



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 PM UTC

PDB ID : 8QH7 / pdb_00008qh7
Title : Crystal structure of respiratory Complex I subunits NuoEF from *Aquifex aeolicus* bound to reduced 3-acetylpyridine adenine dinucleotide (without reducing agent)
Authors : Wohlwend, D.; Friedrich, T.
Deposited on : 2023-09-06
Resolution : 1.85 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

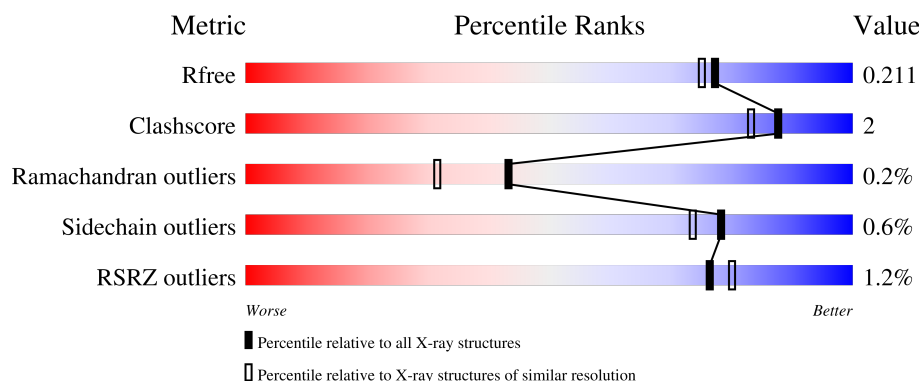
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	
1	C	160	
2	B	434	
2	D	434	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10544 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	155	Total	C	N	O	S	0	1	0
			1268	821	206	232	9			

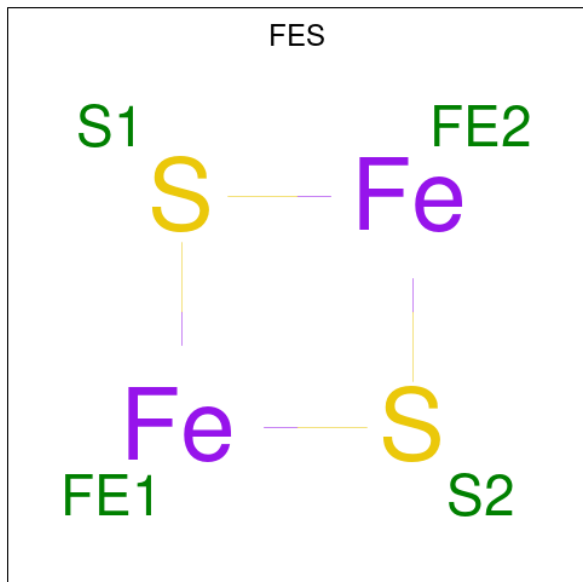
- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	S	0	5	0
			3323	2135	556	619	13			
2	D	417	Total	C	N	O	S	0	9	0
			3367	2161	559	634	13			

There are 16 discrepancies between the modelled and reference sequences:

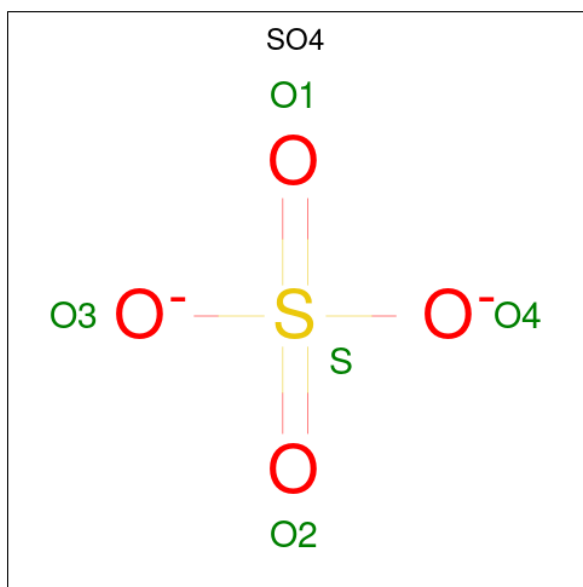
Chain	Residue	Modelled	Actual	Comment	Reference
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag	UNP O66841
B	434	HIS	-	expression tag	UNP O66841
D	427	ALA	-	expression tag	UNP O66841
D	428	GLY	-	expression tag	UNP O66841
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 SULFATE ION (CCD ID: SO4) (formula: O_4S).

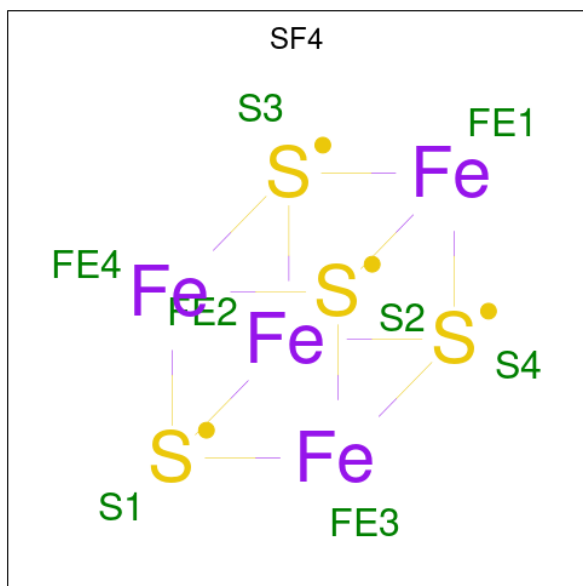


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

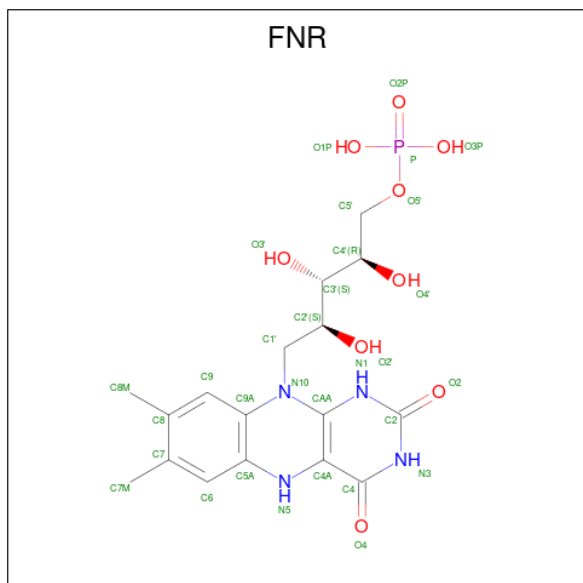
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	4	Total Na 4 4	0	0
5	C	1	Total Na 1 1	0	0
5	D	3	Total Na 3 3	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



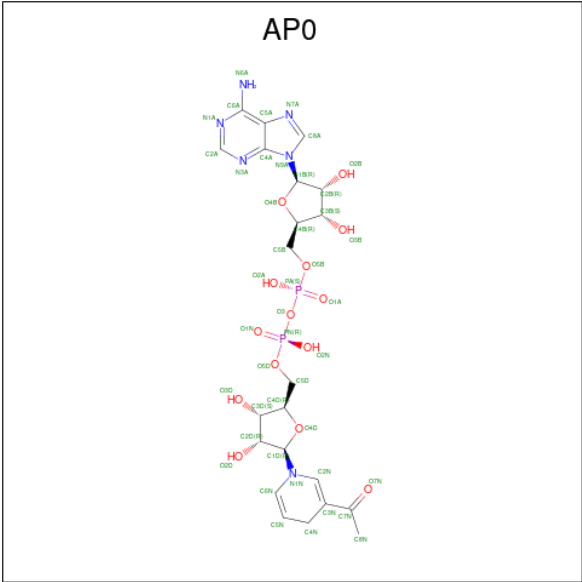
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	D	1	Total	Fe	S	0	0
			8	4	4		

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



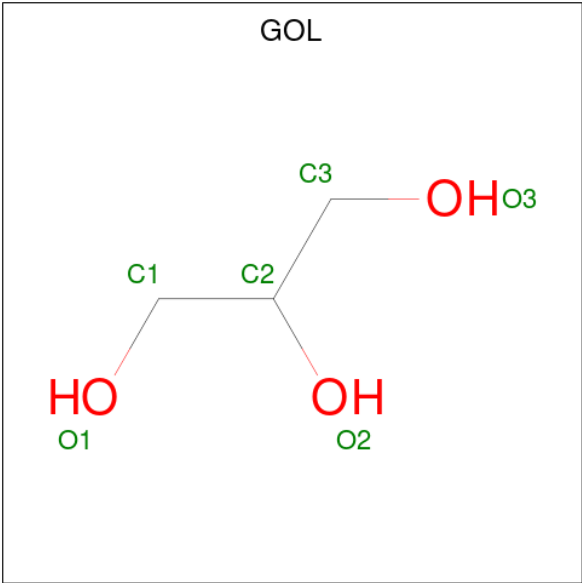
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
7	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 8 is ACETYL PYRIDINE ADENINE DINUCLEOTIDE, REDUCED (CCD ID: AP0) (formula: $C_{22}H_{30}N_6O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 44	C 22	N 6	O 14	P 2	0	0
8	D	1	Total 44	C 22	N 6	O 14	P 2	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



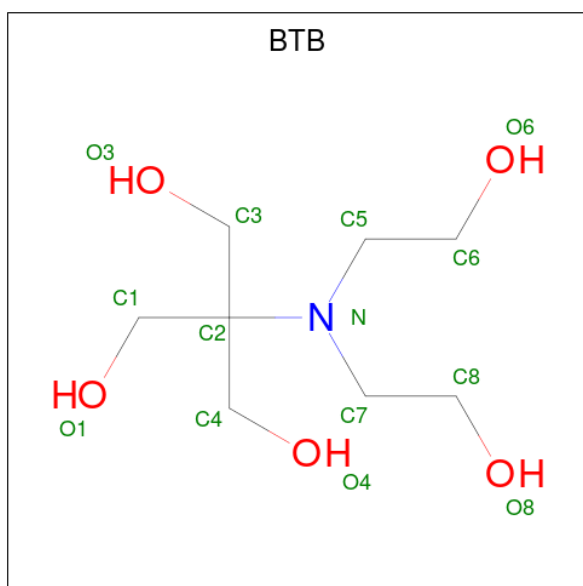
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 10 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	151	Total	O	0	0
			151	151		
11	B	400	Total	O	0	2
			402	402		
11	C	125	Total	O	0	0
			125	125		
11	D	389	Total	O	0	1
			390	390		

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.

