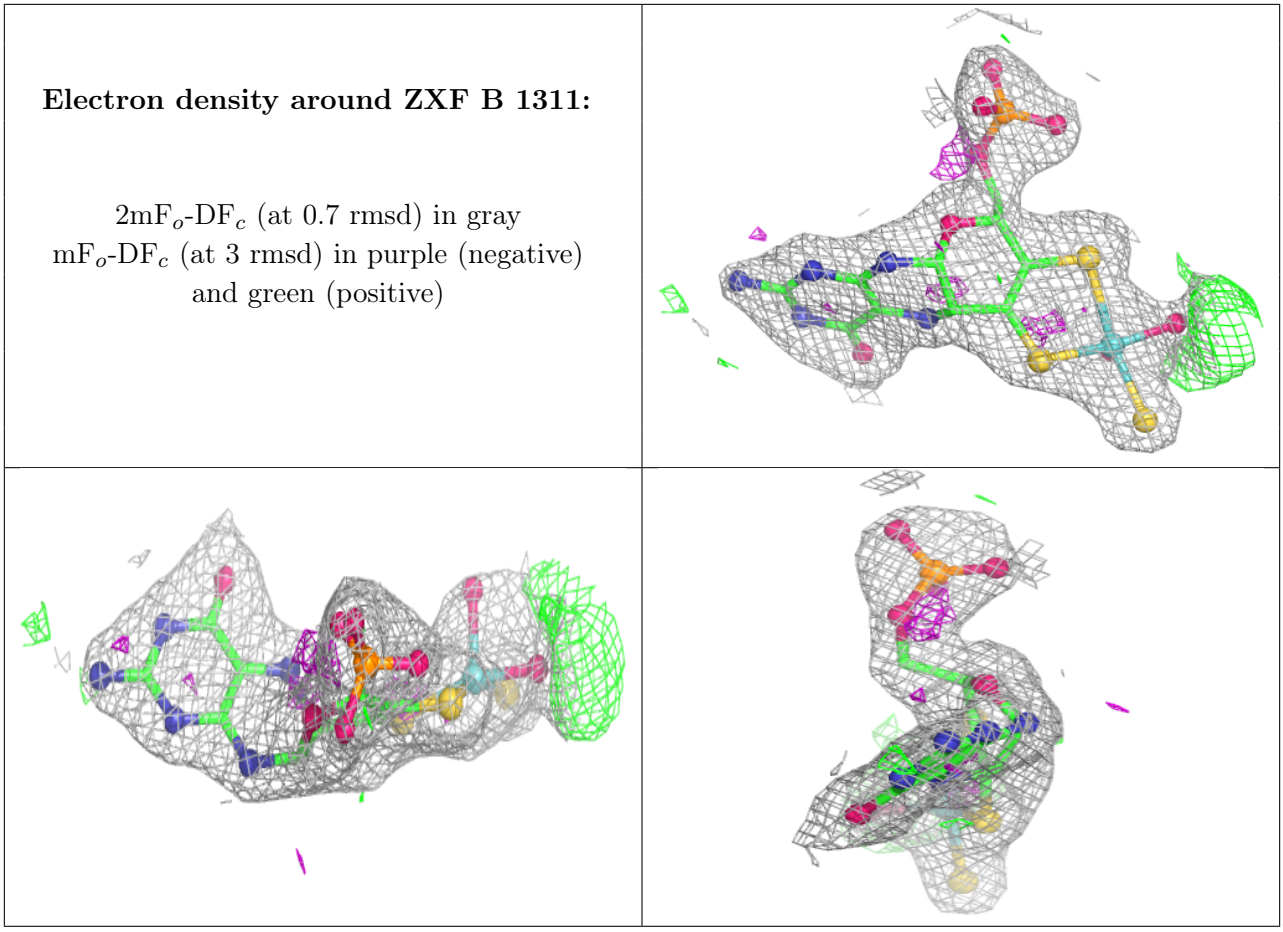
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NH4	D	1308	1/1	0.94	0.20	22,22,22,22	0
4	GOL	C	1306	6/6	0.95	0.07	28,29,31,34	0
6	ZXF	C	1308	28/28	0.95	0.10	31,46,55,58	4
4	GOL	B	1307	6/6	0.96	0.07	33,37,38,40	0
3	FAD	C	1305	53/53	0.96	0.06	22,31,34,35	0
3	FAD	A	1305	53/53	0.97	0.05	19,22,25,26	0
3	FAD	B	1305	53/53	0.97	0.06	20,25,29,30	0
2	FES	C	1301	4/4	0.99	0.03	22,22,23,23	0
2	FES	C	1302	4/4	0.99	0.02	23,23,24,25	0
2	FES	D	1301	4/4	0.99	0.03	27,28,29,32	0
2	FES	D	1302	4/4	0.99	0.04	31,31,31,35	0
2	FES	A	1301	4/4	0.99	0.02	19,19,19,21	0
2	FES	A	1302	4/4	0.99	0.02	17,18,18,18	0
2	FES	B	1301	4/4	0.99	0.02	21,21,22,23	0
2	FES	B	1302	4/4	1.00	0.02	20,21,21,22	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.

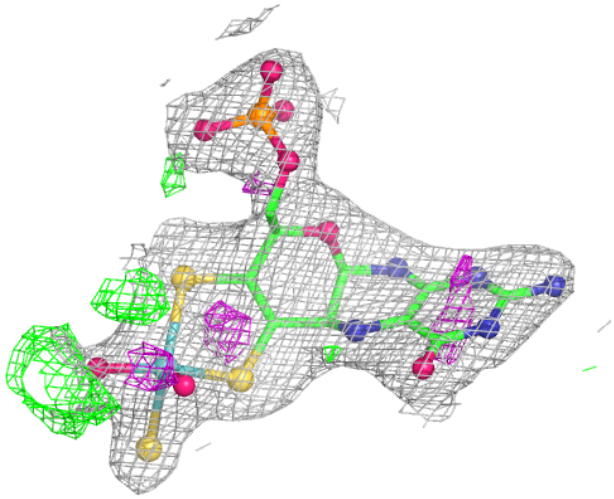
Electron density around ZXF B 1311:

