Full wwPDB EM Validation Report

Mar 10, 2025 – 06:14 am GMT

PDB ID	:	9ERI
EMDB ID	:	EMD-19915
Title	:	Cryo-EM structure of sodium pumping Rnf complex from Acetobacterium woodii bound to NADH
Authors	:	Kumar, A.; Schuller, J.M.
Deposited on	:	2024-03-23
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

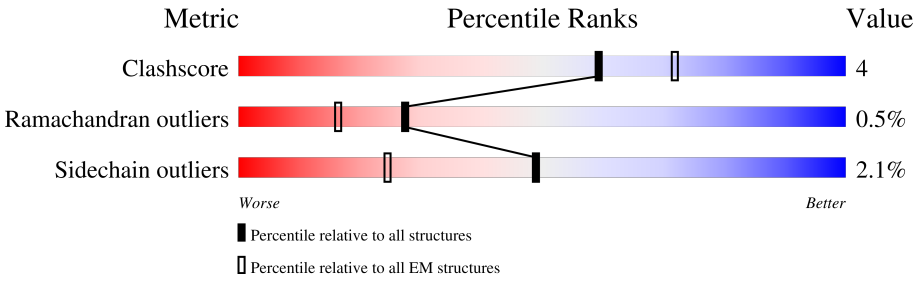
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	191	89% 10% •
2	B	333	85% 14% •
3	C	443	86% 14%
4	D	318	90% 10% •
5	E	196	93% 7%
6	G	207	84% 16%

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
11	RBF	D	401	-	X	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 12704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	191	Total	C	N	O	S	0	0
			1433	959	218	247	9		

- Molecule 2 is a protein called Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	333	Total	C	N	O	S	0	0
			2394	1490	406	453	45		

- Molecule 3 is a protein called Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	443	Total	C	N	O	S	0	0
			3287	2069	567	620	31		

- Molecule 4 is a protein called Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	318	Total	C	N	O	S	0	0
			2374	1566	379	415	14		

- Molecule 5 is a protein called Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit E.

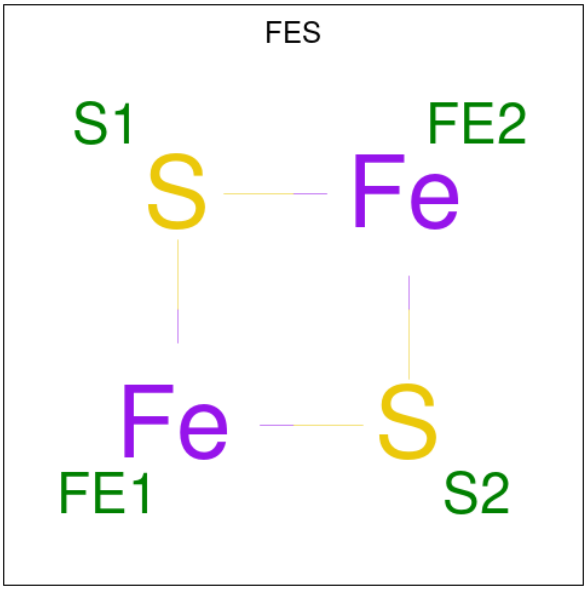
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1439	954	230	243	12		

- Molecule 6 is a protein called Na(+)-translocating ferredoxin:NAD(+) oxidoreductase com-

plex subunit G.

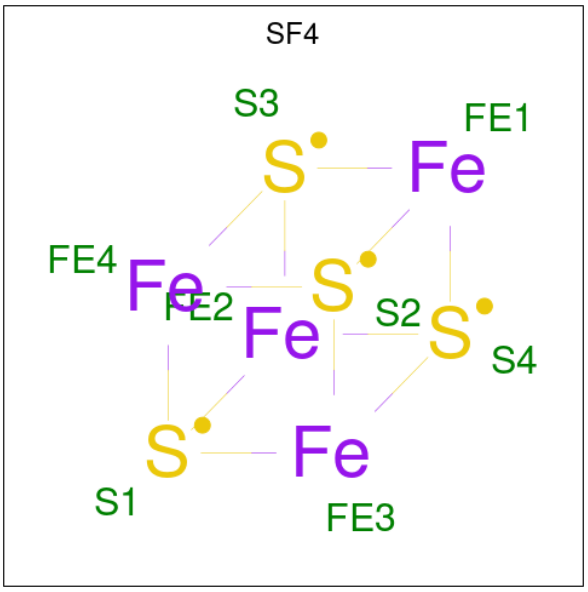
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	207	Total	C	N	O	S	0	0
			1531	968	247	311	5		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



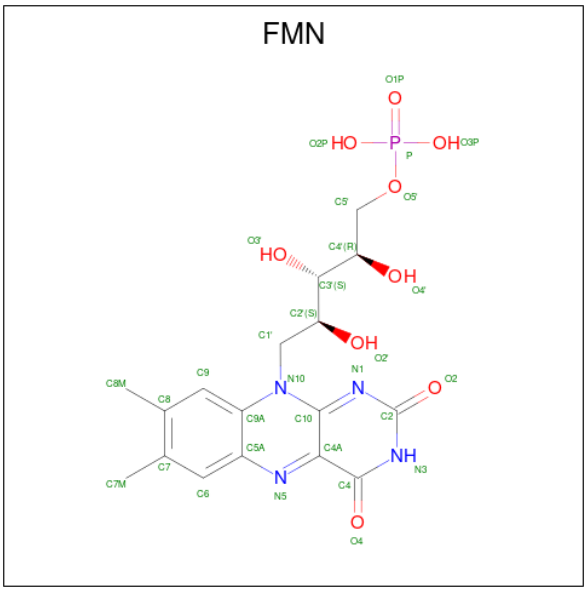
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Fe	S	0
			4	2	2	

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



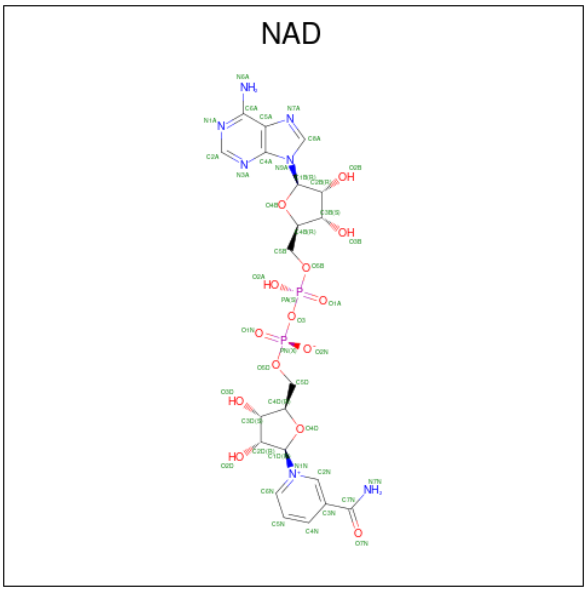
Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	B	1	Total Fe S 8 4 4	0
8	C	1	Total Fe S 8 4 4	0
8	C	1	Total Fe S 8 4 4	0

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



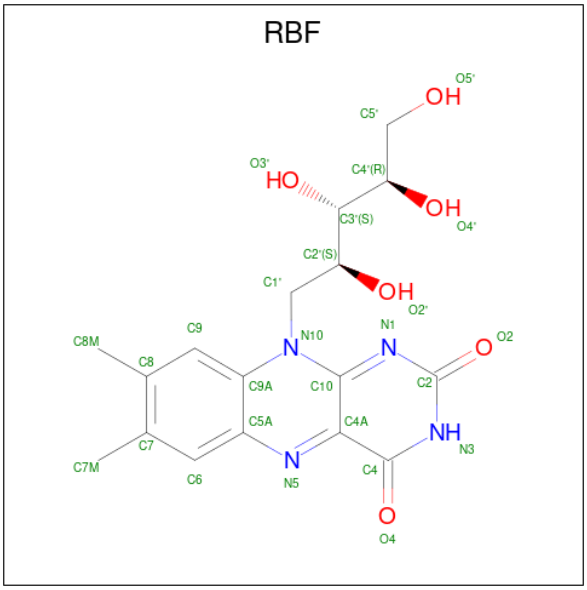
Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
9	D	1	Total	C	N	O	P	0
			30	17	4	8	1	
9	G	1	Total	C	N	O	P	0
			30	17	4	8	1	

- Molecule 10 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 11 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



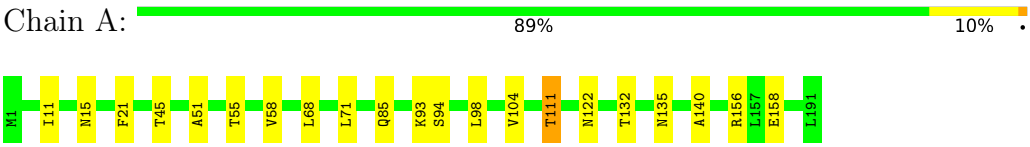
Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	N	O	0
			27	17	4	6	

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. 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. 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.

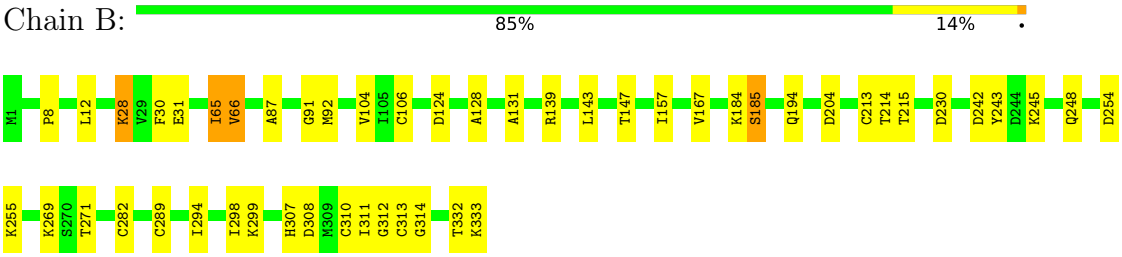
• Molecule 1: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit A

Chain A:



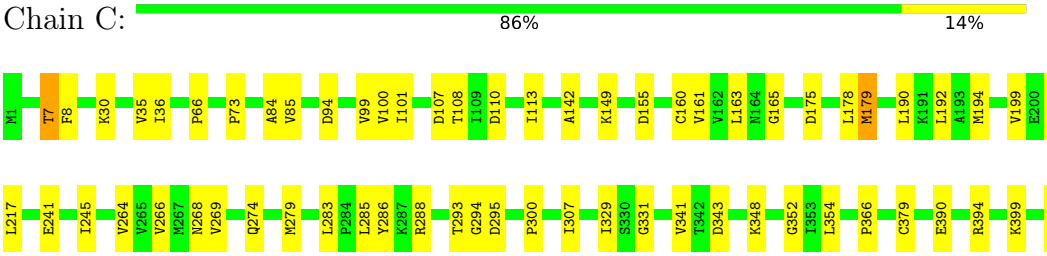
• Molecule 2: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit B

Chain B:



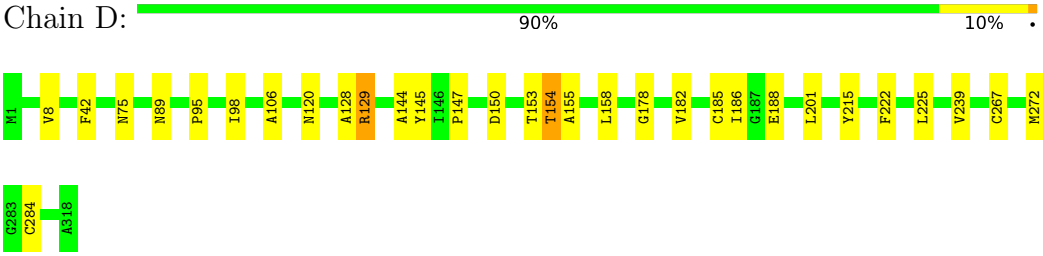
• Molecule 3: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit C

Chain C:



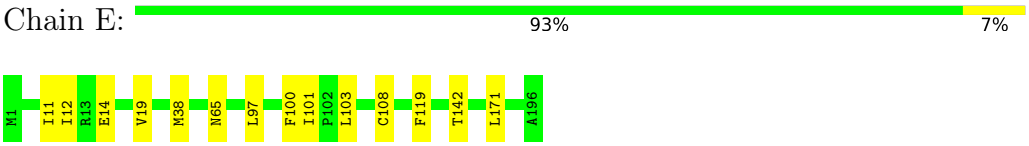
• Molecule 4: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit D

Chain D:



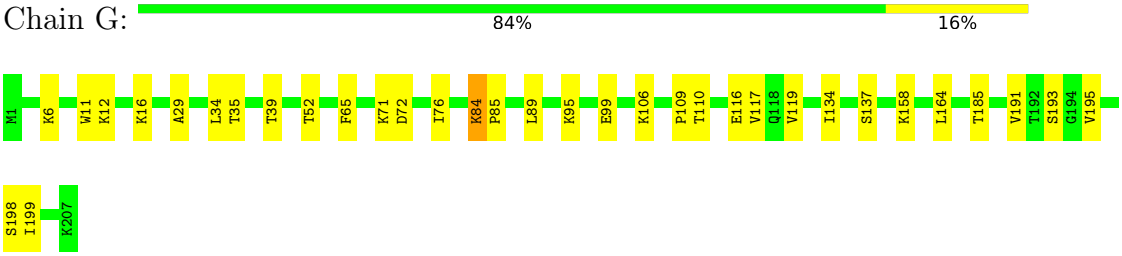
• Molecule 5: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit E

Chain E:



• Molecule 6: Na(+)-translocating ferredoxin:NAD(+) oxidoreductase complex subunit G