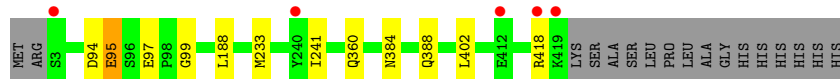
- Molecule 1: NADH-quinone oxidoreductase subunit E



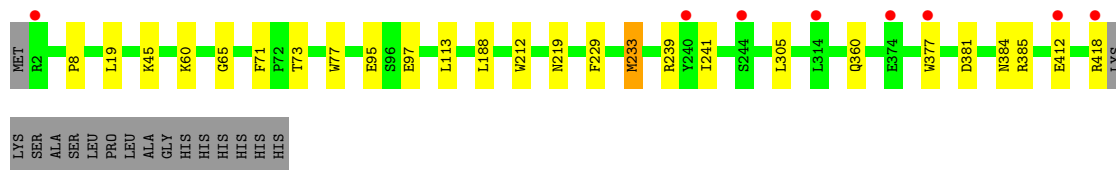
- Molecule 1: NADH-quinone oxidoreductase subunit E



- 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	63.23Å 116.45Å 190.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 1.85 49.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-1.85) 99.9 (49.70-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.171 , 0.201 0.182 , 0.211	Depositor DCC
R_{free} test set	6201 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	0.460	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10544	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 48.20 % 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 8.8964e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FNR, AP0, BTB, FES, GOL, SF4, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1297	0.83	0/1752
1	C	0.46	0/1297	0.80	0/1752
2	B	0.49	0/3404	0.84	0/4605
2	D	0.48	0/3449	0.83	0/4666
All	All	0.48	0/9447	0.83	0/12775

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1268	0	1269	4	0
1	C	1268	0	1268	5	0
2	B	3323	0	3290	9	0
2	D	3367	0	3312	19	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	10	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	4	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
6	B	8	0	0	0	0
6	D	8	0	0	0	0
7	B	31	0	22	0	0
7	D	31	0	22	0	0
8	B	44	0	29	2	0
8	D	44	0	29	2	0
9	B	18	0	24	0	0
9	D	12	0	16	0	0
10	B	12	0	16	1	0
11	A	151	0	0	1	0
11	B	402	0	0	2	0
11	C	125	0	0	0	0
11	D	390	0	0	4	0
All	All	10544	0	9297	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (37) 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:73:THR:OG1	11:D:601:HOH:O	2.01	0.78
2:D:381:ASP:OD2	2:D:385[B]:ARG:NH2	2.19	0.75
2:D:71:PHE:O	11:D:601:HOH:O	2.04	0.75
2:D:360:GLN:NE2	2:D:384:ASN:HD22	1.97	0.62
1:C:133:GLU:HG3	2:D:8:PRO:HB2	1.84	0.59
2:B:360:GLN:NE2	2:B:384:ASN:HD22	1.99	0.59
2:D:77:TRP:HE1	2:D:219:ASN:HD21	1.51	0.59
10:B:511:BTB:H81	11:B:646:HOH:O	2.06	0.54
2:D:77:TRP:HE1	2:D:219:ASN:ND2	2.06	0.53
2:D:377:TRP:HB3	2:D:418:ARG:NH1	2.23	0.53
2:D:65:GLY:N	11:D:601:HOH:O	2.41	0.53
2:B:233:MET:HE1	2:B:241:ILE:HD11	1.90	0.52
1:A:23:PHE:HB2	11:A:387:HOH:O	2.09	0.52
1:C:50:LYS:HB3	1:C:51:PRO:HD3	1.92	0.51
2:B:402:LEU:C	2:B:402:LEU:HD23	2.37	0.50
2:D:97:GLU:HB2	8:D:503:AP0:H42	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:MET:HE1	2:D:241:ILE:HD11	1.97	0.47
2:D:360:GLN:HE21	2:D:384:ASN:HD22	1.62	0.47
2:B:388:GLN:HG3	11:B:612:HOH:O	2.16	0.46
8:B:503:AP0:H81	8:B:503:AP0:H2	1.82	0.46
2:B:188:LEU:C	2:B:188:LEU:HD23	2.41	0.45
2:D:188:LEU:C	2:D:188:LEU:HD23	2.41	0.45
1:A:50:LYS:HB3	1:A:51:PRO:HD3	1.97	0.45
2:D:60:LYS:O	2:D:239:ARG:HD2	2.15	0.45
2:D:377:TRP:HB3	2:D:418:ARG:HH12	1.81	0.44
2:D:229:PHE:O	2:D:233:MET:HG3	2.17	0.44
1:C:25:LYS:HD2	2:D:212:TRP:CZ2	2.53	0.44
2:D:19:LEU:HD13	2:D:113:LEU:HD21	1.99	0.44
2:B:97:GLU:HB2	8:B:503:AP0:H42	2.00	0.43
2:B:94:ASP:O	2:B:95:GLU:C	2.61	0.43
8:D:503:AP0:H2	8:D:503:AP0:H81	1.81	0.43
1:C:91:CYS:HA	1:C:134:ALA:HB1	2.01	0.42
2:D:45:LYS:NZ	11:D:624:HOH:O	2.53	0.42
1:C:133:GLU:HB3	1:C:145:LYS:HB2	2.02	0.41
2:B:418[B]:ARG:HG2	2:B:418[B]:ARG:O	2.21	0.41
1:A:110:LYS:HB3	1:A:111:PRO:HD2	2.03	0.40
1:A:131:CYS:SG	2:B:99:GLY:HA2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	154/160 (96%)	149 (97%)	5 (3%)	0	100	100
1	C	154/160 (96%)	149 (97%)	5 (3%)	0	100	100
2	B	420/434 (97%)	412 (98%)	7 (2%)	1 (0%)	43	31
2	D	424/434 (98%)	415 (98%)	8 (2%)	1 (0%)	43	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1152/1188 (97%)	1125 (98%)	25 (2%)	2 (0%)	43 31

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%)	141 (99%)	1 (1%)	76 70
1	C	141/146 (97%)	139 (99%)	2 (1%)	59 49
2	B	346/357 (97%)	346 (100%)	0	100 100
2	D	351/357 (98%)	347 (99%)	4 (1%)	65 57
All	All	980/1006 (97%)	973 (99%)	7 (1%)	78 70

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

Mol	Chain	Res	Type
1	A	47	GLU
1	C	15	LYS
1	C	47	GLU
2	D	233	MET
2	D	305	LEU
2	D	412[A]	GLU
2	D	412[B]	GLU

