



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 09:45 pm GMT

PDB ID : 9HEM / pdb_00009hem
Title : Crystal structure of the oxidized respiratory complex I subunit NuoEF from Aquifex aeolicus, mutation V136M(NuoE), bound to NAD⁺
Authors : Wohlwend, D.; Friedrich, T.
Deposited on : 2024-11-14
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

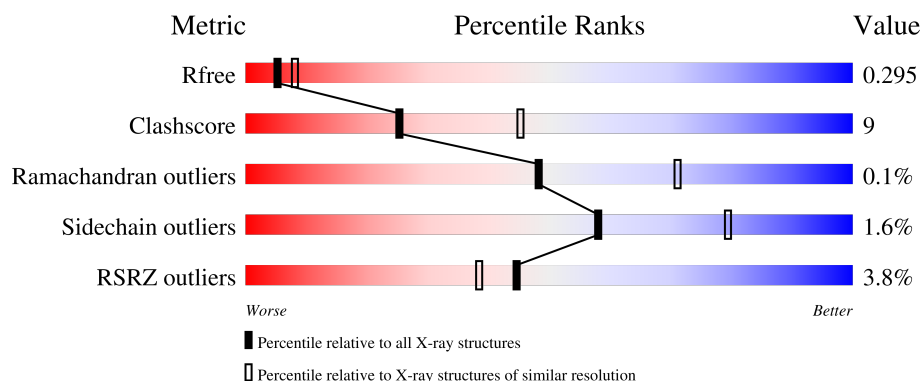
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	160	<div> <div>10%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	C	160	<div> <div>6%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
2	B	434	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>.</div> </div>
2	D	434	<div> <div>2%</div> <div>77%</div> <div>18%</div> <div>.</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9414 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
1	A	155	Total	C	N	O	S	0	0	0
			1260	816	203	231	10			
1	C	156	Total	C	N	O	S	0	0	0
			1263	817	202	234	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	MET	VAL	engineered mutation	UNP O66842
C	136	MET	VAL	engineered mutation	UNP O66842

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3273	2105	543	612	13			
2	D	416	Total	C	N	O	S	0	0	0
			3269	2102	542	612	13			

There are 16 discrepancies between the modelled and reference sequences:

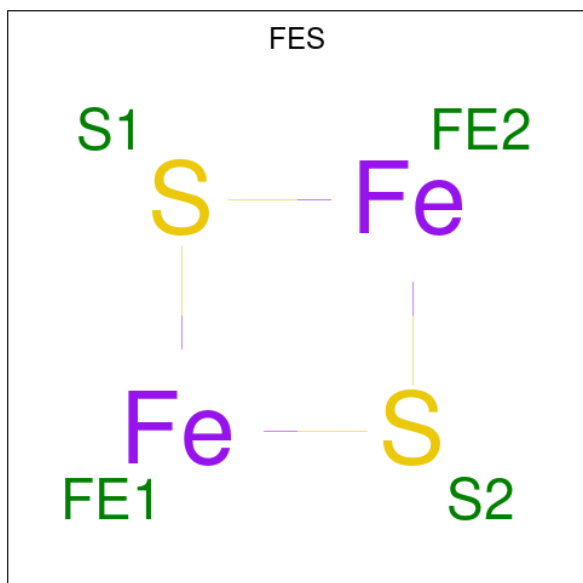
Chain	Residue	Modelled	Actual	Comment	Reference
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	3	Total	Cl	0	0
			3	3		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

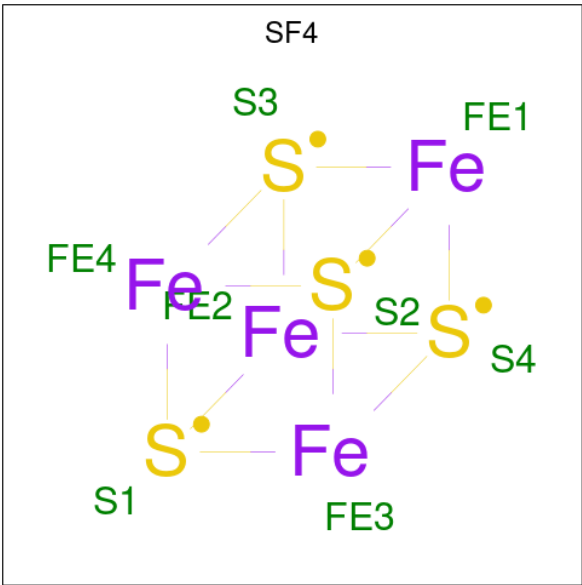


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

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

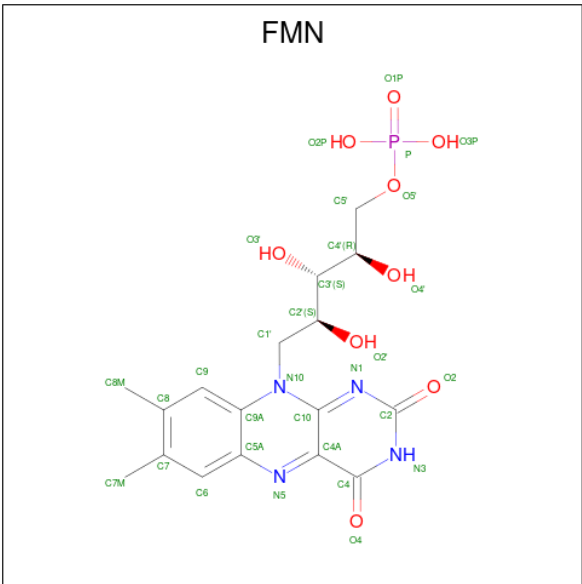
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



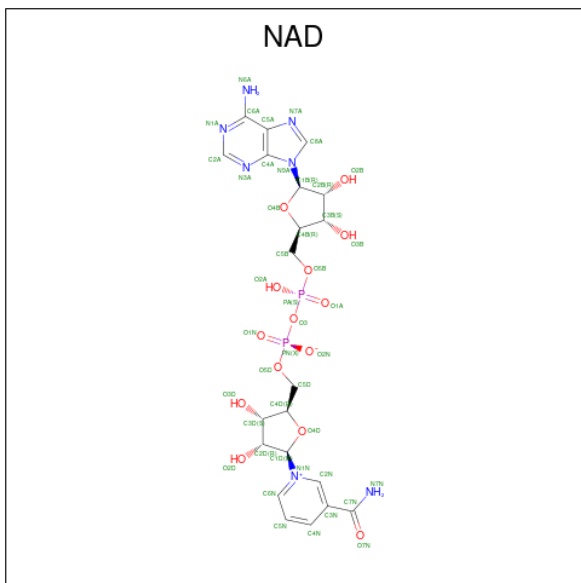
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 9 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 34	C 14	N 5	O 13	P 2	0	0
9	D	1	Total 32	C 13	N 5	O 12	P 2	0	0

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

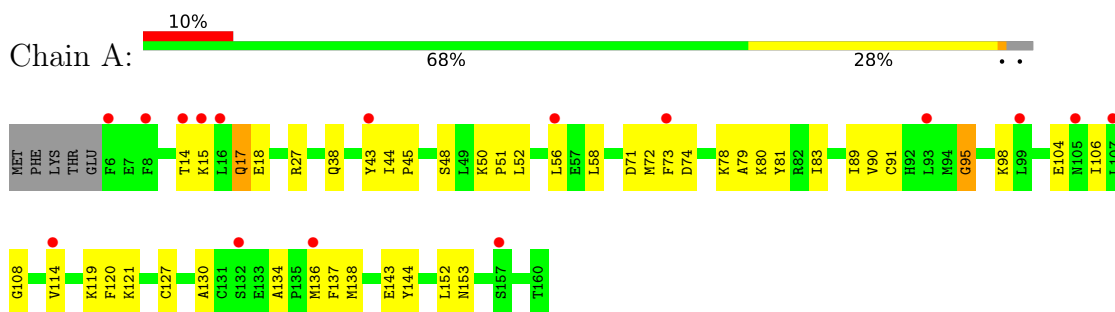
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	19	Total	O	0	0
			19	19		
11	B	51	Total	O	0	0
			51	51		
11	C	32	Total	O	0	0
			32	32		
11	D	51	Total	O	0	0
			51	51		

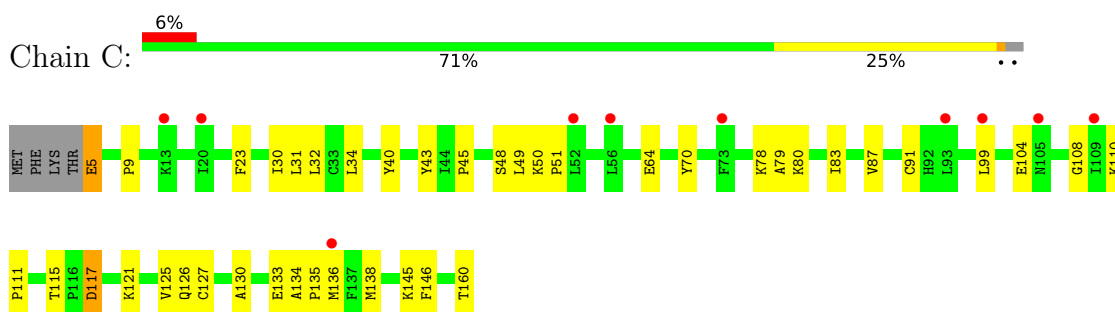
3 Residue-property plots [i](#)

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.