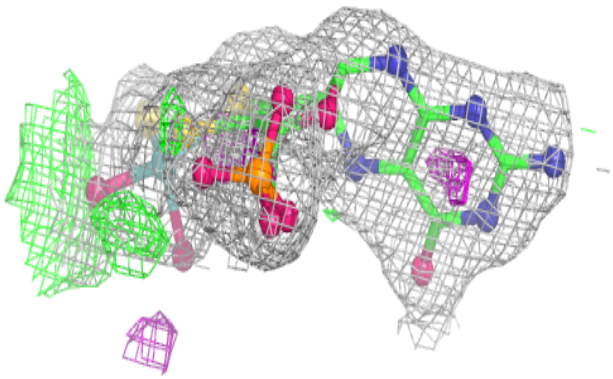
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

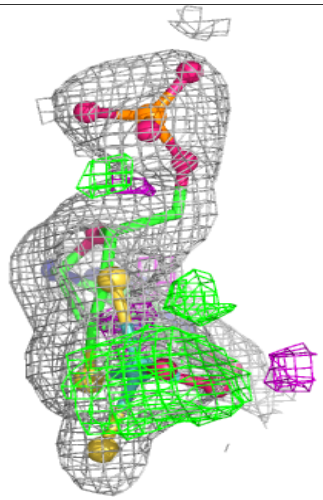


Electron density around ZXF D 1309:

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

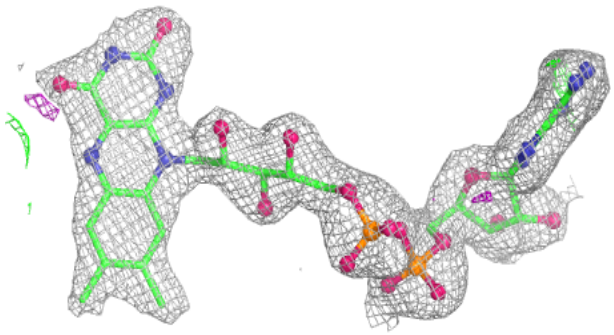


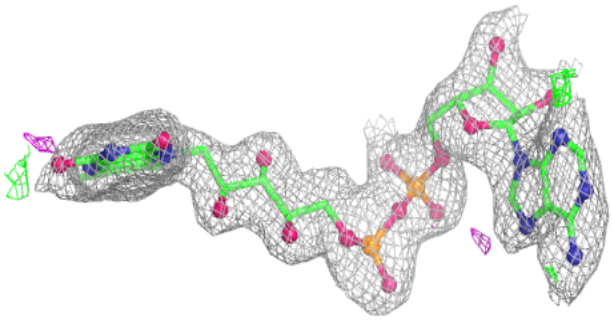


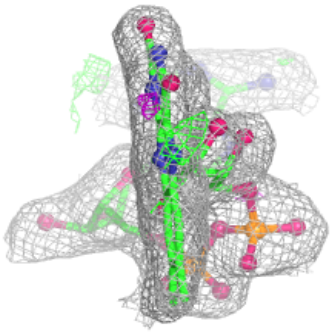


Electron density around FAD D 1305:

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

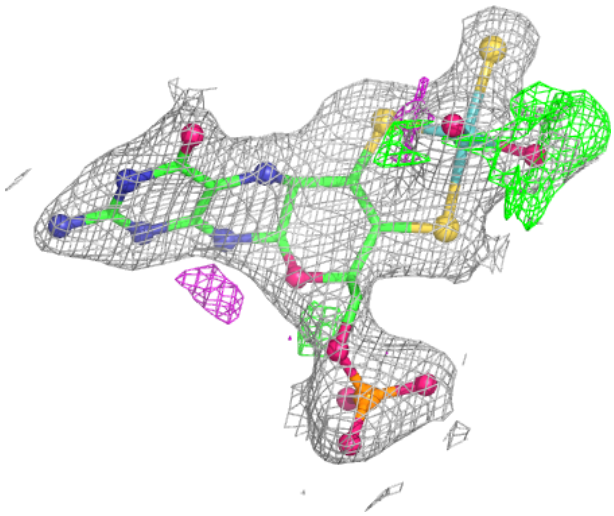


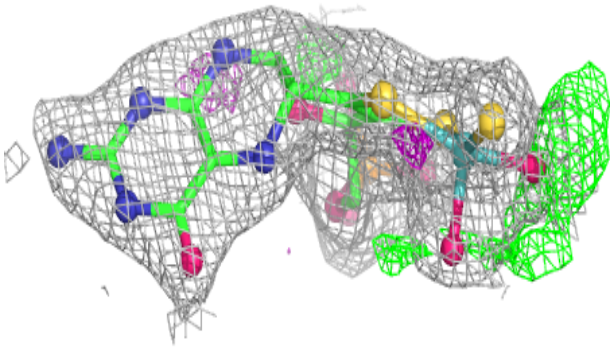


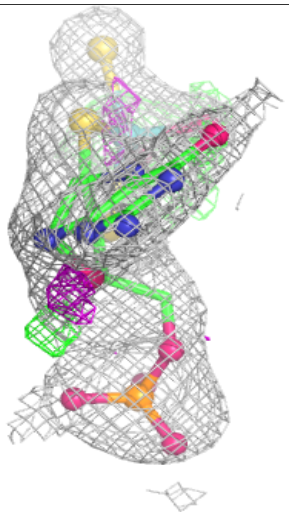


Electron density around ZXF A 1312:

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

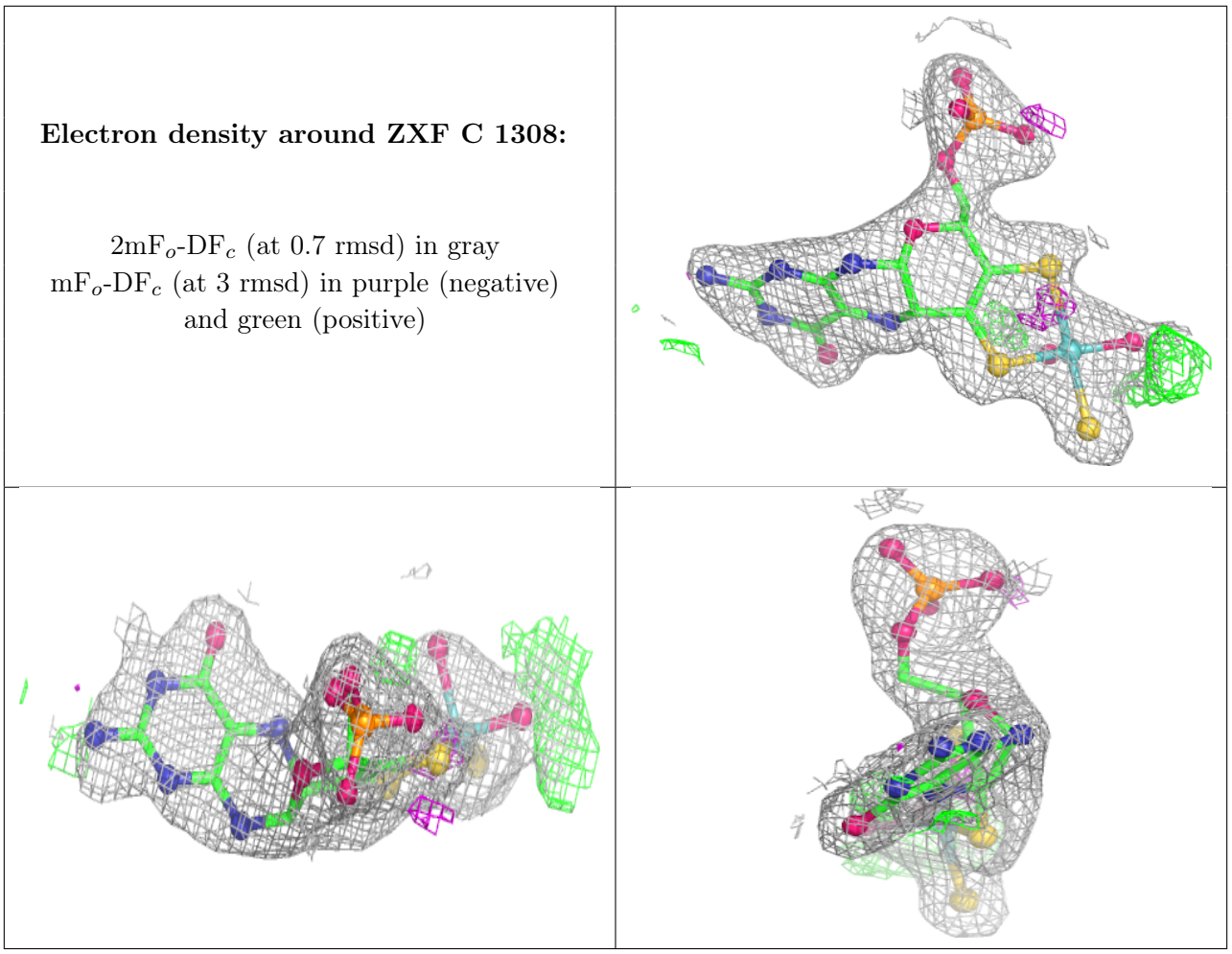






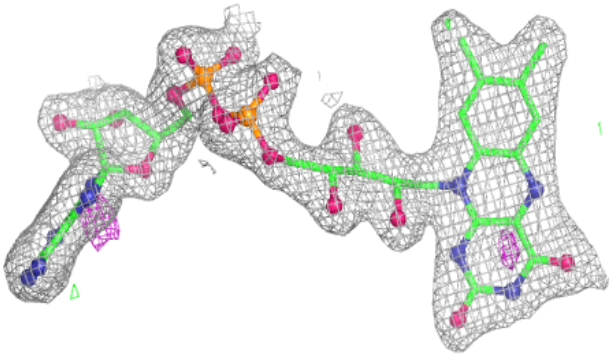
Electron density around ZXF C 1308:

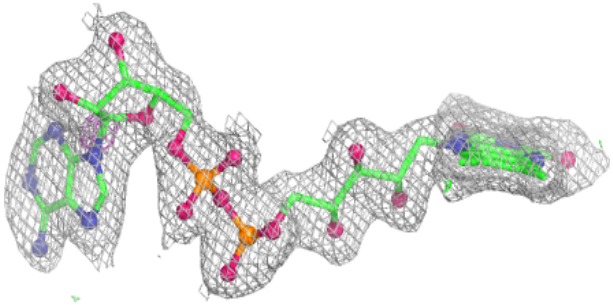
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

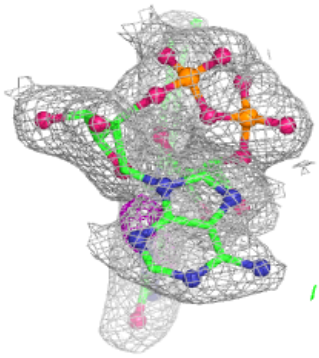


Electron density around FAD C 1305:

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

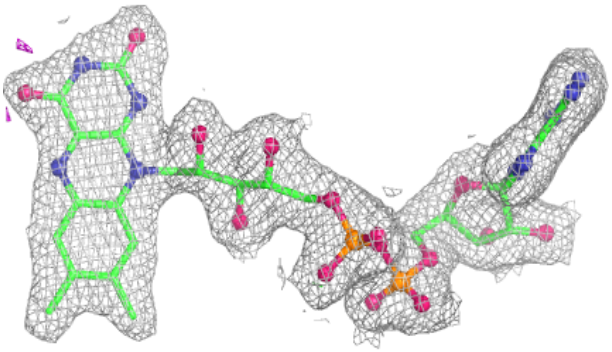


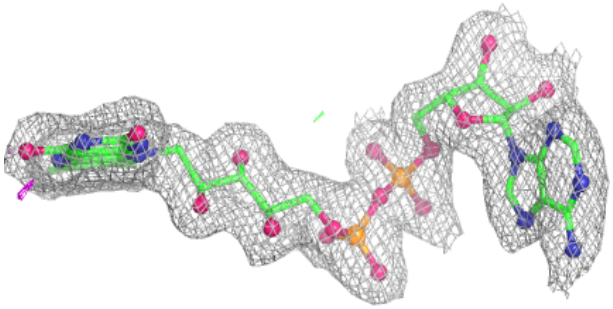


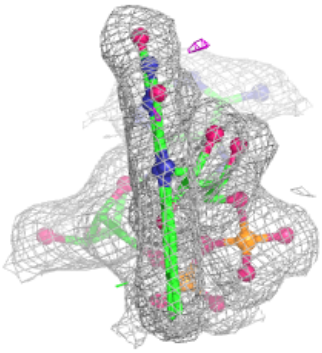


Electron density around FAD A 1305:

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

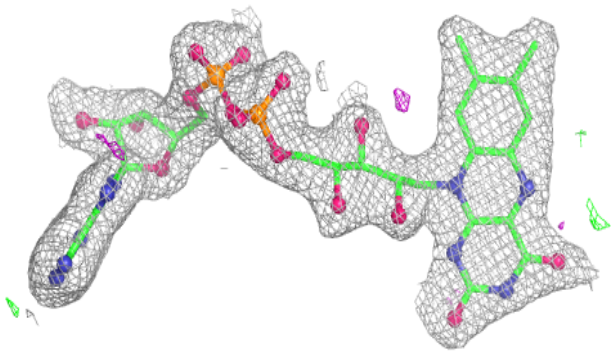


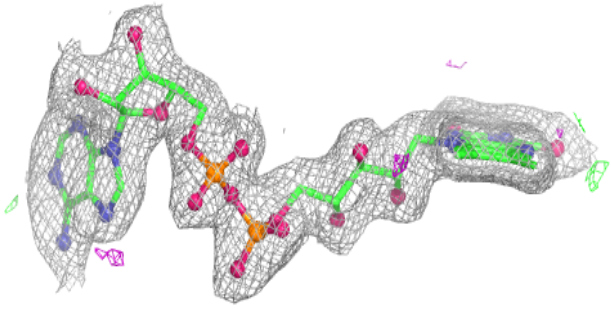


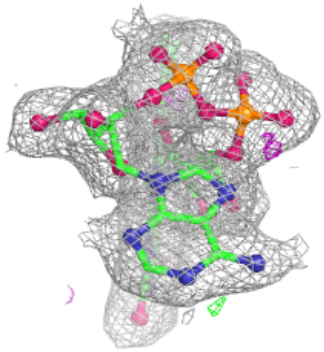


Electron density around FAD B 1305:

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

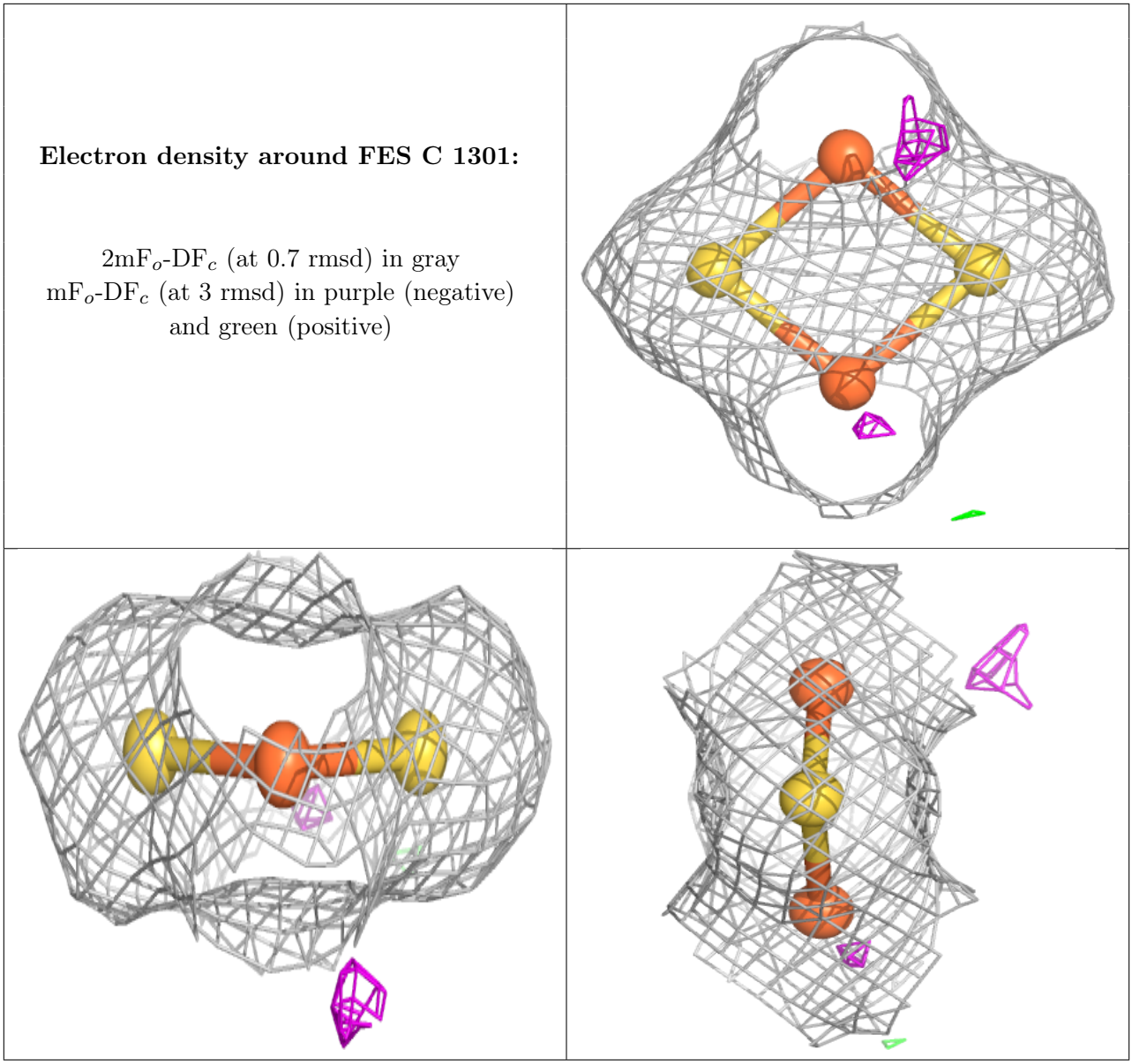






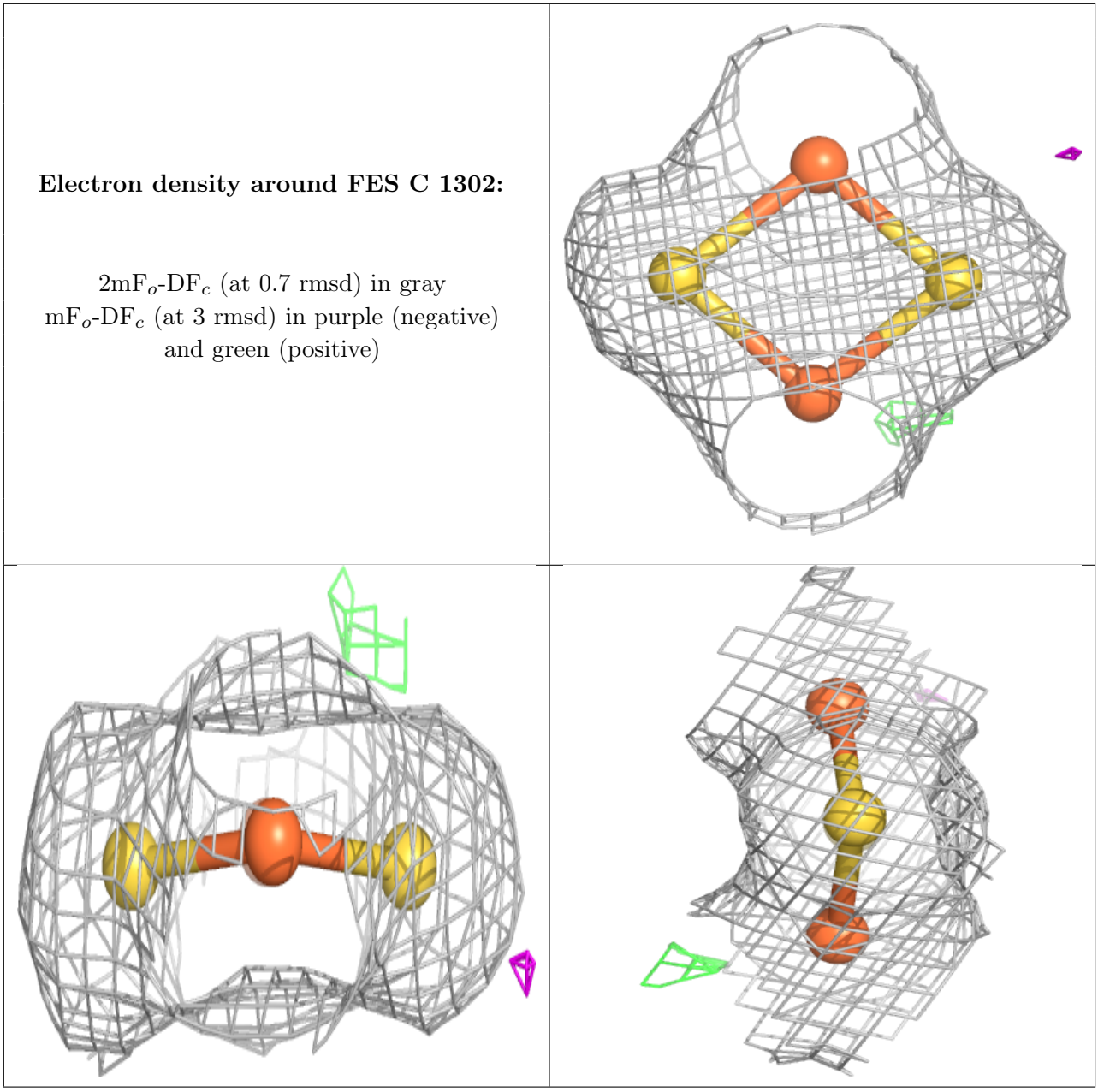
Electron density around FES C 1301:

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



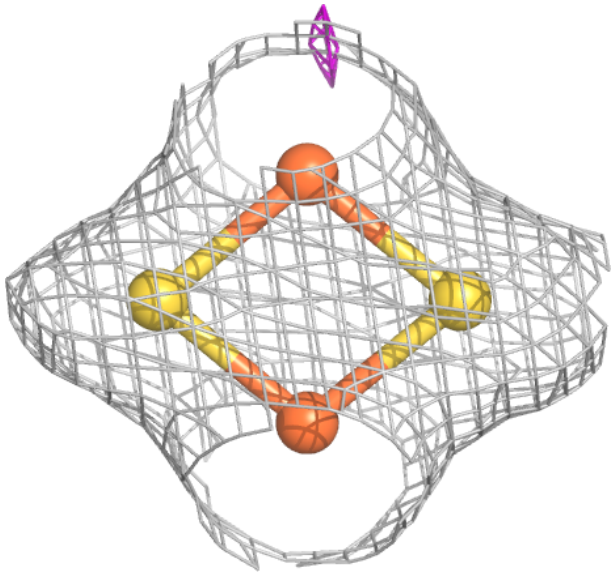
Electron density around FES C 1302:

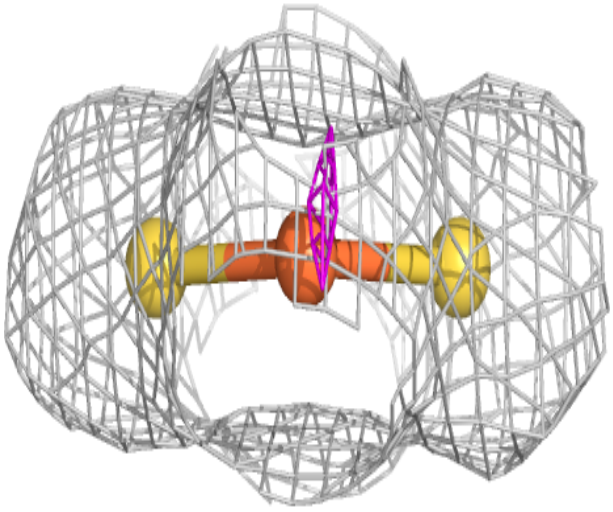
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