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

Mol	Chain	Res	Type
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	153	ASN
2	B	41	GLN
2	B	83	ASN
2	B	128	ASN
2	B	220	ASN
2	B	344	HIS
2	B	360	GLN
2	B	362	ASN
1	C	61	ASN
1	C	97	ASN
1	C	153	ASN
2	D	208	GLN
2	D	219	ASN
2	D	360	GLN
2	D	362	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 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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
9	GOL	B	506	-	5,5,5	0.17	0	5,5,5	0.45	0
4	SO4	C	202	-	4,4,4	0.30	0	6,6,6	0.11	0
9	GOL	B	505	-	5,5,5	0.12	0	5,5,5	0.32	0
4	SO4	A	203	-	4,4,4	0.31	0	6,6,6	0.07	0
9	GOL	B	504	-	5,5,5	0.09	0	5,5,5	0.22	0
9	GOL	D	504	-	5,5,5	0.07	0	5,5,5	0.22	0
4	SO4	D	506	-	4,4,4	0.32	0	6,6,6	0.15	0
4	SO4	C	203	-	4,4,4	0.31	0	6,6,6	0.09	0
7	FNR	D	502	-	32,33,33	0.44	0	41,50,50	0.59	0
7	FNR	B	502	-	32,33,33	0.36	0	41,50,50	0.49	0
3	FES	C	201	1	0,4,4	-	-	-	-	-
6	SF4	D	501	2	0,12,12	-	-	-	-	-
10	BTB	B	511	-	11,11,13	1.18	2 (18%)	11,12,16	0.65	0
6	SF4	B	501	2	0,12,12	-	-	-	-	-
4	SO4	A	202	-	4,4,4	0.31	0	6,6,6	0.11	0
3	FES	A	201	1	0,4,4	-	-	-	-	-
8	AP0	D	503	-	47,48,48	0.43	0	65,73,73	0.47	0
9	GOL	D	505	-	5,5,5	0.12	0	5,5,5	0.34	0
8	AP0	B	503	-	47,48,48	0.39	0	65,73,73	0.47	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
7	FNR	B	502	-	-	2/18/18/18	0/3/3/3
3	FES	A	201	1	-	-	0/1/1/1
9	GOL	B	506	-	-	3/4/4/4	-
6	SF4	B	501	2	-	-	0/6/5/5
9	GOL	B	504	-	-	0/4/4/4	-
9	GOL	D	504	-	-	2/4/4/4	-
3	FES	C	201	1	-	-	0/1/1/1
6	SF4	D	501	2	-	-	0/6/5/5
8	AP0	D	503	-	-	1/30/72/72	0/5/5/5
7	FNR	D	502	-	-	2/18/18/18	0/3/3/3
9	GOL	D	505	-	-	0/4/4/4	-
9	GOL	B	505	-	-	4/4/4/4	-
10	BTB	B	511	-	-	4/14/14/21	-
8	AP0	B	503	-	-	1/30/72/72	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	511	BTB	C5-N	2.44	1.51	1.47
10	B	511	BTB	C7-N	2.39	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	505	GOL	O1-C1-C2-C3
9	B	505	GOL	C1-C2-C3-O3
9	B	505	GOL	O2-C2-C3-O3
9	B	506	GOL	O1-C1-C2-C3
9	B	505	GOL	O1-C1-C2-O2
9	B	506	GOL	O1-C1-C2-O2
9	B	506	GOL	O2-C2-C3-O3
8	D	503	AP0	O4D-C1D-N1N-C2N
10	B	511	BTB	C1-C2-N-C5
10	B	511	BTB	C1-C2-N-C7
10	B	511	BTB	C3-C2-N-C7
8	B	503	AP0	O4D-C1D-N1N-C2N
7	B	502	FNR	C4'-C5'-O5'-P
7	D	502	FNR	C4'-C5'-O5'-P
9	D	504	GOL	O2-C2-C3-O3
9	D	504	GOL	C1-C2-C3-O3
10	B	511	BTB	N-C2-C3-O3
7	B	502	FNR	N10-C1'-C2'-O2'
7	D	502	FNR	N10-C1'-C2'-O2'

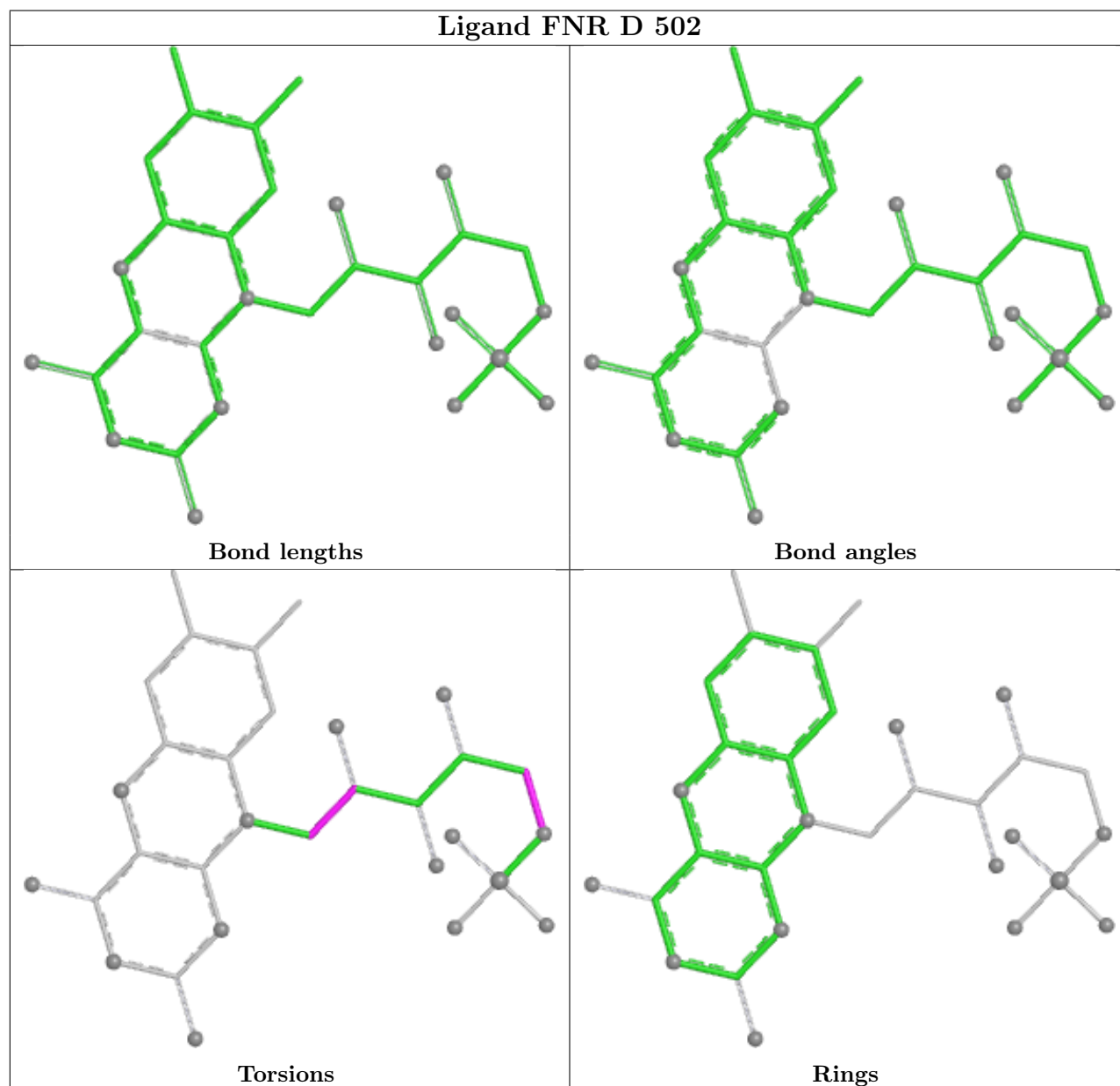
There are no ring outliers.

3 monomers are involved in 5 short contacts:

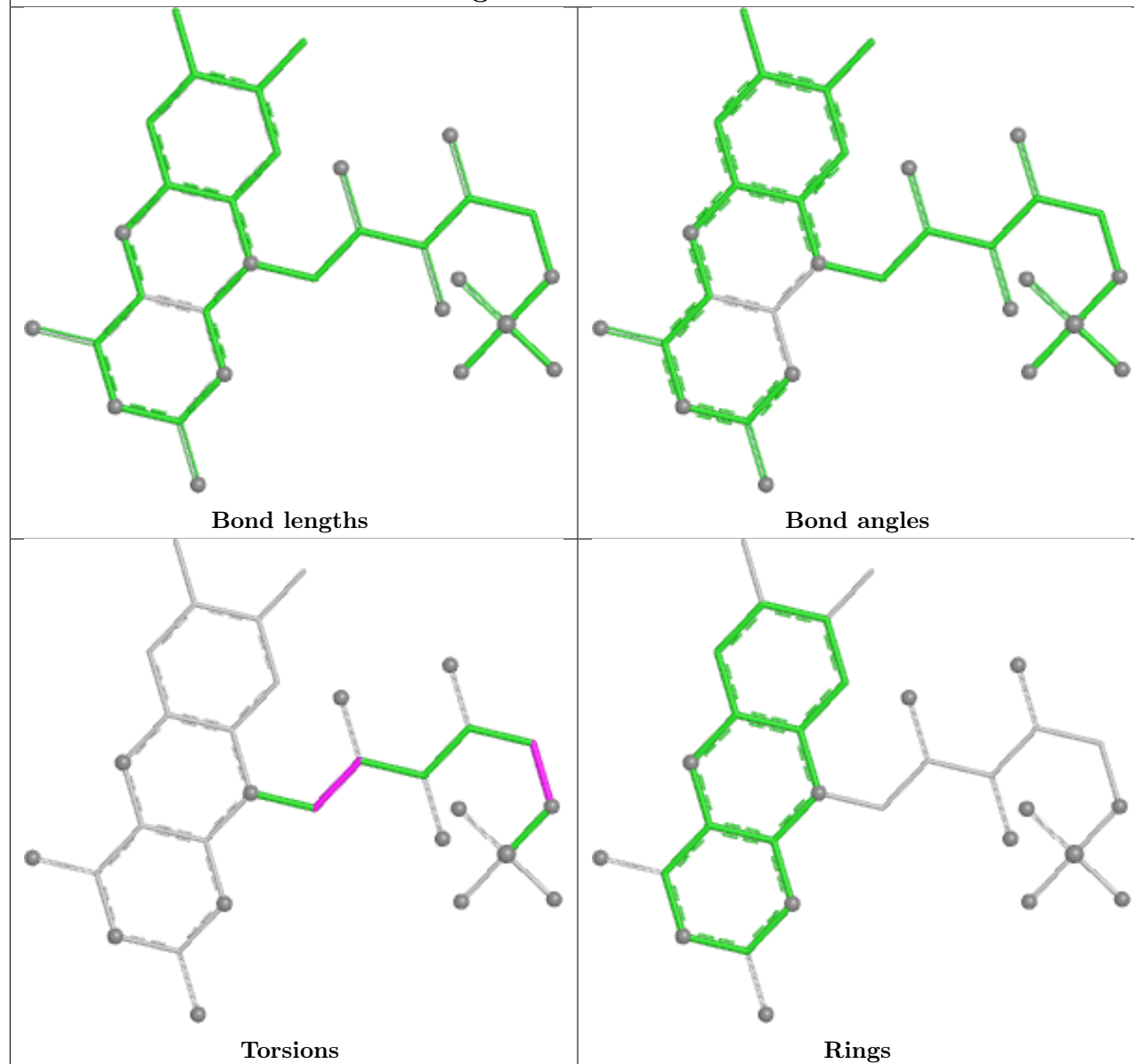
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	511	BTB	1	0
8	D	503	AP0	2	0
8	B	503	AP0	2	0

