Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2026 – 03:56 pm BST

PDB ID	:	9FDV / pdb_00009fdv
Title	:	Crystal Structure of reduced NuoEF variant R66G(NuoF) from Aquifex aeolicus
Authors	:	Wohlwend, D.; Friedrich, T.; Goeppert-Asadollahpour, S.
Deposited on	:	2024-05-17
Resolution	:	1.99 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:

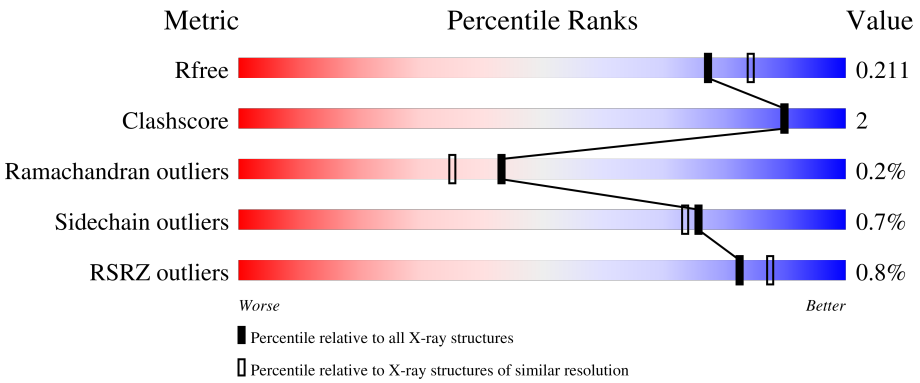
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.99 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	160	92% 6% •
1	C	160	% 95% • •
2	B	434	% 90% 6% •
2	D	434	% 92% • •

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10153 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 NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1268	821	204	234	9	0	0	0
1	C	156	1268	821	204	234	9	0	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3300	2123	546	618	13	0	2	0
2	D	418	3294	2121	544	616	13	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	GLY	ARG	engineered mutation	UNP O66841
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag	UNP O66841
B	434	HIS	-	expression tag	UNP O66841
D	66	GLY	ARG	engineered mutation	UNP O66841
D	427	ALA	-	expression tag	UNP O66841
D	428	GLY	-	expression tag	UNP O66841
D	429	HIS	-	expression tag	UNP O66841
D	430	HIS	-	expression tag	UNP O66841
D	431	HIS	-	expression tag	UNP O66841
D	432	HIS	-	expression tag	UNP O66841

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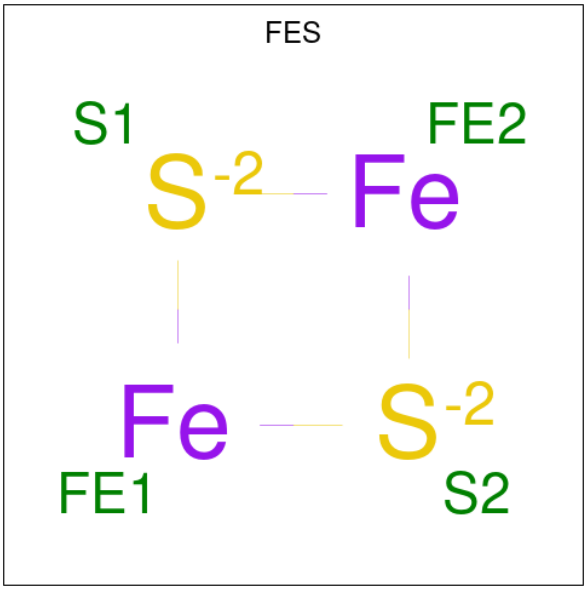
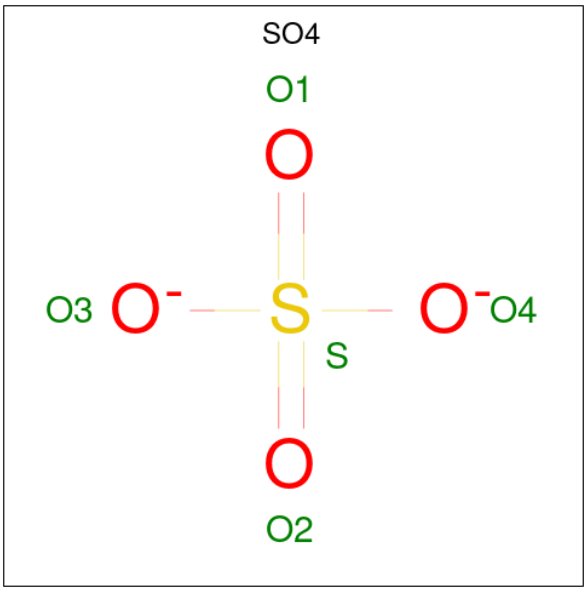
Chain	Residue	Modelled	Actual	Comment	Reference
D	433	HIS	-	expression tag	UNP O66841
D	434	HIS	-	expression tag	UNP O66841

- Molecule 3 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
			Total	Fe	S			
3	A	1	4	2	2		0	0
			Total	Fe	S			
3	C	1	4	2	2		0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

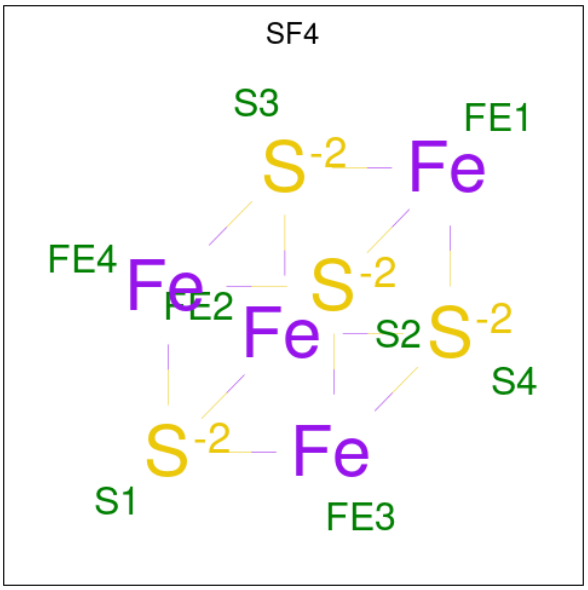
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

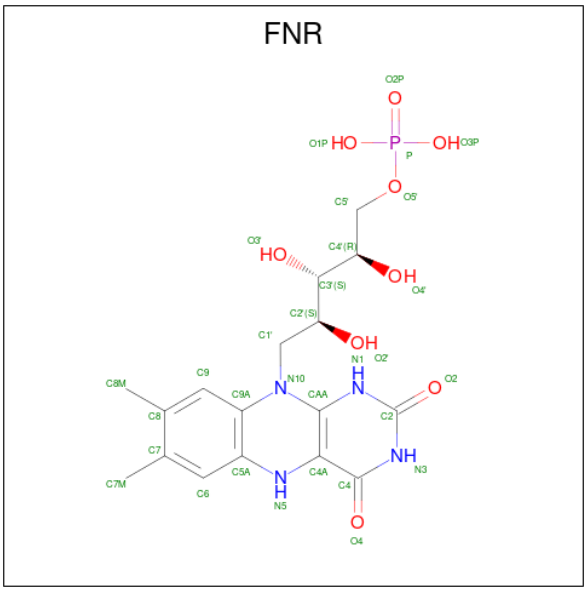
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
			Total	Na		
6	B	8	8	8	0	0
			Total	Na		
6	C	2	2	2	0	0
			Total	Na		
6	D	4	4	4	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



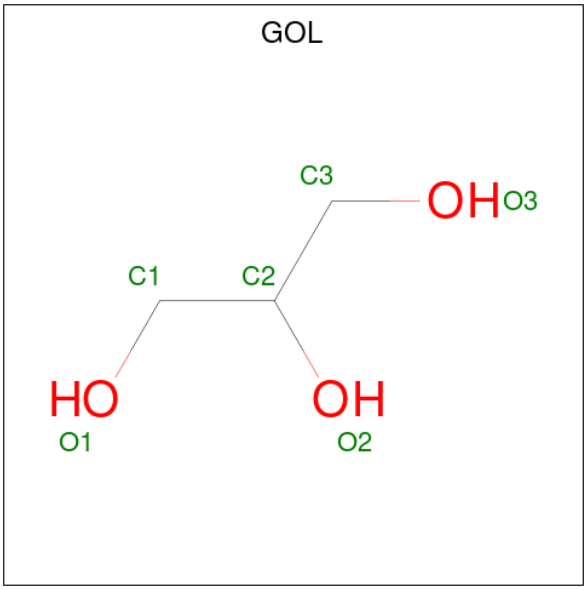
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	8	4	4	0	0
			Total	Fe	S		
7	D	1	8	4	4	0	0