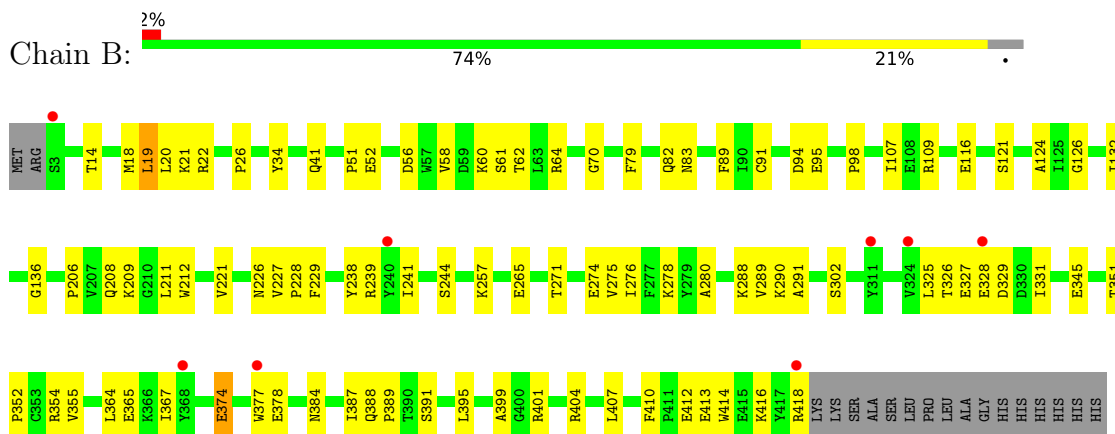
- Molecule 1: NADH-quinone oxidoreductase subunit E



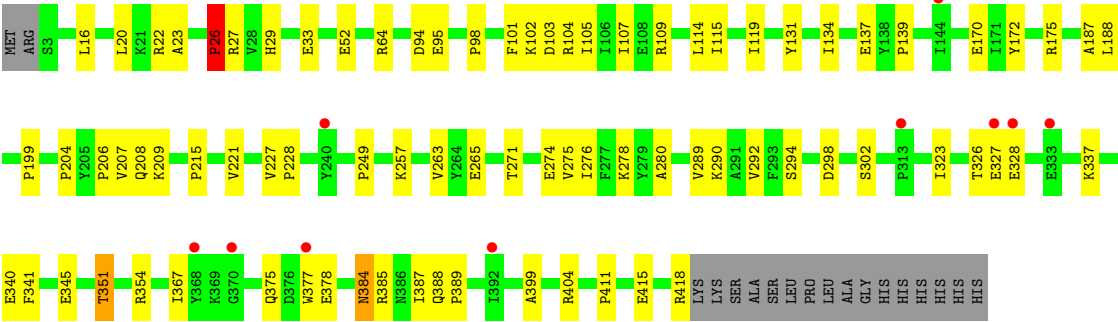
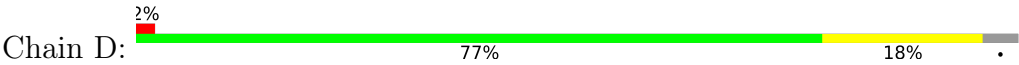
- Molecule 1: NADH-quinone oxidoreductase subunit E



- Molecule 2: NADH-quinone oxidoreductase subunit F



- Molecule 2: NADH-quinone oxidoreductase subunit F



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.72Å 63.37Å 123.43Å 90.00° 107.26° 90.00°	Depositor
Resolution (Å)	46.20 – 2.60 46.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.20-2.60) 99.3 (46.20-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.246 , 0.290 0.252 , 0.295	Depositor DCC
R_{free} test set	2154 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 21.62 % 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 6.7563e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, SF4, SO4, FMN, CL, GOL, NA, 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	0.50	0/1289	1.04	2/1740 (0.1%)
1	C	0.48	0/1292	0.97	0/1746
2	B	0.49	0/3354	0.96	0/4539
2	D	0.50	0/3350	0.95	1/4535 (0.0%)
All	All	0.49	0/9285	0.97	3/12560 (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
2	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLN	N-CA-CB	-10.38	94.76	110.33
2	D	26	PRO	N-CA-CB	-5.22	98.36	102.28
1	A	74	ASP	CA-CB-CG	5.06	117.66	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	64	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	1260	0	1263	30	0
1	C	1263	0	1251	28	0
2	B	3273	0	3244	58	0
2	D	3269	0	3233	57	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	1	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
6	A	1	0	0	0	0
7	B	8	0	0	1	0
7	D	8	0	0	0	0
8	B	31	0	19	2	0
8	D	31	0	19	3	0
9	B	34	0	18	2	0
9	D	32	0	16	4	0
10	B	6	0	8	0	0
10	D	6	0	8	0	0
11	A	19	0	0	2	0
11	B	51	0	0	2	0
11	C	32	0	0	0	0
11	D	51	0	0	3	0
All	All	9414	0	9079	174	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 9.