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	645102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SF4, RBF, FMN, NAD

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	0.27	0/1458	0.47	0/1984
2	B	0.26	0/2429	0.55	2/3281 (0.1%)
3	C	0.26	0/3346	0.49	0/4530
4	D	0.26	0/2427	0.46	0/3315
5	E	0.26	0/1464	0.48	0/1989
6	G	0.26	0/1548	0.51	0/2098
All	All	0.26	0/12672	0.50	2/17197 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	230	ASP	CB-CG-OD1	6.52	124.17	118.30
2	B	254	ASP	CB-CG-OD1	5.24	123.02	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	LEU	Peptide
2	B	289	CYS	Peptide

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	1433	0	1534	14	0
2	B	2394	0	2386	28	0
3	C	3287	0	3363	36	0
4	D	2374	0	2502	18	0
5	E	1439	0	1554	7	0
6	G	1531	0	1575	19	0
7	A	4	0	0	0	0
8	B	64	0	0	1	0
8	C	16	0	0	0	0
9	C	31	0	19	1	0
9	D	30	0	19	1	0
9	G	30	0	19	0	0
10	C	44	0	22	2	0
11	D	27	0	18	0	0
All	All	12704	0	13011	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (112) 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)
6:G:109:PRO:HG3	6:G:117:VAL:H	1.43	0.82
3:C:142:ALA:HB2	10:C:502:NAD:H52N	1.76	0.67
2:B:271:THR:HG22	2:B:310:CYS:HB2	1.77	0.67
4:D:185:CYS:HB2	4:D:188:GLU:HG2	1.77	0.66
3:C:268:ASN:ND2	9:C:501:FMN:O2	2.30	0.65
6:G:119:VAL:HG12	6:G:134:ILE:HG12	1.79	0.65
1:A:122:ASN:HD22	1:A:132:THR:HG23	1.61	0.64
4:D:158:LEU:HB3	9:D:402:FMN:H5'2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:HD3	6:G:6:LYS:HD2	1.80	0.63
1:A:93:LYS:HD2	2:B:30:PHE:HA	1.81	0.63
3:C:390:GLU:OE1	3:C:394:ARG:NH1	2.32	0.63
2:B:194:GLN:HE21	2:B:243:TYR:HD1	1.45	0.63
1:A:71:LEU:HD11	2:B:8:PRO:HB3	1.82	0.61
2:B:310:CYS:SG	2:B:311:ILE:N	2.75	0.60
2:B:104:VAL:HG12	2:B:106:CYS:H	1.66	0.60
2:B:157:ILE:HG12	2:B:167:VAL:HG22	1.84	0.59
2:B:139:ARG:O	2:B:184:LYS:NZ	2.34	0.58
1:A:158:GLU:OE1	3:C:399:LYS:NZ	2.38	0.57
3:C:163:LEU:HD11	3:C:190:LEU:HB2	1.87	0.57
2:B:242:ASP:OD2	2:B:245:LYS:NZ	2.38	0.56
1:A:122:ASN:OD1	1:A:135:ASN:ND2	2.31	0.56
3:C:288:ARG:NH1	3:C:348:LYS:O	2.38	0.56
3:C:241:GLU:HG3	3:C:266:VAL:HG11	1.87	0.55
2:B:185:SER:O	2:B:185:SER:OG	2.25	0.54
6:G:89:LEU:HD12	6:G:106:LYS:HD3	1.88	0.54
6:G:158:LYS:HD2	6:G:164:LEU:HD21	1.89	0.54
2:B:124:ASP:OD1	2:B:147:THR:OG1	2.25	0.54
3:C:85:VAL:HG13	3:C:99:VAL:HG22	1.89	0.54
3:C:212:ASP:N	3:C:212:ASP:OD1	2.39	0.54
3:C:295:ASP:OD1	3:C:295:ASP:N	2.32	0.53
5:E:38:MET:SD	5:E:142:THR:OG1	2.65	0.53
3:C:36:ILE:HG12	3:C:100:VAL:HG23	1.91	0.53
3:C:341:VAL:HG13	3:C:343:ASP:H	1.73	0.52
3:C:293:THR:OG1	3:C:294:GLY:N	2.41	0.52
6:G:72:ASP:O	6:G:76:ILE:HD12	2.09	0.52
4:D:42:PHE:HE2	4:D:186:ILE:HA	1.74	0.52
2:B:332:THR:HG22	2:B:333:LYS:HD3	1.90	0.52
1:A:85:GLN:NE2	5:E:65:ASN:O	2.41	0.51
3:C:175:ASP:O	3:C:179:MET:HG3	2.10	0.51
4:D:106:ALA:HB2	4:D:128:ALA:HB2	1.93	0.51
6:G:119:VAL:HG11	6:G:191:VAL:HG13	1.92	0.51
3:C:35:VAL:HG23	3:C:101:ILE:HG23	1.92	0.51
4:D:239:VAL:HG23	4:D:275:ARG:HH22	1.74	0.51
4:D:154:THR:OG1	4:D:155:ALA:N	2.44	0.50
2:B:12:LEU:HD12	6:G:29:ALA:HB2	1.93	0.50
5:E:97:LEU:HD13	5:E:101:ILE:HD11	1.95	0.49
4:D:178:GLY:HA2	4:D:182:VAL:HG11	1.94	0.49
4:D:282:GLU:OE1	4:D:284:CYS:N	2.36	0.49
3:C:194:MET:HG2	3:C:199:VAL:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:ILE:HD12	3:C:354:LEU:HD23	1.95	0.48
4:D:95:PRO:HD2	4:D:98:ILE:HD12	1.95	0.48
3:C:149:LYS:NZ	10:C:502:NAD:O3B	2.45	0.48
6:G:117:VAL:HG12	6:G:137:SER:HA	1.95	0.48
2:B:214:THR:HG23	2:B:215:THR:HG23	1.95	0.48
4:D:147:PRO:HD2	4:D:150:ASP:HA	1.95	0.47
2:B:271:THR:OG1	2:B:307:HIS:ND1	2.40	0.47
2:B:294:ILE:O	2:B:299:LYS:NZ	2.43	0.47
3:C:293:THR:HA	3:C:300:PRO:HB3	1.96	0.47
4:D:215:TYR:HE1	4:D:267:CYS:HB3	1.80	0.47
1:A:156:ARG:NH1	4:D:120:ASN:O	2.48	0.46
1:A:68:LEU:HB3	1:A:71:LEU:HD12	1.97	0.46
6:G:84:LYS:O	6:G:84:LYS:HD2	2.16	0.46
3:C:7:THR:OG1	3:C:8:PHE:N	2.49	0.46
1:A:45:THR:HA	1:A:140:ALA:HB1	1.97	0.46
1:A:51:ALA:O	1:A:55:THR:HG23	2.16	0.45
3:C:66:PRO:HD3	3:C:73:PRO:HG3	1.98	0.45
3:C:245:ILE:HD13	3:C:245:ILE:HA	1.86	0.45
5:E:100:PHE:HA	5:E:103:LEU:HB2	1.99	0.45
6:G:6:LYS:HB2	6:G:11:TRP:CD1	2.51	0.45
1:A:11:ILE:O	1:A:15:ASN:ND2	2.45	0.44
2:B:255:LYS:HE2	2:B:255:LYS:HB2	1.80	0.44
2:B:312:GLY:O	2:B:314:GLY:N	2.50	0.44
6:G:95:LYS:HA	6:G:95:LYS:HD2	1.81	0.44
4:D:222:PHE:HB3	4:D:272:MET:HG2	2.00	0.44
6:G:12:LYS:HD2	6:G:12:LYS:HA	1.68	0.44
2:B:213:CYS:HB3	8:B:401:SF4:S4	2.57	0.44
6:G:52:THR:HG23	6:G:65:PHE:HZ	1.82	0.43
6:G:95:LYS:HZ3	6:G:99:GLU:N	2.16	0.43
2:B:87:ALA:O	2:B:91:GLY:N	2.51	0.43
2:B:194:GLN:HA	2:B:248:GLN:NE2	2.34	0.43
5:E:11:ILE:HG22	5:E:12:ILE:HG13	2.00	0.43
3:C:283:LEU:HD23	3:C:283:LEU:HA	1.91	0.43
2:B:269:LYS:HA	2:B:310:CYS:HB3	2.01	0.43
3:C:165:GLY:HA3	3:C:179:MET:HE3	2.02	0.42
2:B:128:ALA:HB3	2:B:143:LEU:HD13	2.01	0.42
2:B:131:ALA:HB1	4:D:8:VAL:HG12	2.01	0.42
3:C:160:CYS:SG	3:C:264:VAL:HG12	2.59	0.42
6:G:35:THR:O	6:G:39:THR:HG22	2.19	0.42
1:A:94:SER:HB2	2:B:30:PHE:CE2	2.55	0.42
3:C:366:PRO:HB3	3:C:422:ARG:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:CYS:HB3	3:C:201:LYS:HB2	2.02	0.42
3:C:274:GLN:HG2	3:C:285:LEU:HD13	2.02	0.42
2:B:12:LEU:HD23	2:B:12:LEU:HA	1.87	0.42
3:C:217:LEU:HD23	3:C:217:LEU:HA	1.93	0.42
4:D:147:PRO:HG3	4:D:153:THR:HG23	2.01	0.42
3:C:84:ALA:HB3	3:C:100:VAL:HG12	2.01	0.42
6:G:195:VAL:O	6:G:199:ILE:HG22	2.20	0.42
6:G:16:LYS:HA	6:G:16:LYS:HD2	1.84	0.41
3:C:110:ASP:HB3	3:C:113:ILE:HG12	2.03	0.41
3:C:331:GLY:N	3:C:352:GLY:O	2.54	0.41
2:B:65:ILE:O	2:B:66:VAL:HG13	2.20	0.41
1:A:55:THR:HA	1:A:58:VAL:HG12	2.03	0.41
3:C:192:LEU:HD11	3:C:279:MET:HG3	2.03	0.41
1:A:111:THR:HG21	5:E:108:CYS:HA	2.03	0.41
5:E:14:GLU:O	5:E:19:VAL:HB	2.20	0.41
6:G:71:LYS:HA	6:G:71:LYS:HD3	1.79	0.40
4:D:89:ASN:O	4:D:129:ARG:NH2	2.54	0.40
3:C:161:VAL:HG23	3:C:199:VAL:HG21	2.04	0.40
3:C:178:LEU:HD23	3:C:269:VAL:HG12	2.03	0.40
4:D:225:LEU:HD23	4:D:225:LEU:HA	1.98	0.40
3:C:286:TYR:HA	3:C:307:ILE:HD12	2.03	0.40
4:D:201:LEU:HD23	4:D:201:LEU:HA	1.94	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 PDB entries followed by that with respect to all EM entries.

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	189/191 (99%)	180 (95%)	8 (4%)	1 (0%)	25 56
2	B	331/333 (99%)	294 (89%)	33 (10%)	4 (1%)	11 38
3	C	441/443 (100%)	431 (98%)	10 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	316/318 (99%)	297 (94%)	17 (5%)	2 (1%)	22 53
5	E	194/196 (99%)	185 (95%)	9 (5%)	0	100 100
6	G	205/207 (99%)	189 (92%)	14 (7%)	2 (1%)	13 42
All	All	1676/1688 (99%)	1576 (94%)	91 (5%)	9 (0%)	27 56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	VAL
6	G	110	THR
2	B	298	ILE
2	B	313	CYS
4	D	154	THR
4	D	144	ALA
6	G	85	PRO
2	B	65	ILE
1	A	104	VAL

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 PDB entries followed by that with respect to all EM entries.

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	153/153 (100%)	151 (99%)	2 (1%)	65 79
2	B	257/257 (100%)	250 (97%)	7 (3%)	40 65
3	C	365/365 (100%)	357 (98%)	8 (2%)	47 69
4	D	252/252 (100%)	249 (99%)	3 (1%)	67 80
5	E	152/152 (100%)	150 (99%)	2 (1%)	65 79
6	G	168/168 (100%)	162 (96%)	6 (4%)	30 57
All	All	1347/1347 (100%)	1319 (98%)	28 (2%)	49 70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	111	THR
2	B	28	LYS
2	B	31	GLU
2	B	92	MET
2	B	185	SER
2	B	204	ASP
2	B	282	CYS
2	B	308	ASP
3	C	7	THR
3	C	30	LYS
3	C	94	ASP
3	C	107	ASP
3	C	108	THR
3	C	155	ASP
3	C	179	MET
3	C	379	CYS
4	D	75	ASN
4	D	129	ARG
4	D	145	TYR
5	E	119	PHE
5	E	171	LEU
6	G	34	LEU
6	G	84	LYS
6	G	116	GLU
6	G	185	THR
6	G	193	SER
6	G	198	SER

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

Mol	Chain	Res	Type
1	A	122	ASN
1	A	135	ASN
2	B	194	GLN
2	B	248	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)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FES	A	201	1,5	0,4,4	-	-	-		
8	SF4	B	405	2	0,12,12	-	-	-		
8	SF4	B	408	2	0,12,12	-	-	-		
8	SF4	B	406	2	0,12,12	-	-	-		
8	SF4	B	401	2	0,12,12	-	-	-		
9	FMN	D	402	4	29,32,33	0.58	0	40,47,50	0.69	0
8	SF4	B	404	2	0,12,12	-	-	-		
9	FMN	G	301	6	29,32,33	0.58	0	40,47,50	0.66	1 (2%)
10	NAD	C	502	-	42,48,48	1.65	9 (21%)	50,73,73	3.63	26 (52%)
8	SF4	B	403	2	0,12,12	-	-	-		
8	SF4	B	407	2	0,12,12	-	-	-		
11	RBF	D	401	-	29,29,29	4.43	18 (62%)	41,43,43	5.17	25 (60%)
9	FMN	C	501	-	33,33,33	0.60	0	48,50,50	0.66	1 (2%)
8	SF4	C	504	3	0,12,12	-	-	-		
8	SF4	C	503	3	0,12,12	-	-	-		
8	SF4	B	402	2	0,12,12	-	-	-		

