



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:44 AM UTC

PDB ID : 9FIL / pdb_00009fil
Title : Crystal Structure of reduced NuoEF variant E222K(NuoF) from Aquifex aeolicus bound to NAD⁺
Authors : Wohlwend, D.; Friedrich, T.; Goeppert-Asadollahpour, S.
Deposited on : 2024-05-29
Resolution : 2.54 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

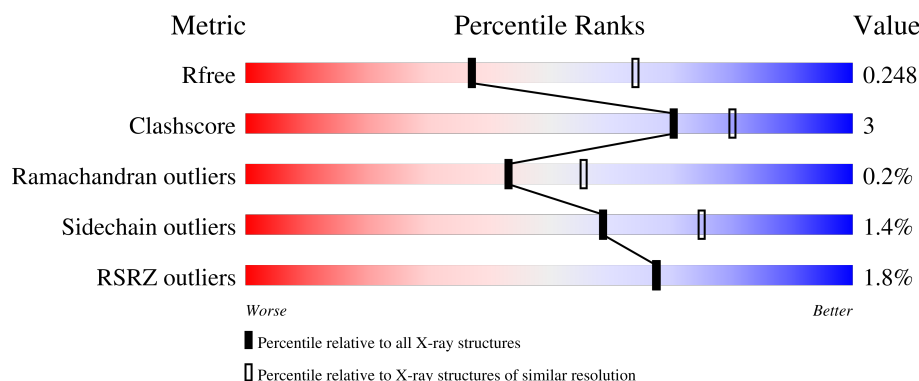
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	0% 86% 11% .
1	C	160	0% 84% 12% ..
2	B	434	2% 86% 10% .
2	D	434	2% 86% 9% .

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
9	CL	D	505	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9682 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	156	Total	C	N	O	S	0	0	0
			1268	821	204	234	9			
1	C	156	Total	C	N	O	S	0	0	0
			1268	821	204	234	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	2	0
			3274	2103	548	609	14			
2	D	418	Total	C	N	O	S	0	1	0
			3268	2098	548	608	14			

There are 18 discrepancies between the modelled and reference sequences:

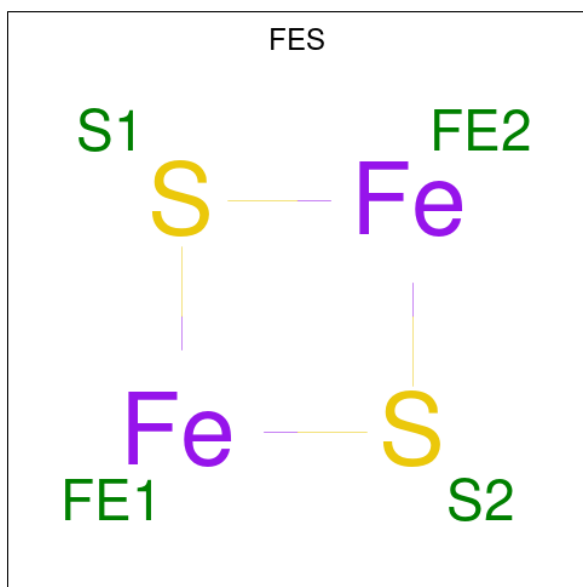
Chain	Residue	Modelled	Actual	Comment	Reference
B	222	LYS	GLU	engineered mutation	UNP O66841
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag	UNP O66841
B	434	HIS	-	expression tag	UNP O66841
D	222	LYS	GLU	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).

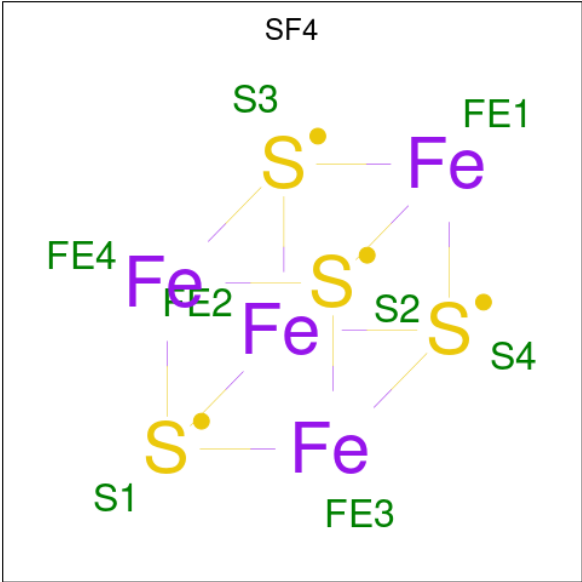


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

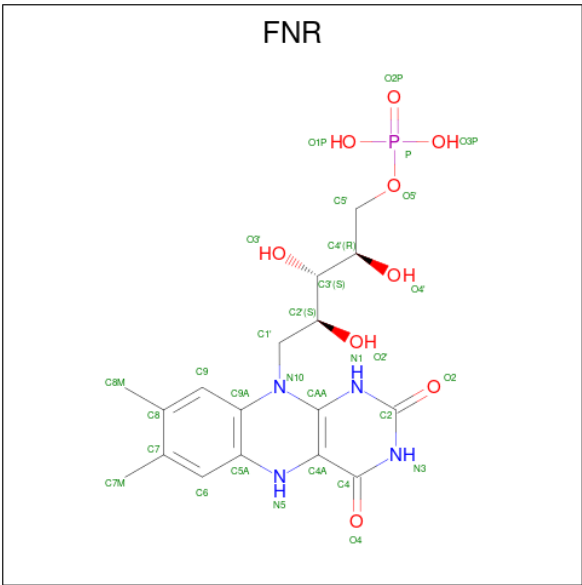
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	5	Total	Na	0	0
			5	5		
4	C	2	Total	Na	0	0
			2	2		
4	D	2	Total	Na	0	0
			2	2		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PT ERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: C₁₇H₂₃N₄O₉P) (labeled as "Ligand of Interest" by depositor).



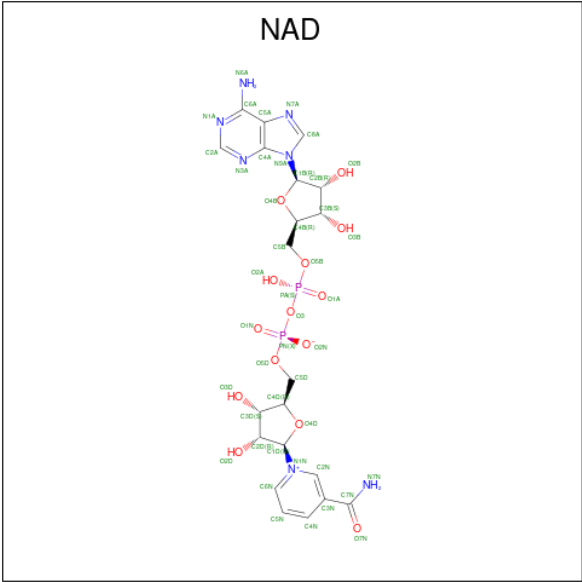
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 7 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
7	D	1	Total	C	N	O	P	0	0
			33	14	5	12	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		
9	D	2	Total	Cl	0	0
			2	2		

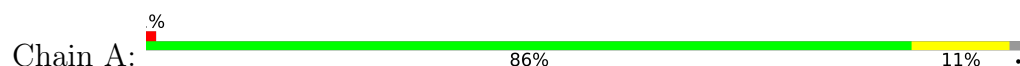
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	56	Total	O	0	0
			56	56		
10	B	156	Total	O	0	0
			156	156		
10	C	69	Total	O	0	0
			69	69		
10	D	137	Total	O	0	0
			137	137		

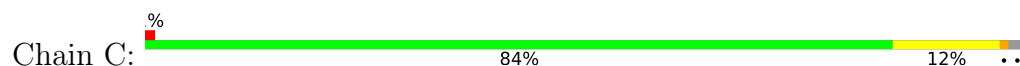
3 Residue-property plots [i](#)

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.