All (174) 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:C:135:PRO:HG2	1:C:146:PHE:HB3	1.68	0.76
2:B:288:LYS:N	2:B:327:GLU:OE1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:LYS:HE3	2:B:327:GLU:HA	1.73	0.70
1:A:114:VAL:HG22	1:A:121:LYS:HG3	1.73	0.70
1:A:138:MET:HG2	1:A:143:GLU:HG3	1.76	0.67
2:B:326:THR:N	2:B:329:ASP:OD2	2.27	0.67
2:B:58:VAL:O	2:B:61:SER:OG	2.13	0.67
2:B:21:LYS:HE3	2:B:22:ARG:HH12	1.59	0.66
8:D:501:FMN:H9	9:D:502:NAD:H52N	1.78	0.66
2:B:79:PHE:O	2:B:82:GLN:HG2	1.96	0.65
2:D:377:TRP:HE3	2:D:418:ARG:HH11	1.46	0.62
2:B:351:THR:OG1	2:B:354:ARG:NH2	2.32	0.62
1:C:43:TYR:HB3	1:C:78:LYS:HA	1.81	0.62
2:B:64:ARG:NH2	2:B:70:GLY:O	2.33	0.61
2:B:384:ASN:HD22	2:B:404:ARG:HH21	1.49	0.60
1:C:43:TYR:O	1:C:45:PRO:HD3	2.01	0.60
1:A:72:MET:HE1	2:B:136:GLY:HA3	1.82	0.60
2:D:257:LYS:NZ	2:D:328:GLU:OE1	2.34	0.60
1:A:15:LYS:O	1:A:18:GLU:HB3	2.02	0.59
2:D:22:ARG:O	2:D:29:HIS:CE1	2.58	0.57
2:B:52:GLU:OE1	2:B:52:GLU:N	2.29	0.57
1:A:104:GLU:O	1:A:108:GLY:HA2	2.05	0.57
1:A:43:TYR:HB3	1:A:78:LYS:HA	1.85	0.57
2:B:391:SER:HB2	7:B:501:SF4:S1	2.45	0.57
2:D:137:GLU:C	2:D:139:PRO:HD3	2.30	0.56
1:A:106:ILE:HD12	1:A:152:LEU:HD23	1.86	0.56
2:B:412:GLU:H	2:B:412:GLU:CD	2.13	0.56
2:B:331:ILE:HG22	2:B:413:GLU:CD	2.31	0.56
2:D:16:LEU:HD12	2:D:265:GLU:HG2	1.88	0.55
2:D:341:PHE:O	2:D:345:GLU:HG2	2.06	0.55
1:C:133:GLU:O	1:C:145:LYS:HG3	2.07	0.55
2:D:105:ILE:HD11	2:D:263:VAL:HG11	1.89	0.55
2:B:21:LYS:HE3	2:B:22:ARG:NH1	2.22	0.54
2:B:351:THR:O	2:B:355:VAL:HG22	2.07	0.54
2:D:351:THR:OG1	2:D:354:ARG:NH2	2.40	0.54
2:D:377:TRP:CE3	2:D:418:ARG:NH1	2.76	0.54
2:B:388:GLN:N	2:B:389:PRO:CD	2.71	0.54
2:D:115:ILE:O	2:D:119:ILE:HG13	2.08	0.53
2:D:345:GLU:HA	2:D:345:GLU:OE1	2.07	0.53
2:D:274:GLU:O	2:D:278:LYS:HB3	2.09	0.53
1:C:115:THR:OG1	1:C:117:ASP:OD1	2.21	0.52
8:B:502:FMN:H9	9:B:503:NAD:H52N	1.91	0.52
2:B:345:GLU:HA	2:B:345:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:LYS:HA	2:D:340:GLU:OE1	2.08	0.52
1:A:91:CYS:HA	1:A:134:ALA:HB1	1.91	0.52
2:D:377:TRP:HE3	2:D:418:ARG:NH1	2.08	0.52
2:B:289:VAL:O	2:B:302:SER:HB3	2.10	0.51
2:B:352:PRO:HG2	2:B:389:PRO:O	2.10	0.51
1:A:38:GLN:OE1	1:A:44:ILE:HG12	2.10	0.51
1:A:43:TYR:O	1:A:45:PRO:HD3	2.10	0.51
1:A:50:LYS:HB3	1:A:51:PRO:HD3	1.92	0.51
2:B:407:LEU:HD23	2:B:414:TRP:CD2	2.46	0.51
2:D:341:PHE:CE1	2:D:345:GLU:HG3	2.45	0.51
1:A:52:LEU:O	1:A:56:LEU:HG	2.11	0.51
2:D:276:ILE:O	2:D:280:ALA:HB3	2.11	0.51
2:D:294:SER:HB3	2:D:298:ASP:HB2	1.93	0.51
2:D:134:ILE:O	2:D:175:ARG:HA	2.11	0.50
2:B:19:LEU:HD12	2:B:229:PHE:CE2	2.47	0.50
2:D:102:LYS:NZ	2:D:103:ASP:OD1	2.41	0.50
1:A:72:MET:CE	2:B:136:GLY:HA3	2.42	0.50
2:D:384:ASN:ND2	2:D:404:ARG:HH21	2.09	0.50
2:B:367:ILE:HG23	2:B:377:TRP:CZ2	2.47	0.49
2:B:374:GLU:H	2:B:374:GLU:CD	2.20	0.49
1:C:45:PRO:O	1:C:48:SER:OG	2.22	0.49
2:D:27:ARG:NH1	2:D:33:GLU:OE2	2.42	0.49
2:D:388:GLN:N	2:D:389:PRO:CD	2.75	0.49
2:B:34:TYR:OH	2:B:116:GLU:OE1	2.21	0.49
2:D:52:GLU:H	2:D:52:GLU:CD	2.20	0.48
1:A:72:MET:HG2	11:A:309:HOH:O	2.13	0.48
1:C:79:ALA:CB	1:C:121:LYS:HB3	2.44	0.48
2:D:375:GLN:NE2	2:D:375:GLN:HA	2.29	0.48
1:C:49:LEU:HD23	1:C:64:GLU:HG3	1.96	0.48
8:D:501:FMN:C9	9:D:502:NAD:H52N	2.42	0.47
2:D:207:VAL:O	2:D:215:PRO:HB3	2.15	0.47
2:B:83:ASN:OD1	2:B:208:GLN:HA	2.15	0.47
2:D:137:GLU:O	2:D:139:PRO:HD3	2.15	0.47
2:D:170:GLU:HA	11:D:607:HOH:O	2.15	0.47
2:D:411:PRO:O	2:D:415:GLU:HG2	2.15	0.47
2:D:290:LYS:HE3	2:D:327:GLU:HA	1.95	0.47
2:B:14:THR:CB	2:B:265:GLU:HB3	2.45	0.47
2:D:114:LEU:HD13	2:D:221:VAL:HG13	1.97	0.47
1:C:127:CYS:SG	2:D:98:PRO:HA	2.55	0.46
2:D:384:ASN:HD21	2:D:404:ARG:HE	1.63	0.46
2:B:211:LEU:HG	2:B:212:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HG2	1:C:40:TYR:CE2	2.51	0.46
1:C:130:ALA:HB3	1:C:136:MET:HG3	1.99	0.45
2:B:206:PRO:HA	2:B:209:LYS:O	2.16	0.45
2:B:226:ASN:OD1	2:B:238:TYR:OH	2.23	0.45
1:C:49:LEU:HD23	1:C:64:GLU:CG	2.46	0.45
2:D:271:THR:O	2:D:275:VAL:HG23	2.17	0.45
2:B:387:ILE:HG21	2:B:399:ALA:HB3	1.99	0.45
1:A:114:VAL:HG22	1:A:121:LYS:CG	2.44	0.45
2:B:56:ASP:OD2	2:B:60:LYS:HE2	2.17	0.45
1:C:104:GLU:O	1:C:108:GLY:HA2	2.17	0.45
2:B:257:LYS:HB2	2:B:326:THR:HG23	1.99	0.44
2:D:206:PRO:HA	2:D:209:LYS:O	2.17	0.44
1:A:127:CYS:SG	2:B:98:PRO:HA	2.57	0.44
2:D:94:ASP:O	2:D:95:GLU:C	2.59	0.44
1:A:83:ILE:HD11	1:A:120:PHE:CD1	2.52	0.44
2:D:207:VAL:HG21	9:D:502:NAD:H2A	1.98	0.44
2:B:351:THR:HB	2:B:352:PRO:HD3	2.00	0.44
2:D:101:PHE:O	2:D:104:ARG:HG2	2.18	0.44
2:D:227:VAL:HB	2:D:228:PRO:HD3	1.99	0.44
2:D:289:VAL:O	2:D:302:SER:HB3	2.18	0.44
2:B:89:PHE:CE1	2:B:121:SER:HB3	2.52	0.44
2:B:107:ILE:HD11	2:B:221:VAL:HG21	1.99	0.44
2:B:276:ILE:HA	2:B:280:ALA:HB3	1.99	0.44
1:C:80:LYS:NZ	1:C:160:THR:O	2.47	0.44
2:D:107:ILE:HD11	2:D:221:VAL:HG21	2.00	0.43
2:D:20:LEU:HA	2:D:23:ALA:HB3	1.99	0.43
1:A:48:SER:C	1:A:51:PRO:HD2	2.43	0.43
2:D:257:LYS:HG3	2:D:326:THR:OG1	2.18	0.43
2:D:387:ILE:HG21	2:D:399:ALA:HB3	2.01	0.43
2:D:26:PRO:HA	2:D:109:ARG:NE	2.33	0.43
1:A:71:ASP:HA	11:A:315:HOH:O	2.17	0.43
2:B:26:PRO:HA	2:B:109:ARG:NE	2.34	0.43
1:A:14:THR:O	1:A:17:GLN:HB3	2.18	0.43
2:B:327:GLU:H	2:B:327:GLU:HG2	1.71	0.43
1:A:136:MET:CE	1:A:143:GLU:HG2	2.49	0.43
1:C:48:SER:C	1:C:51:PRO:HD2	2.44	0.43
1:C:99:LEU:HD13	1:C:146:PHE:CD1	2.54	0.43
1:A:95:GLY:HA3	1:A:98:LYS:HE2	2.00	0.42
2:B:41:GLN:HB2	11:B:639:HOH:O	2.18	0.42
1:C:87:VAL:HG22	1:C:125:VAL:O	2.19	0.42
2:D:95:GLU:OE2	2:D:103:ASP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:VAL:HA	2:D:323:ILE:O	2.19	0.42
2:B:395:LEU:C	2:B:395:LEU:HD23	2.44	0.42
1:C:91:CYS:HA	1:C:134:ALA:HB1	2.01	0.42
1:C:83:ILE:HA	1:C:138:MET:O	2.19	0.42
2:B:20:LEU:HD12	2:B:265:GLU:HB2	2.01	0.42
2:D:131:TYR:HA	2:D:172:TYR:O	2.19	0.42
2:B:91:CYS:HB3	2:B:132:ILE:HG12	2.00	0.42
2:B:227:VAL:N	2:B:228:PRO:CD	2.82	0.42
1:C:110:LYS:HB3	1:C:111:PRO:HD2	2.02	0.42
2:D:290:LYS:CE	2:D:327:GLU:HA	2.50	0.42
1:C:49:LEU:CD2	1:C:64:GLU:HG2	2.50	0.42
2:D:188:LEU:C	2:D:188:LEU:HD23	2.45	0.42
1:C:5:GLU:HG2	1:C:5:GLU:O	2.19	0.42
2:B:126:GLY:HA2	11:B:633:HOH:O	2.20	0.42
2:B:377:TRP:CH2	2:B:418:ARG:HG3	2.55	0.41
1:A:79:ALA:HB2	1:A:121:LYS:HB2	2.00	0.41
2:B:51:PRO:HB3	2:B:124:ALA:O	2.21	0.41
1:C:23:PHE:HE2	1:C:32:LEU:HD12	1.85	0.41
2:D:367:ILE:HG23	2:D:377:TRP:CZ2	2.55	0.41
2:D:16:LEU:CD1	2:D:249:PRO:HA	2.50	0.41
2:D:16:LEU:HD13	2:D:249:PRO:HB3	2.01	0.41
1:A:137:PHE:CZ	1:A:144:TYR:HB2	2.55	0.41
2:B:94:ASP:O	2:B:95:GLU:C	2.63	0.41
2:B:291:ALA:HB2	2:B:410:PHE:CZ	2.55	0.41
2:D:204:PRO:HB2	2:D:208:GLN:OE1	2.20	0.41
2:D:385:ARG:NH2	11:D:604:HOH:O	2.52	0.41
8:B:502:FMN:C9	9:B:503:NAD:H52N	2.50	0.41
1:A:89:ILE:HG23	1:A:90:VAL:H	1.86	0.41
2:B:271:THR:O	2:B:275:VAL:HG23	2.21	0.41
1:C:126:GLN:O	1:C:127:CYS:C	2.64	0.41
1:A:130:ALA:HB3	1:A:136:MET:HG3	2.02	0.41
2:B:62:THR:HG21	2:B:239:ARG:HH11	1.86	0.41
2:D:187:ALA:HB2	2:D:199:PRO:HG3	2.03	0.41
1:A:80:LYS:HD3	1:A:81:TYR:CE2	2.56	0.41
2:B:18:MET:SD	2:B:241:ILE:HD13	2.61	0.41
2:B:274:GLU:O	2:B:278:LYS:HB3	2.20	0.41
2:B:325:LEU:N	2:B:325:LEU:HD12	2.35	0.41
2:B:227:VAL:HB	2:B:228:PRO:HD3	2.02	0.41
1:C:30:ILE:O	1:C:34:LEU:HG	2.21	0.41
2:D:16:LEU:CD1	2:D:249:PRO:HB3	2.50	0.41
1:A:27:ARG:HB2	1:A:58:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LYS:N	1:C:51:PRO:CD	2.84	0.40
1:A:81:TYR:N	1:A:119:LYS:O	2.50	0.40
2:D:337:LYS:NZ	11:D:603:HOH:O	2.49	0.40
1:C:31:LEU:HD21	1:C:70:TYR:CE2	2.57	0.40
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.37	0.40
1:C:104:GLU:O	1:C:108:GLY:N	2.51	0.40
8:D:501:FMN:H1'1	9:D:502:NAD:H52N	2.04	0.40
1:A:44:ILE:HG13	1:A:73:PHE:HB3	2.03	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	153/160 (96%)	149 (97%)	3 (2%)	1 (1%)	19	38
1	C	154/160 (96%)	149 (97%)	5 (3%)	0	100	100
2	B	414/434 (95%)	402 (97%)	12 (3%)	0	100	100
2	D	414/434 (95%)	405 (98%)	9 (2%)	0	100	100
All	All	1135/1188 (96%)	1105 (97%)	29 (3%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLY

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	141/146 (97%)	140 (99%)	1 (1%)	81	93
1	C	140/146 (96%)	138 (99%)	2 (1%)	62	82
2	B	342/357 (96%)	334 (98%)	8 (2%)	45	71
2	D	341/357 (96%)	337 (99%)	4 (1%)	67	85
All	All	964/1006 (96%)	949 (98%)	15 (2%)	58	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
2	B	19	LEU
2	B	244	SER
2	B	328	GLU
2	B	364	LEU
2	B	365	GLU
2	B	374	GLU
2	B	378	GLU
2	B	416	LYS
1	C	5	GLU
1	C	117	ASP
2	D	26	PRO
2	D	351	THR
2	D	378	GLU
2	D	384	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	151	GLN
2	B	286	ASN
2	B	349	GLN
2	B	360	GLN
2	B	375	GLN
2	B	384	ASN
1	C	126	GLN
2	D	29	HIS
2	D	41	GLN

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Mol	Chain	Res	Type
2	D	362	ASN
2	D	384	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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	$\# Z > 2$
8	FMN	D	501	-	33,33,33	0.48	0	48,50,50	0.40	0
9	NAD	D	502	-	29,34,48	0.61	0	31,51,73	0.73	1 (3%)
10	GOL	D	504	-	5,5,5	0.11	0	5,5,5	0.26	0
5	SO4	B	505	-	4,4,4	0.36	0	6,6,6	0.07	0
7	SF4	D	503	2	0,12,12	-	-	-	-	-
10	GOL	B	504	-	5,5,5	0.10	0	5,5,5	0.31	0
5	SO4	A	203	-	4,4,4	0.35	0	6,6,6	0.06	0
9	NAD	B	503	-	31,36,48	0.63	0	34,54,73	1.15	3 (8%)
3	FES	A	201	1	0,4,4	-	-	-	-	-
7	SF4	B	501	2	0,12,12	-	-	-	-	-
3	FES	C	201	1	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	204	-	4,4,4	0.35	0	6,6,6	0.05	0
5	SO4	B	506	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	C	205	-	4,4,4	0.34	0	6,6,6	0.07	0
8	FMN	B	502	-	33,33,33	0.42	0	48,50,50	0.43	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
8	FMN	D	501	-	-	5/18/18/18	0/3/3/3
9	NAD	D	502	-	-	0/20/40/62	0/3/3/5
10	GOL	D	504	-	-	0/4/4/4	-
7	SF4	D	503	2	-	-	0/6/5/5
10	GOL	B	504	-	-	2/4/4/4	-
9	NAD	B	503	-	-	3/24/44/62	0/3/3/5
3	FES	A	201	1	-	-	0/1/1/1
7	SF4	B	501	2	-	-	0/6/5/5
3	FES	C	201	1	-	-	0/1/1/1
8	FMN	B	502	-	-	4/18/18/18	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	NAD	C2D-C3D-C4D	-4.67	102.97	113.11
9	D	502	NAD	C5A-C6A-N6A	2.46	124.08	120.35
9	B	503	NAD	C5A-C6A-N6A	2.18	123.67	120.35
9	B	503	NAD	O4D-C4D-C3D	-2.18	105.25	109.72