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
7	FES	A	201	1,5	-	-	0/1/1/1
8	SF4	B	405	2	-	-	0/6/5/5
8	SF4	B	408	2	-	-	0/6/5/5
8	SF4	B	406	2	-	-	0/6/5/5
8	SF4	B	401	2	-	-	0/6/5/5
9	FMN	D	402	4	-	7/15/17/18	0/3/3/3
9	FMN	G	301	6	-	2/15/17/18	0/3/3/3
8	SF4	B	404	2	-	-	0/6/5/5
8	SF4	B	402	2	-	-	0/6/5/5
8	SF4	B	403	2	-	-	0/6/5/5
8	SF4	B	407	2	-	-	0/6/5/5
11	RBF	D	401	-	-	8/14/14/14	0/3/3/3
9	FMN	C	501	-	-	1/18/18/18	0/3/3/3
8	SF4	C	504	3	-	-	0/6/5/5
8	SF4	C	503	3	-	-	0/6/5/5
10	NAD	C	502	-	-	16/26/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	401	RBF	C4-N3	-12.58	1.15	1.38
11	D	401	RBF	C2-N3	-7.14	1.22	1.39
11	D	401	RBF	C9-C8	-7.12	1.29	1.39
11	D	401	RBF	O4-C4	-6.86	1.10	1.23
11	D	401	RBF	C8M-C8	-6.71	1.37	1.51
11	D	401	RBF	C6-C5A	-6.69	1.29	1.40
11	D	401	RBF	C6-C7	-6.40	1.30	1.39
11	D	401	RBF	O2-C2	-5.48	1.14	1.24
10	C	502	NAD	C3D-C4D	-4.77	1.40	1.53
10	C	502	NAD	C2D-C1D	-4.01	1.47	1.53
11	D	401	RBF	O2'-C2'	-3.84	1.35	1.43
11	D	401	RBF	C1'-C2'	3.47	1.57	1.52
10	C	502	NAD	O4B-C4B	-3.34	1.37	1.45
11	D	401	RBF	C7M-C7	-3.28	1.44	1.51
10	C	502	NAD	O3D-C3D	-3.25	1.35	1.43
11	D	401	RBF	C9-C9A	-3.19	1.34	1.39
11	D	401	RBF	O4'-C4'	-3.07	1.36	1.43
11	D	401	RBF	C2-N1	-2.90	1.29	1.36
10	C	502	NAD	C2D-C3D	-2.62	1.46	1.53
11	D	401	RBF	C8-C7	-2.61	1.34	1.40
11	D	401	RBF	C5'-C4'	-2.49	1.45	1.52
10	C	502	NAD	C4N-C3N	-2.46	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	502	NAD	PA-O2A	-2.32	1.44	1.55
11	D	401	RBF	C5A-N5	-2.28	1.35	1.39
10	C	502	NAD	C2N-C3N	2.18	1.42	1.39
10	C	502	NAD	C3B-C4B	-2.04	1.47	1.53
11	D	401	RBF	C10-N1	-2.00	1.29	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	401	RBF	O4-C4-N3	-16.81	87.89	120.12
11	D	401	RBF	C4-C4A-N5	12.00	135.31	118.23
11	D	401	RBF	C1'-C2'-C3'	11.06	140.71	109.79
11	D	401	RBF	O2'-C2'-C3'	-10.29	84.09	109.10
10	C	502	NAD	O4D-C1D-C2D	-10.09	92.19	106.93
10	C	502	NAD	C6N-N1N-C2N	-9.09	113.68	121.97
10	C	502	NAD	O4B-C1B-C2B	-8.89	93.93	106.93
11	D	401	RBF	O4-C4-C4A	7.08	145.38	126.60
10	C	502	NAD	C3B-C2B-C1B	-6.79	90.76	100.98
10	C	502	NAD	C1B-N9A-C4A	-6.57	115.10	126.64
11	D	401	RBF	C4A-C10-N10	6.47	125.94	116.48
10	C	502	NAD	N3A-C2A-N1A	-6.28	118.86	128.68
11	D	401	RBF	O4'-C4'-C5'	-6.26	94.47	109.14
11	D	401	RBF	O2'-C2'-C1'	-6.11	95.04	109.80
11	D	401	RBF	O2-C2-N1	-5.88	112.09	121.83
10	C	502	NAD	C3D-C2D-C1D	5.45	109.19	100.98
11	D	401	RBF	C10-C4A-N5	-5.34	113.53	124.86
11	D	401	RBF	C5'-C4'-C3'	5.12	123.52	112.41
10	C	502	NAD	C5D-C4D-C3D	-5.05	96.26	115.18
11	D	401	RBF	N3-C2-N1	5.02	129.23	119.38
11	D	401	RBF	C4A-C4-N3	4.96	125.79	113.19
11	D	401	RBF	C4-N3-C2	-4.85	116.68	125.64
10	C	502	NAD	O4B-C4B-C3B	-4.41	96.39	105.11
10	C	502	NAD	O5D-C5D-C4D	4.16	123.30	108.99
11	D	401	RBF	C4A-C10-N1	-3.99	115.48	124.73
10	C	502	NAD	C4N-C3N-C7N	-3.94	110.50	121.04
10	C	502	NAD	C5N-C6N-N1N	3.85	125.93	120.40
10	C	502	NAD	O3D-C3D-C4D	-3.67	100.44	111.05
10	C	502	NAD	C2N-N1N-C1D	3.38	126.66	119.14
11	D	401	RBF	C4-C4A-C10	-3.35	111.16	116.79
10	C	502	NAD	C5N-C4N-C3N	-3.32	116.42	120.34
10	C	502	NAD	O5B-C5B-C4B	3.31	120.39	108.99
10	C	502	NAD	C2N-C3N-C7N	3.31	129.07	119.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	401	RBF	O3'-C3'-C2'	-3.23	101.02	108.81
10	C	502	NAD	O2B-C2B-C1B	3.21	122.70	110.85
10	C	502	NAD	O2D-C2D-C1D	3.13	122.43	110.85
11	D	401	RBF	C5A-N5-C4A	2.93	122.94	118.07
10	C	502	NAD	C3N-C2N-N1N	2.82	123.18	120.43
10	C	502	NAD	O7N-C7N-N7N	2.79	126.54	122.58
11	D	401	RBF	C9A-N10-C10	-2.67	116.61	120.77
11	D	401	RBF	C8M-C8-C7	-2.66	115.28	120.74
11	D	401	RBF	C9A-C5A-N5	2.55	125.21	122.43
10	C	502	NAD	C2A-N1A-C6A	2.45	122.94	118.75
11	D	401	RBF	C7M-C7-C6	-2.44	114.97	119.49
10	C	502	NAD	C4A-C5A-N7A	-2.37	106.92	109.40
11	D	401	RBF	C7M-C7-C8	2.34	125.54	120.74
11	D	401	RBF	C9-C8-C7	2.22	122.84	119.67
10	C	502	NAD	O2B-C2B-C3B	-2.17	104.81	111.82
10	C	502	NAD	O7N-C7N-C3N	-2.12	117.09	119.63
11	D	401	RBF	C5A-C9A-N10	-2.11	115.78	117.95
10	C	502	NAD	O4D-C4D-C5D	2.08	116.20	109.37
9	C	501	FMN	C4-N3-C2	-2.04	121.88	125.64
9	G	301	FMN	C4-N3-C2	-2.03	121.89	125.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	402	FMN	N10-C1'-C2'-O2'
9	D	402	FMN	N10-C1'-C2'-C3'
9	D	402	FMN	O3'-C3'-C4'-C5'
9	D	402	FMN	C4'-C5'-O5'-P
10	C	502	NAD	C5B-O5B-PA-O3
10	C	502	NAD	O4B-C4B-C5B-O5B
10	C	502	NAD	O4D-C1D-N1N-C2N
10	C	502	NAD	O4D-C1D-N1N-C6N
10	C	502	NAD	C2D-C1D-N1N-C2N
11	D	401	RBF	N10-C1'-C2'-O2'
11	D	401	RBF	C1'-C2'-C3'-O3'
11	D	401	RBF	C2'-C3'-C4'-O4'
11	D	401	RBF	C3'-C4'-C5'-O5'
11	D	401	RBF	O4'-C4'-C5'-O5'
10	C	502	NAD	O4D-C4D-C5D-O5D
11	D	401	RBF	C2'-C3'-C4'-C5'
10	C	502	NAD	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	402	FMN	C2'-C3'-C4'-C5'
11	D	401	RBF	O3'-C3'-C4'-O4'
9	D	402	FMN	O3'-C3'-C4'-O4'
9	G	301	FMN	O2'-C2'-C3'-C4'
9	D	402	FMN	C2'-C3'-C4'-O4'
9	C	501	FMN	C5'-O5'-P-O1P
11	D	401	RBF	O3'-C3'-C4'-C5'
10	C	502	NAD	C2N-C3N-C7N-O7N
10	C	502	NAD	C4N-C3N-C7N-O7N
10	C	502	NAD	PA-O3-PN-O5D
10	C	502	NAD	C4N-C3N-C7N-N7N
10	C	502	NAD	C5B-O5B-PA-O1A
10	C	502	NAD	C5B-O5B-PA-O2A
10	C	502	NAD	C2N-C3N-C7N-N7N
9	G	301	FMN	C4'-C5'-O5'-P
10	C	502	NAD	C3D-C4D-C5D-O5D
10	C	502	NAD	C2D-C1D-N1N-C6N

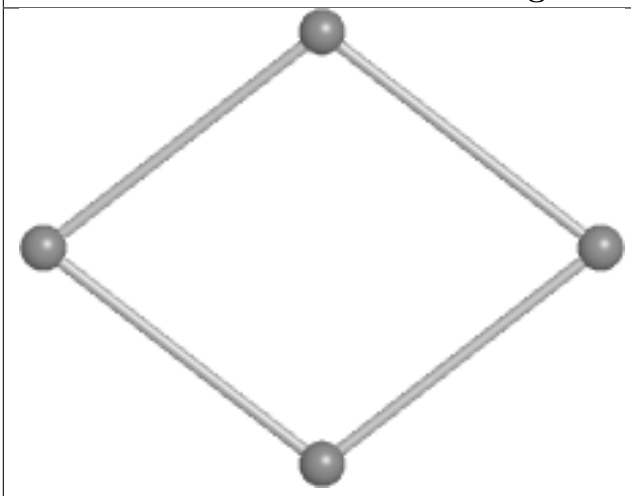
There are no ring outliers.

4 monomers are involved in 5 short contacts:

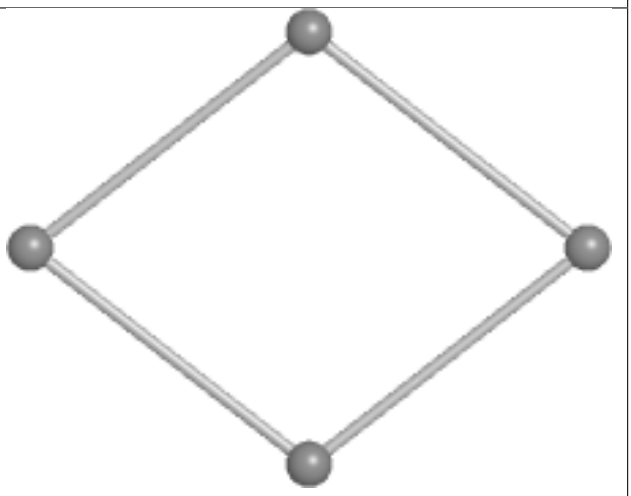
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	401	SF4	1	0
9	D	402	FMN	1	0
10	C	502	NAD	2	0
9	C	501	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