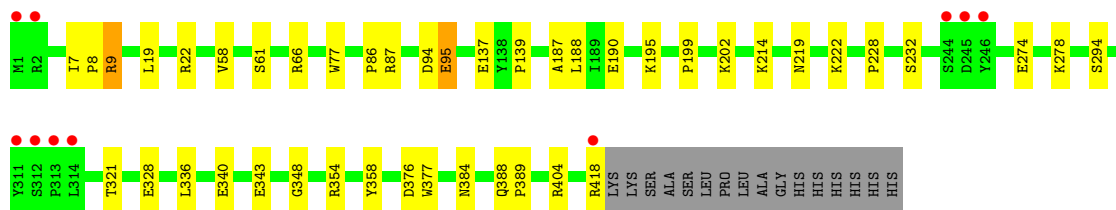
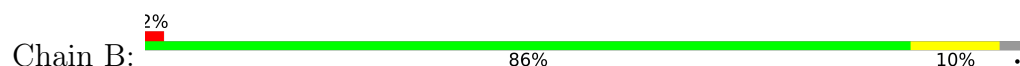
- Molecule 1: NADH-quinone oxidoreductase subunit E



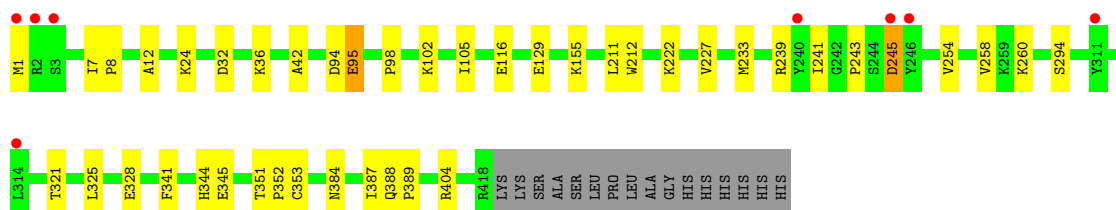
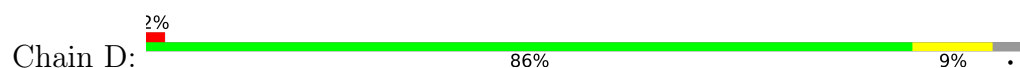
- Molecule 1: NADH-quinone oxidoreductase subunit E



- 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 115.54Å 189.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.54 49.40 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.40-2.54) 99.0 (49.40-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.201 , 0.248 0.206 , 0.248	Depositor DCC
R_{free} test set	2370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtrriage
Anisotropy	0.767	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9682	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.62 % 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 9.6714e-05. 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: CL, NAD, NA, FES, GOL, SF4, FNR

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	0.54	0/1297	1.00	1/1752 (0.1%)
1	C	0.55	0/1297	1.03	0/1752
2	B	0.55	0/3353	1.02	1/4540 (0.0%)
2	D	0.55	0/3347	1.02	3/4530 (0.1%)
All	All	0.55	0/9294	1.02	5/12574 (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
1	C	0	2
2	B	0	3
2	D	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	129	GLU	CB-CA-C	6.84	120.68	110.14
1	A	74	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	376	ASP	CA-CB-CG	5.15	117.75	112.60
2	D	245	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	227	VAL	N-CA-CB	5.03	114.37	110.45

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	ARG	Sidechain
2	B	22	ARG	Sidechain
2	B	87	ARG	Sidechain
2	B	9	ARG	Sidechain
1	C	75	ARG	Sidechain
1	C	82	ARG	Sidechain
2	D	239	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	8	0
1	C	1268	0	1269	11	0
2	B	3274	0	3227	24	0
2	D	3268	0	3227	25	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	1	0	0	0	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	8	0	0	0	0
5	D	8	0	0	0	0
6	B	31	0	22	0	0
6	D	31	0	22	0	0
7	B	36	0	20	0	0
7	D	33	0	16	0	0
8	B	12	0	16	2	0
8	D	6	0	8	0	0
9	B	1	0	0	0	0
9	D	2	0	0	2	0
10	A	56	0	0	0	0
10	B	156	0	0	1	0
10	C	69	0	0	1	0
10	D	137	0	0	1	0
All	All	9682	0	9096	62	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 3.

All (62) 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:D:222:LYS:HE2	9:D:505:CL:CL	2.16	0.82
2:D:233:MET:HE1	2:D:241:ILE:HD11	1.69	0.73
2:D:384:ASN:HD22	2:D:404:ARG:HH21	1.35	0.73
2:D:222:LYS:CE	9:D:505:CL:CL	2.78	0.68
2:B:202:LYS:HD3	10:B:645:HOH:O	1.98	0.62
2:B:384:ASN:HD22	2:B:404:ARG:HH21	1.49	0.60
1:C:93:LEU:HD21	2:D:325:LEU:HG	1.86	0.56
2:B:377:TRP:CZ2	2:B:418:ARG:HG2	2.42	0.54
2:B:343:GLU:HG3	2:B:358:TYR:HA	1.92	0.52
1:C:75:ARG:HD2	10:C:344:HOH:O	2.09	0.51
1:A:43:TYR:O	1:A:45:PRO:HD3	2.10	0.51
2:B:77:TRP:HE1	2:B:219:ASN:ND2	2.10	0.50
2:D:94:ASP:O	2:D:95:GLU:C	2.54	0.50
2:B:336:LEU:O	2:B:340:GLU:HG3	2.12	0.50
2:B:94:ASP:O	2:B:95:GLU:C	2.55	0.49
2:B:9:ARG:HD2	2:D:155:LYS:O	2.13	0.49
2:B:77:TRP:HE1	2:B:219:ASN:HD21	1.58	0.49
2:D:353:CYS:HA	2:D:387:ILE:HG23	1.96	0.48
1:A:90:VAL:O	1:A:94:MET:HG2	2.15	0.47
2:B:190:GLU:OE1	2:B:195:LYS:HE2	2.14	0.47
1:A:138:MET:HG2	1:A:143:GLU:HG3	1.96	0.46
2:B:348:GLY:HA2	2:B:354[B]:ARG:HB2	1.97	0.46
2:B:188:LEU:C	2:B:188:LEU:HD23	2.41	0.46
2:D:294:SER:HA	2:D:321:THR:O	2.15	0.46
2:D:102:LYS:HD2	2:D:222:LYS:HE3	1.98	0.46
1:C:127:CYS:SG	2:D:98:PRO:HA	2.56	0.45
1:C:100:LEU:HD22	1:C:111:PRO:HG3	1.98	0.45
1:A:91:CYS:HA	1:A:134:ALA:HB1	1.98	0.45
2:B:294:SER:HA	2:B:321:THR:O	2.16	0.45
2:D:341:PHE:O	2:D:345:GLU:HG2	2.17	0.45
2:B:187:ALA:HB2	2:B:199:PRO:HG3	1.98	0.45
2:D:388:GLN:N	2:D:389:PRO:CD	2.80	0.45
1:C:71:ASP:OD2	2:D:344[B]:HIS:CE1	2.71	0.44
2:B:228:PRO:HB3	8:B:504:GOL:H32	1.99	0.44
2:D:243:PRO:HB2	2:D:245:ASP:OD1	2.18	0.44
1:C:135:PRO:HG2	1:C:146:PHE:HB3	2.00	0.44
2:D:254:VAL:HG12	2:D:258:VAL:HG21	1.99	0.43
2:D:42:ALA:HB3	2:D:116:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HB2	1:C:138:MET:HB2	2.00	0.43
1:A:23:PHE:HE2	1:A:32:LEU:HD12	1.83	0.43
1:C:143:GLU:HB3	2:D:8:PRO:HD3	2.01	0.43
2:D:102:LYS:O	2:D:105:ILE:HG12	2.18	0.43
1:C:50:LYS:N	1:C:51:PRO:HD2	2.34	0.42
2:B:86:PRO:HD2	2:B:214:LYS:HE2	2.02	0.42
2:B:274:GLU:O	2:B:278:LYS:HB3	2.19	0.42
2:D:328:GLU:HB2	10:D:658:HOH:O	2.20	0.42
1:A:135:PRO:HG2	1:A:146:PHE:HB3	2.02	0.41
2:D:211:LEU:HG	2:D:212:TRP:CD1	2.56	0.41
1:C:63:VAL:O	1:C:67:VAL:HG23	2.20	0.41
2:D:260:LYS:HB3	2:D:260:LYS:HE2	1.92	0.41
2:B:58:VAL:O	2:B:61:SER:OG	2.36	0.41
2:D:32:ASP:O	2:D:36:LYS:HG3	2.20	0.41
2:B:377:TRP:CH2	2:B:418:ARG:HG2	2.55	0.41
2:D:12:ALA:HB3	2:D:24:LYS:HA	2.02	0.41
1:A:133:GLU:HG3	2:B:8:PRO:HB2	2.02	0.41
1:C:27:ARG:HB2	1:C:58:LEU:HD11	2.02	0.41
2:D:351:THR:HB	2:D:352:PRO:HD3	2.02	0.41
2:B:66:ARG:HB3	2:B:222:LYS:HE2	2.02	0.40
1:A:45:PRO:HA	1:A:46:PRO:HD3	1.96	0.40
2:B:137:GLU:C	2:B:139:PRO:HD3	2.46	0.40
2:B:388:GLN:N	2:B:389:PRO:CD	2.85	0.40
2:B:228:PRO:CB	8:B:504:GOL:H32	2.51	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%)	150 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	154/160 (96%)	148 (96%)	6 (4%)	0	100	100
2	B	418/434 (96%)	405 (97%)	12 (3%)	1 (0%)	43	56
2	D	417/434 (96%)	406 (97%)	10 (2%)	1 (0%)	43	56
All	All	1143/1188 (96%)	1109 (97%)	32 (3%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/146 (97%)	140 (99%)	2 (1%)	59	75
1	C	142/146 (97%)	137 (96%)	5 (4%)	32	48
2	B	336/357 (94%)	332 (99%)	4 (1%)	63	78
2	D	337/357 (94%)	335 (99%)	2 (1%)	78	87
All	All	957/1006 (95%)	944 (99%)	13 (1%)	59	75