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	501	FMN	C5'-O5'-P-O1P
8	D	501	FMN	C5'-O5'-P-O3P
10	B	504	GOL	C1-C2-C3-O3
10	B	504	GOL	O2-C2-C3-O3
8	B	502	FMN	C5'-O5'-P-O1P

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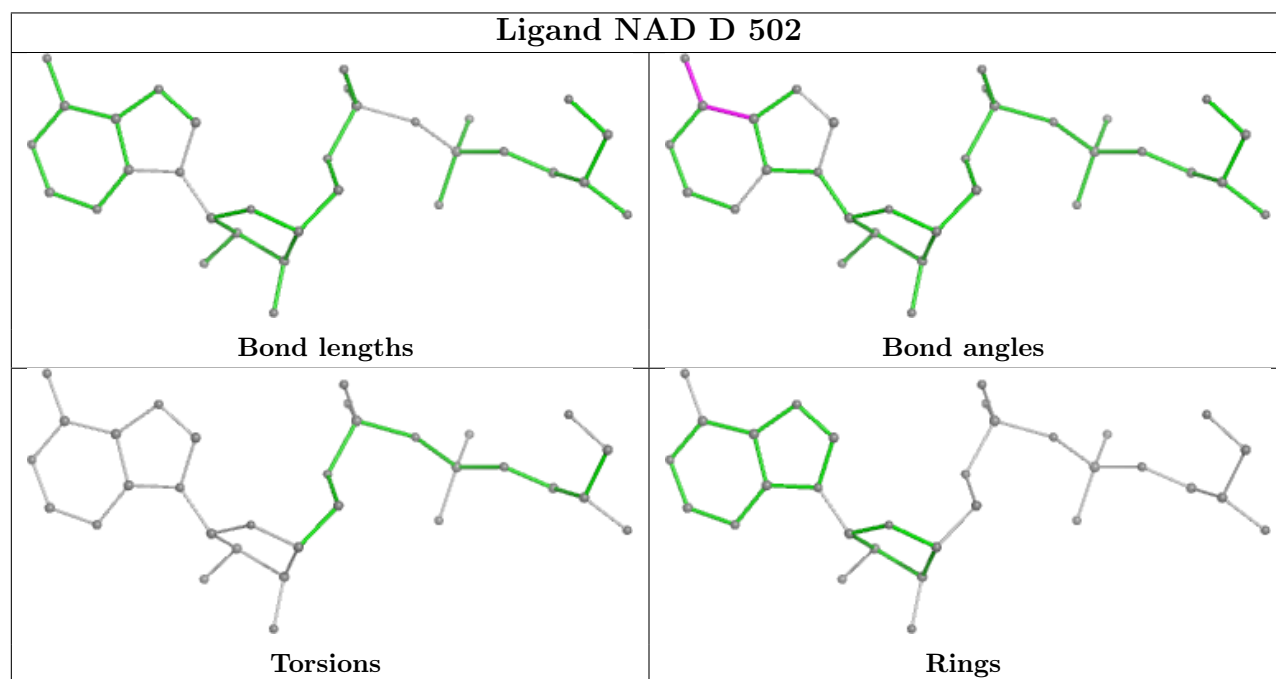
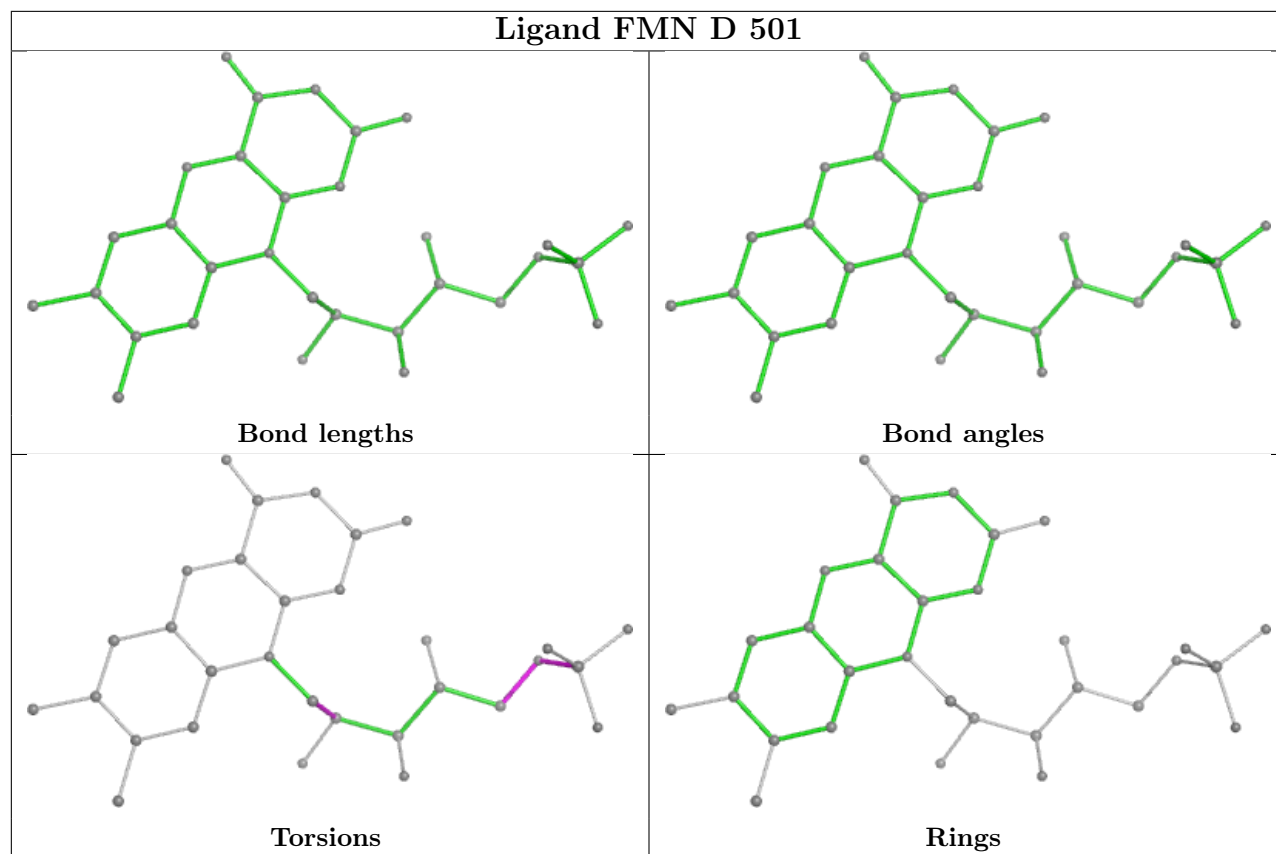
Mol	Chain	Res	Type	Atoms
9	B	503	NAD	C5B-O5B-PA-O3
8	D	501	FMN	N10-C1'-C2'-O2'
8	D	501	FMN	N10-C1'-C2'-C3'
8	B	502	FMN	C4'-C5'-O5'-P
8	D	501	FMN	C4'-C5'-O5'-P
8	B	502	FMN	C5'-O5'-P-O3P
9	B	503	NAD	O3D-C3D-C4D-O4D
9	B	503	NAD	C5B-O5B-PA-O1A
8	B	502	FMN	N10-C1'-C2'-O2'

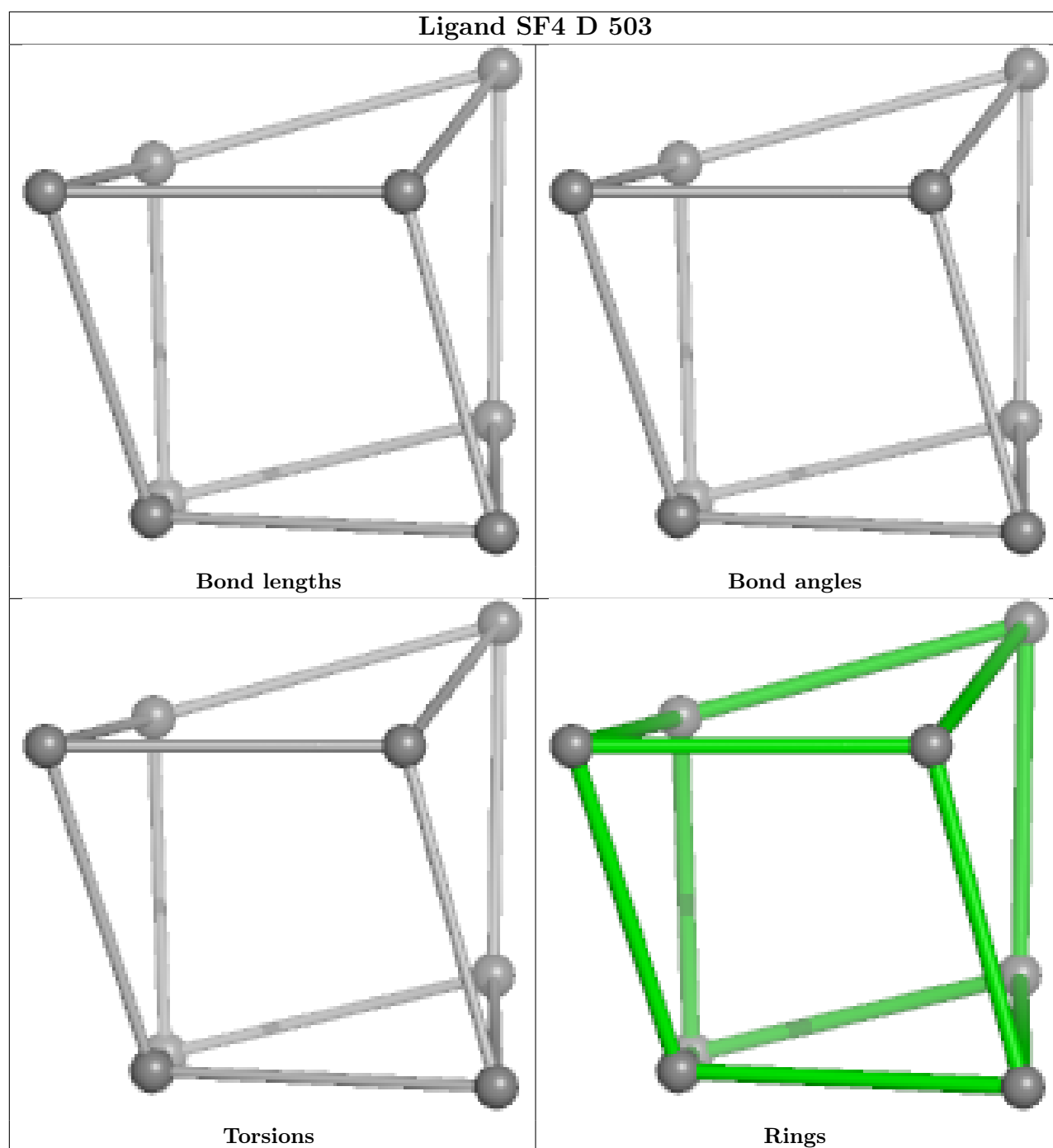
There are no ring outliers.