- Molecule 8 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PTERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: $C_{17}H_{23}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
8	D	1	31	17	4	9	1	0	0

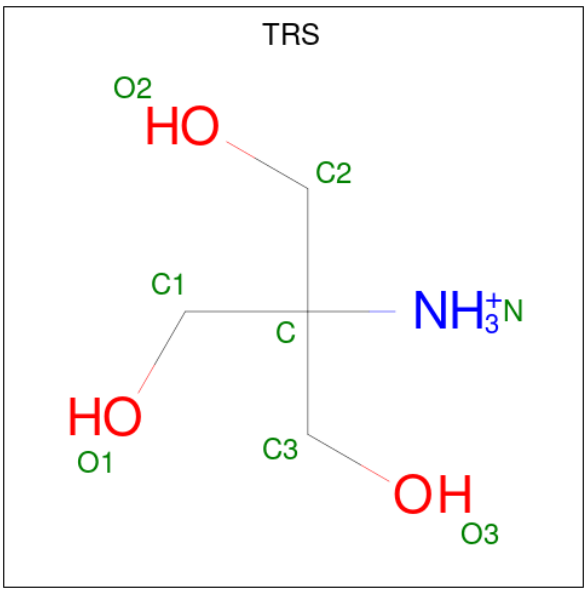
- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	6	3	3	0	0

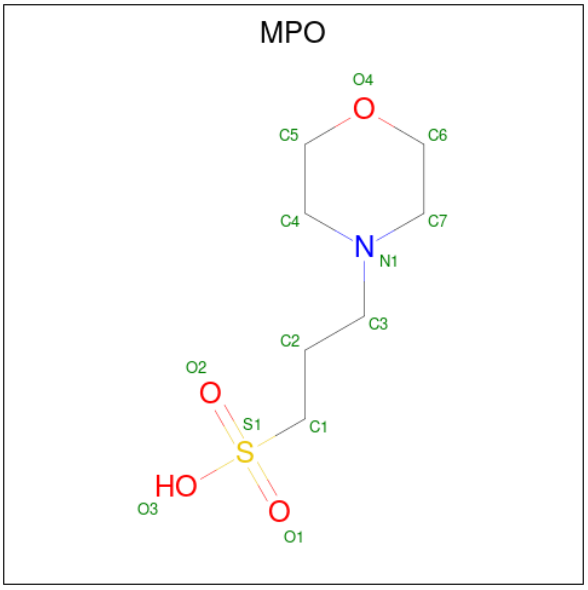
- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	D	1	8	4	1	3	0	0

- Molecule 11 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	D	1	13	7	1	4	1	0	0

- Molecule 12 is water.

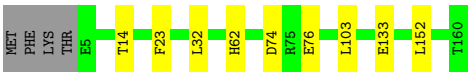
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	110	111	111	0	1
			Total	O		
12	B	306	306	306	0	0
			Total	O		
12	C	121	121	121	0	0
			Total	O		
12	D	312	313	313	0	1

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.

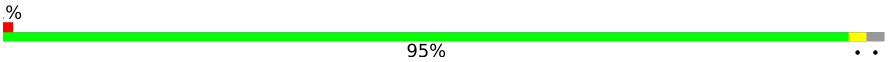
• Molecule 1: NADH-quinone oxidoreductase subunit E

Chain A:



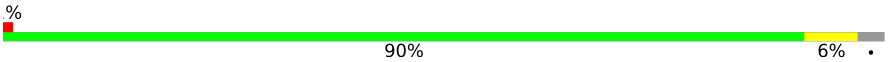
• Molecule 1: NADH-quinone oxidoreductase subunit E

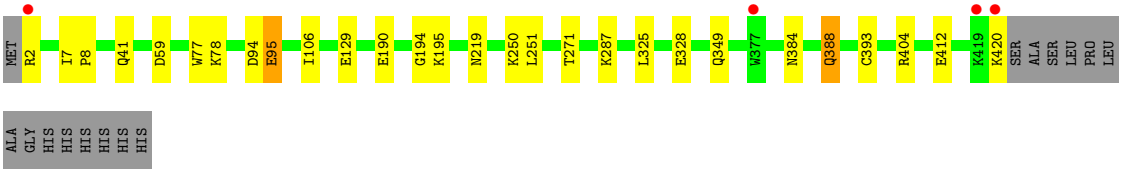
Chain C:



• Molecule 2: NADH-quinone oxidoreductase subunit F

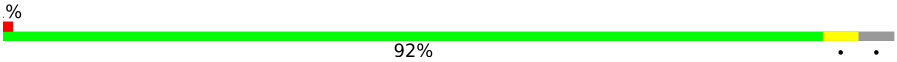
Chain B:

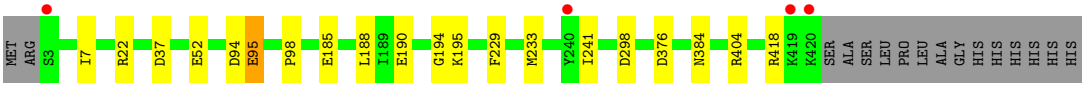




• Molecule 2: NADH-quinone oxidoreductase subunit F

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.30Å 116.22Å 189.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 1.99 49.59 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.59-1.99) 99.3 (49.59-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.165 , 0.201 0.178 , 0.211	Depositor DCC
R_{free} test set	4847 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10153	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % 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 2.5206e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, TRS, NA, FES, CL, FNR, MPO, SO4

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	0.50	0/1297	0.92	2/1752 (0.1%)
1	C	0.52	0/1297	0.92	0/1752
2	B	0.52	0/3381	0.93	3/4576 (0.1%)
2	D	0.53	0/3375	0.93	2/4568 (0.0%)
All	All	0.52	0/9350	0.93	7/12648 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	271	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	74	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	14	THR	CA-CB-OG1	-5.33	101.61	109.60
2	B	129	GLU	CB-CA-C	5.27	118.88	109.65
2	D	298	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	349	GLN	CB-CA-C	-5.16	102.07	110.85
2	D	376	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	22	ARG	Sidechain
2	D	418	ARG	Sidechain

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	1268	0	1269	6	0
1	C	1268	0	1269	3	0
2	B	3300	0	3258	17	0
2	D	3294	0	3262	11	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	B	8	0	0	0	0
6	C	2	0	0	0	0
6	D	4	0	0	0	0
7	B	8	0	0	0	0
7	D	8	0	0	0	0
8	B	31	0	22	0	0
8	D	31	0	22	0	0
9	B	6	0	8	0	0
10	D	8	0	12	1	0
11	D	13	0	15	2	0
12	A	111	0	0	2	0
12	B	306	0	0	5	0
12	C	121	0	0	0	0
12	D	313	0	0	1	0
All	All	10153	0	9137	33	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 2.