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

Mol	Chain	Res	Type
1	A	15	LYS
1	A	76	GLU
2	B	7	ILE
2	B	19	LEU
2	B	232	SER
2	B	328	GLU
1	C	43	TYR
1	C	47	GLU
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	93	LEU
1	C	96	THR
2	D	1	MET
2	D	7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
2	B	41	GLN
2	B	220	ASN
2	B	384	ASN
1	C	62	HIS
1	C	126	GLN
1	C	153	ASN
2	D	29	HIS
2	D	83	ASN
2	D	128	ASN
2	D	220	ASN
2	D	349	GLN
2	D	384	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SF4	B	501	2	0,12,12	-	-	-		
8	GOL	B	505	-	5,5,5	0.17	0	5,5,5	0.49	0
6	FNR	D	502	-	32,33,33	0.44	0	41,50,50	0.55	0
7	NAD	D	503	-	35,35,48	0.62	0	48,52,73	0.68	1 (2%)
7	NAD	B	503	-	38,39,48	0.61	1 (2%)	55,60,73	0.53	0
3	FES	A	201	1	0,4,4	-	-	-		
8	GOL	B	504	-	5,5,5	0.16	0	5,5,5	0.39	0
6	FNR	B	502	-	32,33,33	0.47	0	41,50,50	0.99	4 (9%)
8	GOL	D	504	-	5,5,5	0.17	0	5,5,5	0.21	0
5	SF4	D	501	2	0,12,12	-	-	-		
3	FES	C	201	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	B	501	2	-	-	0/6/5/5
8	GOL	B	505	-	-	1/4/4/4	-
6	FNR	D	502	-	-	3/18/18/18	0/3/3/3
7	NAD	D	503	-	-	1/26/42/62	0/3/3/5
7	NAD	B	503	-	-	3/22/54/62	0/4/4/5
3	FES	A	201	1	-	-	0/1/1/1
8	GOL	B	504	-	-	1/4/4/4	-
6	FNR	B	502	-	-	9/18/18/18	0/3/3/3
8	GOL	D	504	-	-	1/4/4/4	-
5	SF4	D	501	2	-	-	0/6/5/5
3	FES	C	201	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503	NAD	PN-O3	2.27	1.61	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	FNR	O5'-C5'-C4'	-3.25	100.67	109.36
6	B	502	FNR	O5'-P-O2P	2.75	113.86	106.44
6	B	502	FNR	O3P-P-O5'	-2.66	99.74	106.67
7	D	503	NAD	C5D-C4D-C3D	2.43	117.41	111.80
6	B	502	FNR	O1P-P-O5'	-2.32	100.62	106.67

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	FNR	N10-C1'-C2'-O2'
6	B	502	FNR	N10-C1'-C2'-C3'
6	B	502	FNR	C3'-C4'-C5'-O5'
6	B	502	FNR	O4'-C4'-C5'-O5'
6	B	502	FNR	C5'-O5'-P-O1P
6	B	502	FNR	C5'-O5'-P-O3P
7	D	503	NAD	C3D-C4D-O4D-C1D
7	B	503	NAD	O4D-C4D-C5D-O5D
7	B	503	NAD	C3D-C4D-C5D-O5D
8	B	505	GOL	O2-C2-C3-O3
8	D	504	GOL	O1-C1-C2-C3
7	B	503	NAD	C5B-O5B-PA-O1A
6	B	502	FNR	O2'-C2'-C3'-C4'
6	D	502	FNR	C4'-C5'-O5'-P
6	D	502	FNR	O2'-C2'-C3'-C4'
6	B	502	FNR	C5'-O5'-P-O2P
8	B	504	GOL	O1-C1-C2-O2
6	B	502	FNR	O2'-C2'-C3'-O3'
6	D	502	FNR	N10-C1'-C2'-O2'

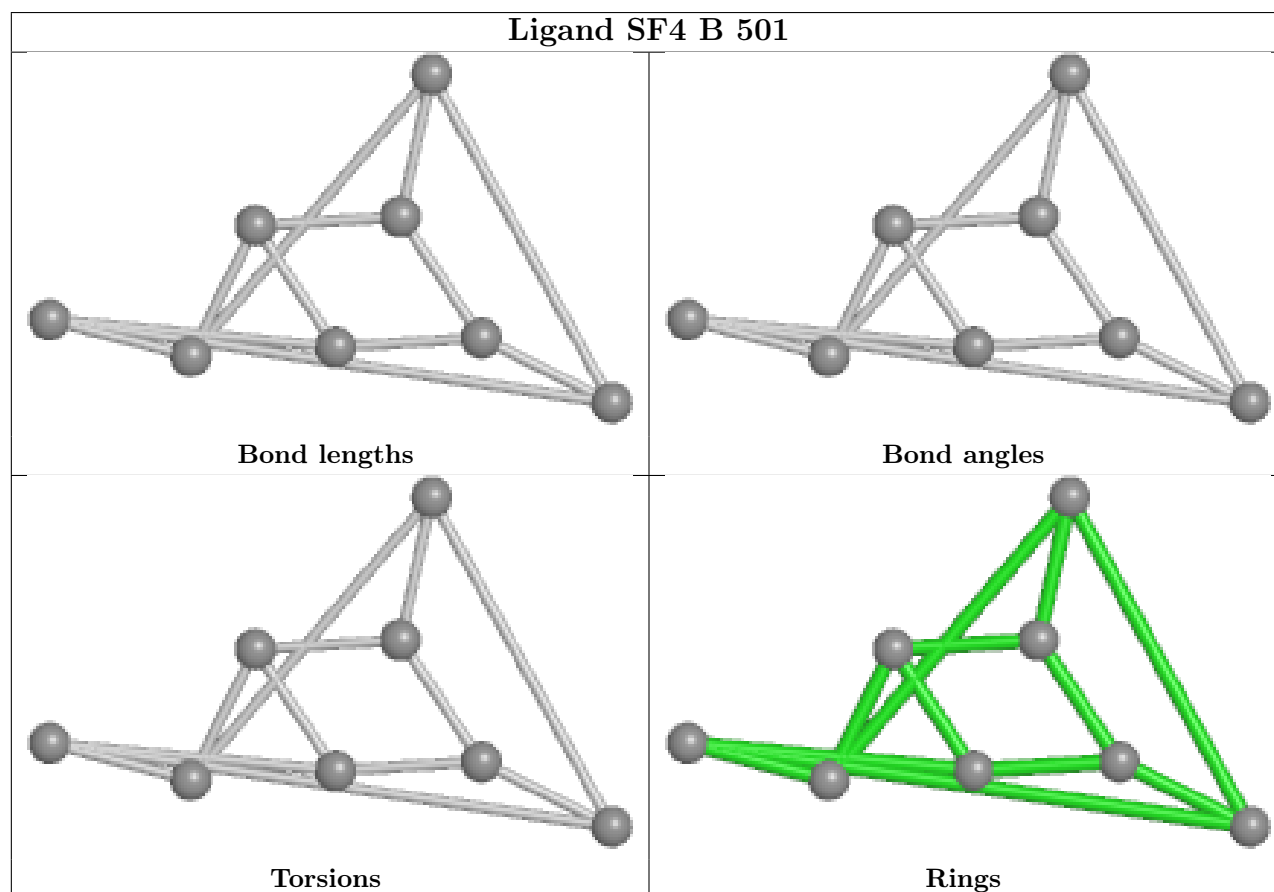
There are no ring outliers.

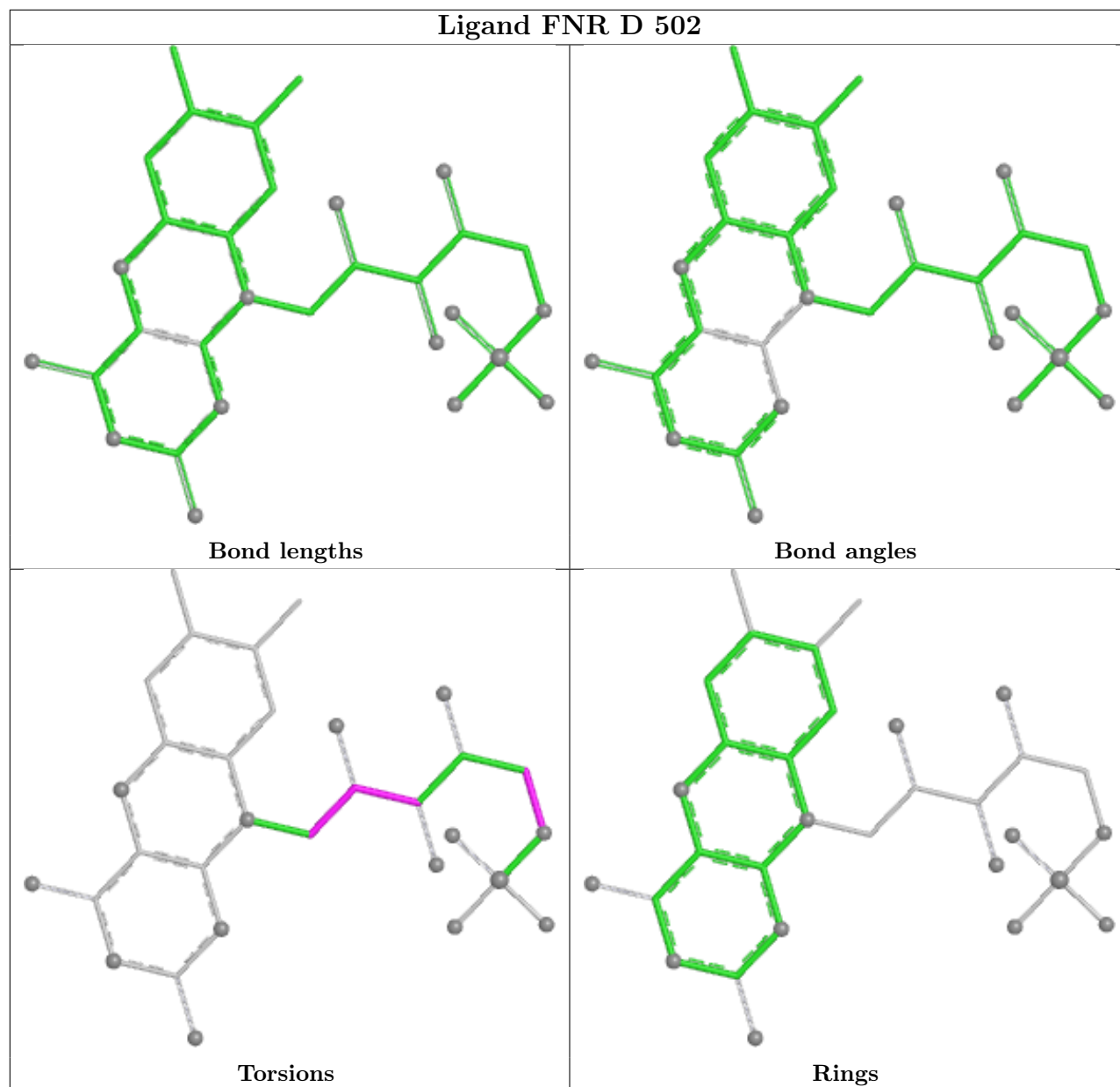
1 monomer is involved in 2 short contacts:

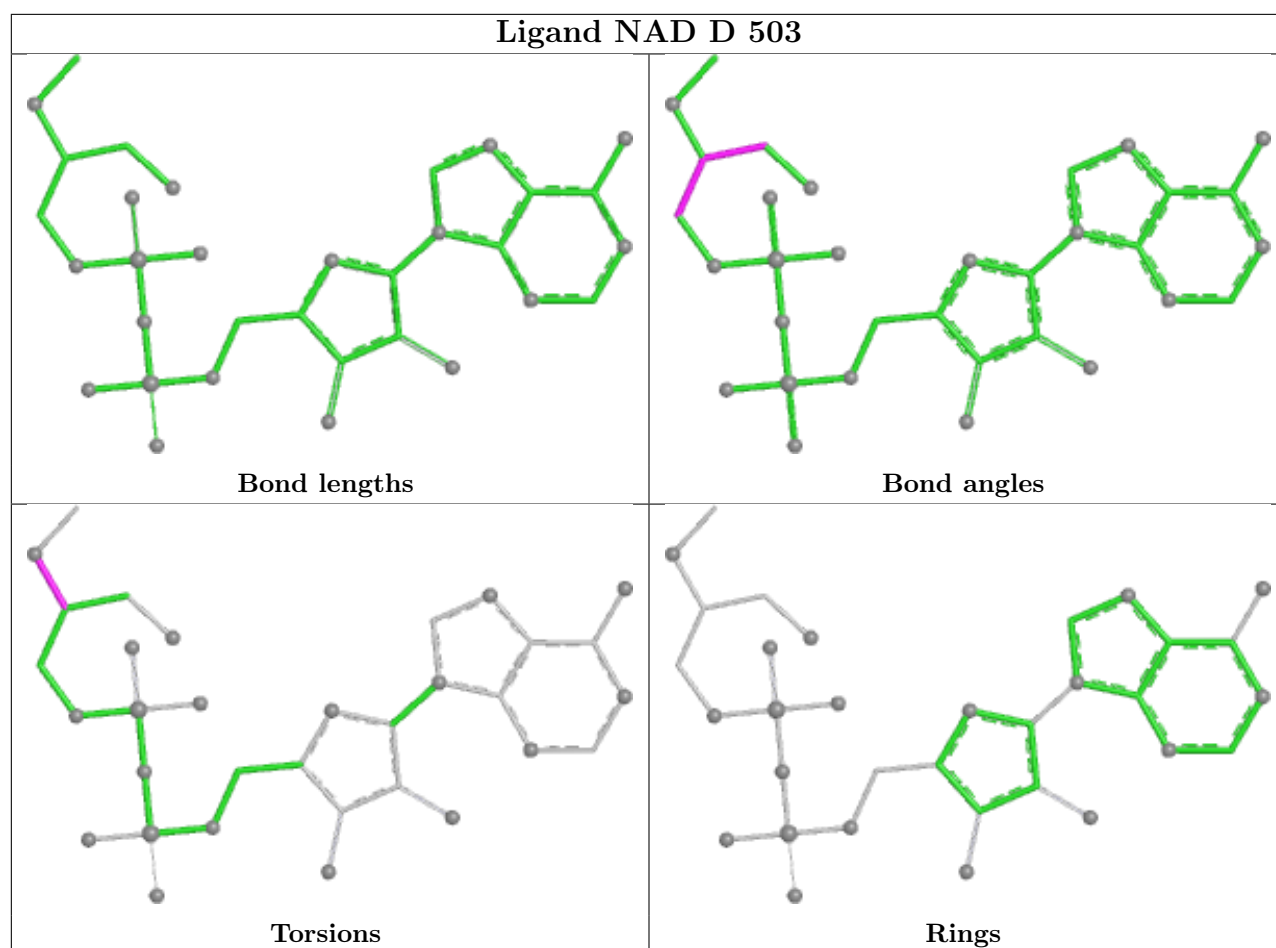
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	504	GOL	2	0

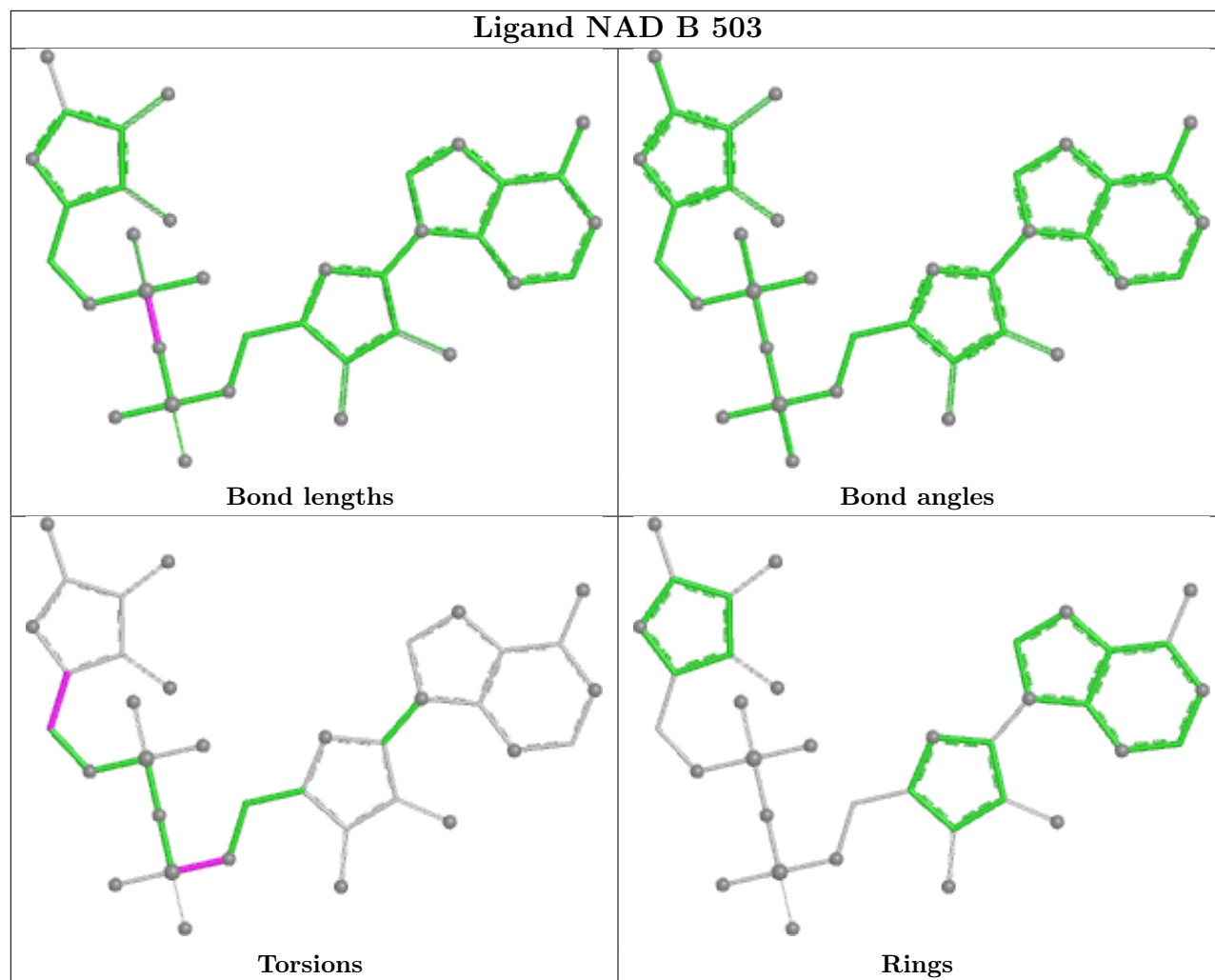
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