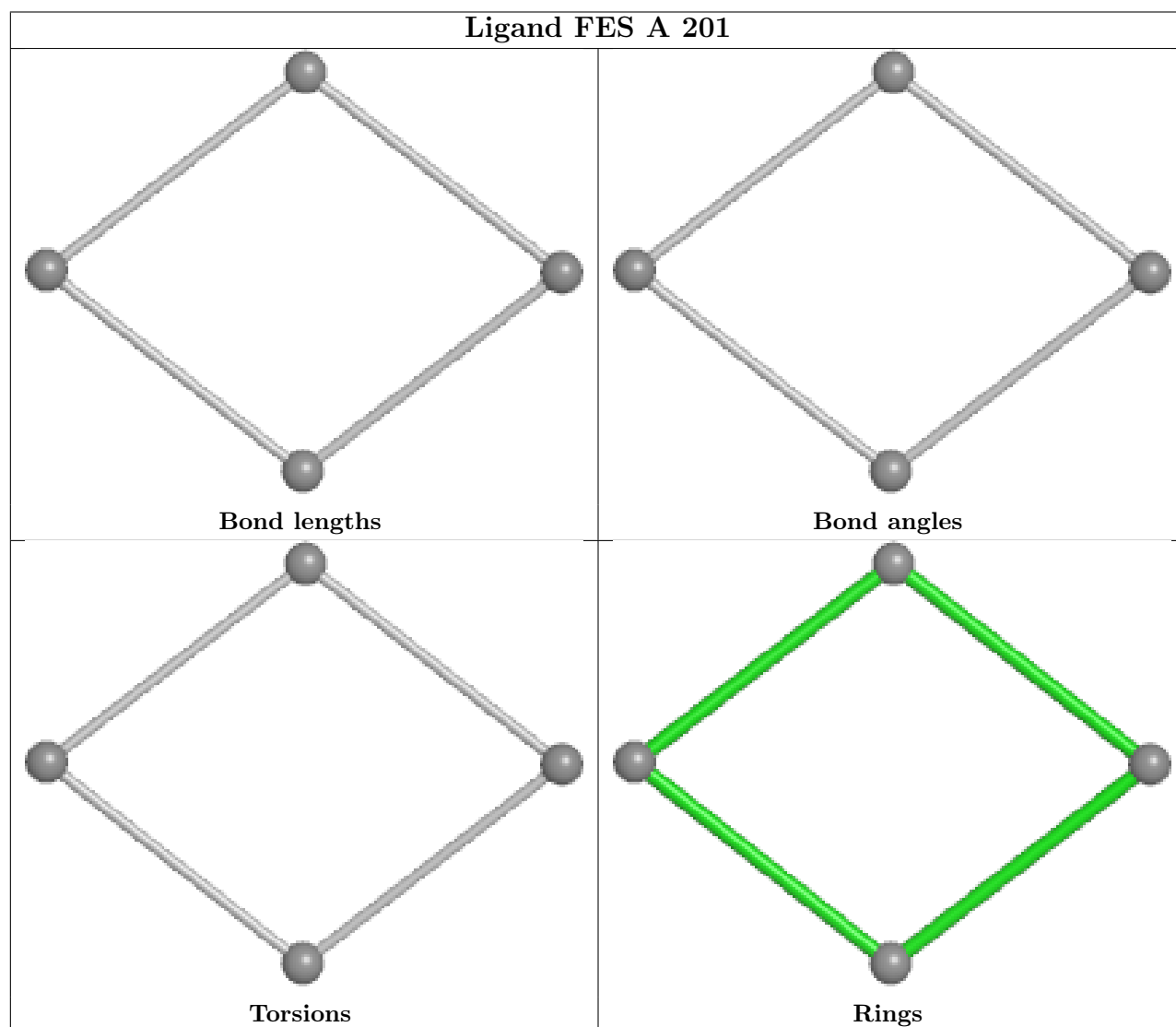
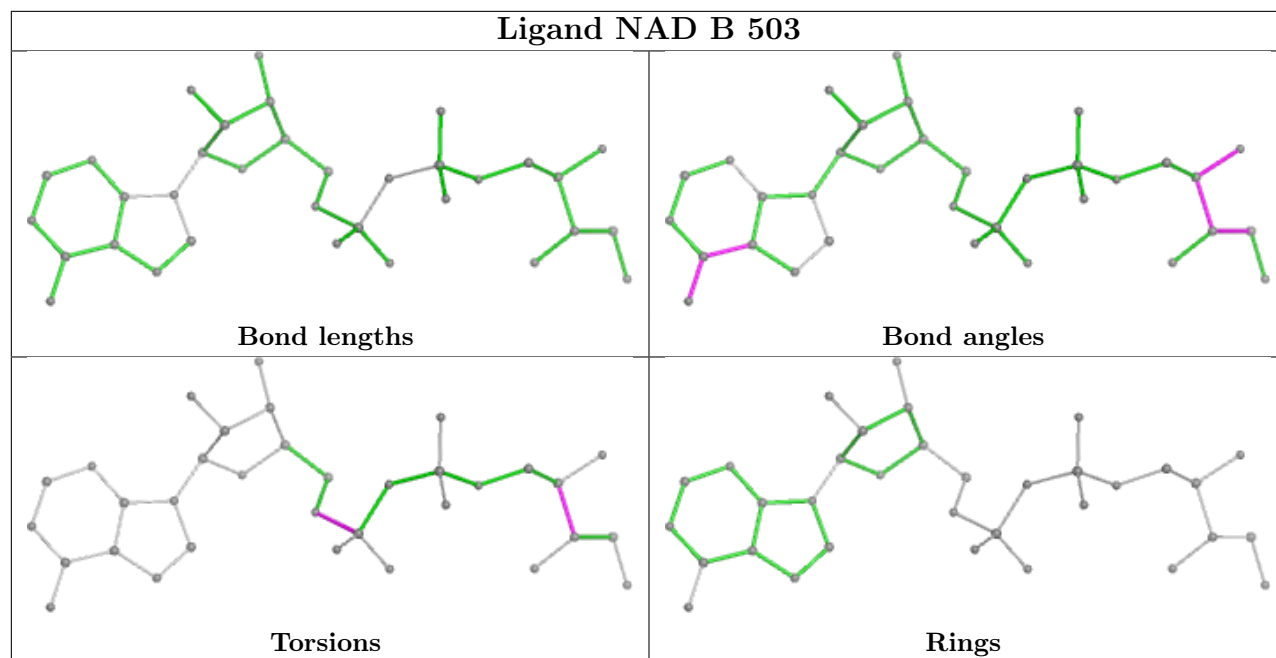
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	FMN	3	0
9	D	502	NAD	4	0
9	B	503	NAD	2	0
7	B	501	SF4	1	0
8	B	502	FMN	2	0

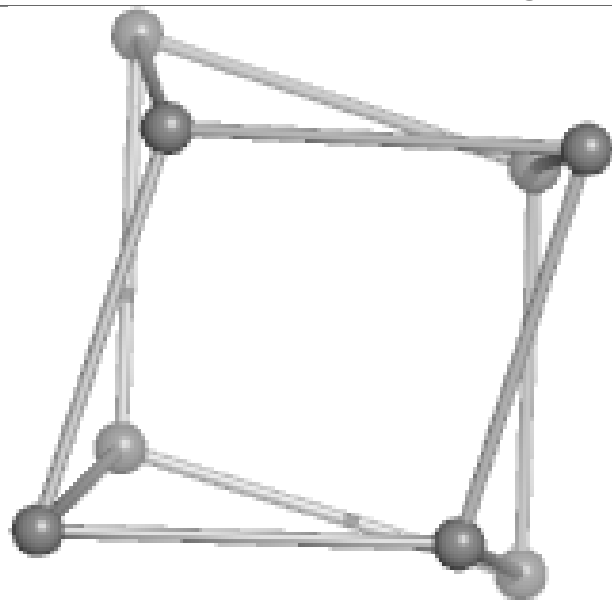
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