All (33) 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)
2:B:250:LYS:HE2	12:B:640:HOH:O	1.73	0.88
2:B:388:GLN:HG3	12:B:831:HOH:O	1.89	0.73
2:D:185:GLU:OE2	11:D:504:MPO:O3	2.08	0.71
2:B:190:GLU:OE1	2:B:195:LYS:HE2	2.00	0.61
1:A:62:HIS:HD2	12:A:402:HOH:O	1.84	0.59
2:B:250:LYS:CE	12:B:640:HOH:O	2.38	0.58
2:B:77:TRP:HE1	2:B:219:ASN:HD21	1.53	0.56
2:D:233:MET:HE1	2:D:241:ILE:HD11	1.88	0.55
2:D:190:GLU:OE1	2:D:195:LYS:HE2	2.08	0.54
1:A:133:GLU:HG3	2:B:8:PRO:HB2	1.93	0.51
1:C:62:HIS:HE1	2:D:194:GLY:O	1.94	0.50
1:A:62:HIS:HE1	2:B:194:GLY:O	1.95	0.48
2:B:77:TRP:HE1	2:B:219:ASN:ND2	2.11	0.48
2:D:384:ASN:HD22	2:D:404:ARG:HH21	1.60	0.48
2:B:325:LEU:N	2:B:325:LEU:HD12	2.31	0.46
1:A:103:LEU:HD23	1:A:152:LEU:HD21	1.99	0.45
2:D:94:ASP:O	2:D:95:GLU:C	2.60	0.44
1:C:127:CYS:SG	2:D:98:PRO:HA	2.57	0.44
2:D:37:ASP:HB3	12:D:702:HOH:O	2.17	0.44
2:B:7:ILE:HG22	2:B:8:PRO:O	2.18	0.43
2:B:2:ARG:NH1	12:B:617:HOH:O	2.52	0.43
1:A:23:PHE:HE2	1:A:32:LEU:HD12	1.84	0.42
2:B:106:ILE:HD11	2:B:251:LEU:HD11	2.01	0.42
2:B:384:ASN:HD22	2:B:404:ARG:HH21	1.67	0.42
1:C:114:VAL:HG22	1:C:121:LYS:HB2	2.02	0.41
2:D:188:LEU:C	2:D:188:LEU:HD23	2.44	0.41
2:B:287:LYS:NZ	2:B:328:GLU:OE1	2.51	0.41
2:B:59:ASP:CG	2:B:78:LYS:HZ3	2.29	0.40
2:B:94:ASP:O	2:B:95:GLU:C	2.64	0.40
2:D:185:GLU:CD	11:D:504:MPO:O3	2.64	0.40
2:B:41:GLN:HG2	12:B:706:HOH:O	2.21	0.40
1:A:62:HIS:CD2	12:A:402:HOH:O	2.67	0.40
2:D:229:PHE:CZ	10:D:503:TRS:H21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	154/160 (96%)	149 (97%)	5 (3%)	0	100	100
1	C	154/160 (96%)	148 (96%)	6 (4%)	0	100	100
2	B	419/434 (96%)	413 (99%)	5 (1%)	1 (0%)	43	35
2	D	418/434 (96%)	408 (98%)	9 (2%)	1 (0%)	43	35
All	All	1145/1188 (96%)	1118 (98%)	25 (2%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	95	GLU
2	D	95	GLU

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	142/146 (97%)	141 (99%)	1 (1%)	76	73
1	C	142/146 (97%)	142 (100%)	0	100	100
2	B	342/356 (96%)	338 (99%)	4 (1%)	63	58
2	D	343/356 (96%)	341 (99%)	2 (1%)	78	76
All	All	969/1004 (96%)	962 (99%)	7 (1%)	76	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
2	B	388	GLN
2	B	393	CYS
2	B	412	GLU
2	B	420	LYS
2	D	7	ILE
2	D	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	153	ASN
2	B	83	ASN
2	B	128	ASN
2	B	219	ASN
2	B	349	GLN
2	B	384	ASN
1	C	62	HIS
1	C	153	ASN
2	D	83	ASN
2	D	128	ASN
2	D	208	GLN
2	D	286	ASN
2	D	349	GLN
2	D	384	ASN
2	D	388	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 19 are monoatomic - leaving 17 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	A	202	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	203	-	4,4,4	0.36	0	6,6,6	0.07	0
10	TRS	D	503	-	7,7,7	0.18	0	9,9,9	0.19	0
8	FNR	D	502	-	32,33,33	0.41	0	40,50,50	0.55	0
4	SO4	A	203	-	4,4,4	0.29	0	6,6,6	0.10	0
7	SF4	D	501	2	0,12,12	-	-	-		
3	FES	A	201	1	0,4,4	-	-	-		
8	FNR	B	502	-	32,33,33	0.35	0	40,50,50	0.72	1 (2%)
3	FES	C	201	1	0,4,4	-	-	-		
4	SO4	D	505	-	4,4,4	0.32	0	6,6,6	0.27	0
9	GOL	B	503	-	5,5,5	0.10	0	5,5,5	0.15	0
4	SO4	B	504	-	4,4,4	0.28	0	6,6,6	0.17	0
7	SF4	B	501	2	0,12,12	-	-	-		
4	SO4	B	505	-	4,4,4	0.36	0	6,6,6	0.09	0
11	MPO	D	504	6	13,13,13	0.54	0	17,17,17	1.58	4 (23%)
4	SO4	C	202	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	A	204	-	4,4,4	0.33	0	6,6,6	0.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	TRS	D	503	-	-	3/9/9/9	-
8	FNR	D	502	-	-	2/18/18/18	0/3/3/3
7	SF4	D	501	2	-	-	0/6/5/5
3	FES	A	201	1	-	-	0/1/1/1
8	FNR	B	502	-	-	3/18/18/18	0/3/3/3
3	FES	C	201	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	B	503	-	-	0/4/4/4	-
11	MPO	D	504	6	-	1/7/15/15	0/1/1/1
7	SF4	B	501	2	-	-	0/6/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	504	MPO	O3-S1-O1	-3.88	101.78	111.27
11	D	504	MPO	O3-S1-C1	-2.90	101.08	105.77
8	B	502	FNR	O3P-P-O5'	-2.79	99.31	106.73
11	D	504	MPO	O2-S1-O1	2.63	123.07	113.95
11	D	504	MPO	O1-S1-C1	2.21	109.58	106.92

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	502	FNR	C4'-C5'-O5'-P
8	D	502	FNR	C4'-C5'-O5'-P
10	D	503	TRS	C3-C-C2-O2
10	D	503	TRS	N-C-C2-O2
10	D	503	TRS	C1-C-C2-O2
8	B	502	FNR	O2'-C2'-C3'-C4'
11	D	504	MPO	C2-C3-N1-C4
8	B	502	FNR	N10-C1'-C2'-O2'
8	D	502	FNR	N10-C1'-C2'-O2'

There are no ring outliers.

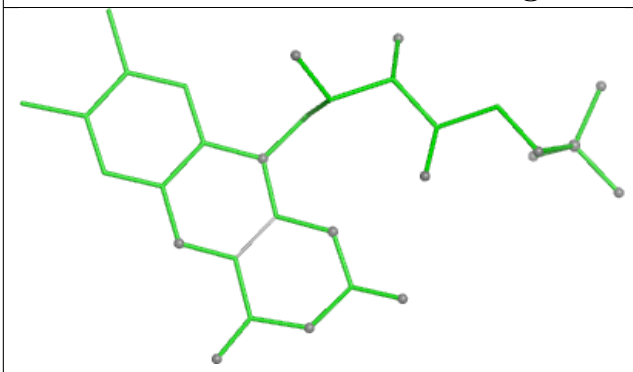
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	TRS	1	0
11	D	504	MPO	2	0

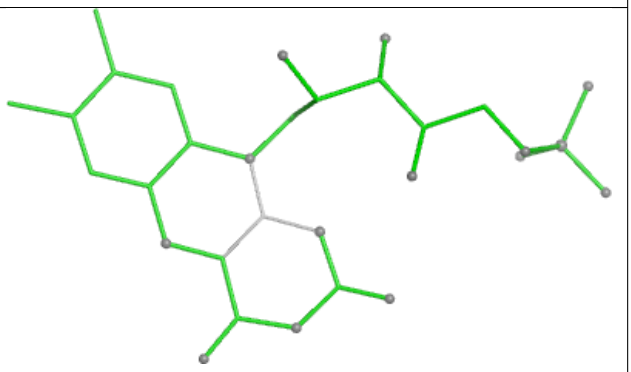
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