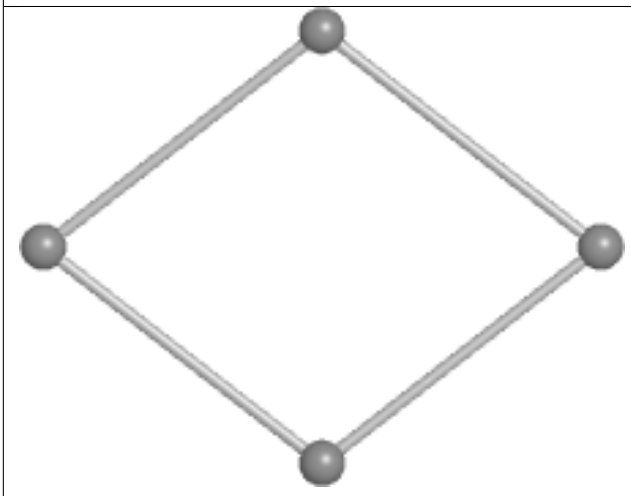
Ligand FES A 201



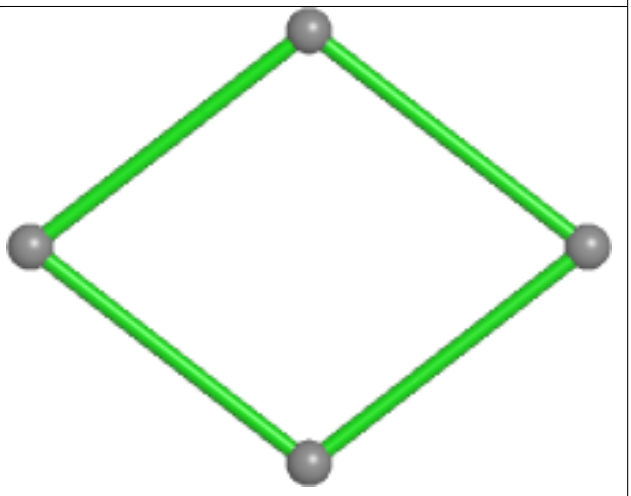
Bond lengths



Bond angles

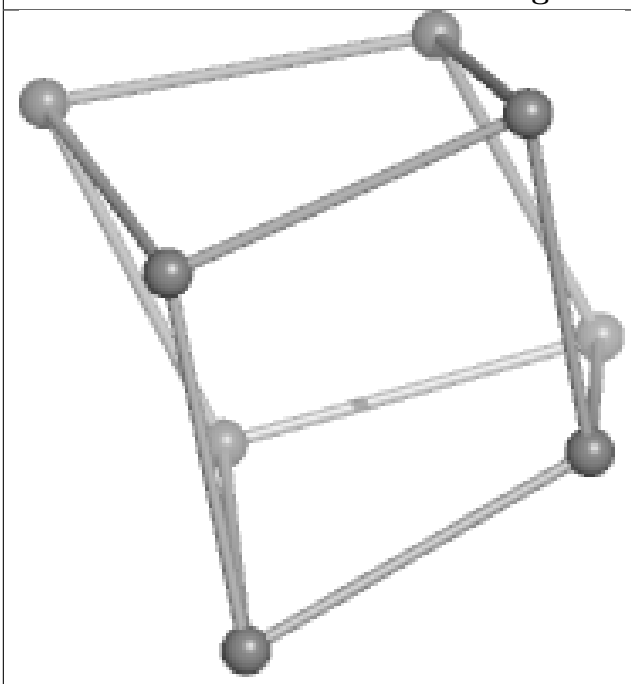


Torsions

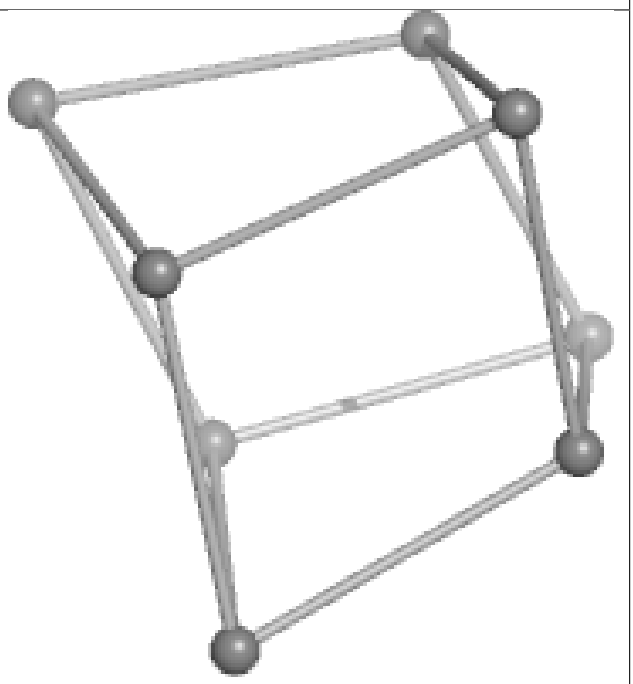


Rings

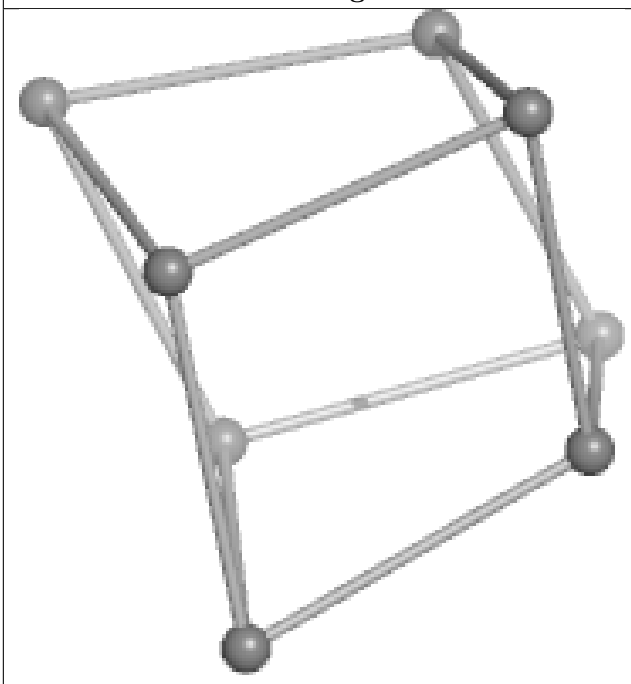
Ligand SF4 B 405



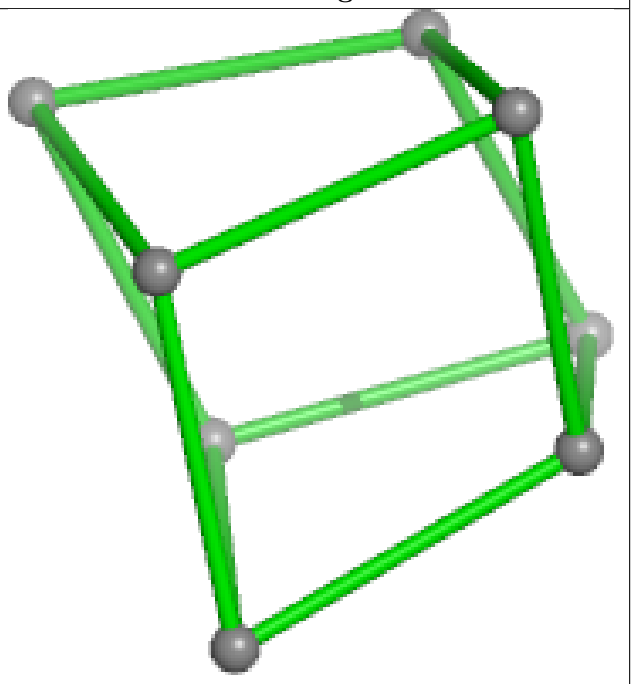
Bond lengths



Bond angles

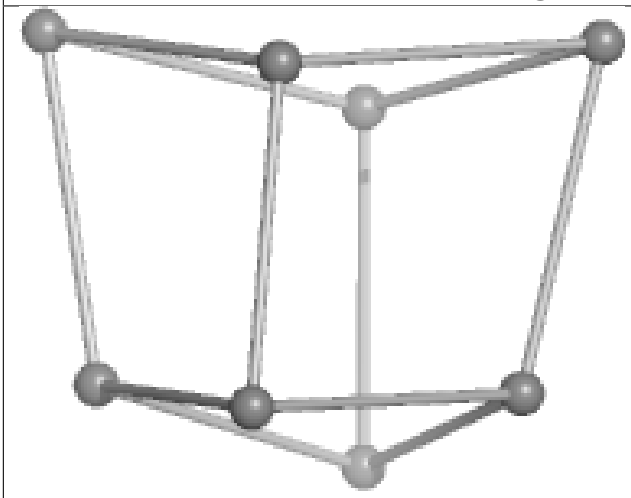


Torsions

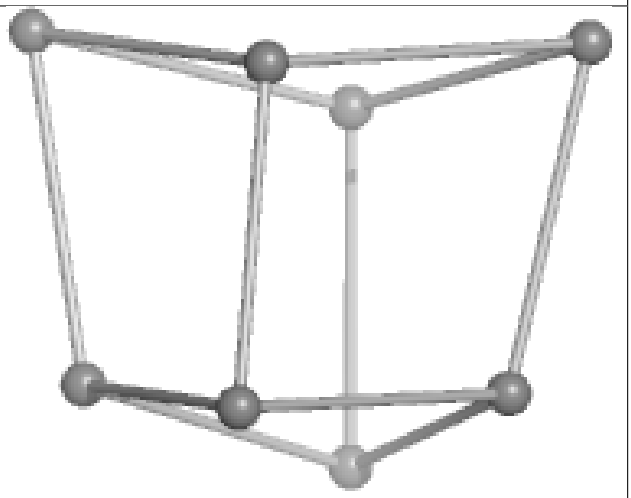


Rings

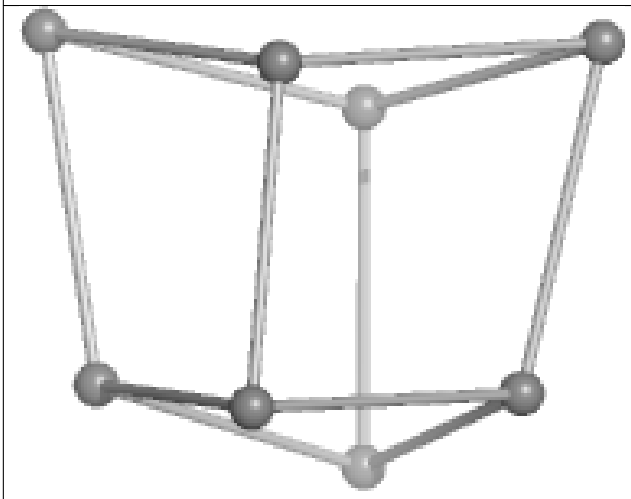
Ligand SF4 B 408



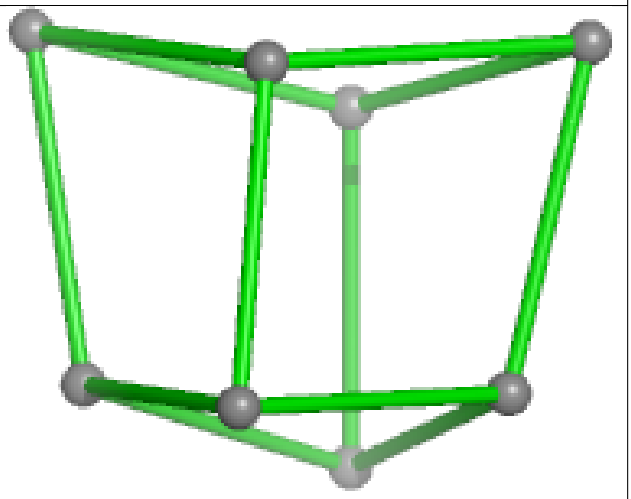
Bond lengths



Bond angles

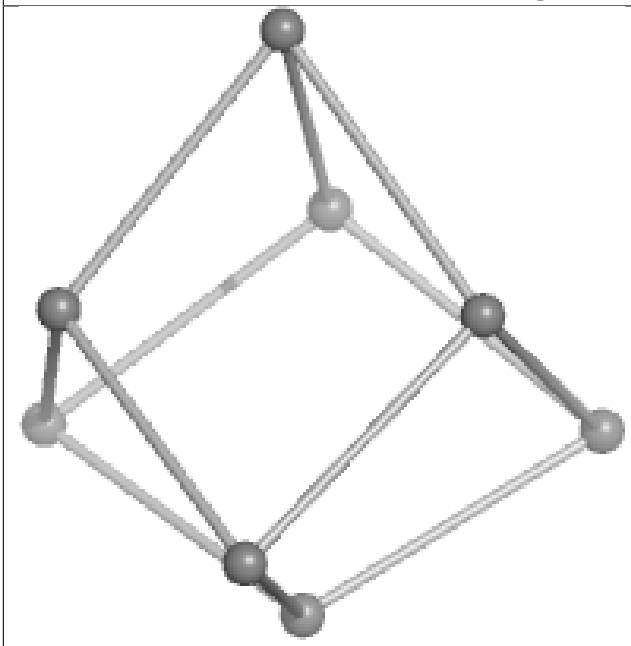


Torsions

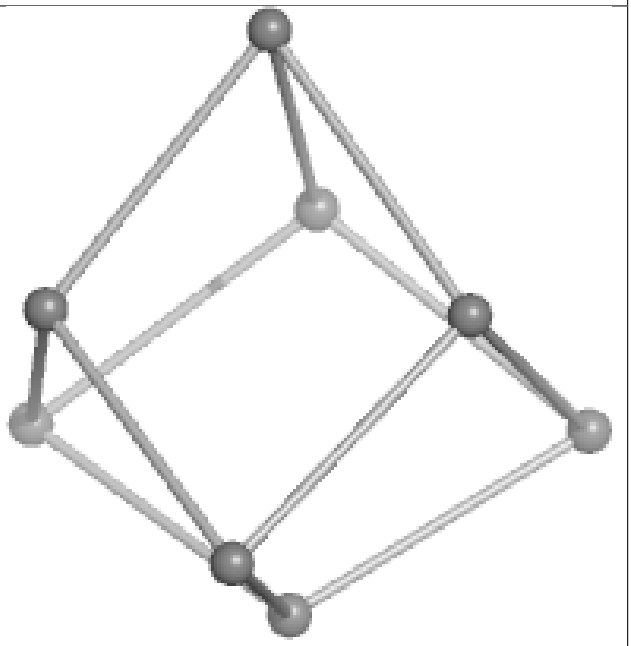


Rings

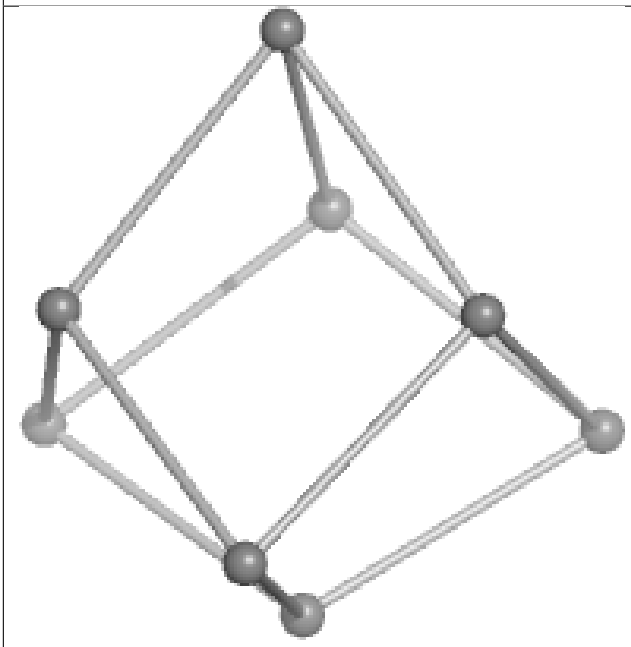