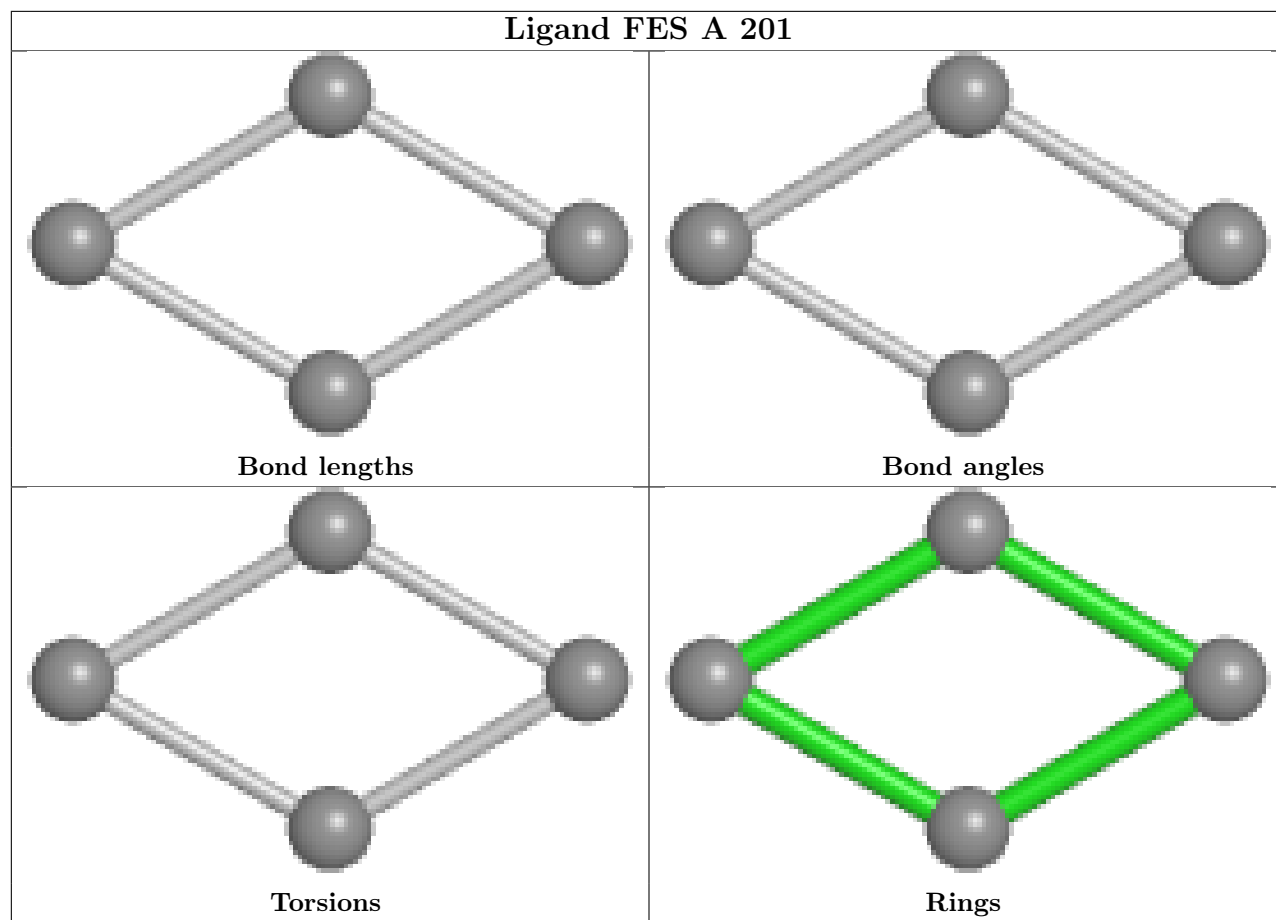
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