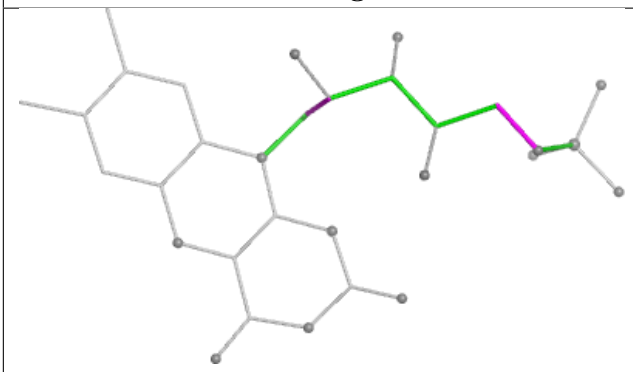
Ligand FNR D 502



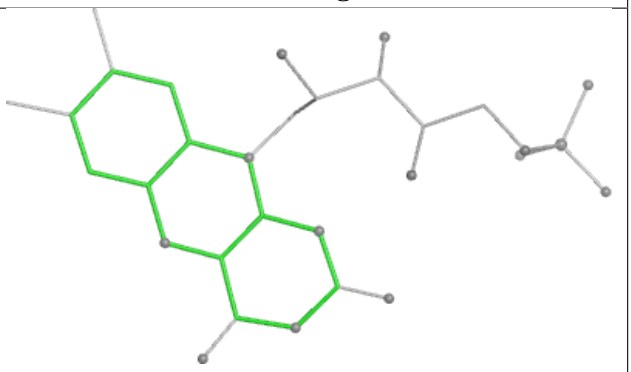
Bond lengths



Bond angles

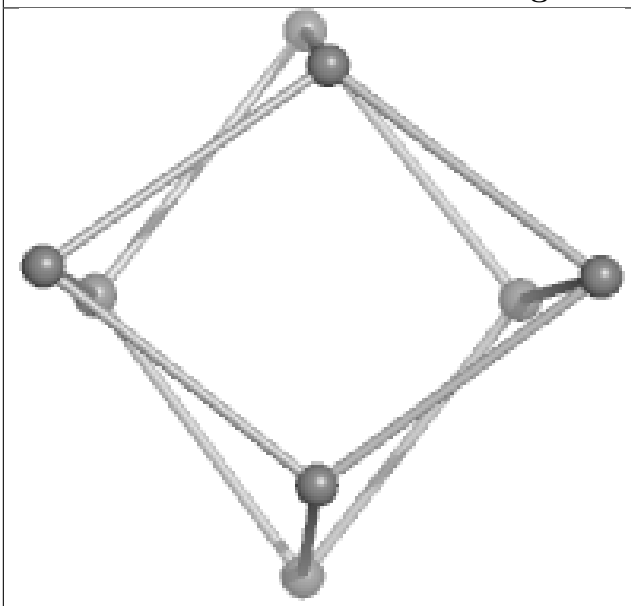


Torsions

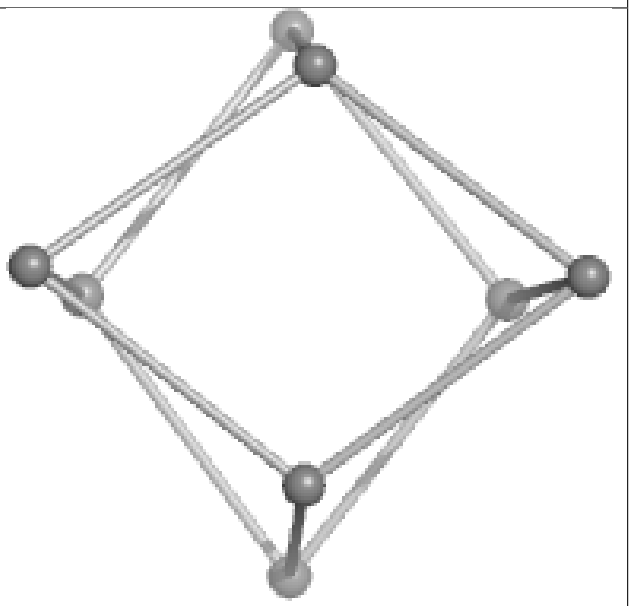


Rings

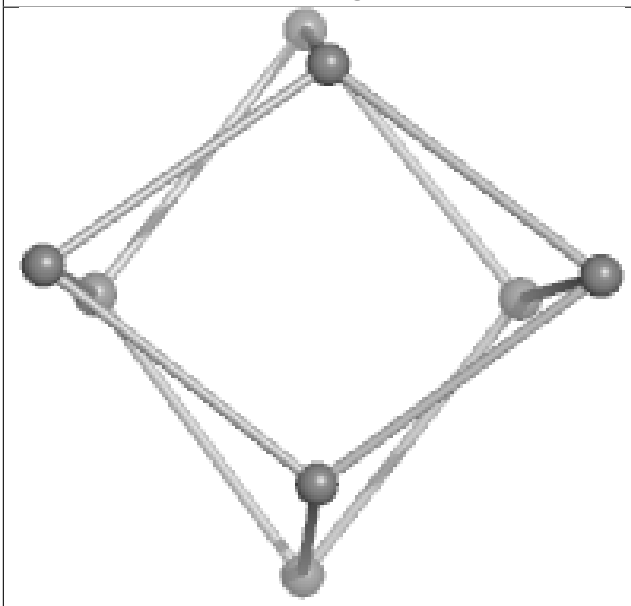
Ligand SF4 D 501



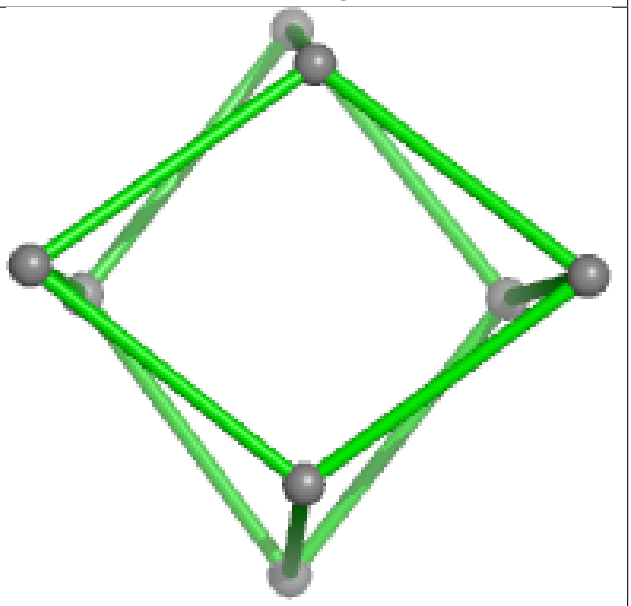
Bond lengths



Bond angles

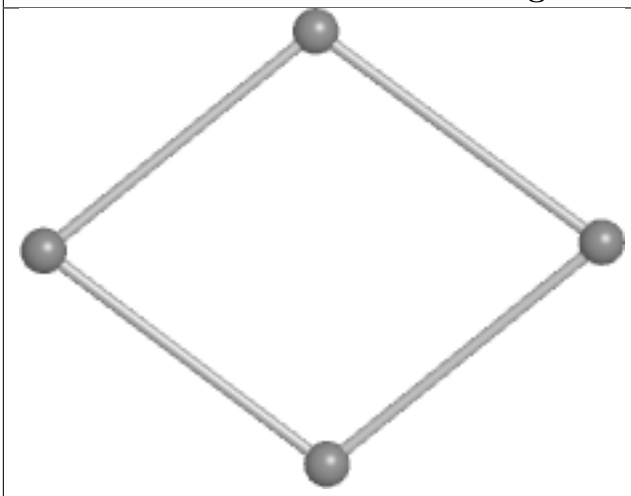


Torsions

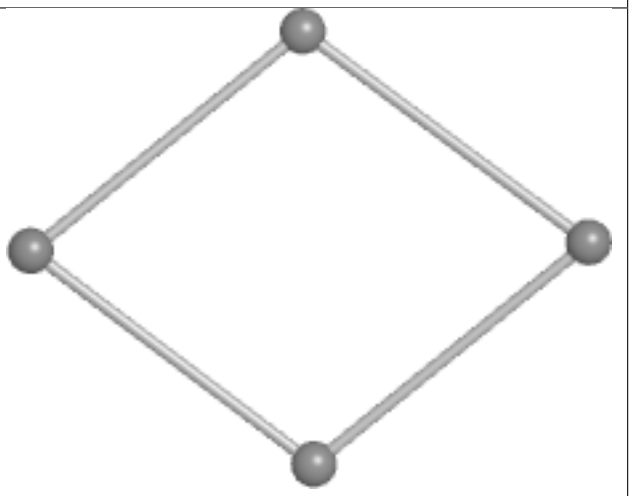


Rings

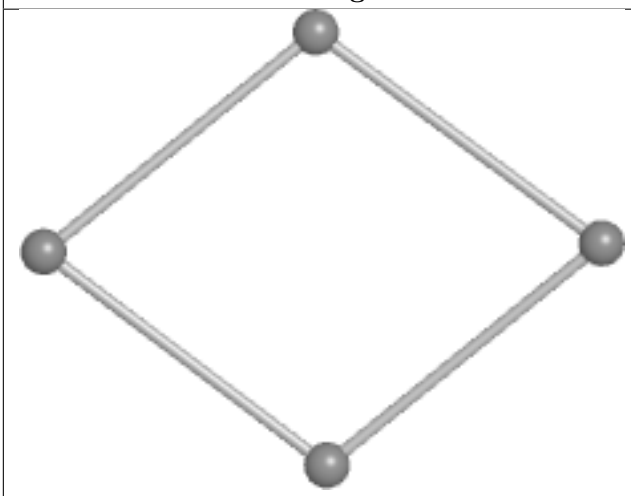
Ligand FES A 201



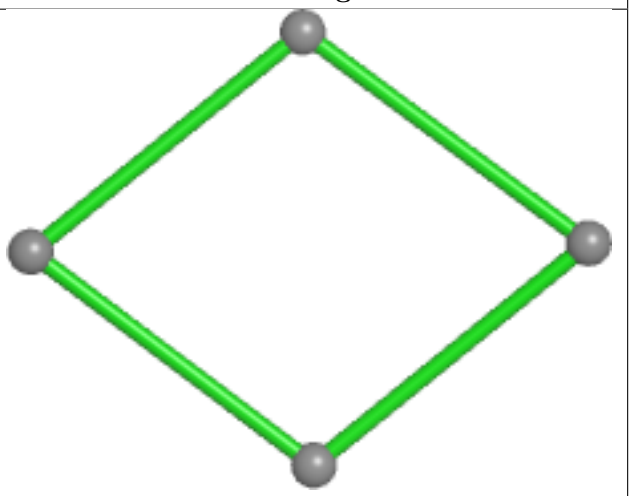
Bond lengths



Bond angles

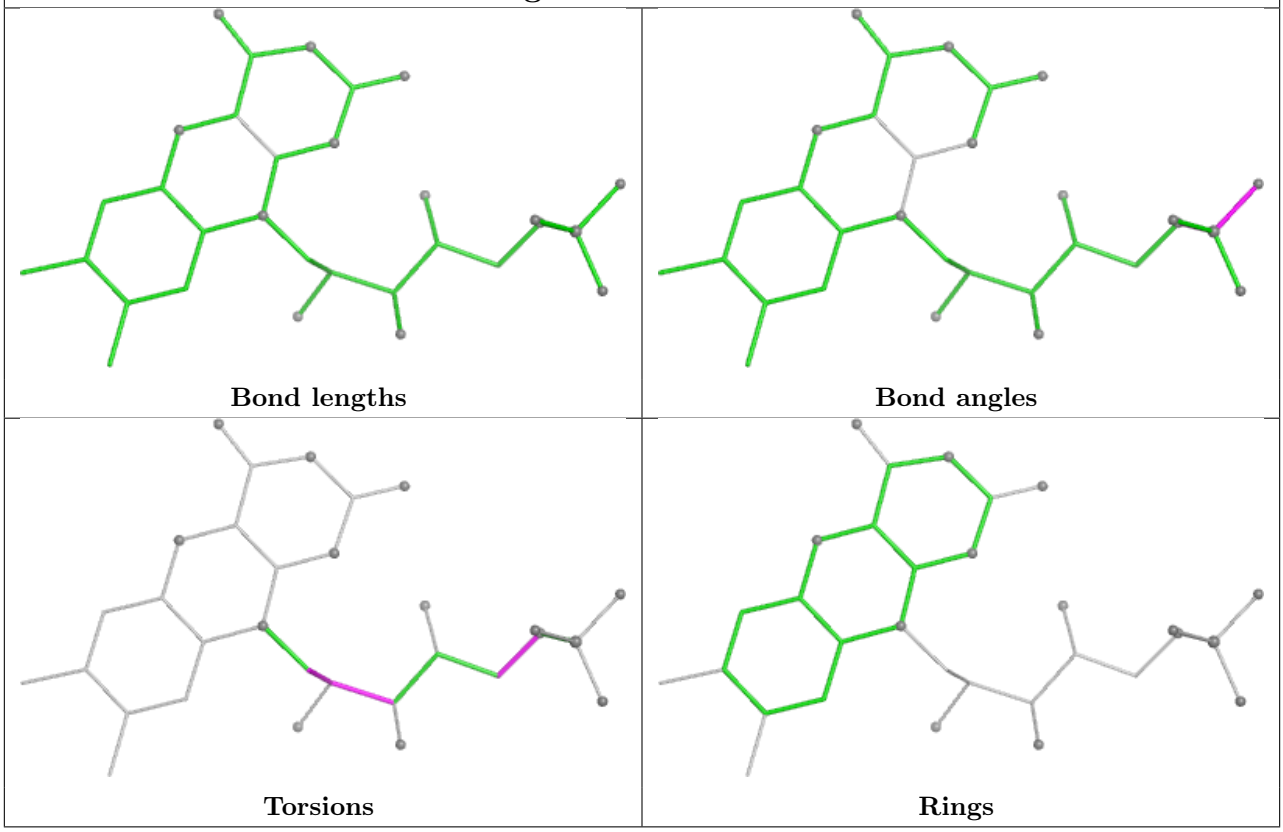


Torsions

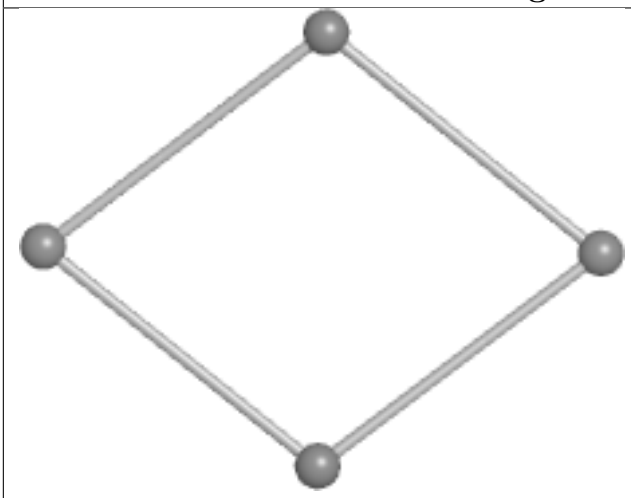


Rings

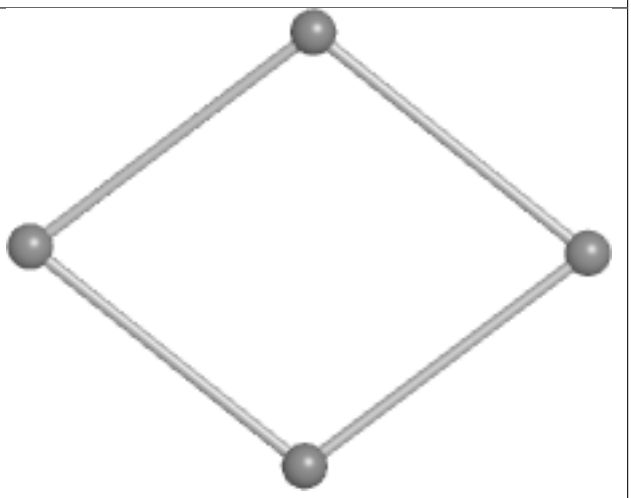
Ligand FNR B 502



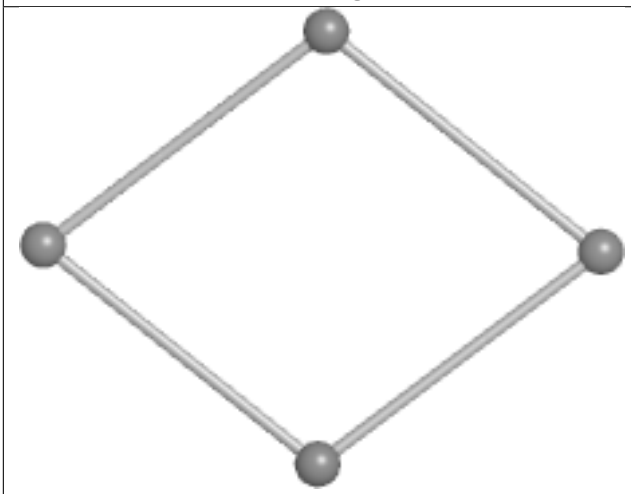
Ligand FES C 201



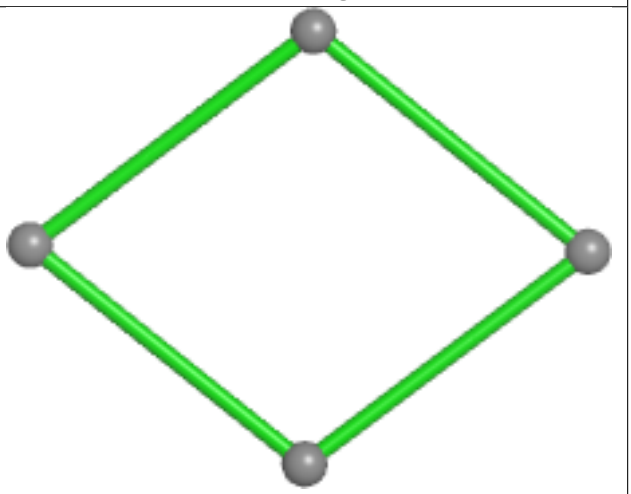
Bond lengths



Bond angles

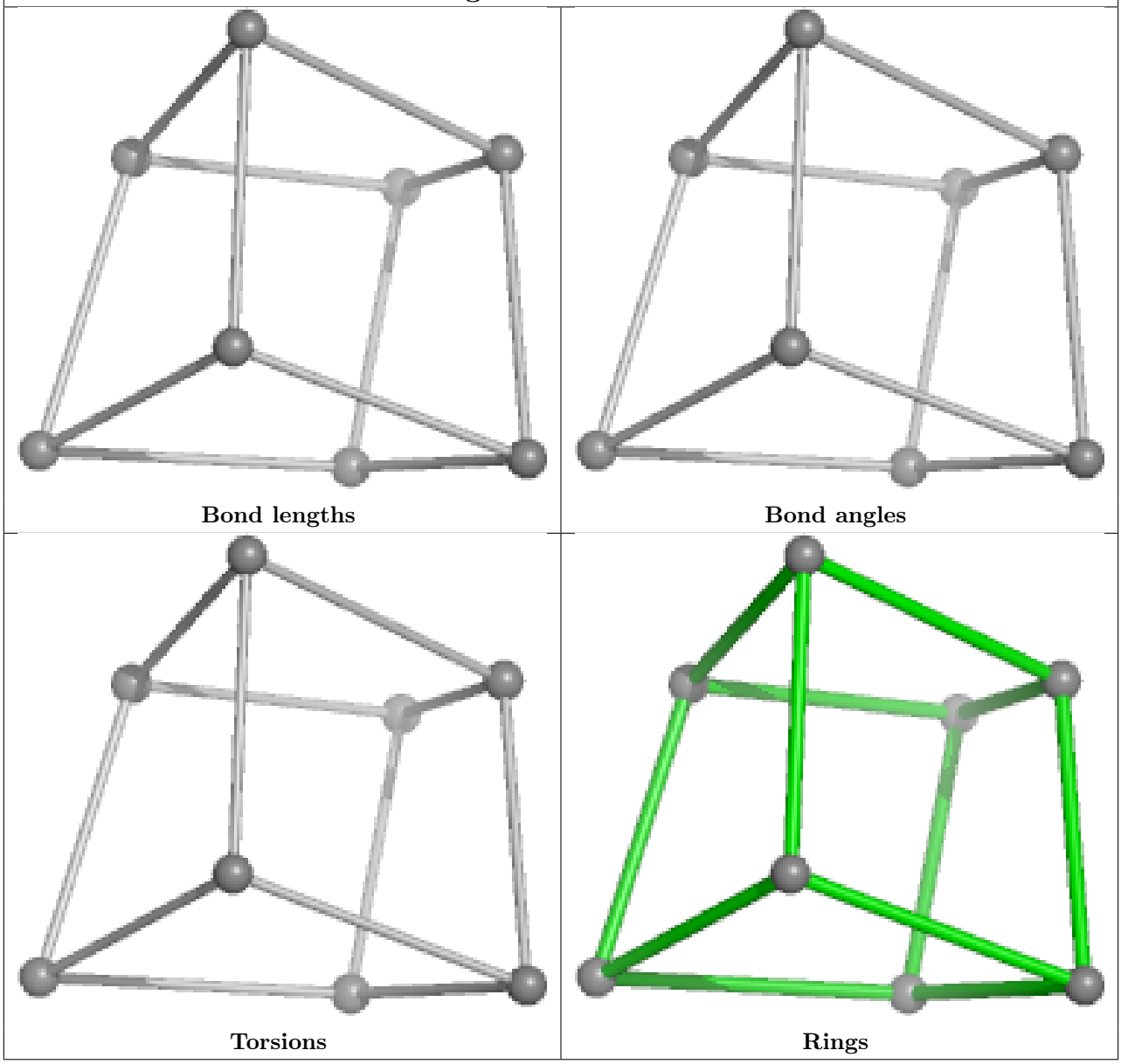


Torsions



Rings

Ligand SF4 B 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	156/160 (97%)	0.01	0	100	100	20, 34, 53, 95	0