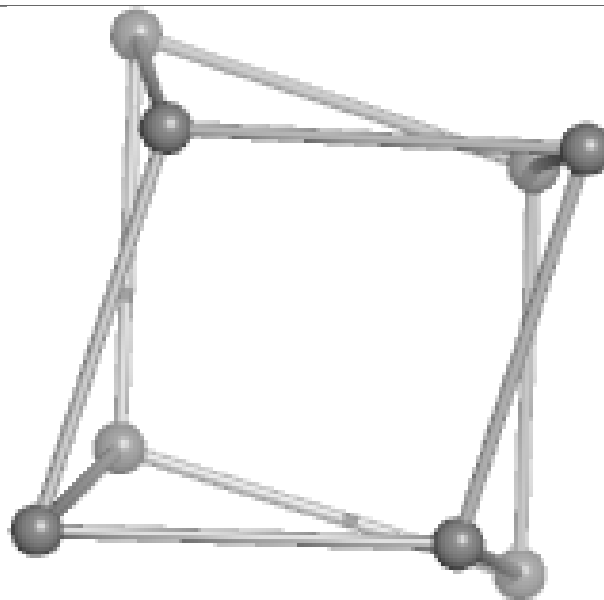




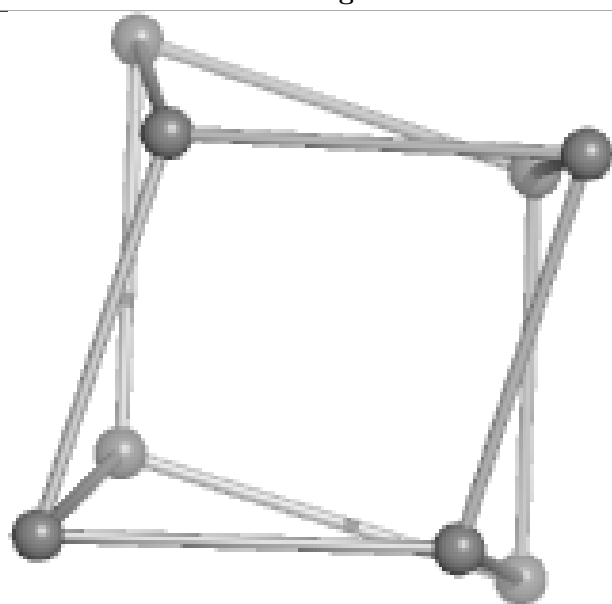
Ligand SF4 B 501



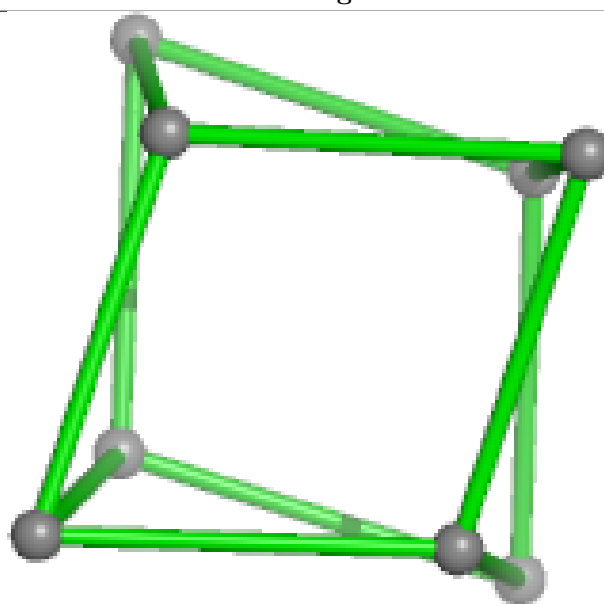
Bond lengths



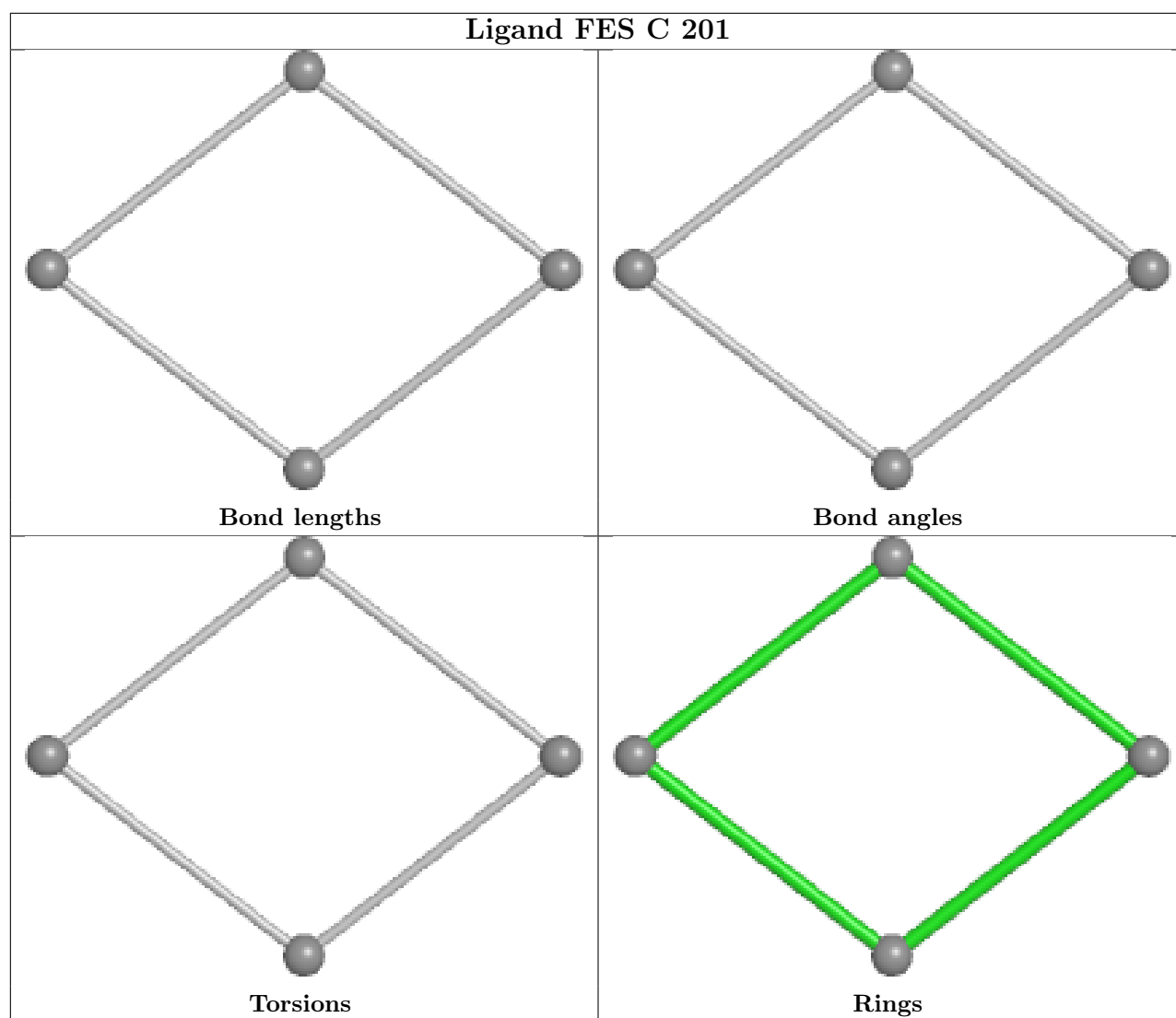
Bond angles

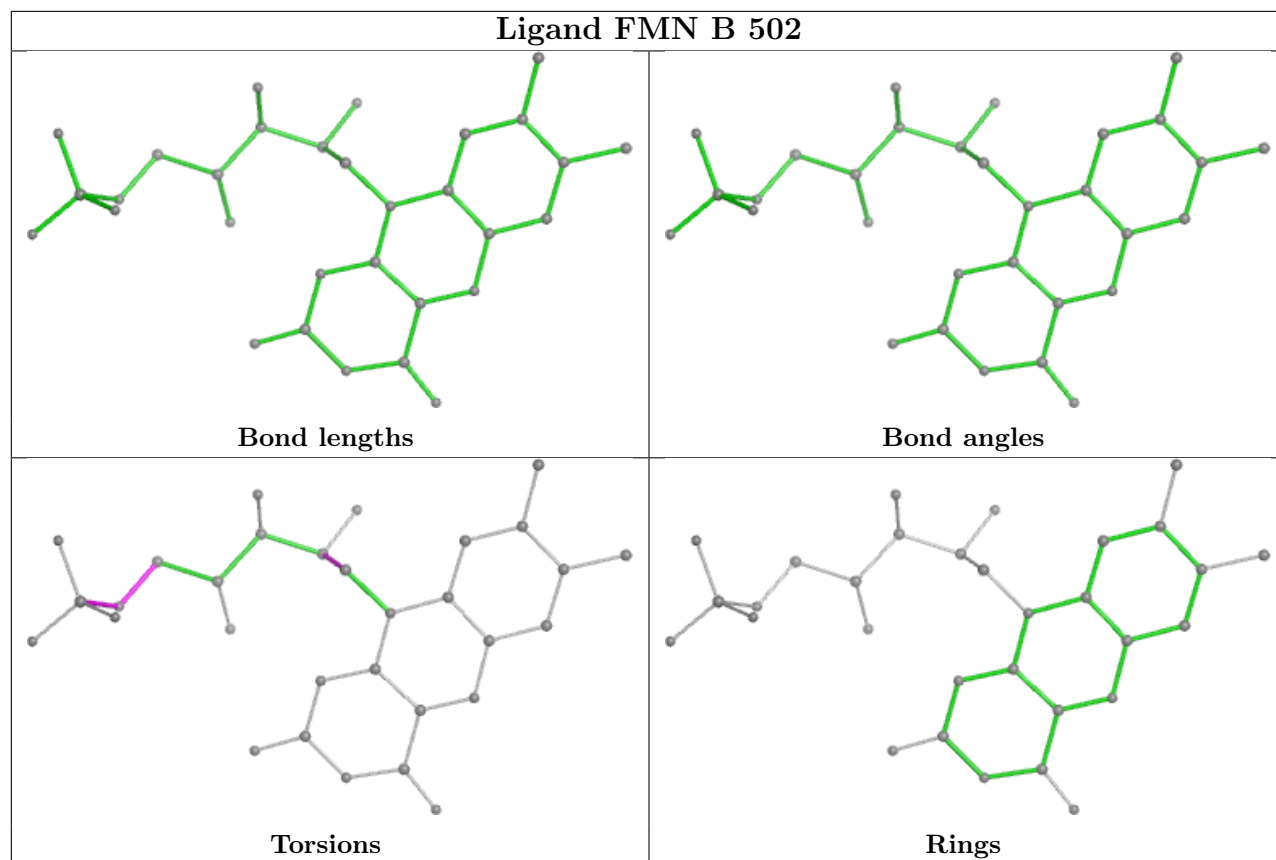


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	155/160 (96%)	0.97	16 (10%)	13 11	33, 53, 78, 94	0
1	C	156/160 (97%)	0.92	10 (6%)	27 21	33, 51, 73, 106	0
2	B	416/434 (95%)	0.31	8 (1%)	66 61	25, 39, 60, 72	0
2	D	416/434 (95%)	0.31	10 (2%)	59 54	24, 39, 59, 77	0
All	All	1143/1188 (96%)	0.48	44 (3%)	44 38	24, 41, 67, 106	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	328	GLU	4.9
1	C	56	LEU	3.4
1	A	56	LEU	3.3
2	D	313	PRO	3.3
1	A	6	PHE	3.2
1	A	157	SER	3.2
1	C	93	LEU	3.0
2	D	328	GLU	2.8
1	C	73	PHE	2.8
1	C	109	ILE	2.7
2	B	368	TYR	2.6
1	A	105	ASN	2.6
2	B	324	VAL	2.6
1	A	14	THR	2.6
2	D	240	TYR	2.6
1	A	73	PHE	2.5
1	A	8	PHE	2.5
1	C	52	LEU	2.5
2	B	418	ARG	2.4
2	D	370	GLY	2.4
2	D	333	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	20	ILE	2.4
2	D	368	TYR	2.4
1	A	93	LEU	2.3
1	A	136	MET	2.3
1	C	99	LEU	2.3
1	C	105	ASN	2.2
2	D	392	ILE	2.2
1	A	15	LYS	2.2
1	C	136	MET	2.2
1	A	99	LEU	2.2
1	A	107	LEU	2.2
1	A	16	LEU	2.2
2	B	377	TRP	2.1
2	D	377	TRP	2.1
2	B	240	TYR	2.1
2	D	144	ILE	2.1
1	C	13	LYS	2.1
1	A	43	TYR	2.1
2	D	327	GLU	2.0
1	A	114	VAL	2.0
1	A	132	SER	2.0
2	B	3	SER	2.0
2	B	311	TYR	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, 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.