Ligand SF4 B 406



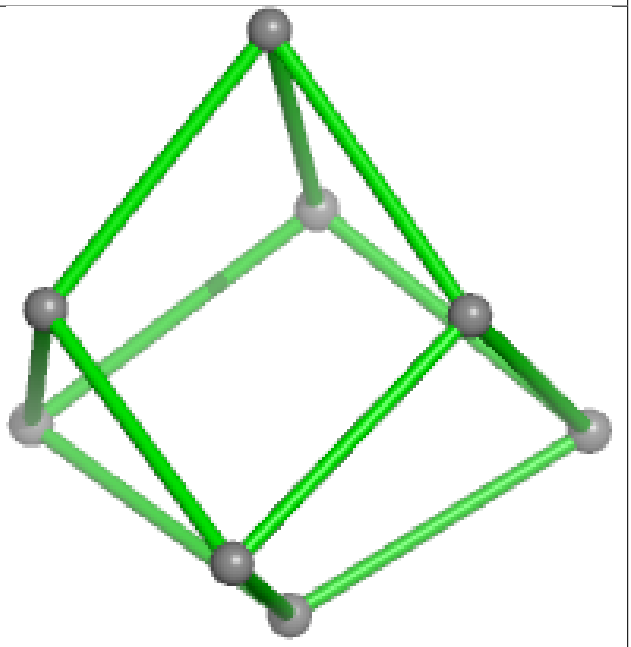
Bond lengths



Bond angles

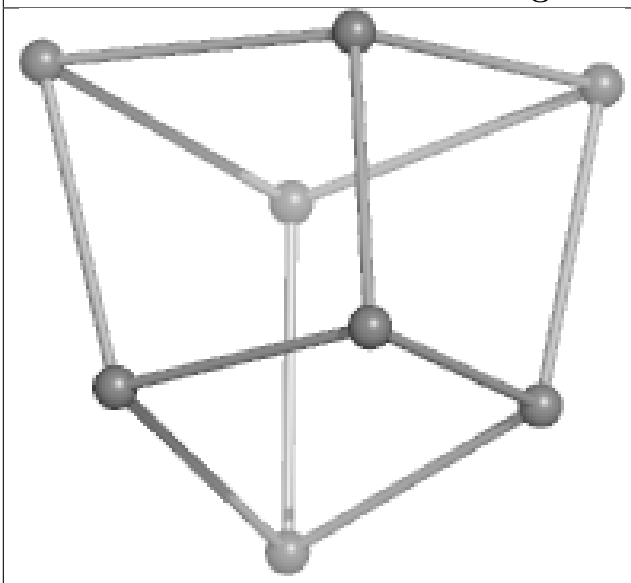


Torsions

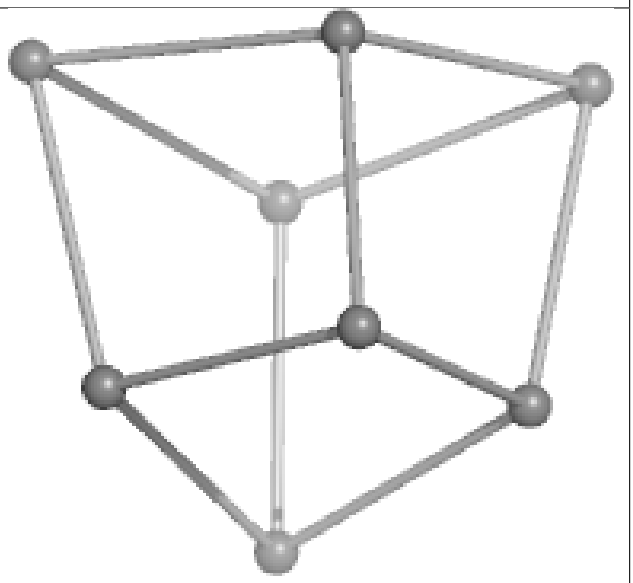


Rings

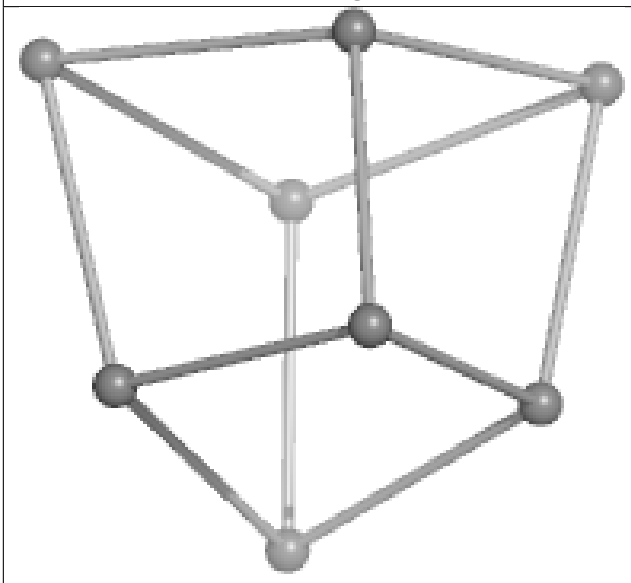
Ligand SF4 B 401



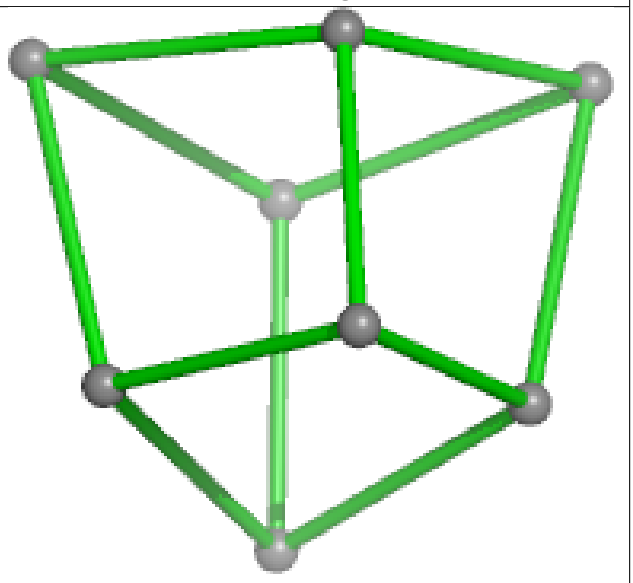
Bond lengths



Bond angles

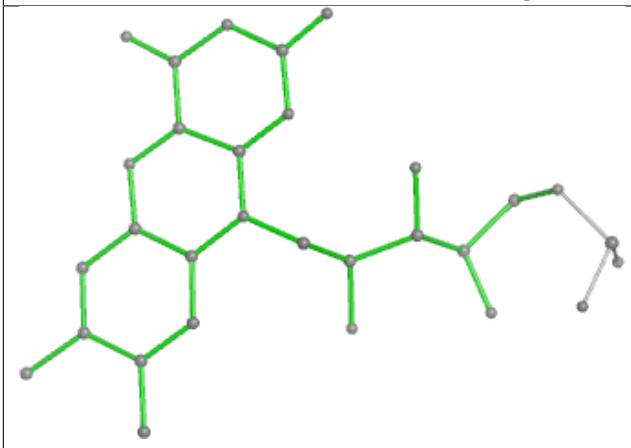


Torsions

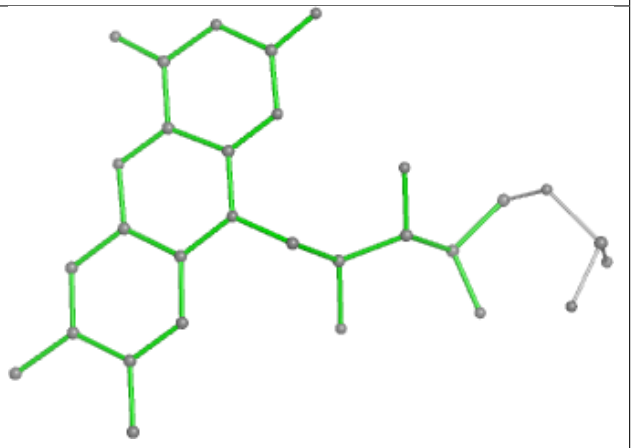


Rings

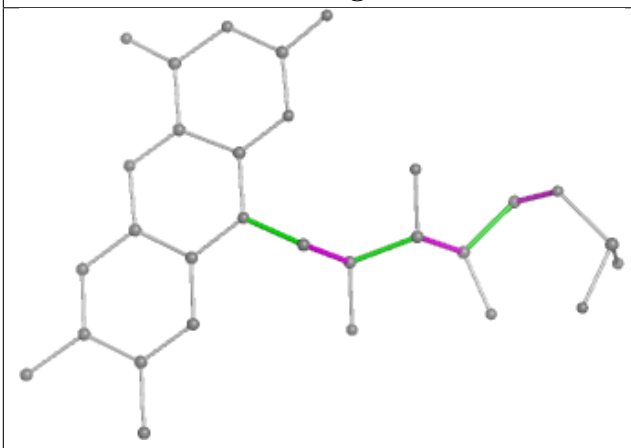
Ligand FMN D 402



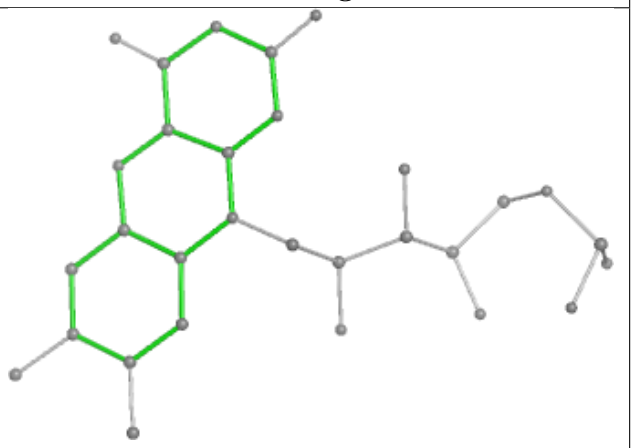
Bond lengths



Bond angles

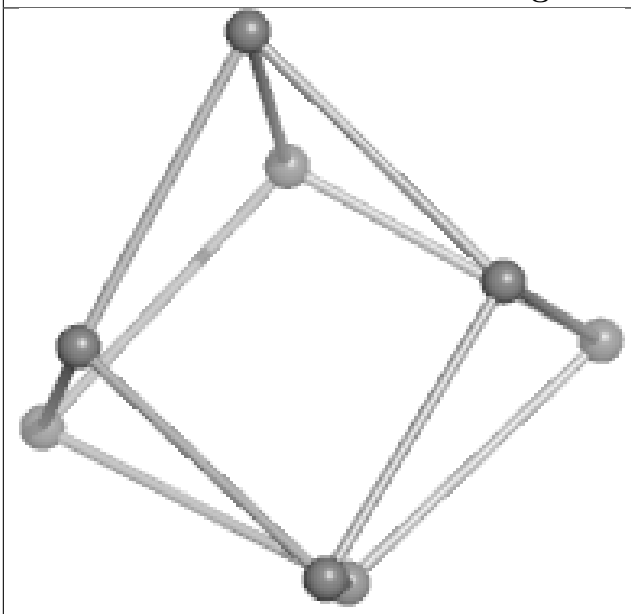


Torsions

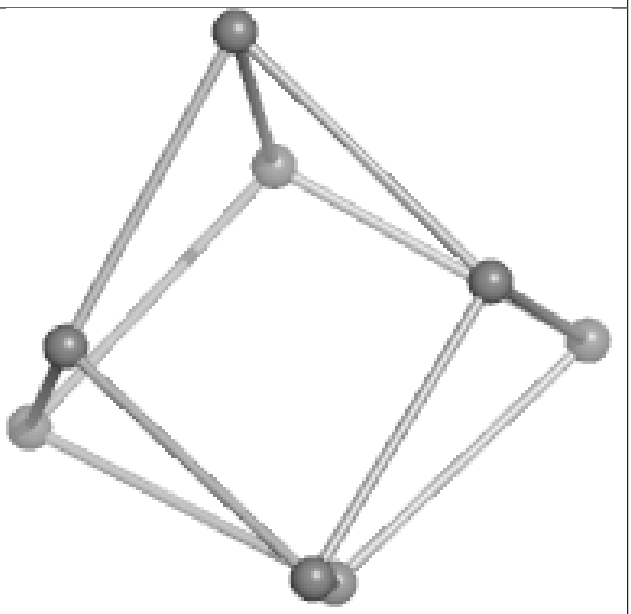


Rings

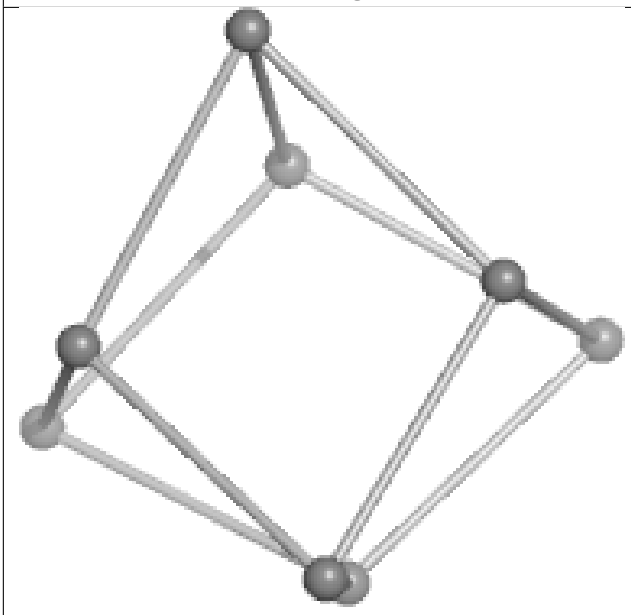
Ligand SF4 B 404