1	C	156/160 (97%)	0.02	1 (0%)	85	90	20, 33, 52, 83	0
2	B	419/434 (96%)	-0.17	4 (0%)	79	86	11, 27, 41, 81	2 (0%)
2	D	418/434 (96%)	-0.27	4 (0%)	79	86	11, 26, 41, 97	2 (0%)
All	All	1149/1188 (96%)	-0.16	9 (0%)	82	87	11, 28, 47, 97	4 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	377	TRP	3.1
2	B	419	LYS	2.9
1	C	5	GLU	2.7
2	B	420	LYS	2.7
2	D	3	SER	2.5
2	D	420	LYS	2.4
2	D	419	LYS	2.3
2	B	2	ARG	2.2
2	D	240	TYR	2.2

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)

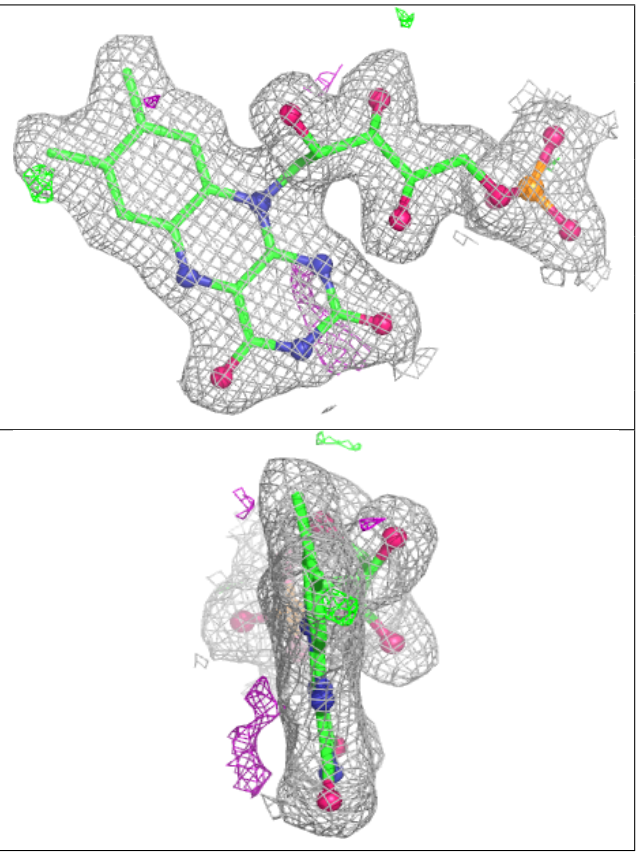
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	B	511	1/1	0.72	0.14	62,62,62,62	0
4	SO4	B	505	5/5	0.74	0.12	86,92,93,97	0
4	SO4	A	202	5/5	0.78	0.11	73,75,81,84	0
4	SO4	B	504	5/5	0.82	0.13	44,57,63,63	0
6	NA	C	205	1/1	0.84	0.16	43,43,43,43	0
4	SO4	C	202	5/5	0.85	0.10	63,64,66,68	0
6	NA	D	507	1/1	0.85	0.13	58,58,58,58	0
11	MPO	D	504	13/13	0.85	0.20	53,59,70,70	0
6	NA	B	510	1/1	0.86	0.26	63,63,63,63	0
6	NA	B	513	1/1	0.89	0.40	72,72,72,72	0
9	GOL	B	503	6/6	0.89	0.13	41,44,45,48	0