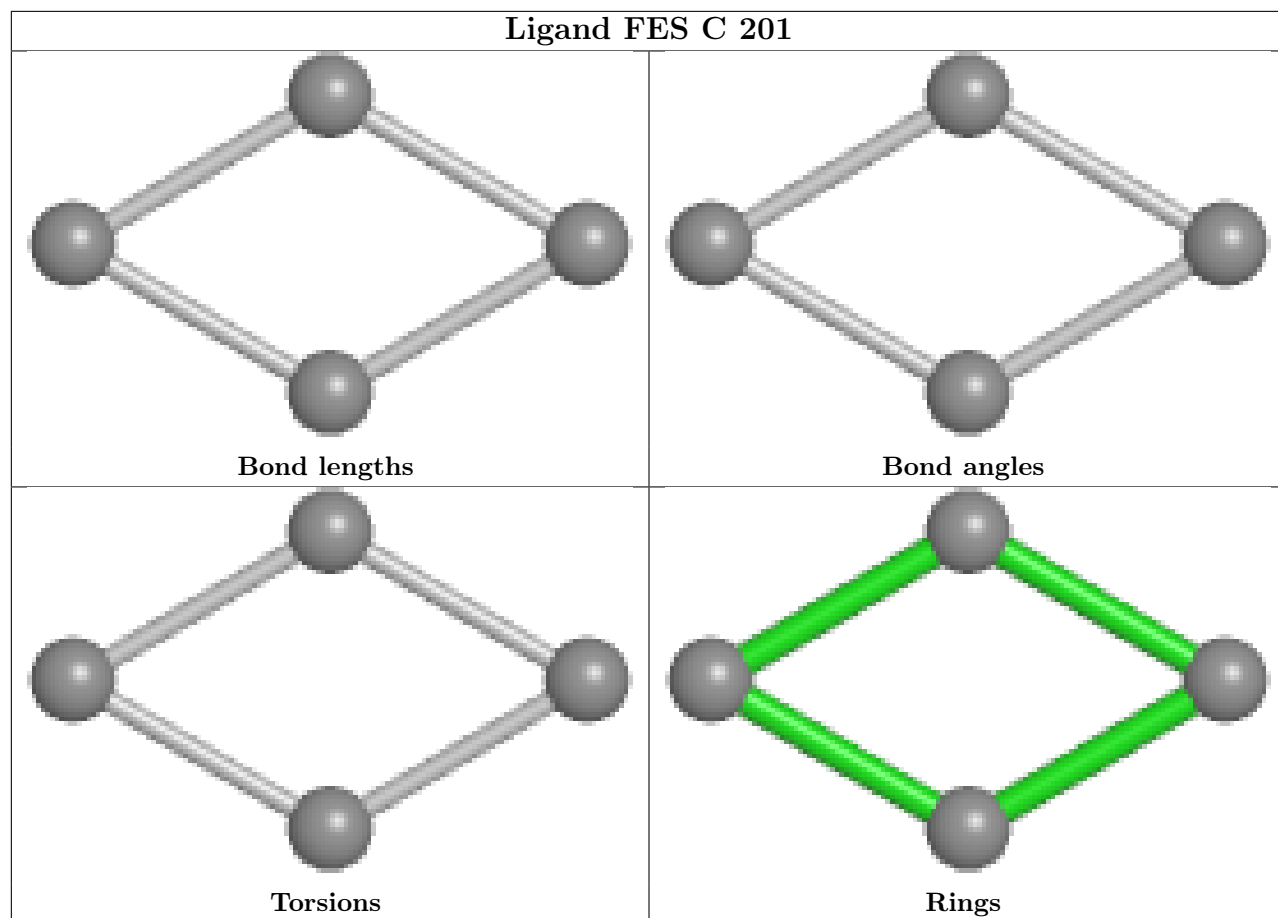
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

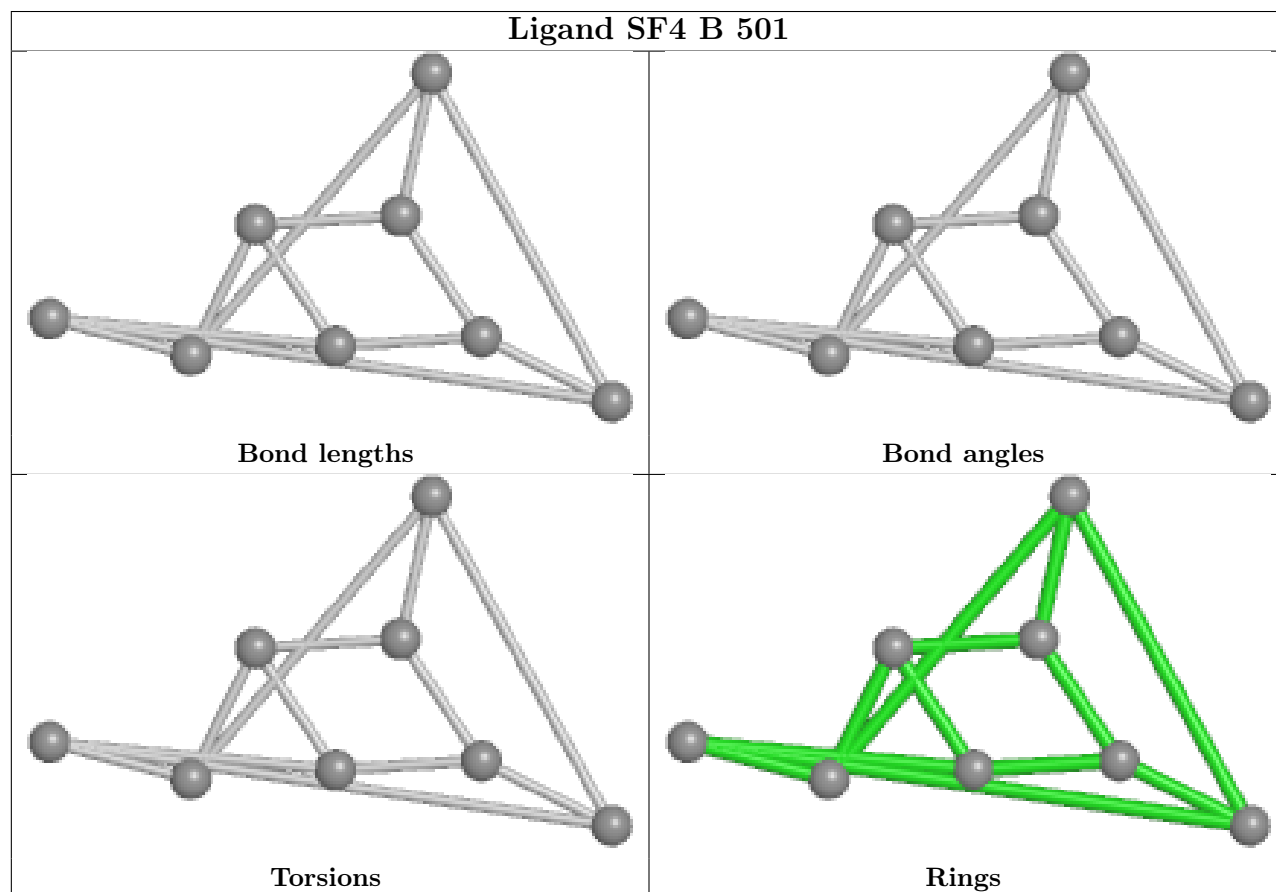
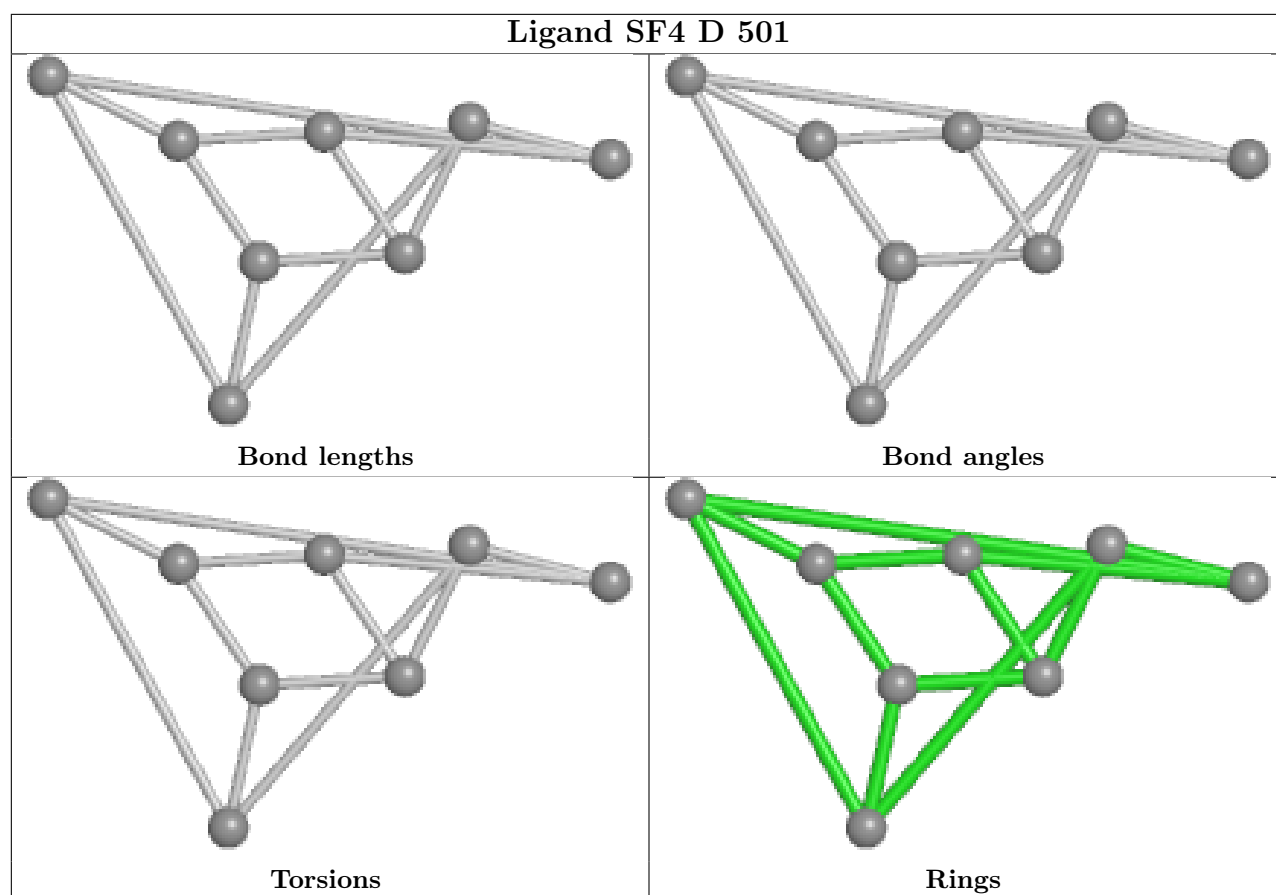
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