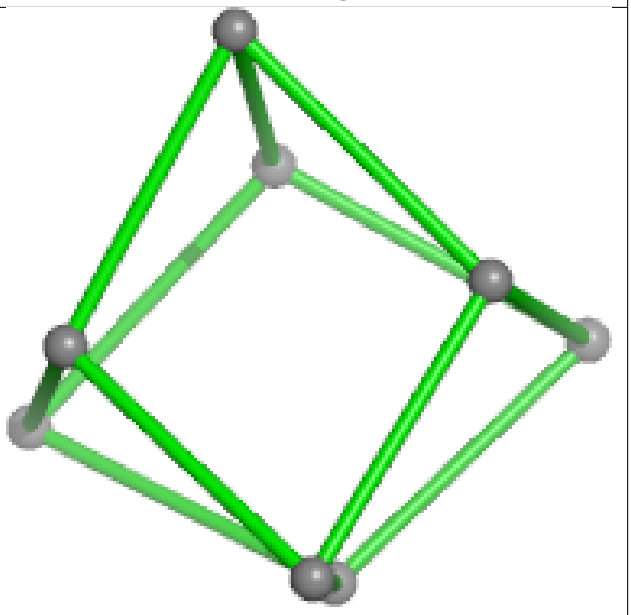
Bond lengths



Bond angles

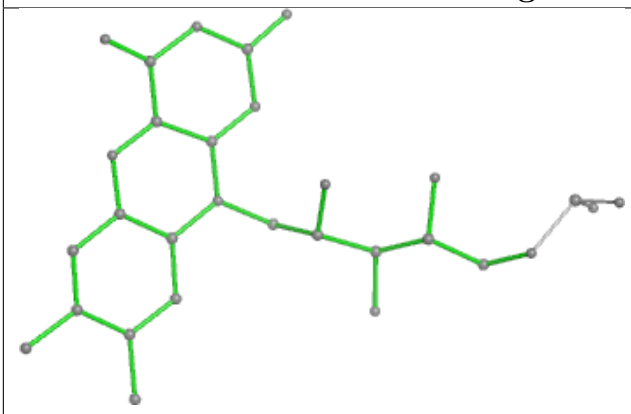


Torsions

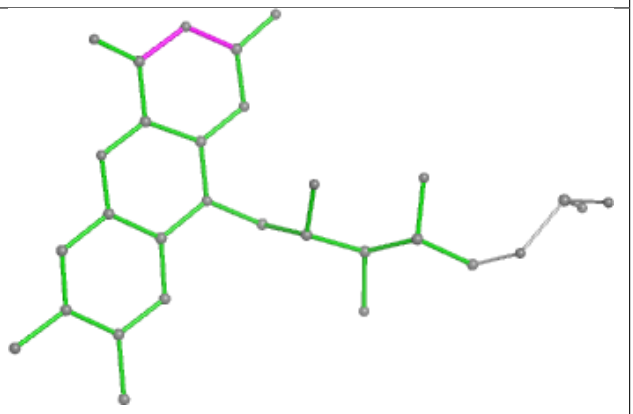


Rings

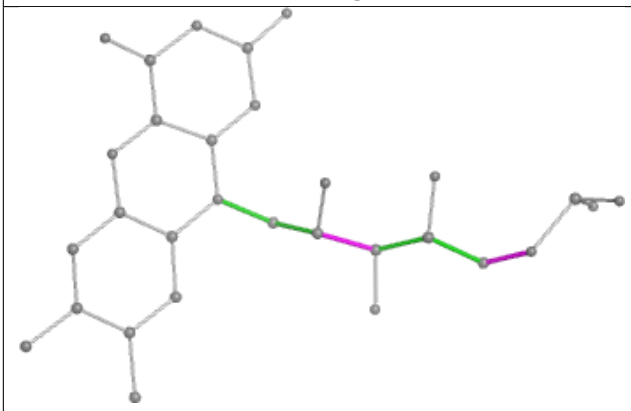
Ligand FMN G 301



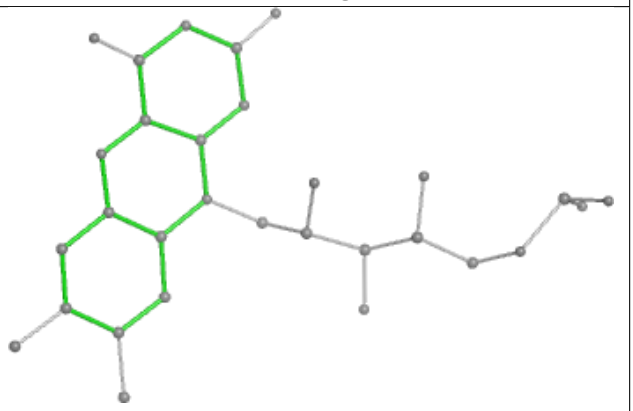
Bond lengths



Bond angles

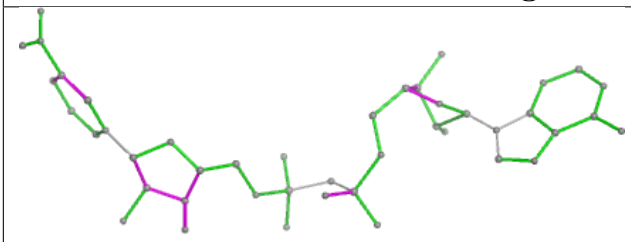


Torsions

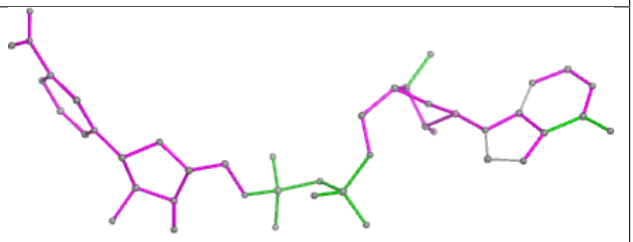


Rings

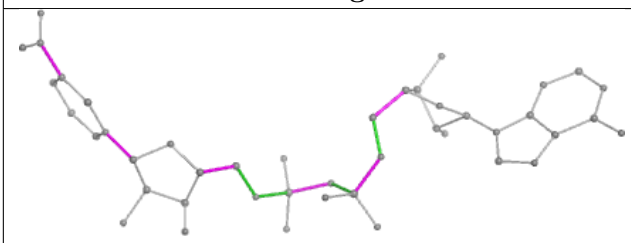
Ligand NAD C 502



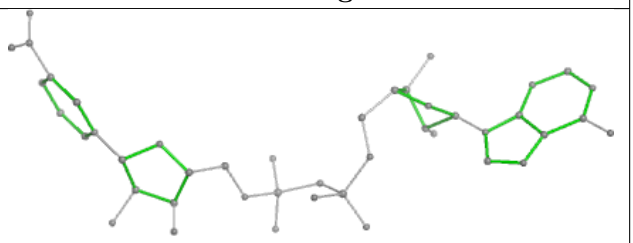
Bond lengths



Bond angles

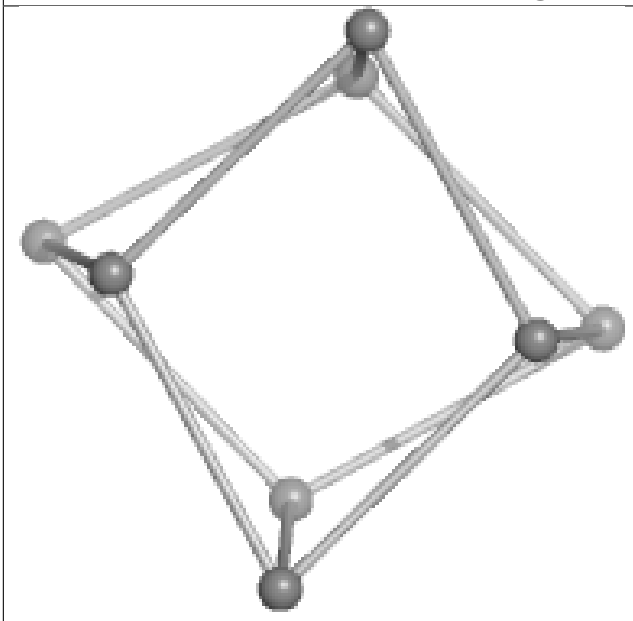


Torsions

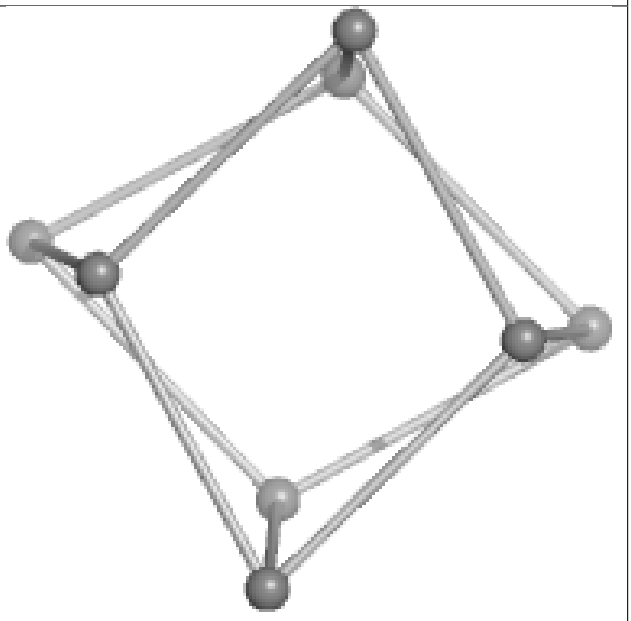


Rings

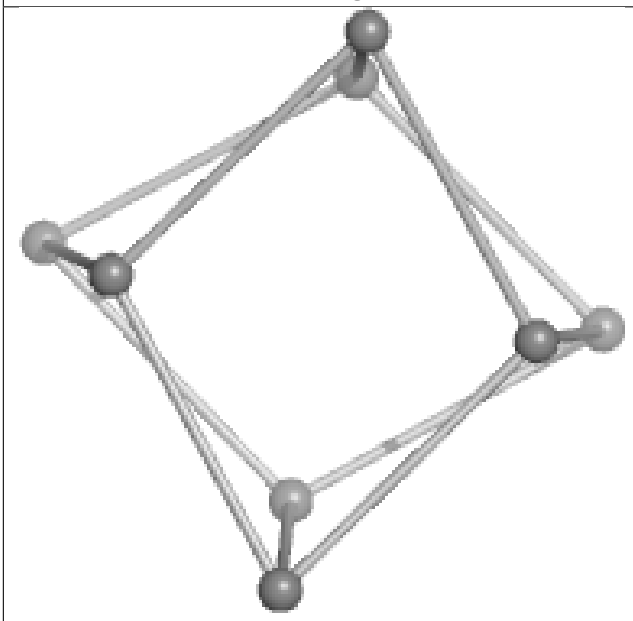
Ligand SF4 B 403



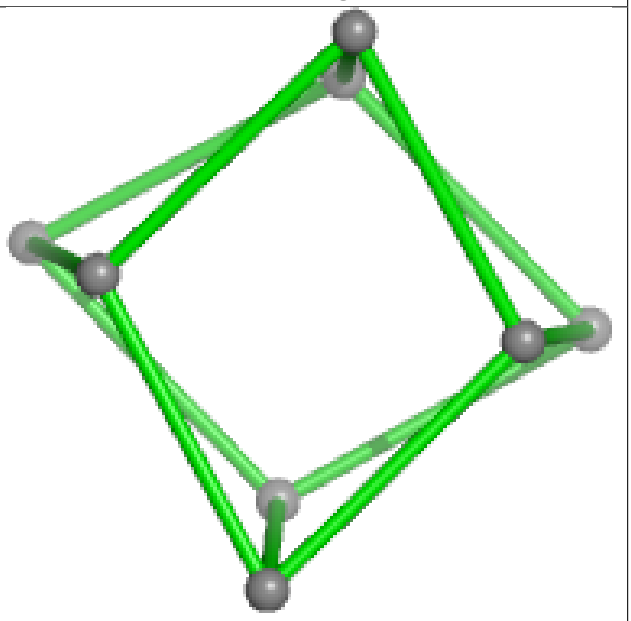