10	TRS	D	503	8/8	0.89	0.14	42,45,51,56	0
6	NA	B	508	1/1	0.89	0.23	44,44,44,44	0
4	SO4	A	203	5/5	0.90	0.10	52,56,62,71	0
6	NA	C	206	1/1	0.91	0.18	48,48,48,48	0
5	CL	B	506	1/1	0.91	0.16	58,58,58,58	0
6	NA	D	508	1/1	0.91	0.13	47,47,47,47	0
6	NA	D	509	1/1	0.91	0.20	55,55,55,55	0
4	SO4	D	505	5/5	0.91	0.13	37,45,46,52	0
6	NA	B	514	1/1	0.91	0.18	53,53,53,53	0
5	CL	A	205	1/1	0.91	0.11	65,65,65,65	0
4	SO4	A	204	5/5	0.92	0.07	56,58,64,64	0
4	SO4	C	203	5/5	0.92	0.10	67,68,71,76	0
5	CL	C	204	1/1	0.94	0.08	58,58,58,58	0
6	NA	B	509	1/1	0.94	0.12	47,47,47,47	0
6	NA	B	512	1/1	0.95	0.08	53,53,53,53	0
6	NA	A	207	1/1	0.96	0.11	38,38,38,38	0
8	FNR	B	502	31/31	0.98	0.05	17,20,22,24	0
8	FNR	D	502	31/31	0.98	0.05	16,20,23,25	0
6	NA	B	507	1/1	0.98	0.04	34,34,34,34	0
6	NA	A	206	1/1	0.98	0.14	32,32,32,32	0
6	NA	D	506	1/1	0.98	0.06	31,31,31,31	0
7	SF4	D	501	8/8	0.99	0.02	18,18,19,20	0
3	FES	A	201	4/4	0.99	0.03	16,17,19,19	0
7	SF4	B	501	8/8	0.99	0.03	17,19,19,19	0
3	FES	C	201	4/4	1.00	0.01	17,18,18,18	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.