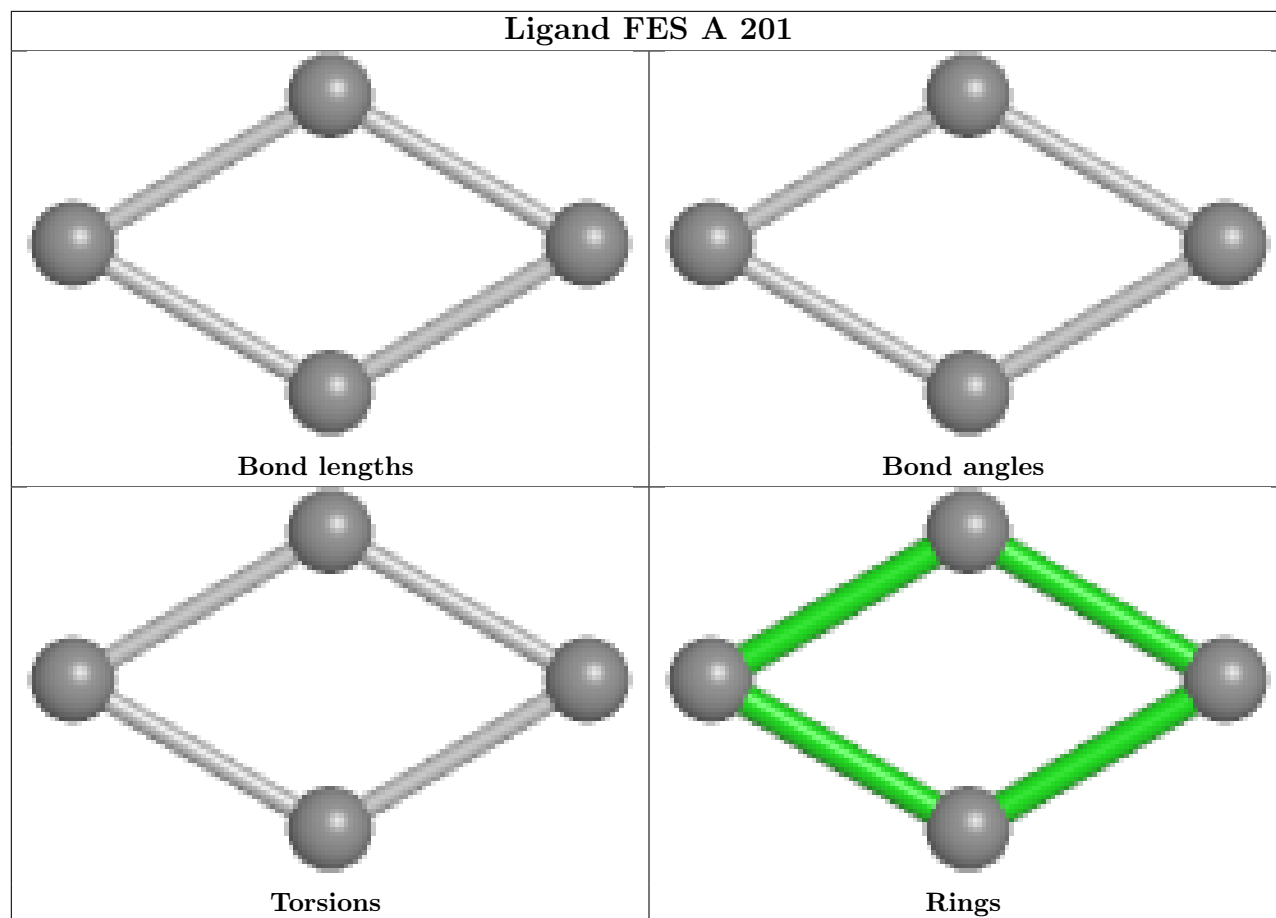


Ligand FNR B 502

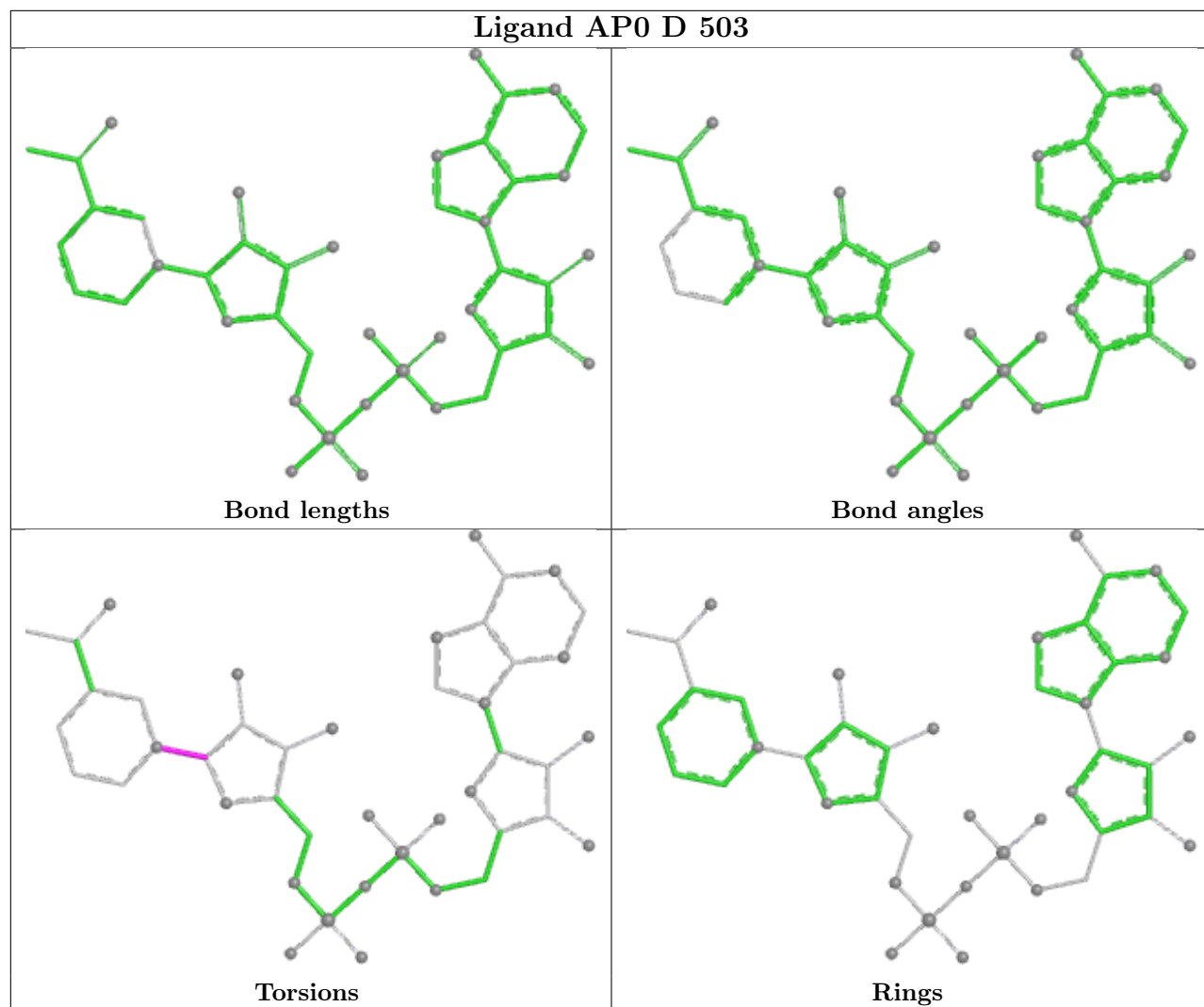


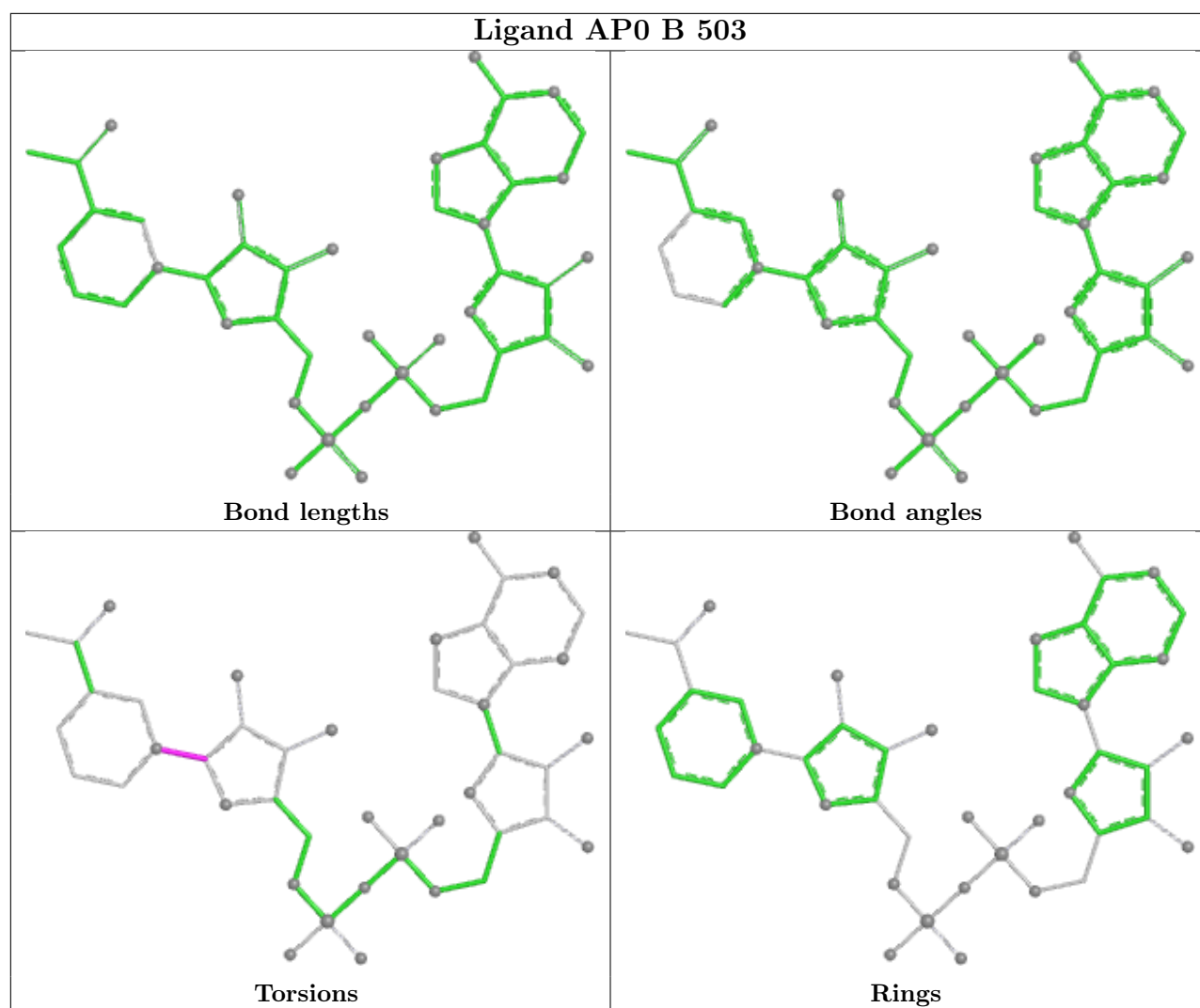






Ligand AP0 D 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/160 (97%)	0.13	1 (0%) 85 88	21, 34, 55, 84	0
1	C	155/160 (96%)	0.03	0 100 100	16, 35, 55, 74	1 (0%)
2	B	417/434 (96%)	-0.26	5 (1%) 76 80	11, 26, 39, 66	5 (1%)
2	D	417/434 (96%)	-0.16	8 (1%) 66 70	11, 27, 42, 67	9 (2%)
All	All	1145/1188 (96%)	-0.13	14 (1%) 76 80	11, 28, 47, 84	15 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	240[A]	TYR	4.8
2	D	418	ARG	3.4
2	B	3	SER	3.1
2	B	418[A]	ARG	3.0
2	D	377	TRP	2.8
2	D	2	ARG	2.6
2	D	244	SER	2.6
2	B	240	TYR	2.6
2	B	419	LYS	2.3
2	D	412[A]	GLU	2.3
2	D	374	GLU	2.2
1	A	6	PHE	2.2
2	D	314	LEU	2.0
2	B	412	GLU	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 ⓘ

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.

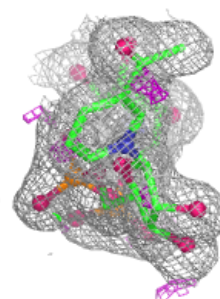
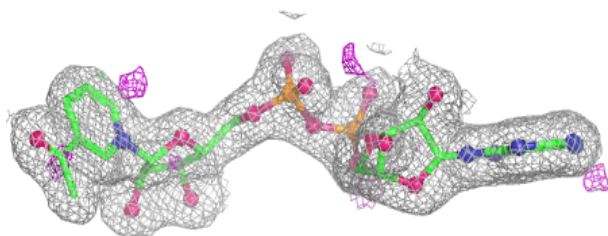
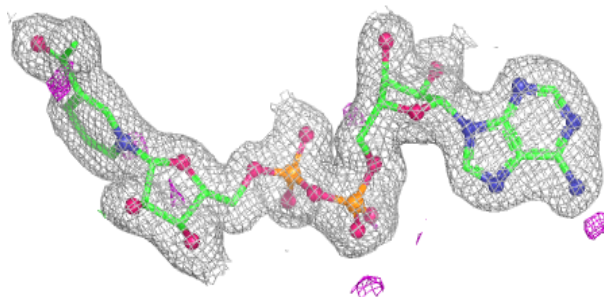
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	B	506	6/6	0.73	0.20	49,52,56,57	0
9	GOL	B	505	6/6	0.74	0.21	34,43,52,53	0