Bond lengths



Bond angles

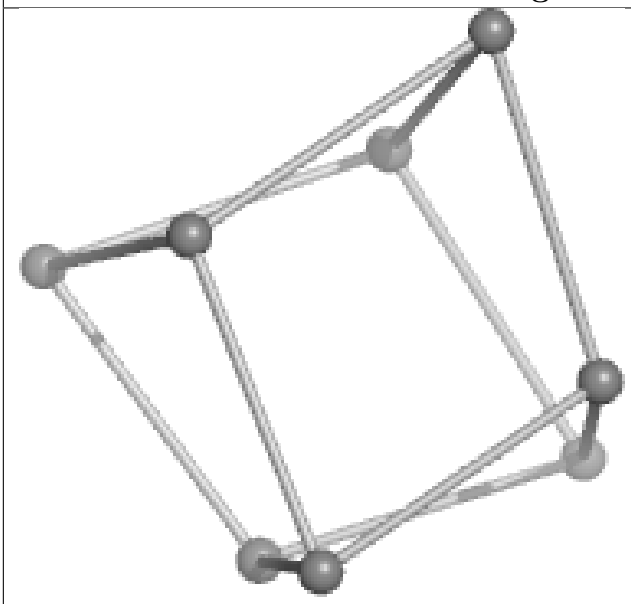


Torsions

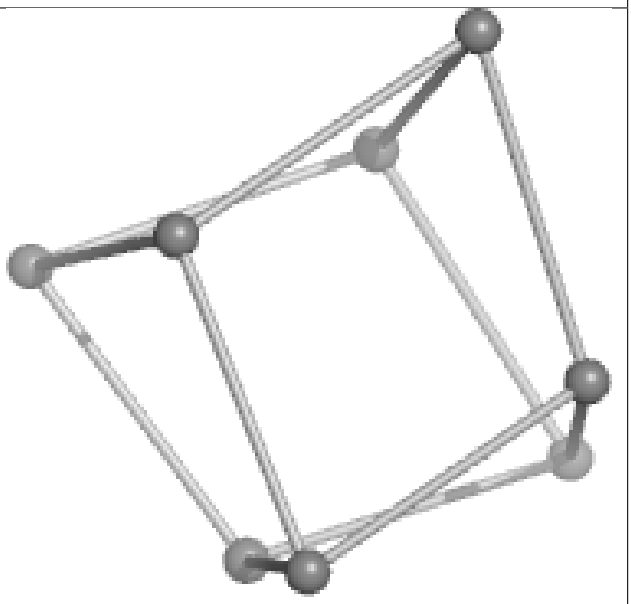


Rings

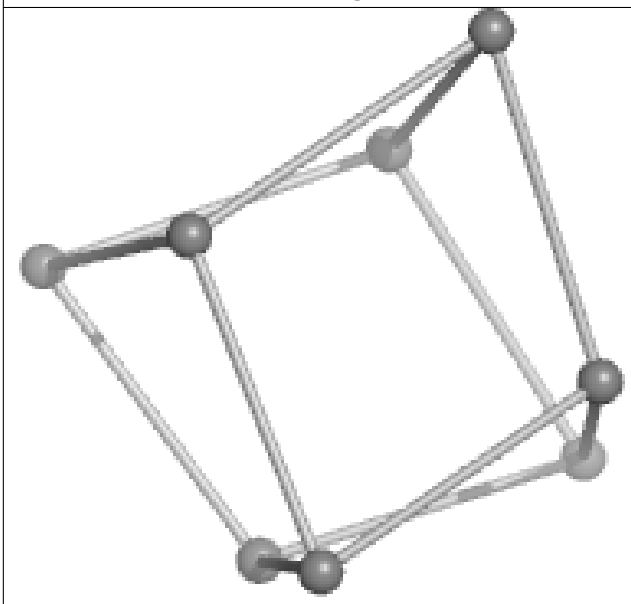
Ligand SF4 B 407



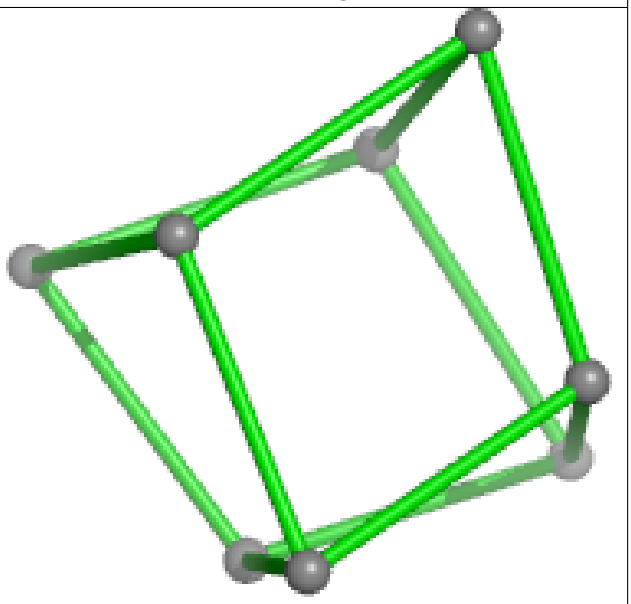
Bond lengths



Bond angles

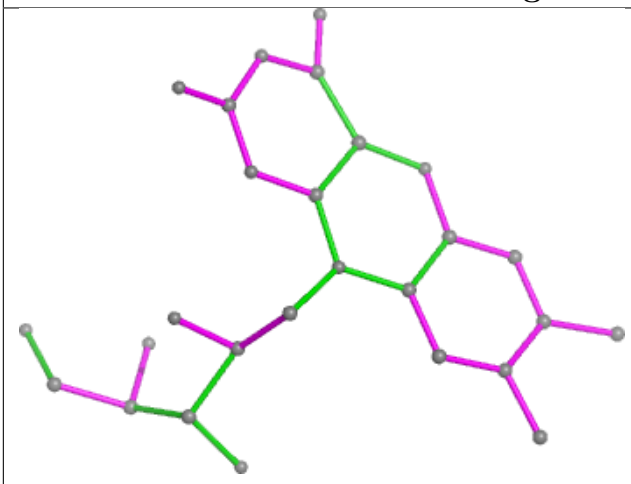


Torsions

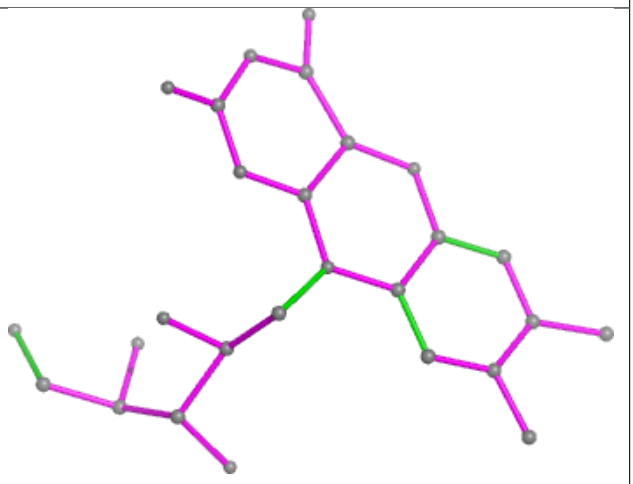


Rings

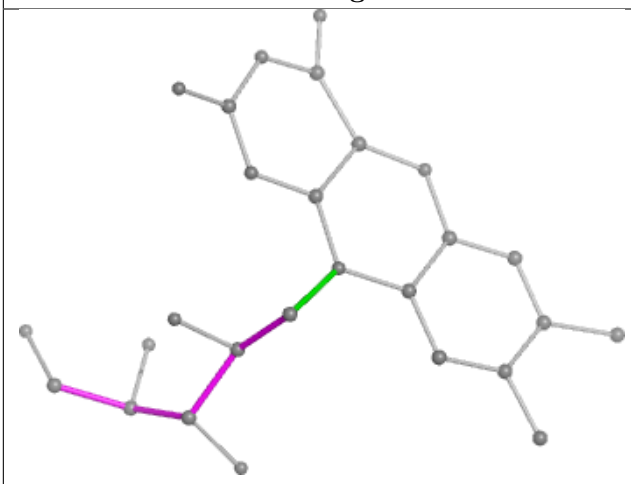
Ligand RBF D 401



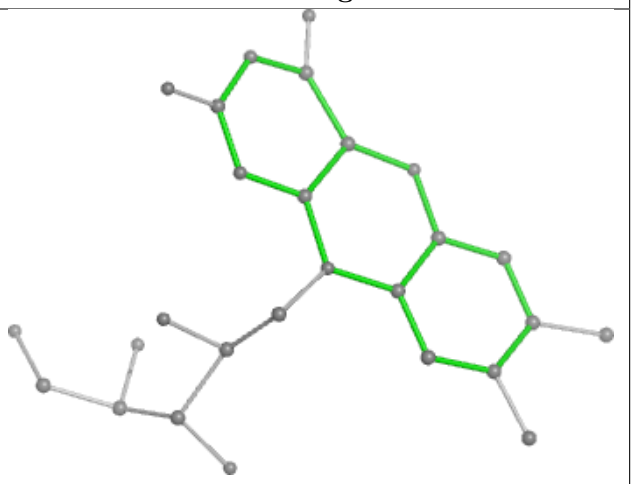
Bond lengths



Bond angles

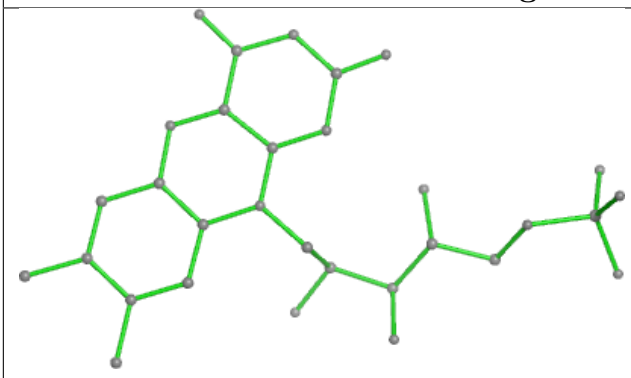


Torsions

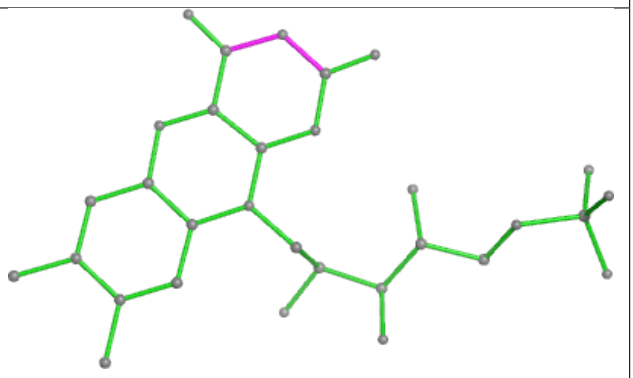


Rings

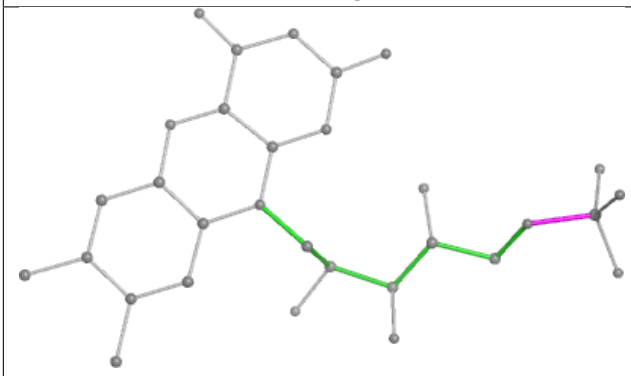
Ligand FMN C 501



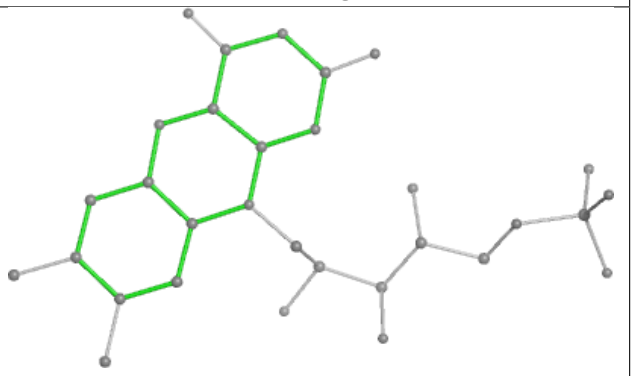
Bond lengths



Bond angles