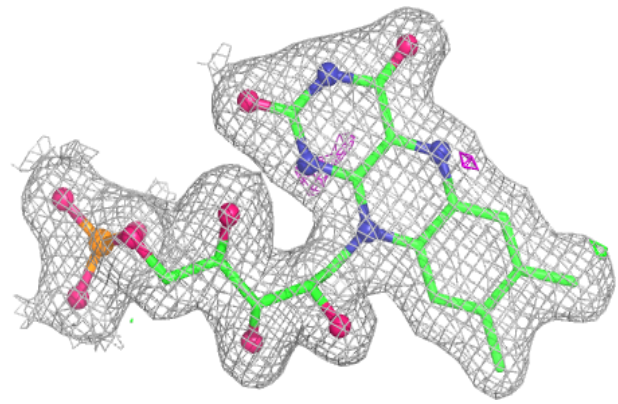
Electron density around FNR B 502:

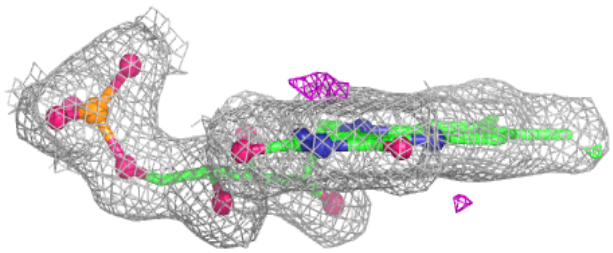
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

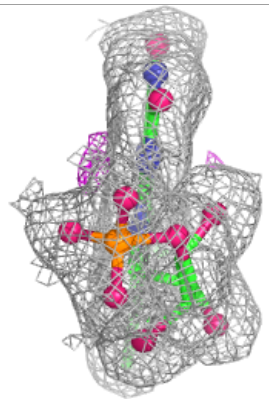


Electron density around FNR D 502:

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

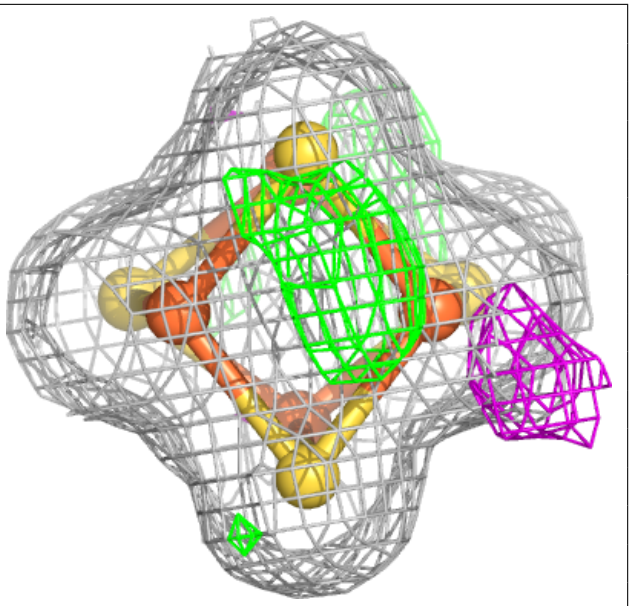


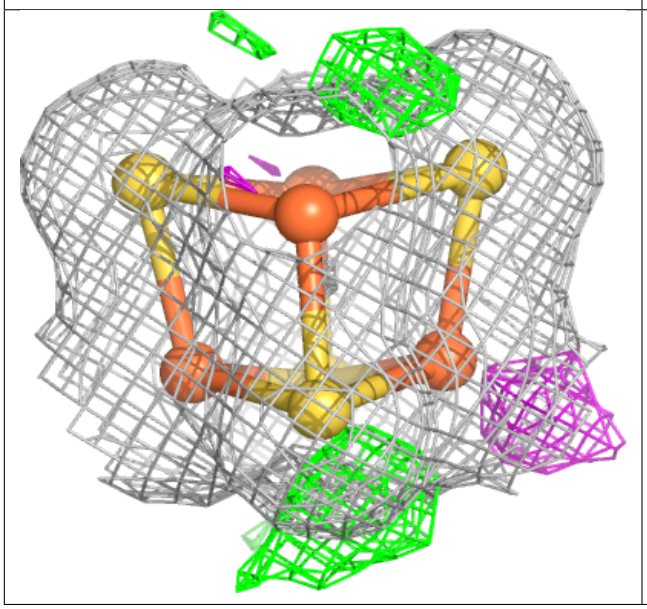


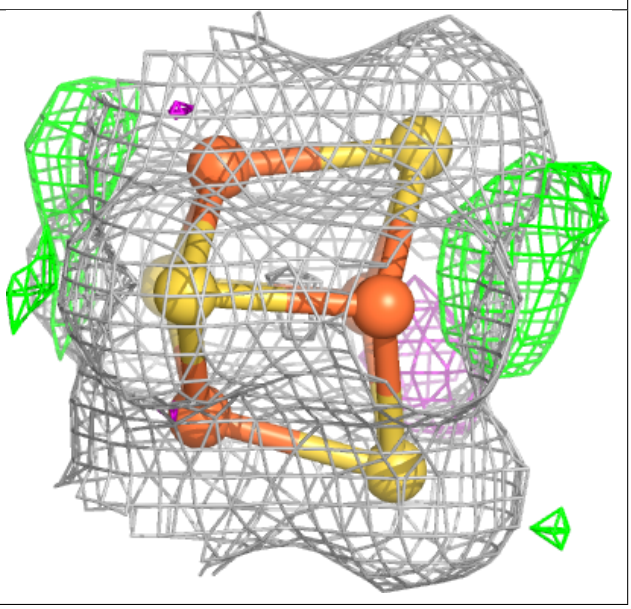


Electron density around SF4 D 501:

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

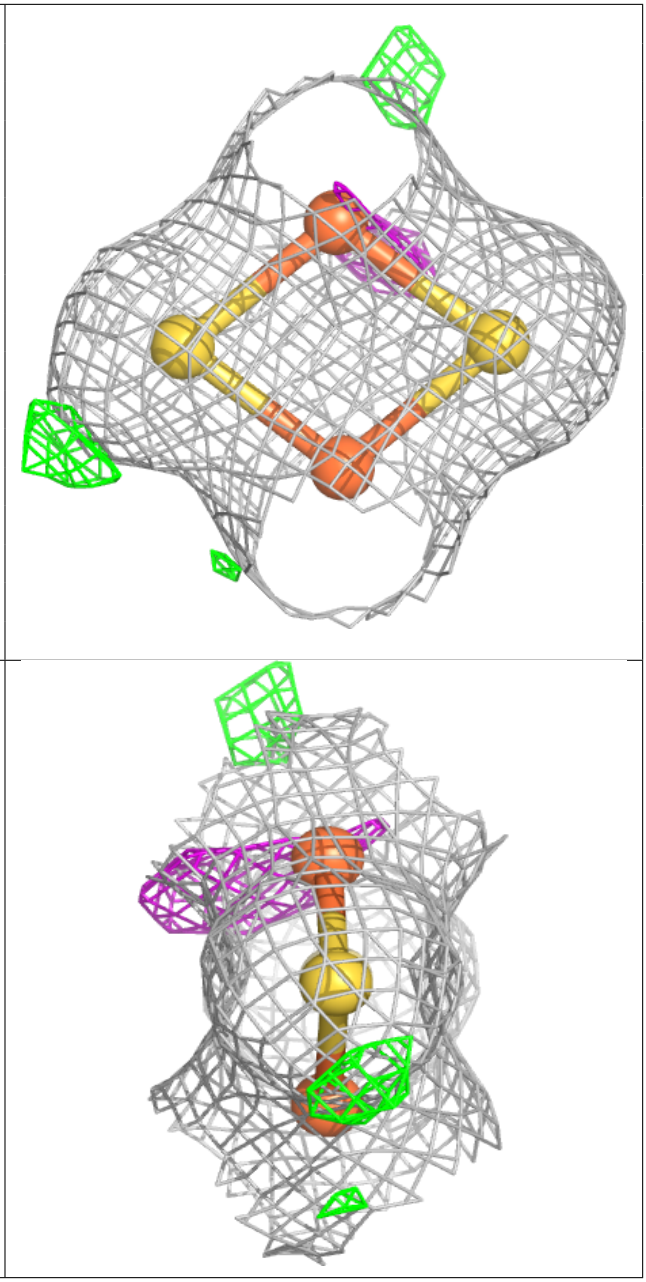






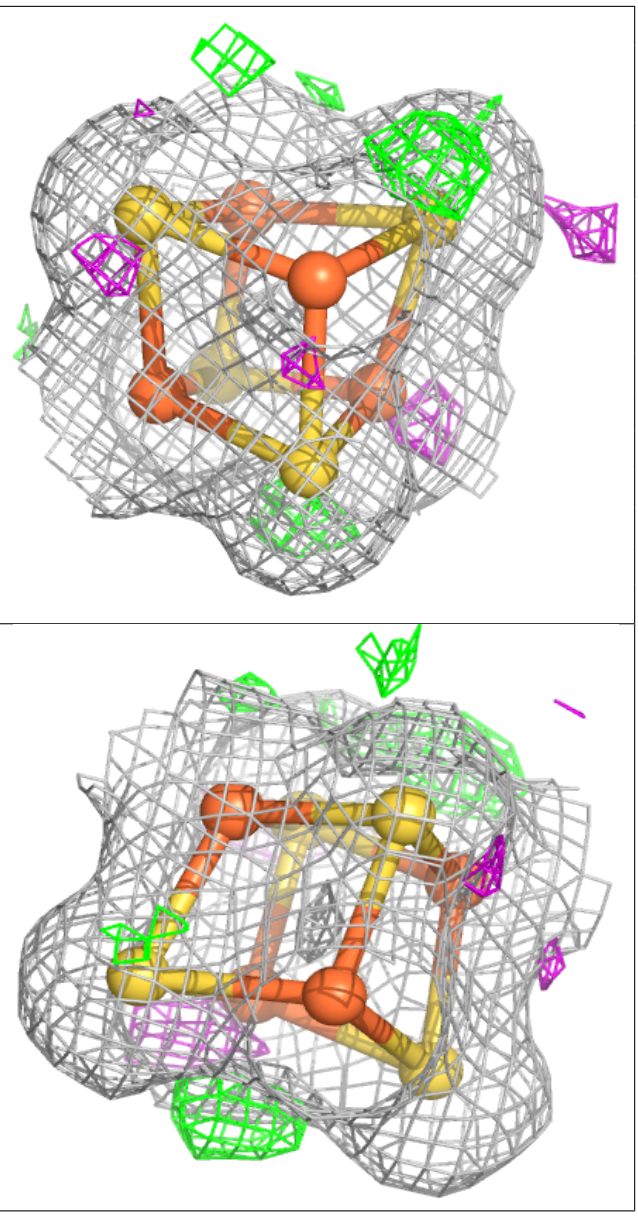
Electron density around FES A 201:

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



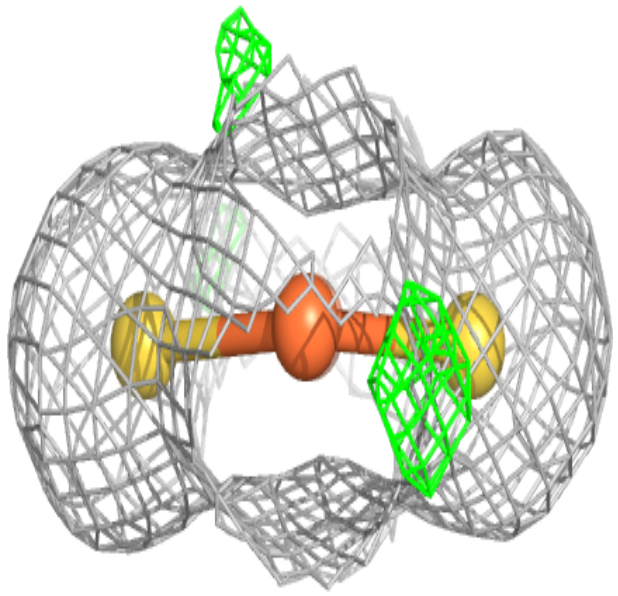
Electron density around SF4 B 501:

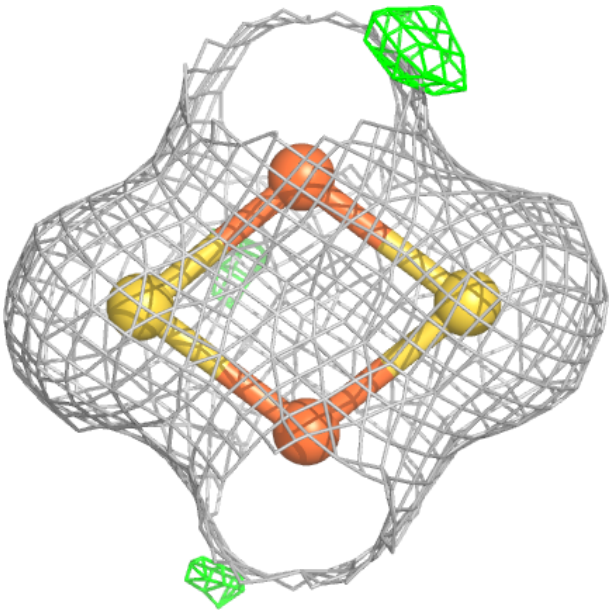
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

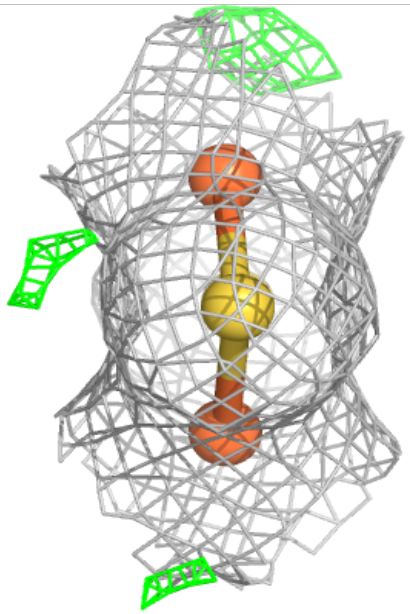


Electron density around FES C 201:

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.