10	BTB	B	511	12/14	0.74	0.18	46,55,61,61	0
9	GOL	D	505	6/6	0.76	0.18	55,58,62,62	0
4	SO4	A	202	5/5	0.77	0.11	73,74,76,78	0
5	NA	B	509	1/1	0.77	0.17	51,51,51,51	0
5	NA	C	204	1/1	0.80	0.18	57,57,57,57	0
4	SO4	C	203	5/5	0.85	0.13	54,61,64,71	0
4	SO4	D	506	5/5	0.85	0.11	38,49,50,52	0
4	SO4	A	203	5/5	0.85	0.12	56,67,73,76	0
4	SO4	C	202	5/5	0.85	0.10	57,60,62,64	0
5	NA	D	507	1/1	0.87	0.38	63,63,63,63	0
5	NA	B	508	1/1	0.88	0.51	53,53,53,53	0
5	NA	D	509	1/1	0.90	0.13	50,50,50,50	0
5	NA	D	508	1/1	0.93	0.11	46,46,46,46	0
9	GOL	B	504	6/6	0.93	0.09	30,33,34,35	0
9	GOL	D	504	6/6	0.94	0.10	28,30,32,32	0
5	NA	B	507	1/1	0.95	0.12	39,39,39,39	0
5	NA	B	510	1/1	0.96	0.19	39,39,39,39	0
8	AP0	D	503	44/44	0.96	0.07	24,28,33,36	0
8	AP0	B	503	44/44	0.97	0.05	21,23,27,28	0
7	FNR	D	502	31/31	0.97	0.05	19,20,20,21	0
7	FNR	B	502	31/31	0.98	0.04	18,19,21,21	0
5	NA	A	204	1/1	0.98	0.09	27,27,27,27	0
6	SF4	B	501	8/8	0.99	0.02	20,20,21,21	0
3	FES	A	201	4/4	1.00	0.02	20,21,21,22	0
6	SF4	D	501	8/8	1.00	0.02	19,20,21,21	0
3	FES	C	201	4/4	1.00	0.02	21,21,22,22	0

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

orientation to approximate a three-dimensional view.