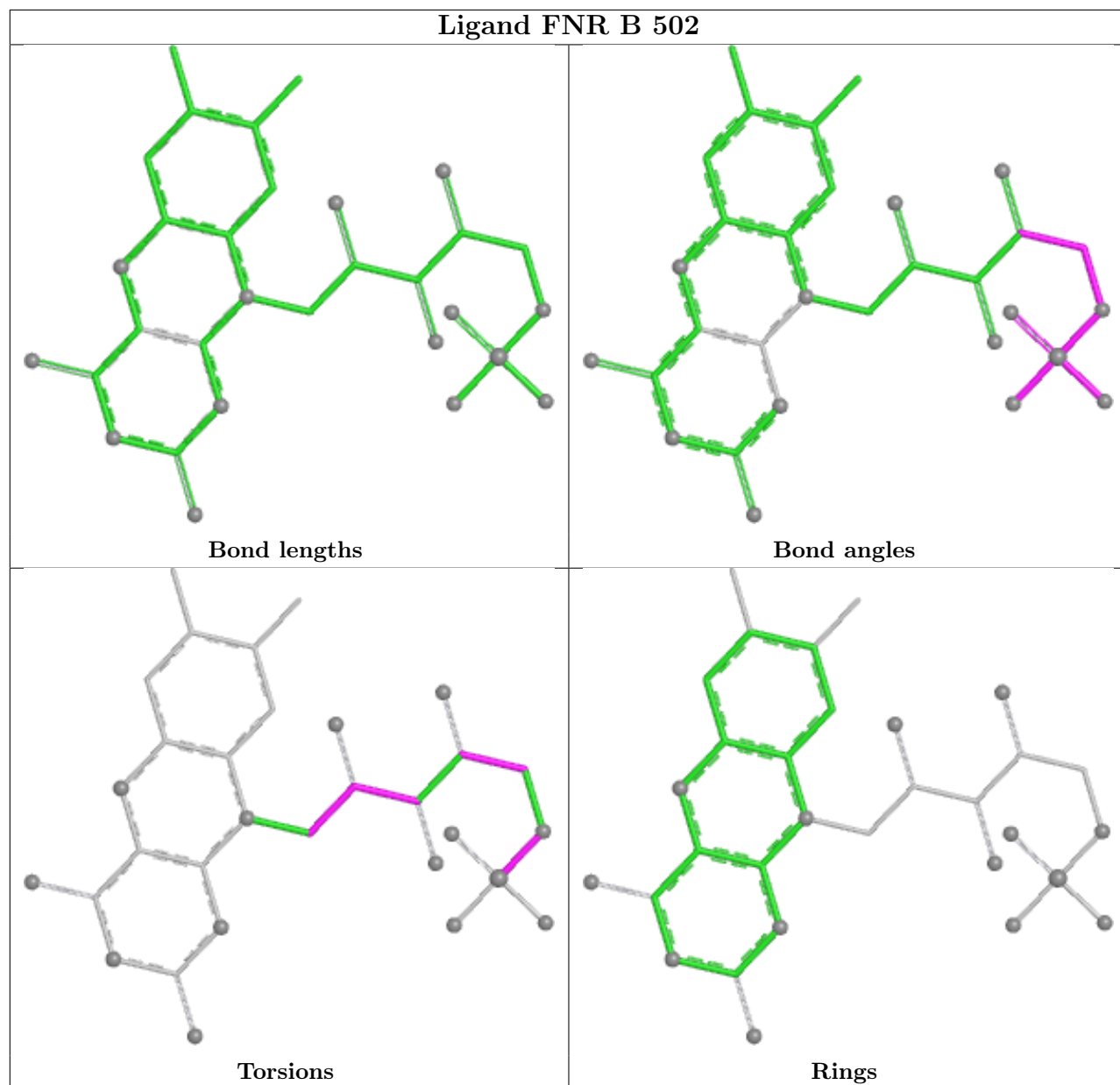


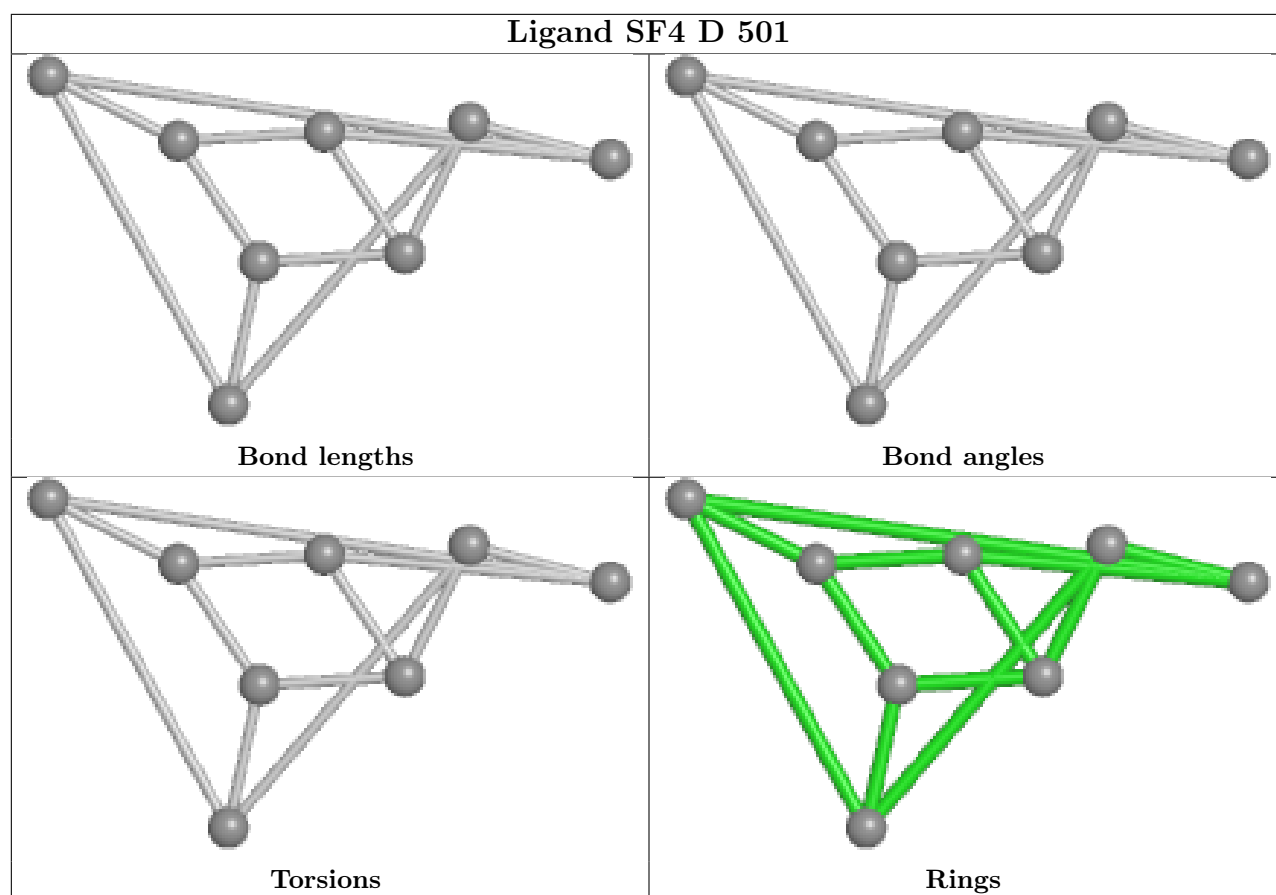


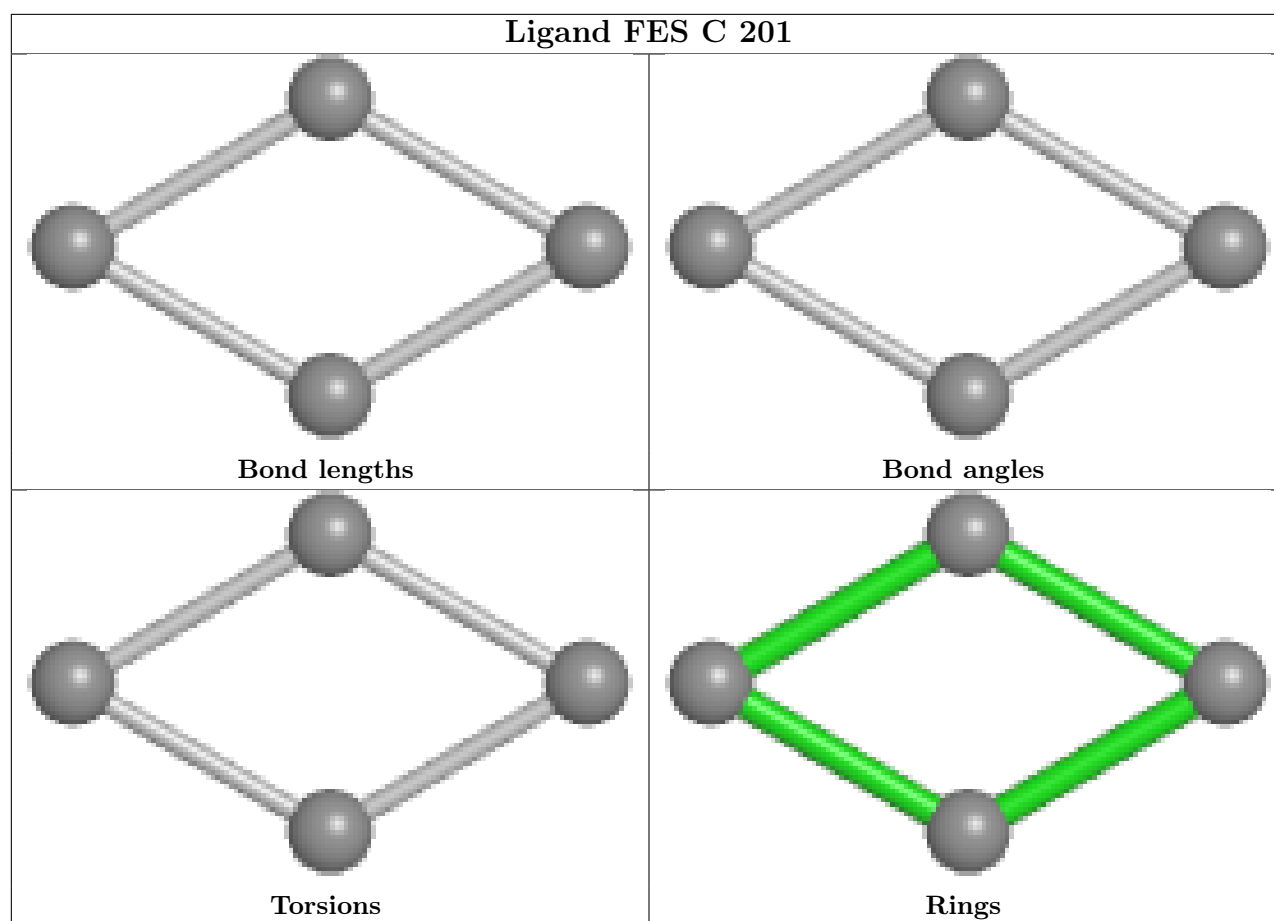




Ligand FNR B 502







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	156/160 (97%)	-0.05	2 (1%) 75 75	11, 24, 44, 78	0
1	C	156/160 (97%)	-0.05	1 (0%) 85 88	11, 23, 43, 72	0
2	B	418/434 (96%)	-0.10	10 (2%) 59 61	6, 18, 39, 81	2 (0%)
2	D	418/434 (96%)	-0.15	8 (1%) 66 66	7, 18, 37, 74	1 (0%)
All	All	1148/1188 (96%)	-0.11	21 (1%) 67 68	6, 19, 40, 81	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	4.4
2	D	1	MET	4.3
2	B	314	LEU	4.3
2	B	311	TYR	4.2
1	A	5	GLU	3.9
2	B	313	PRO	3.9
2	D	311	TYR	3.8
2	D	2	ARG	3.2
1	C	5	GLU	3.0
2	B	245	ASP	2.9
2	B	244	SER	2.6
2	B	246	TYR	2.6
2	B	418	ARG	2.6
2	B	2	ARG	2.5
1	A	10	GLU	2.3
2	D	245	ASP	2.2
2	D	246	TYR	2.2
2	D	3	SER	2.2
2	D	314	LEU	2.1
2	D	240	TYR	2.1
2	B	312	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