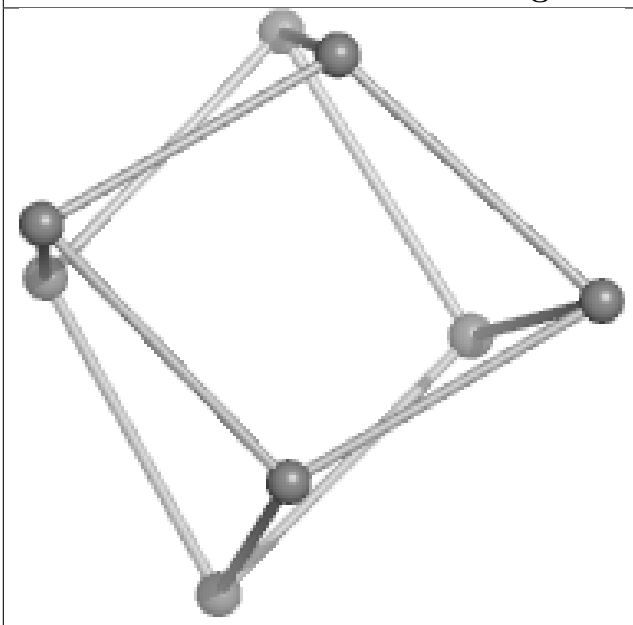


Torsions

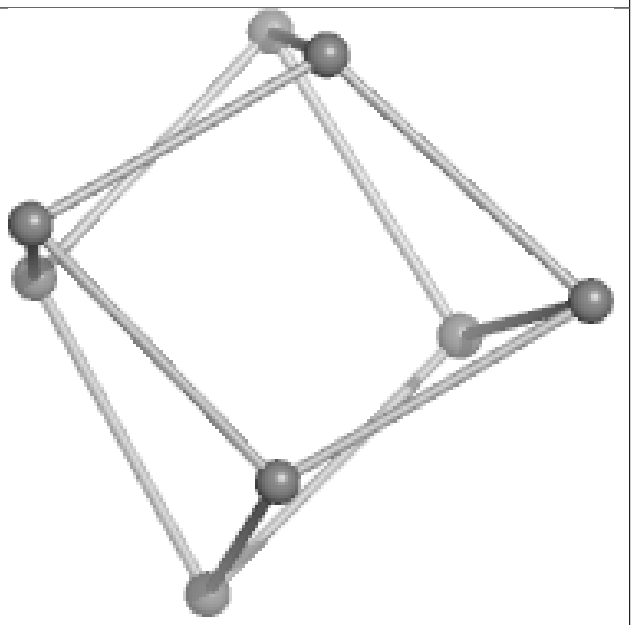


Rings

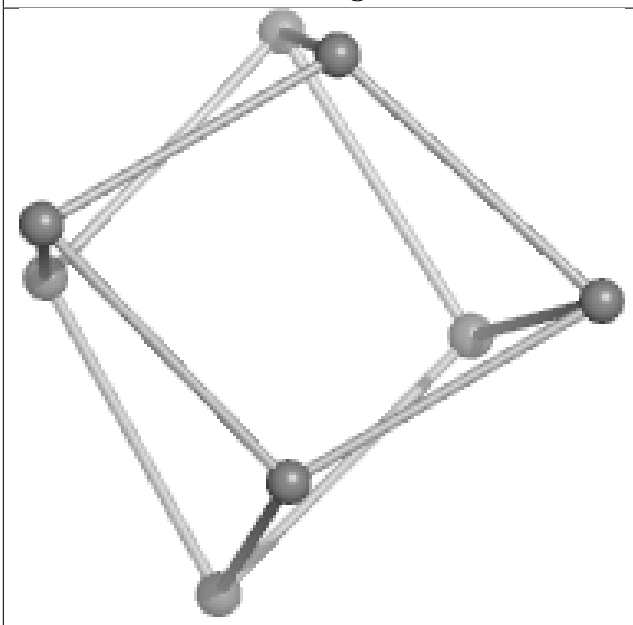
Ligand SF4 C 504



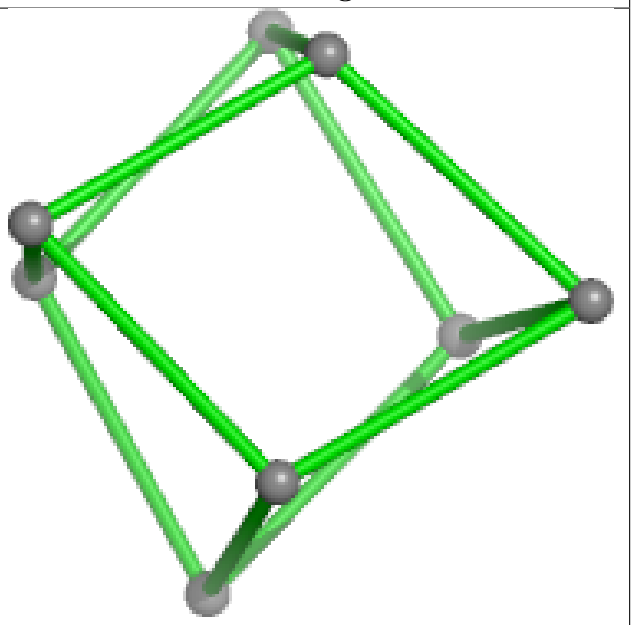
Bond lengths



Bond angles

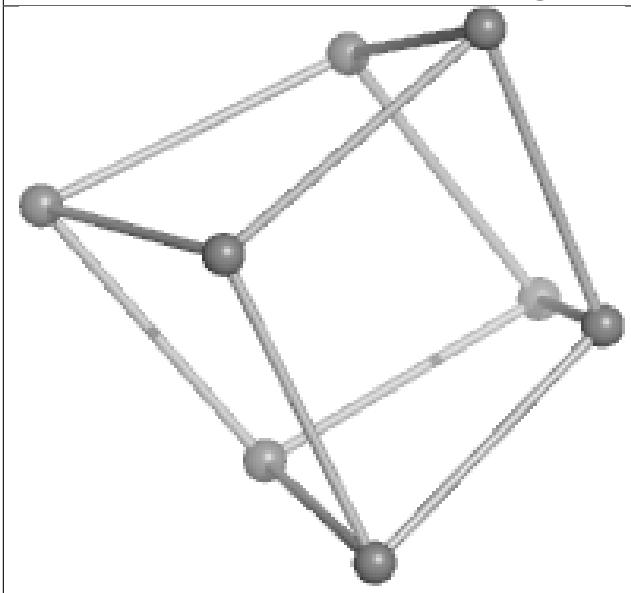


Torsions

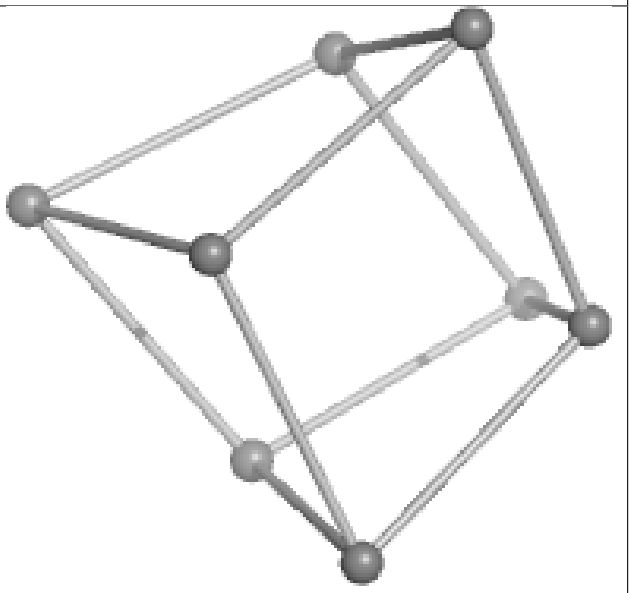


Rings

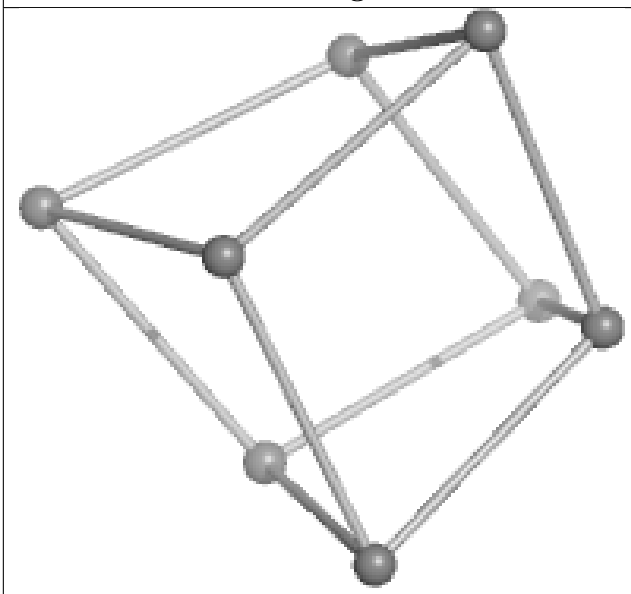
Ligand SF4 C 503



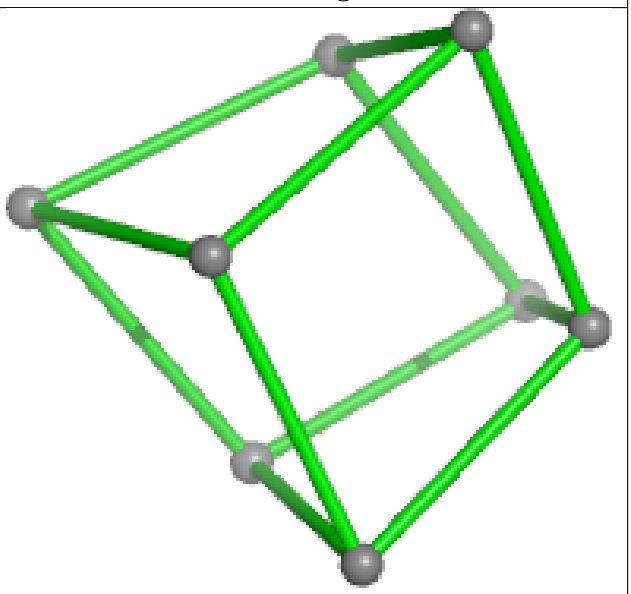
Bond lengths



Bond angles

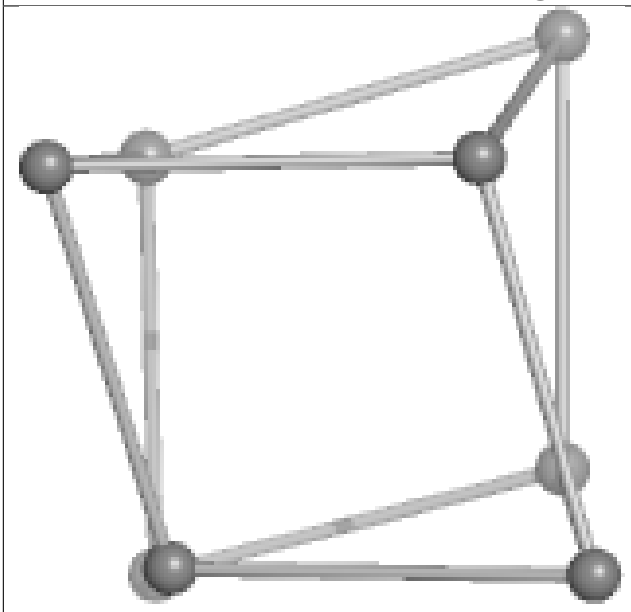


Torsions

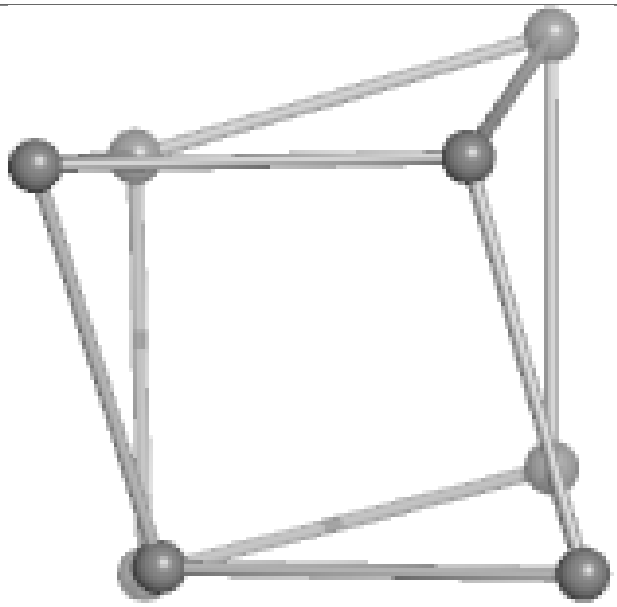


Rings

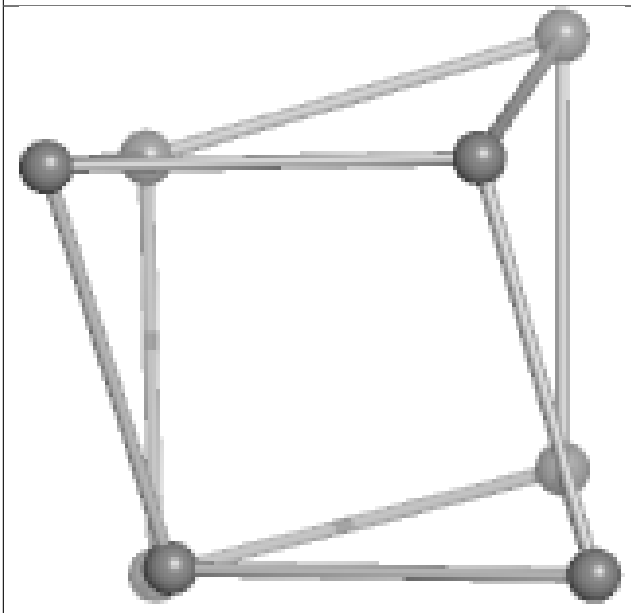
Ligand SF4 B 402



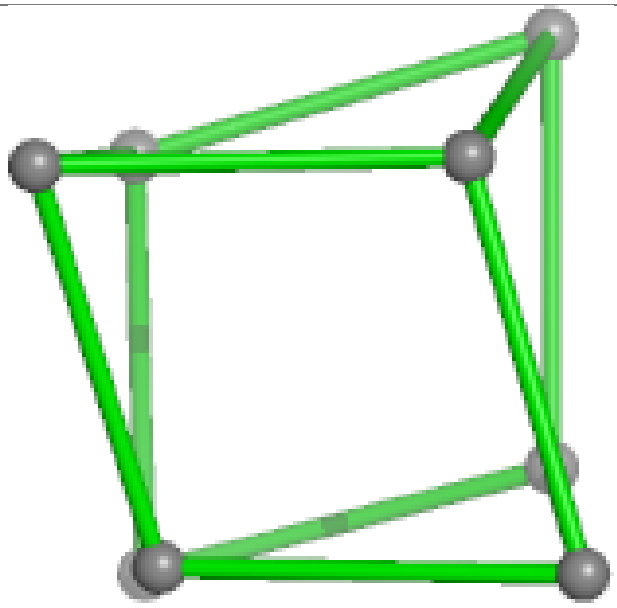
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.