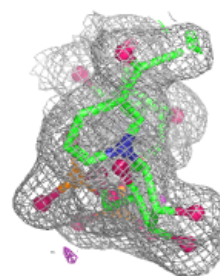
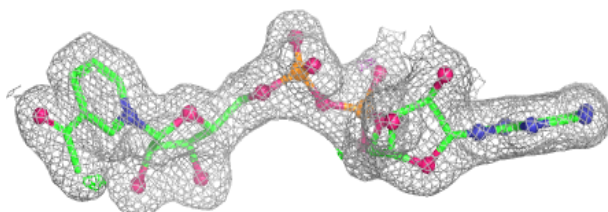
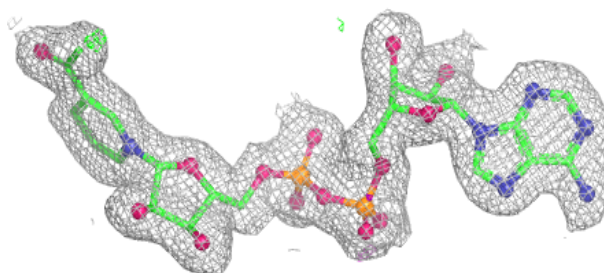
Electron density around AP0 D 503:

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



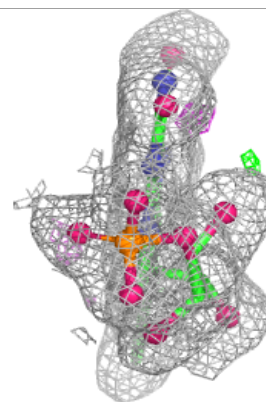
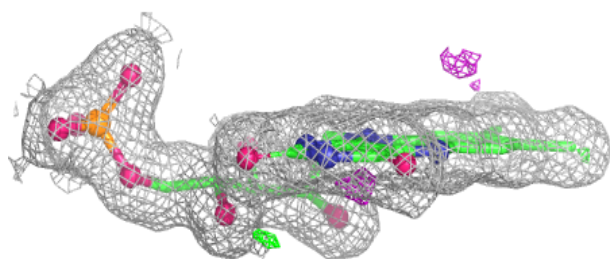
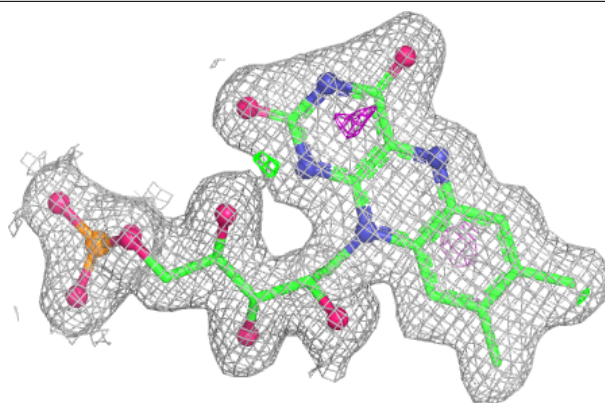
Electron density around AP0 B 503:

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

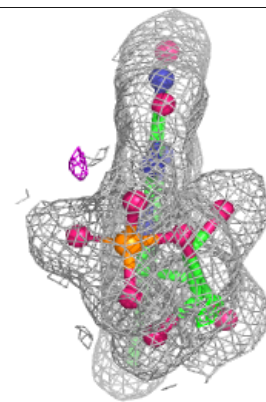
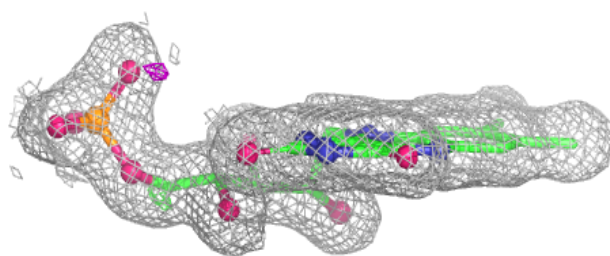
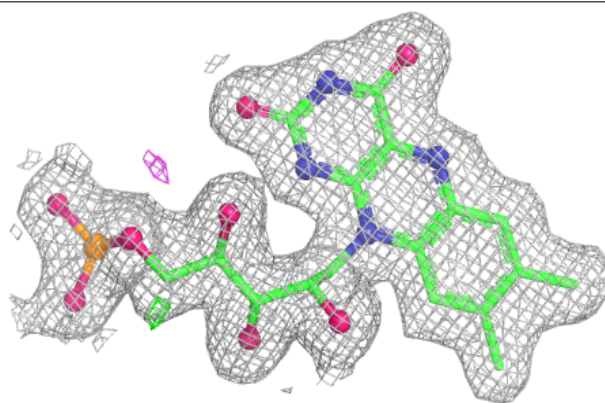


Electron density around FNR D 502:

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

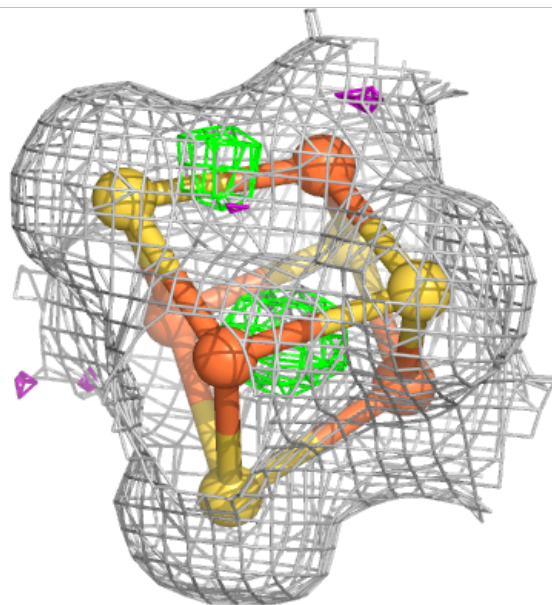
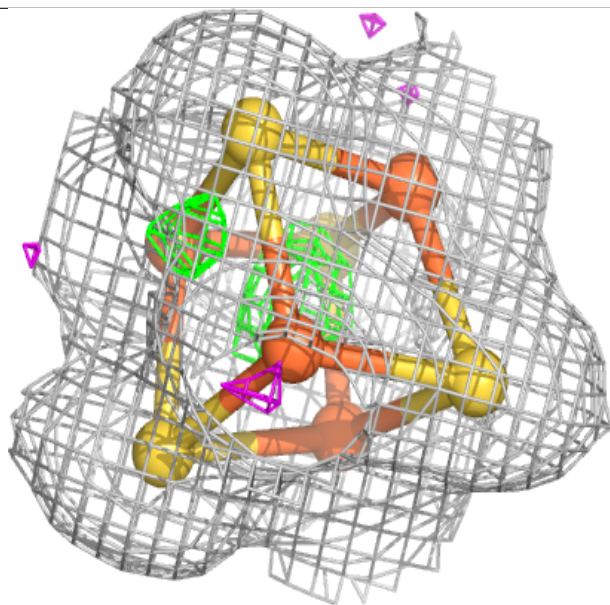
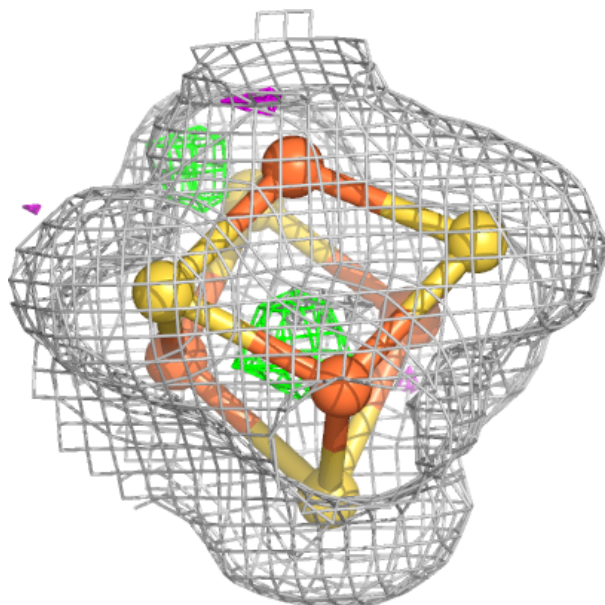
**Electron density around FNR B 502:**