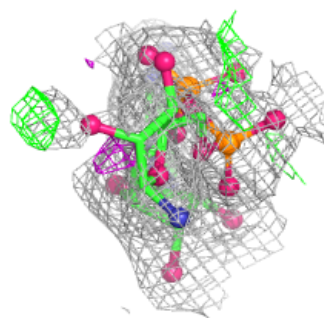
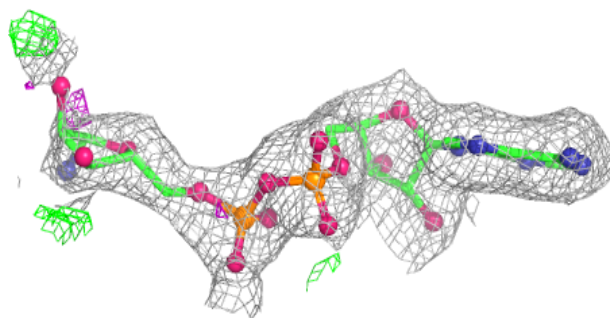
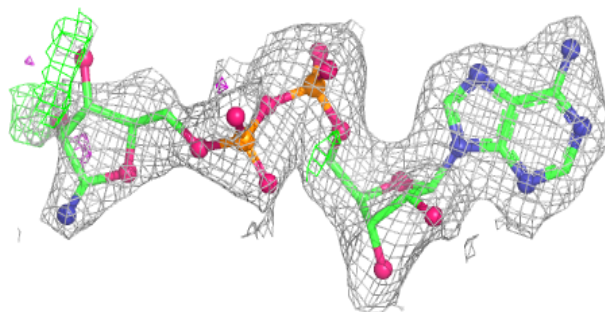
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	505	6/6	0.75	0.19	49,51,53,56	0
4	NA	B	509	1/1	0.79	0.15	37,37,37,37	0
9	CL	D	506	1/1	0.82	0.15	64,64,64,64	0
4	NA	B	511	1/1	0.83	0.11	26,26,26,26	0
8	GOL	D	504	6/6	0.86	0.13	29,31,35,37	0
4	NA	D	508	1/1	0.86	0.12	30,30,30,30	0
4	NA	B	510	1/1	0.88	0.08	35,35,35,35	0
8	GOL	B	504	6/6	0.89	0.10	25,25,25,27	0
4	NA	B	507	1/1	0.92	0.09	19,19,19,19	0
4	NA	B	508	1/1	0.92	0.09	24,24,24,24	0
7	NAD	B	503	36/44	0.93	0.10	19,25,50,55	0
4	NA	C	202	1/1	0.94	0.07	35,35,35,35	0
4	NA	D	507	1/1	0.94	0.11	25,25,25,25	0
4	NA	A	202	1/1	0.95	0.18	22,22,22,22	0
7	NAD	D	503	33/44	0.95	0.09	16,21,36,42	0
9	CL	D	505	1/1	0.95	0.07	21,21,21,21	0
6	FNR	B	502	31/31	0.95	0.08	10,12,13,14	0
6	FNR	D	502	31/31	0.97	0.07	9,11,12,12	0
9	CL	B	506	1/1	0.98	0.04	14,14,14,14	0
4	NA	C	203	1/1	0.99	0.17	12,12,12,12	0
3	FES	C	201	4/4	0.99	0.02	10,10,10,11	0
3	FES	A	201	4/4	0.99	0.02	10,11,11,11	0
5	SF4	B	501	8/8	0.99	0.03	11,13,13,13	0
5	SF4	D	501	8/8	0.99	0.02	11,11,12,12	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.

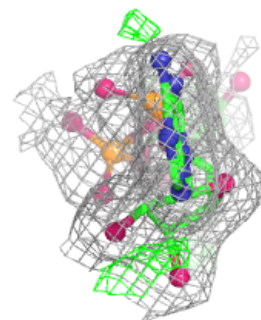
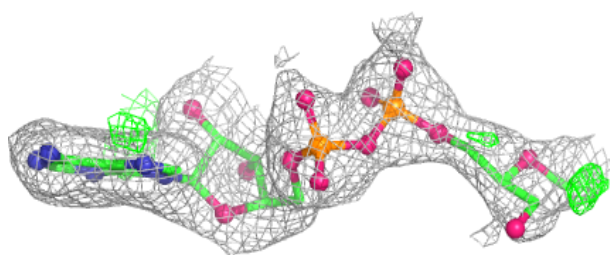
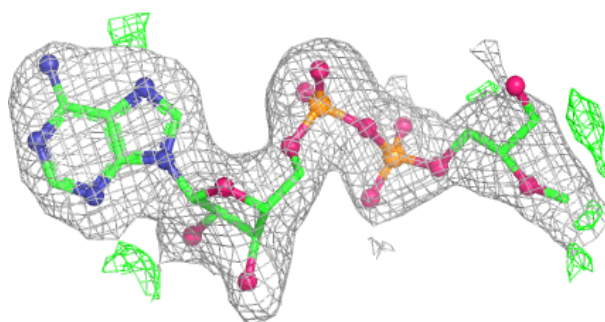
Electron density around NAD B 503:

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



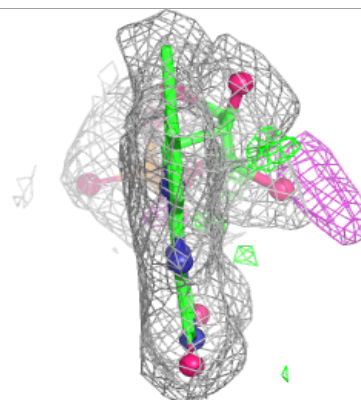
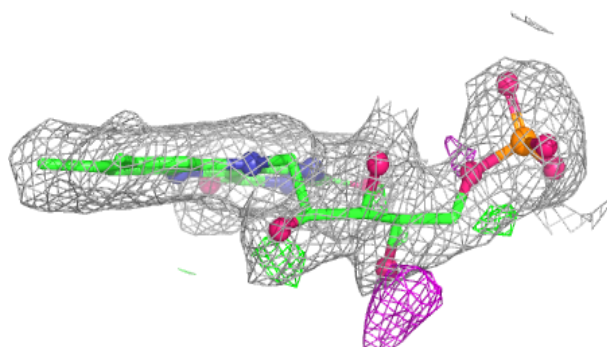
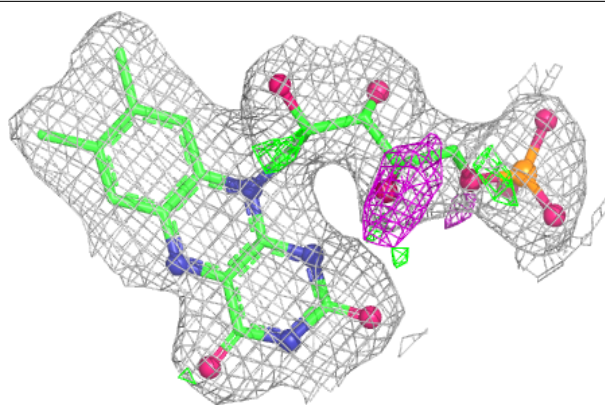
Electron density around NAD D 503:

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

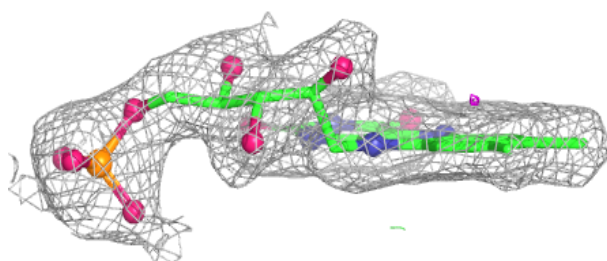
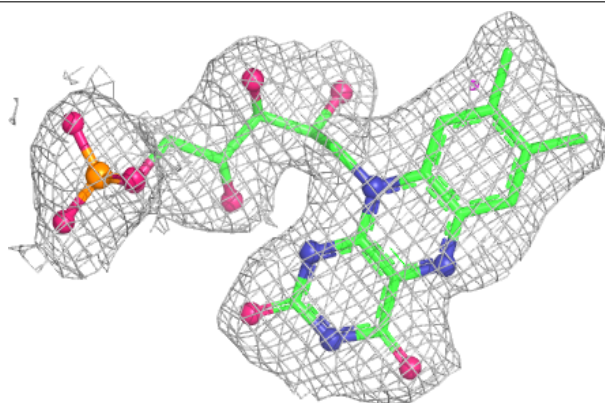


Electron density around FNR B 502:

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

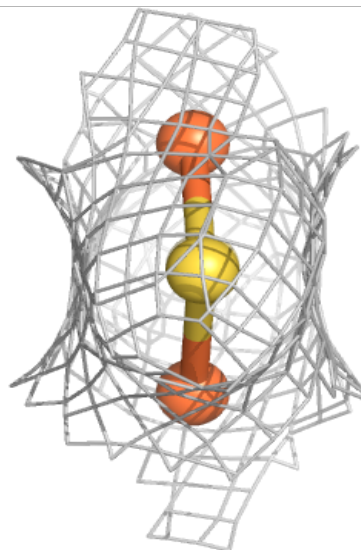
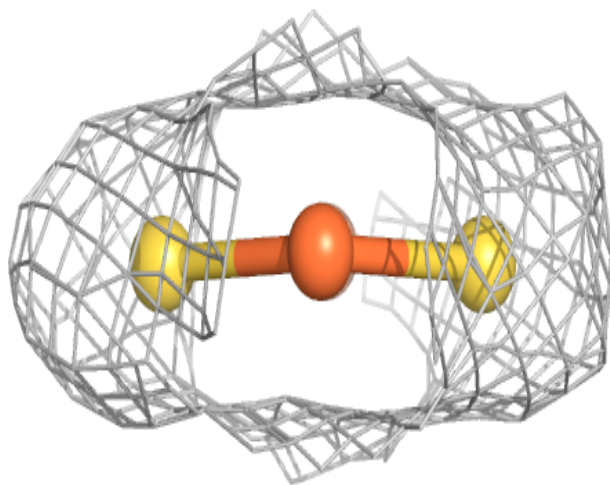
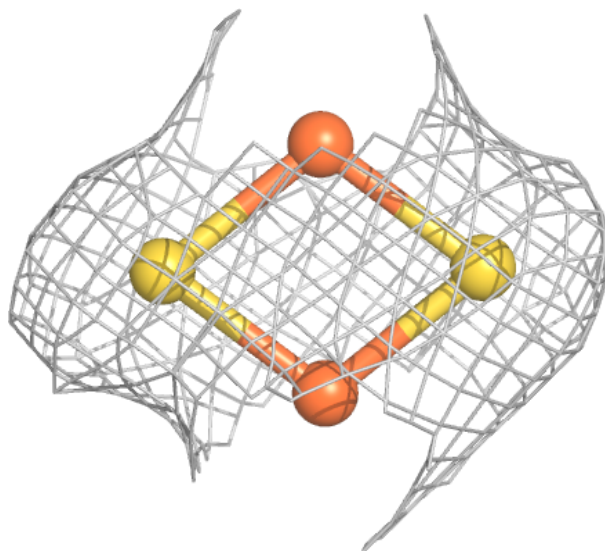
**Electron density around FNR D 502:**