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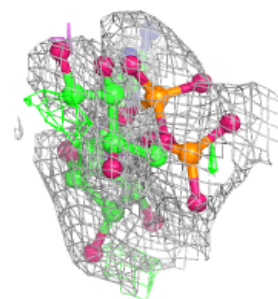
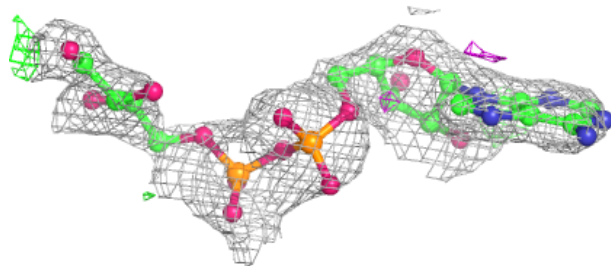
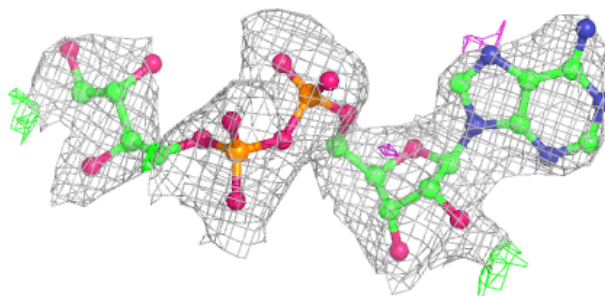
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	203	5/5	0.57	0.15	80,81,83,86	0
5	SO4	C	205	5/5	0.58	0.17	74,80,85,86	0
5	SO4	B	506	5/5	0.64	0.14	80,86,86,88	0
5	SO4	A	204	5/5	0.78	0.21	83,90,92,92	0
9	NAD	B	503	34/44	0.81	0.14	49,59,64,66	0
9	NAD	D	502	32/44	0.83	0.13	45,59,62,64	0
4	CL	C	202	1/1	0.84	0.21	66,66,66,66	0
5	SO4	B	505	5/5	0.84	0.17	62,65,70,72	0
10	GOL	B	504	6/6	0.85	0.11	31,32,33,34	0
6	NA	A	205	1/1	0.87	0.23	46,46,46,46	0
4	CL	D	505	1/1	0.88	0.15	52,52,52,52	0
4	CL	A	202	1/1	0.90	0.11	58,58,58,58	0
8	FMN	B	502	31/31	0.92	0.10	29,31,32,33	0
10	GOL	D	504	6/6	0.92	0.13	35,39,41,43	0
4	CL	C	204	1/1	0.93	0.07	49,49,49,49	0
8	FMN	D	501	31/31	0.93	0.09	26,29,31,32	0
4	CL	C	203	1/1	0.93	0.06	48,48,48,48	0
3	FES	C	201	4/4	0.96	0.10	38,40,41,41	0
3	FES	A	201	4/4	0.96	0.10	36,37,38,42	0
4	CL	D	506	1/1	0.96	0.12	55,55,55,55	0
7	SF4	D	503	8/8	0.98	0.04	33,35,38,39	0
7	SF4	B	501	8/8	0.99	0.04	30,33,37,37	0

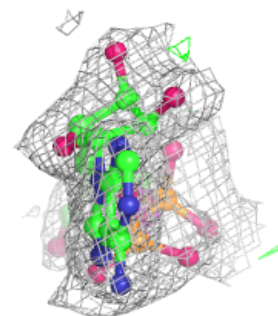
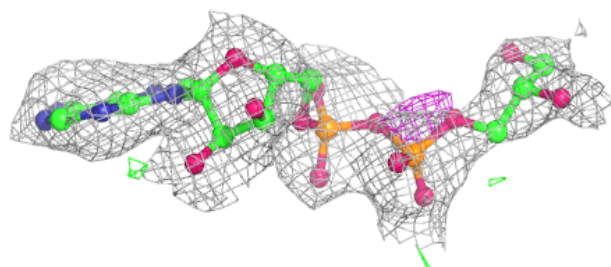
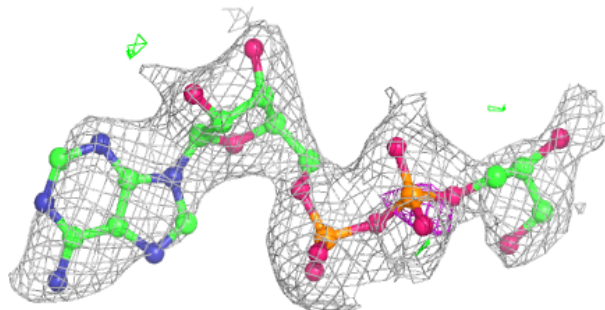
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 503:

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

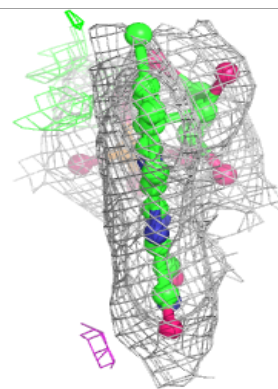
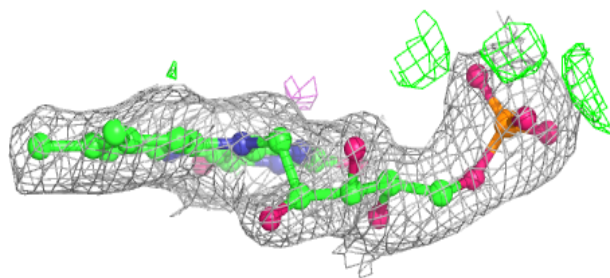
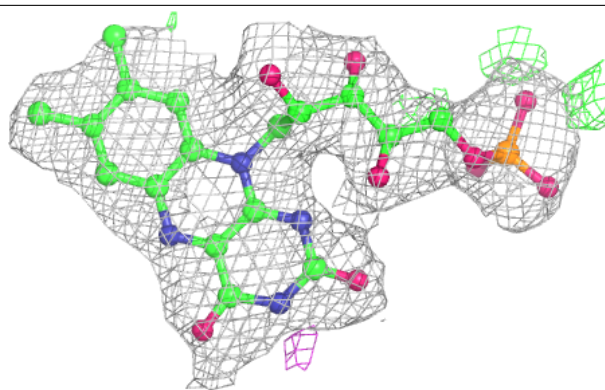
**Electron density around NAD D 502:**

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

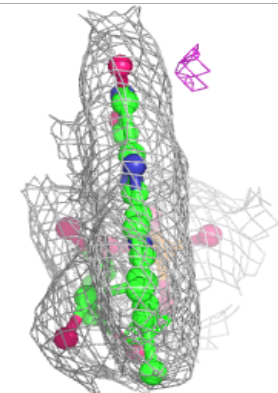
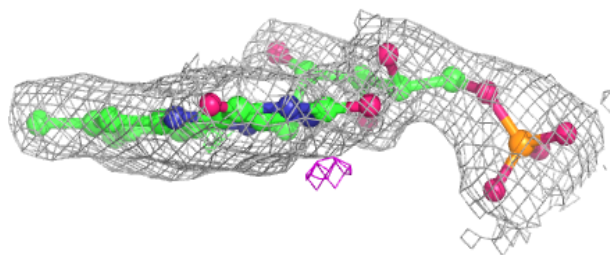
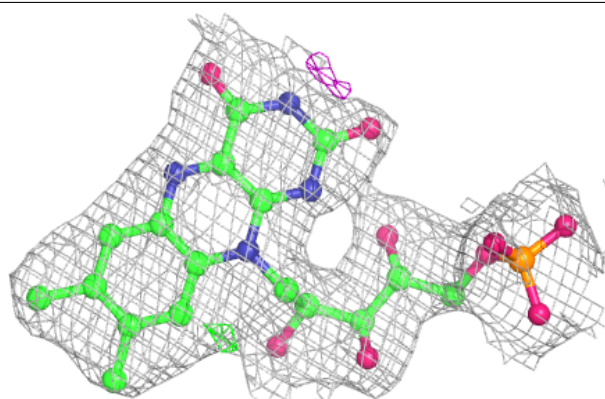


Electron density around FMN B 502:

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

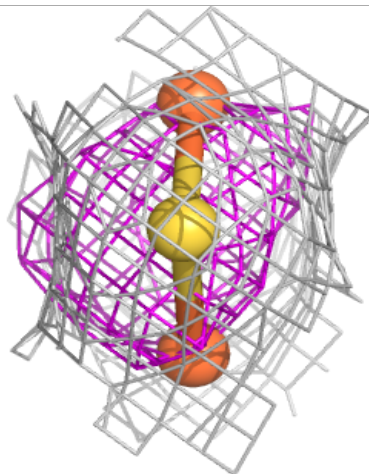
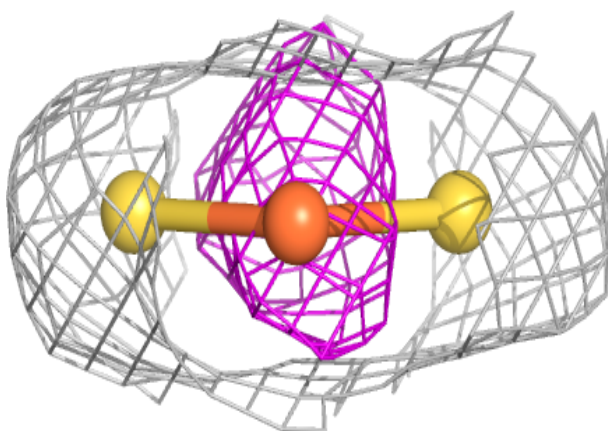
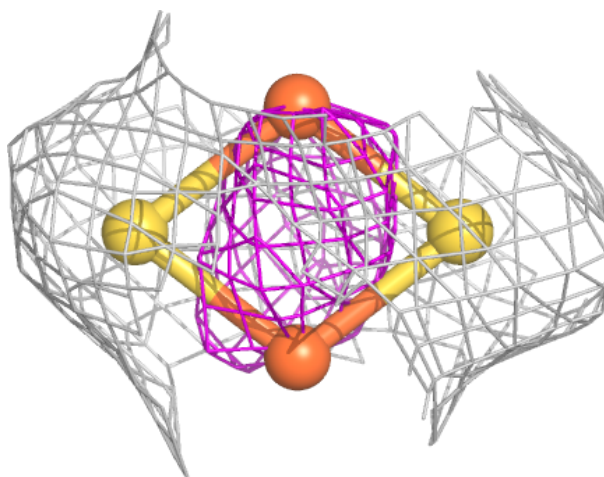
**Electron density around FMN D 501:**

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



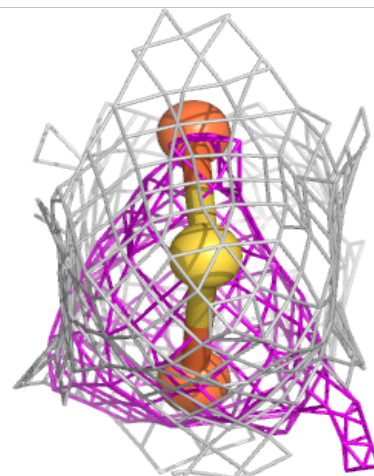
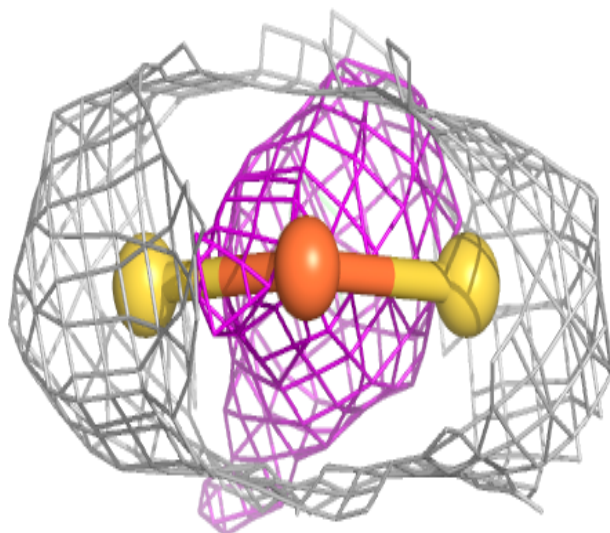
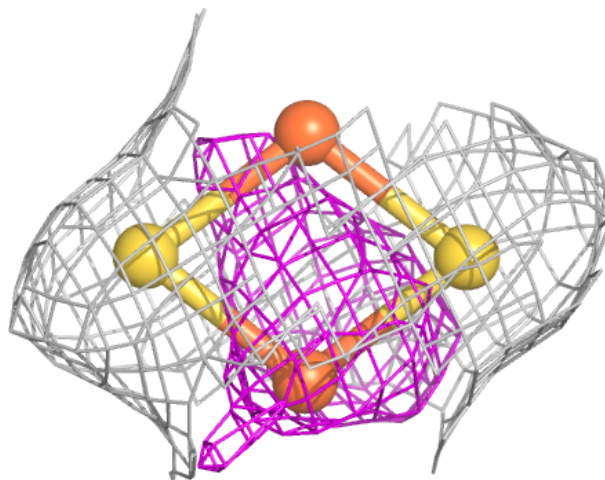
Electron density around FES C 201:

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



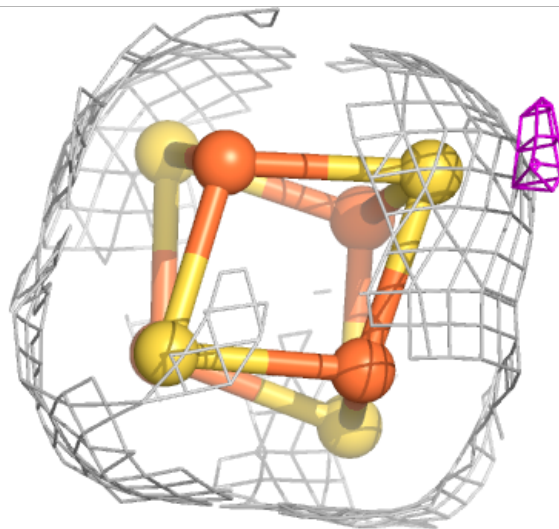
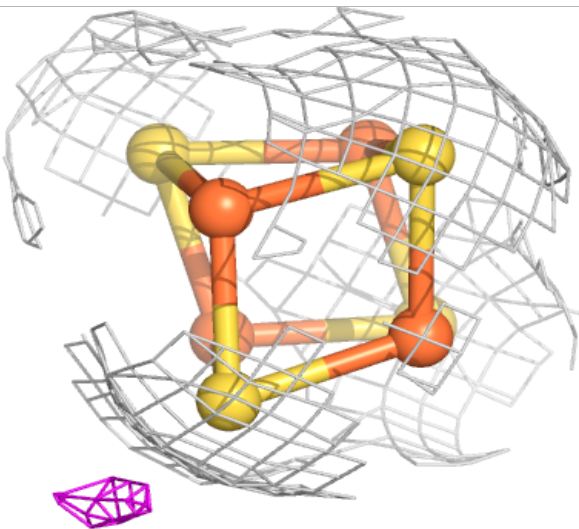
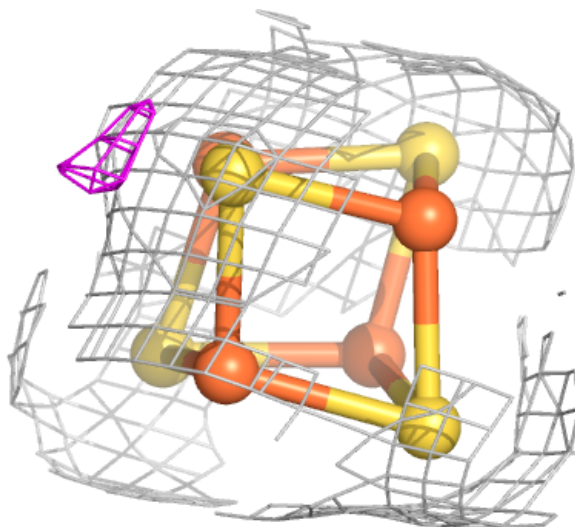
Electron density around FES A 201:

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



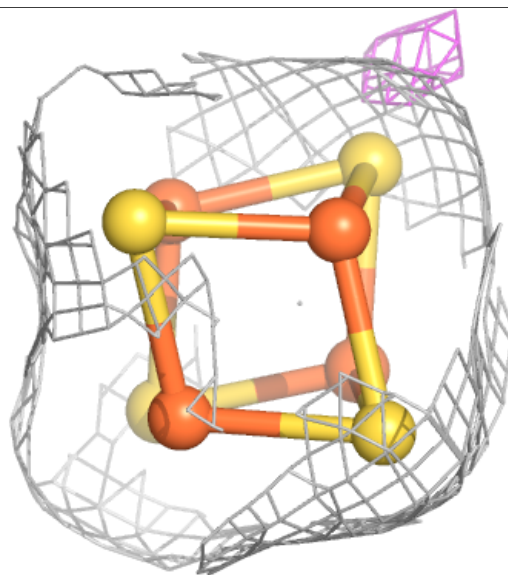
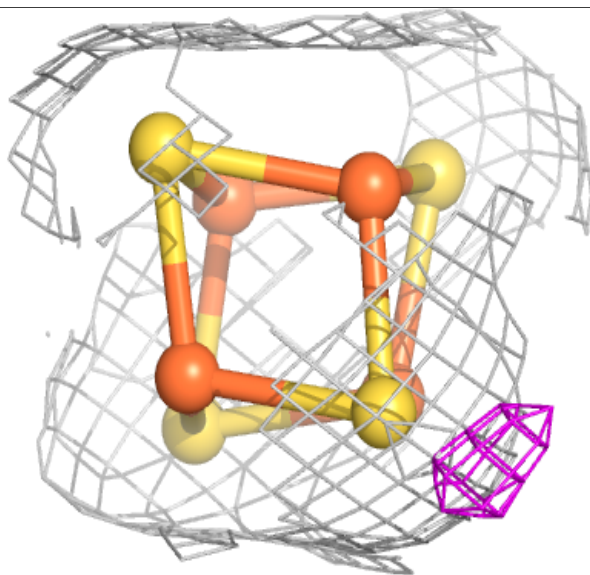
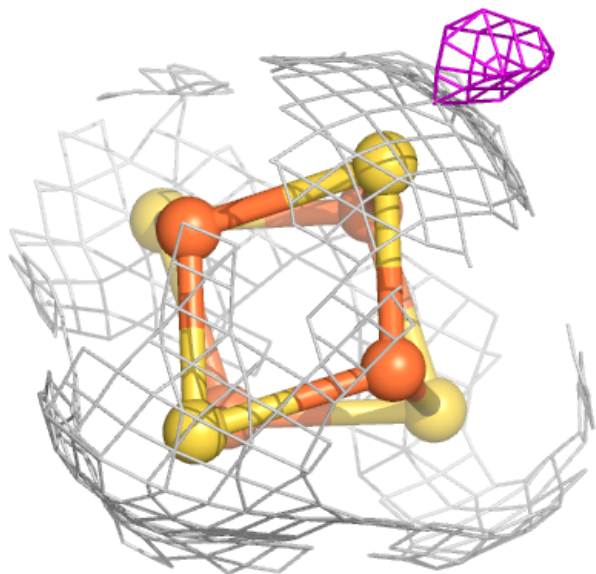
Electron density around SF4 D 503:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.