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



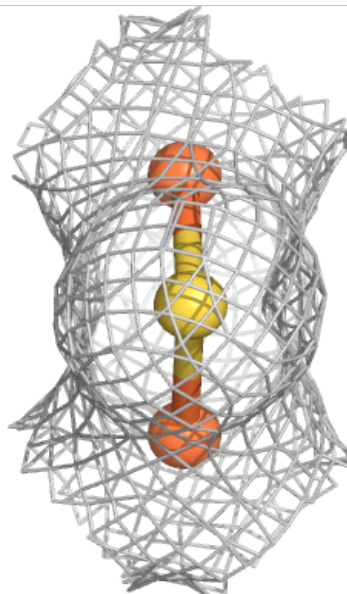
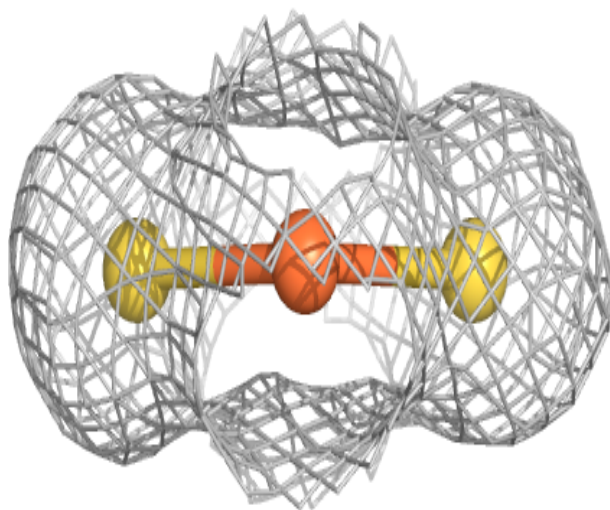
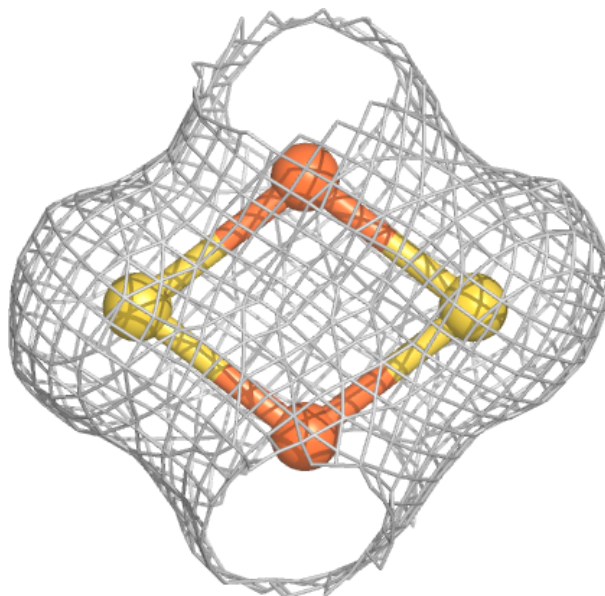
Electron density around SF4 B 501:

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



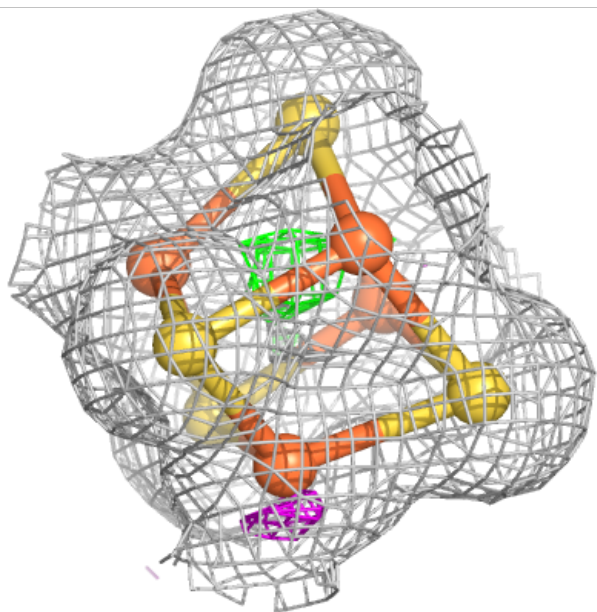
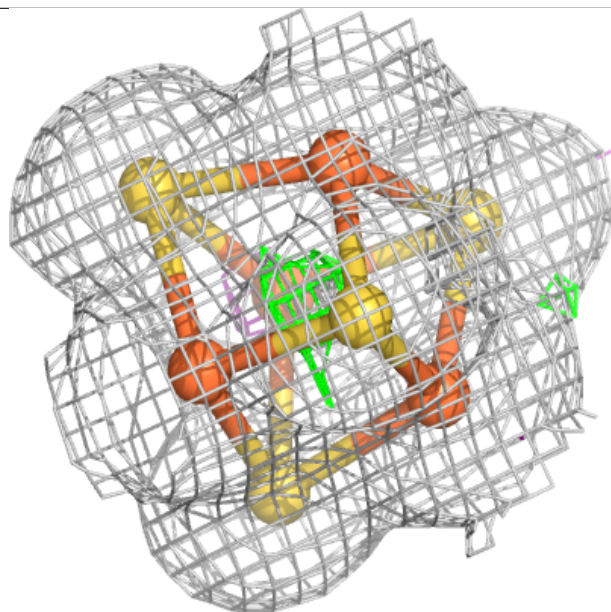
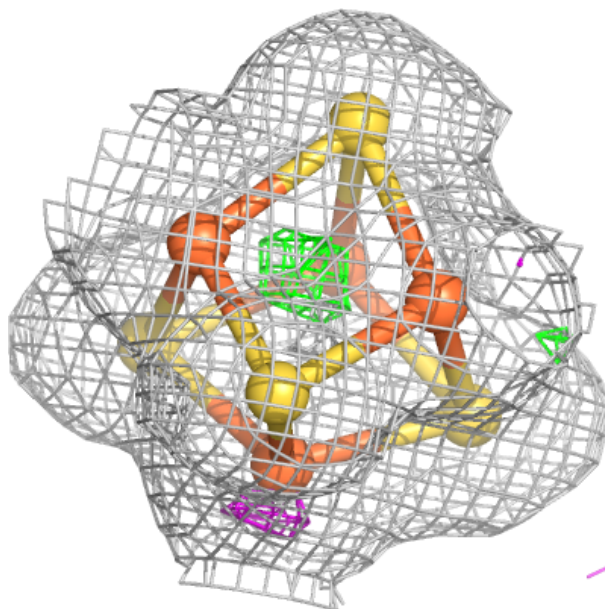
Electron density around FES A 201:

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



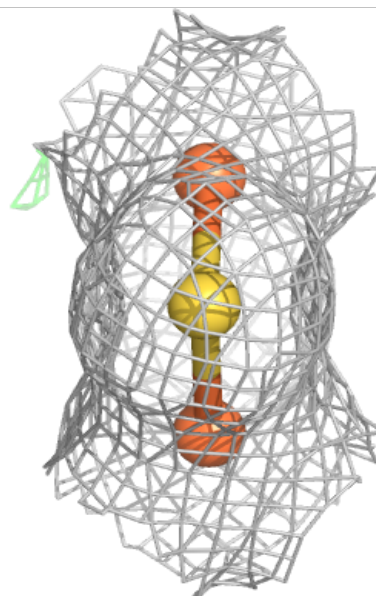
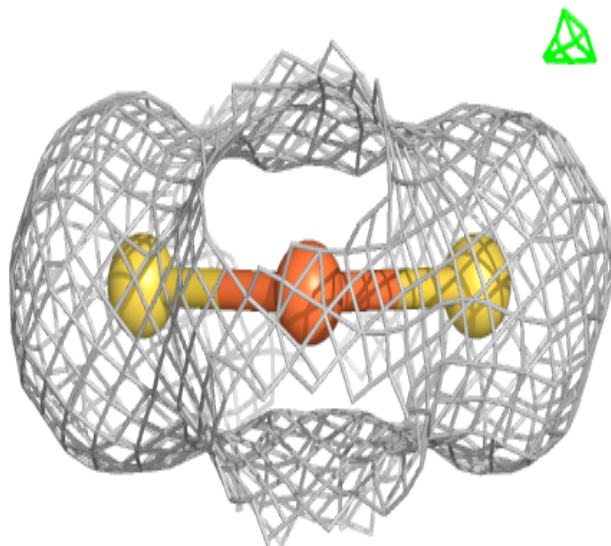
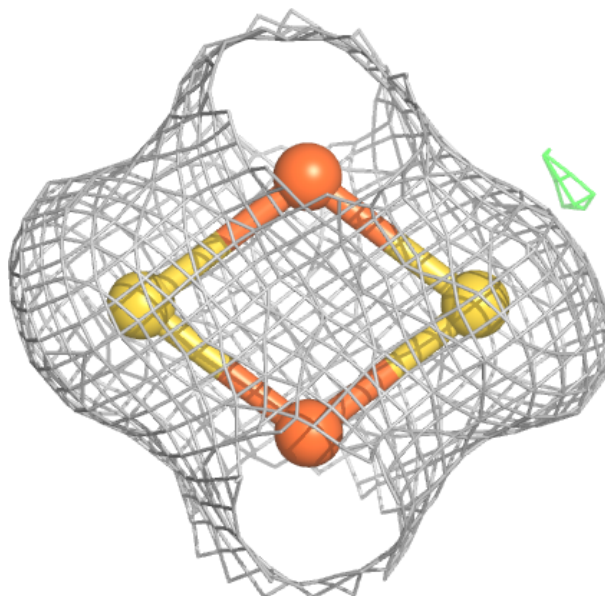
Electron density around SF4 D 501:

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



Electron density around FES C 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.