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



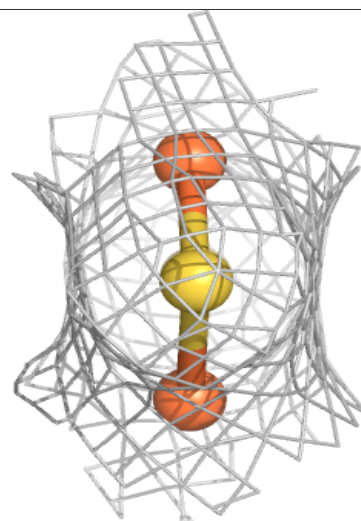
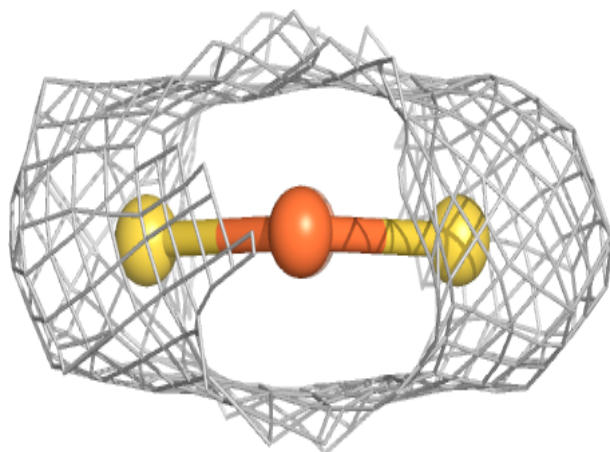
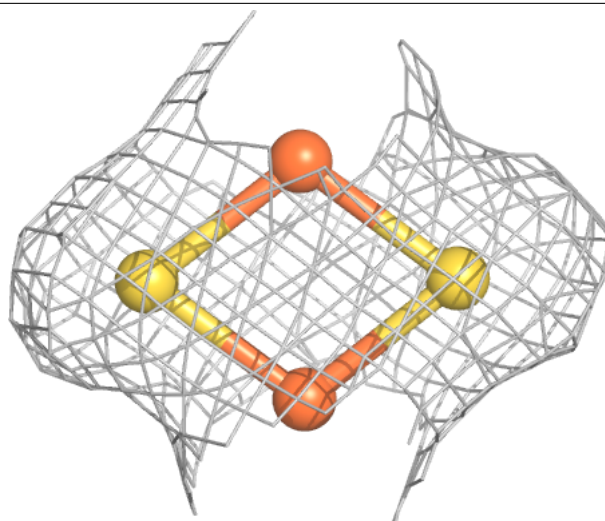
Electron density around FES C 201:

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



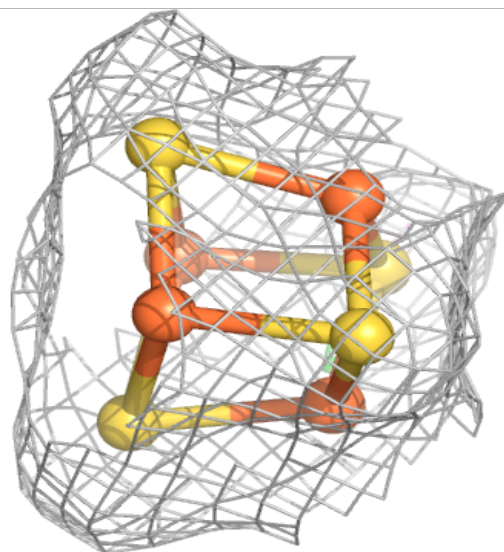
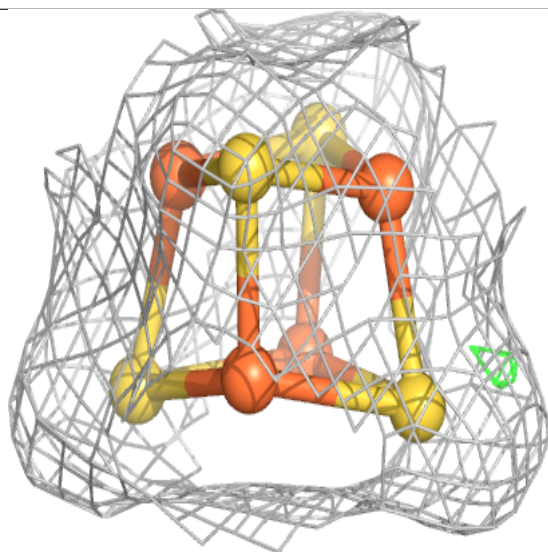
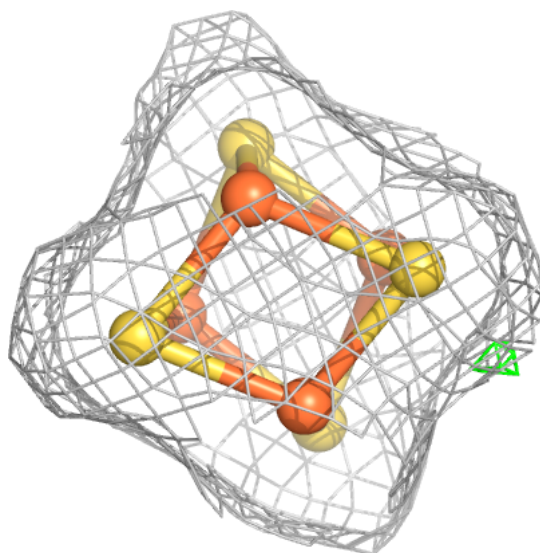
Electron density around FES A 201:

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



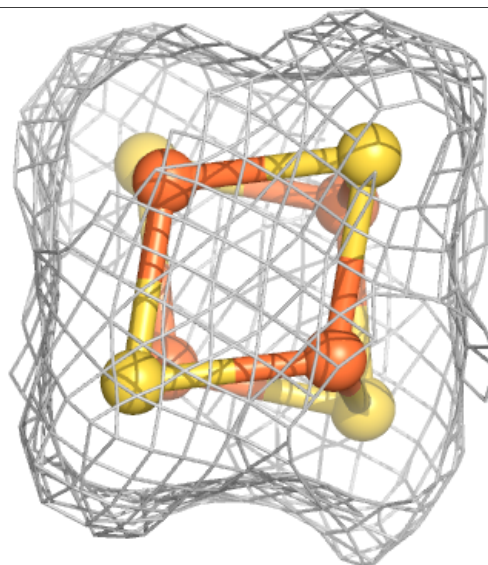
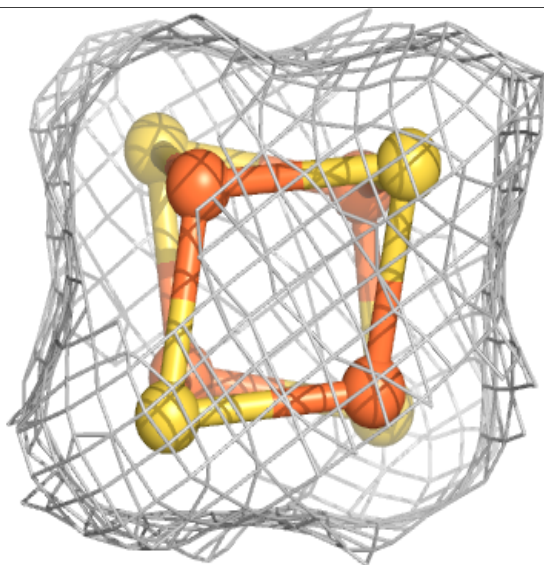
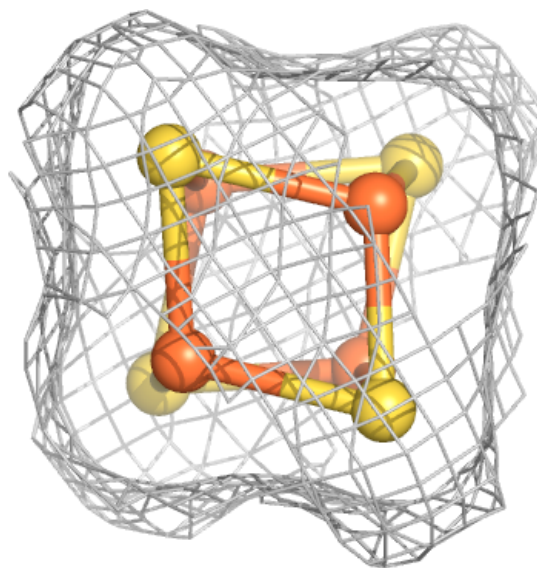
Electron density around SF4 B 501:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.