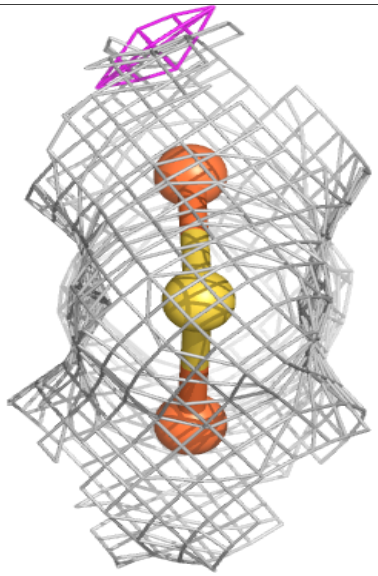


Electron density around FES D 1301:

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

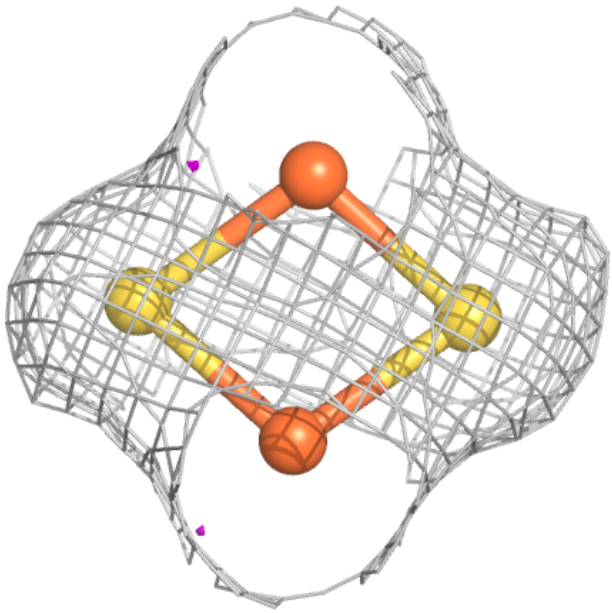


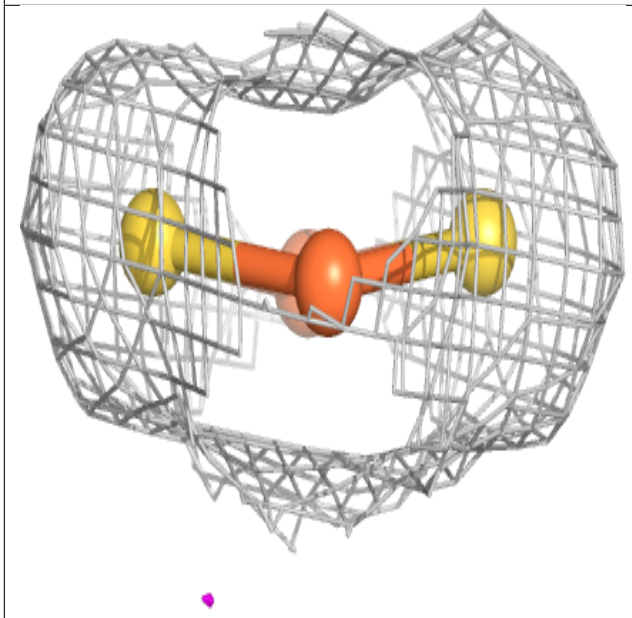


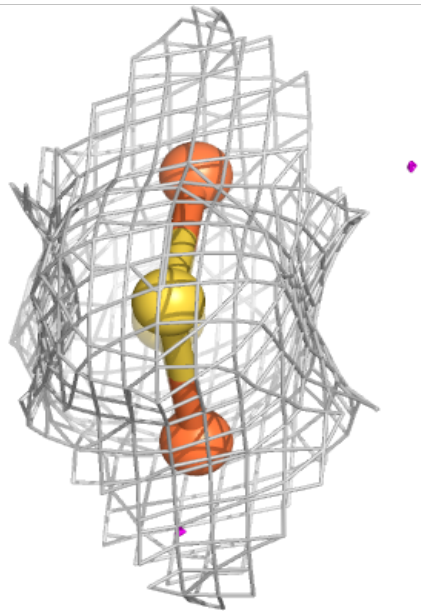


Electron density around FES D 1302:

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

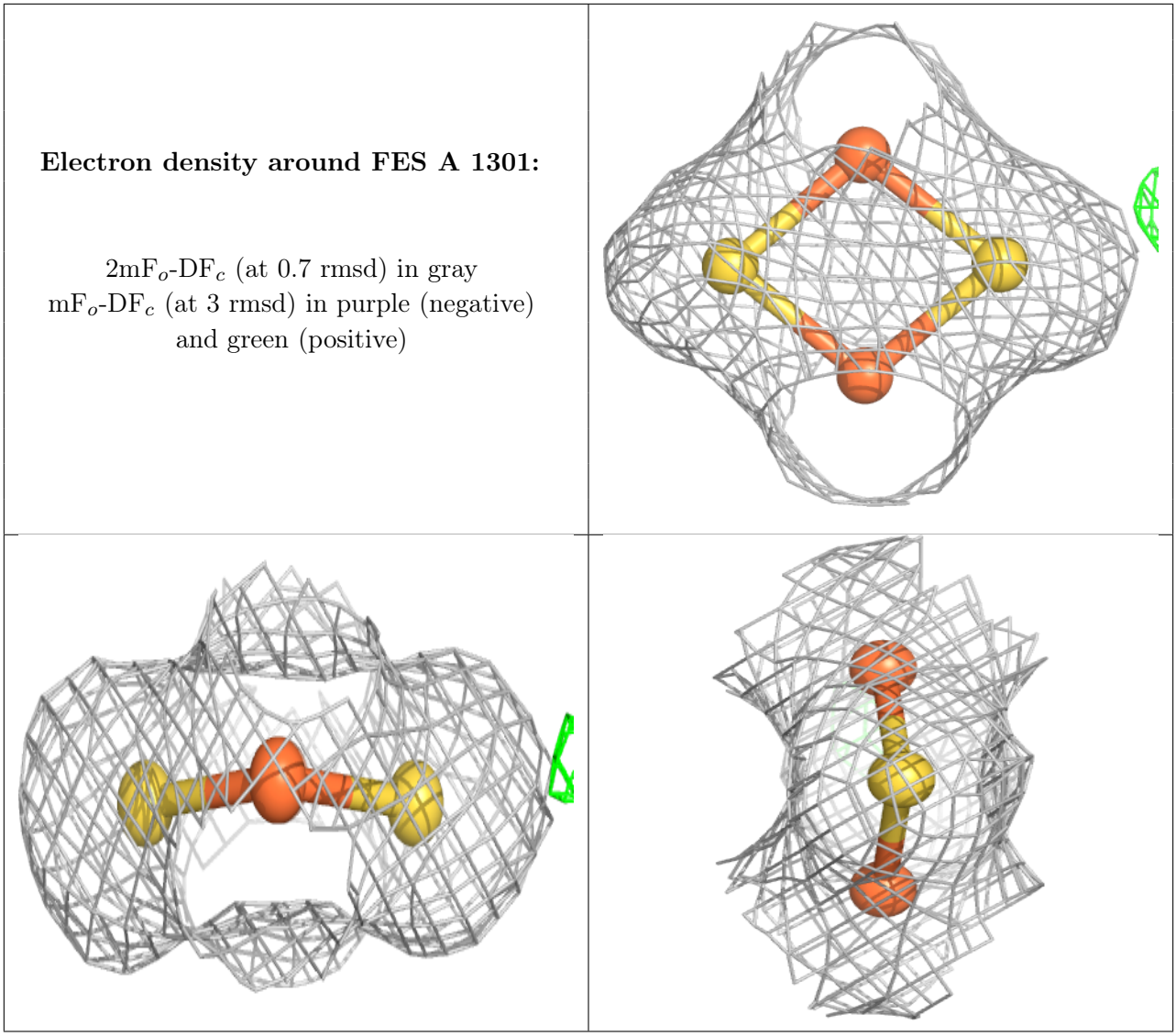






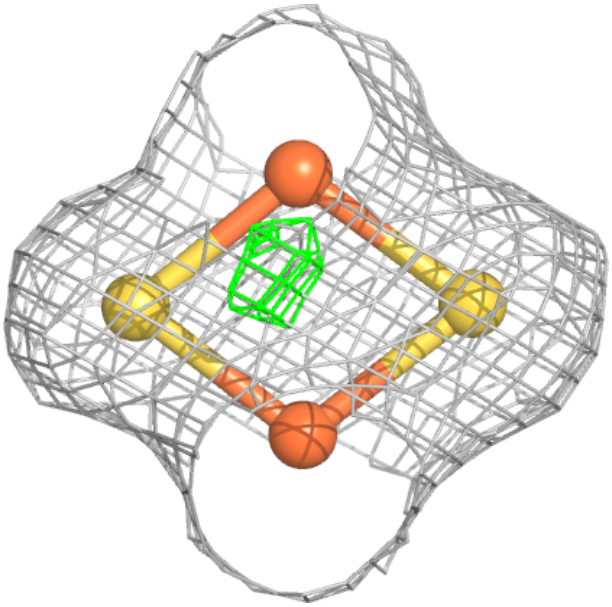
Electron density around FES A 1301:

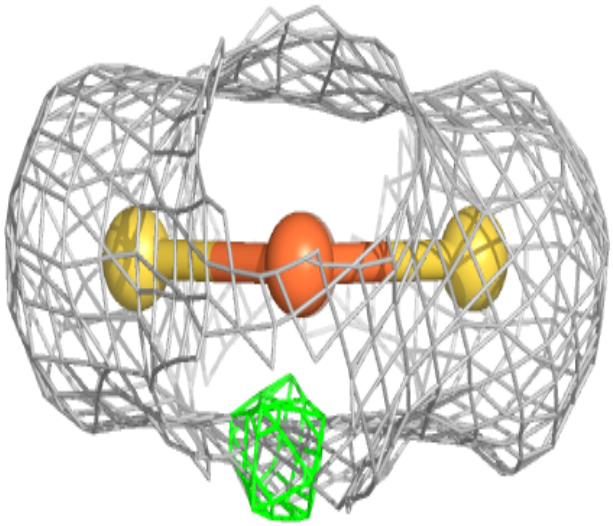
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

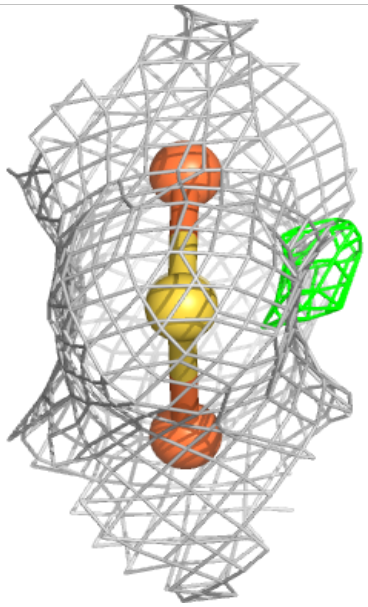


Electron density around FES A 1302:

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

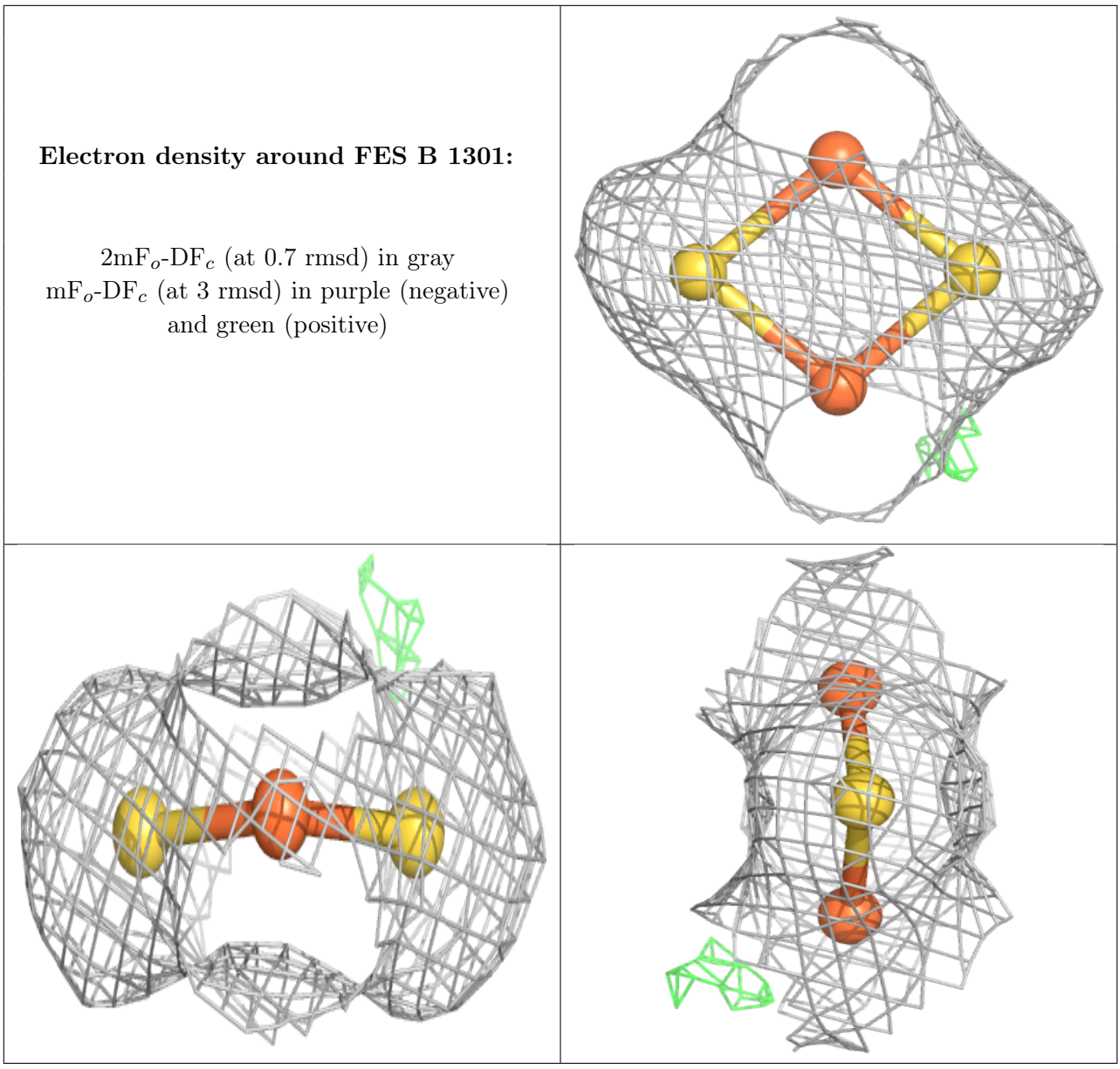






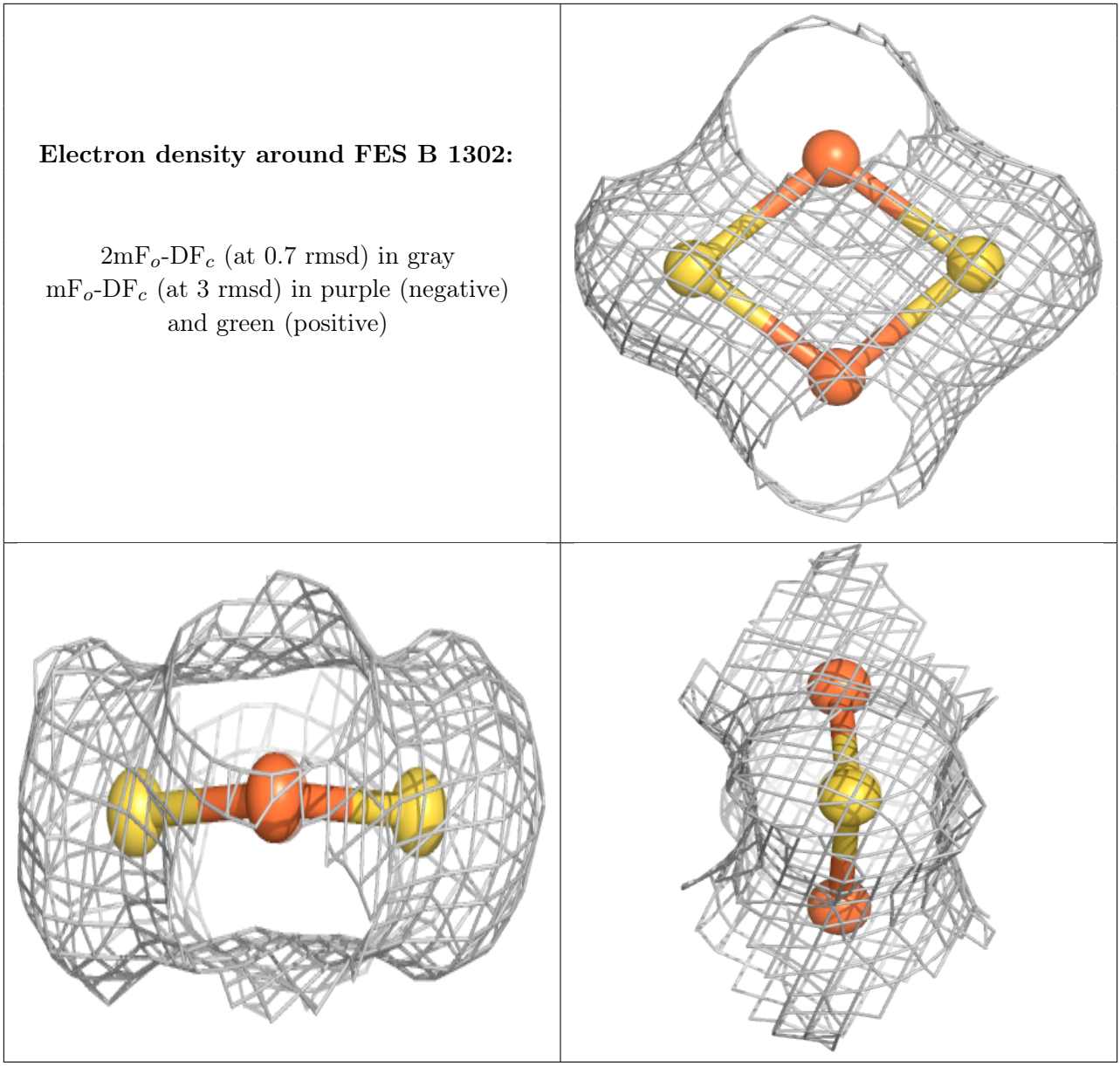
Electron density around FES B 1301:

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



Electron density around FES B 1302:

$2mF_o$-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.