



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 05:50 pm BST

PDB ID : 9HQK / pdb_00009hqk
Title : Bacteroides fragilis lipoprotein XusB bound to ferrichrome
Authors : Silale, A.; van den Berg, B.
Deposited on : 2024-12-16
Resolution : 3.32 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

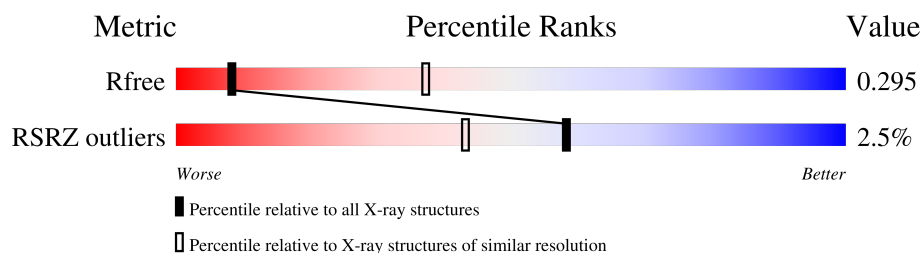
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1066 (3.34-3.30)
RSRZ outliers	164620	1066 (3.34-3.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11810 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 XusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2883	1832	470	568	13			
1	B	377	Total	C	N	O	S	0	0	0
			2900	1843	472	572	13			
1	C	376	Total	C	N	O	S	0	0	0
			2892	1837	471	571	13			
1	D	381	Total	C	N	O	S	0	0	0
			2939	1866	482	578	13			

There are 32 discrepancies between the modelled and reference sequences:

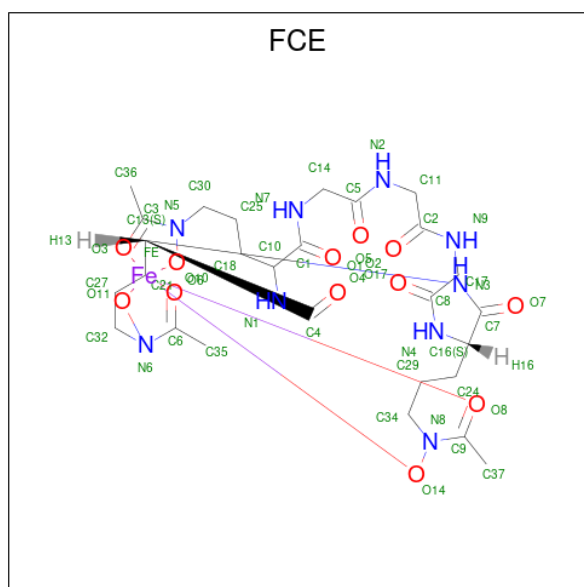
Chain	Residue	Modelled	Actual	Comment	Reference
A	407	LEU	-	expression tag	UNP Q5L7E3
A	408	GLU	-	expression tag	UNP Q5L7E3
A	409	HIS	-	expression tag	UNP Q5L7E3
A	410	HIS	-	expression tag	UNP Q5L7E3
A	411	HIS	-	expression tag	UNP Q5L7E3
A	412	HIS	-	expression tag	UNP Q5L7E3
A	413	HIS	-	expression tag	UNP Q5L7E3
A	414	HIS	-	expression tag	UNP Q5L7E3
B	407	LEU	-	expression tag	UNP Q5L7E3
B	408	GLU	-	expression tag	UNP Q5L7E3
B	409	HIS	-	expression tag	UNP Q5L7E3
B	410	HIS	-	expression tag	UNP Q5L7E3
B	411	HIS	-	expression tag	UNP Q5L7E3
B	412	HIS	-	expression tag	UNP Q5L7E3
B	413	HIS	-	expression tag	UNP Q5L7E3
B	414	HIS	-	expression tag	UNP Q5L7E3
C	407	LEU	-	expression tag	UNP Q5L7E3
C	408	GLU	-	expression tag	UNP Q5L7E3
C	409	HIS	-	expression tag	UNP Q5L7E3
C	410	HIS	-	expression tag	UNP Q5L7E3
C	411	HIS	-	expression tag	UNP Q5L7E3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	412	HIS	-	expression tag	UNP Q5L7E3
C	413	HIS	-	expression tag	UNP Q5L7E3
C	414	HIS	-	expression tag	UNP Q5L7E3
D	407	LEU	-	expression tag	UNP Q5L7E3
D	408	GLU	-	expression tag	UNP Q5L7E3
D	409	HIS	-	expression tag	UNP Q5L7E3
D	410	HIS	-	expression tag	UNP Q5L7E3
D	411	HIS	-	expression tag	UNP Q5L7E3
D	412	HIS	-	expression tag	UNP Q5L7E3
D	413	HIS	-	expression tag	UNP Q5L7E3
D	414	HIS	-	expression tag	UNP Q5L7E3

- Molecule 2 is FERRICHROME (CCD ID: FCE) (formula: $C_{27}H_{42}FeN_9O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			48	27	9	12		
2	B	1	Total	C	N	O	0	0
			48	27	9	12		
2	C	1	Total	C	N	O	0	0
			48	27	9	12		
2	D	1	Total	C	N	O	0	0
			48	27	9	12		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0
3	B	1	Total 1	Fe 1	0	0
3	C	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 155.97Å 89.62Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	58.71 – 3.32 58.71 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (58.71-3.32) 99.1 (58.71-3.32)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.33Å)	Xtriage
Refinement program	PHENIX v1.21	Depositor
R, R_{free}	0.248 , 0.296 0.249 , 0.295	Depositor DCC
R_{free} test set	1148 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 12.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11810	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	FCE	D	501	3	45,48,54	2.21	13 (28%)	51,63,84	1.52	6 (11%)
2	FCE	A	501	3	45,48,54	2.56	18 (40%)	51,63,84	1.84	14 (27%)
2	FCE	B	501	3	45,48,54	2.33	13 (28%)	51,63,84	2.01	14 (27%)
2	FCE	C	501	3	45,48,54	2.36	14 (31%)	51,63,84	1.81	14 (27%)

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
2	FCE	D	501	3	3/3/15/22	22/69/69/111	0/1/1/6
2	FCE	A	501	3	5/5/15/22	22/69/69/111	1/1/1/6
2	FCE	B	501	3	4/4/15/22	25/69/69/111	0/1/1/6
2	FCE	C	501	3	4/4/15/22	26/69/69/111	0/1/1/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FCE	O14-N8	-8.01	1.34	1.40
2	B	501	FCE	O14-N8	-7.51	1.34	1.40
2	A	501	FCE	O14-N8	-7.35	1.34	1.40
2	D	501	FCE	O14-N8	-6.92	1.35	1.40
2	D	501	FCE	O11-N6	-6.16	1.35	1.40
2	A	501	FCE	O11-N6	-6.06	1.35	1.40
2	C	501	FCE	O10-N5	-5.94	1.35	1.40
2	B	501	FCE	O11-N6	-5.94	1.35	1.40
2	A	501	FCE	O10-N5	-5.73	1.35	1.40
2	C	501	FCE	O11-N6	-5.62	1.36	1.40
2	B	501	FCE	O10-N5	-5.61	1.36	1.40
2	D	501	FCE	O10-N5	-5.37	1.36	1.40
2	A	501	FCE	C30-N5	3.76	1.53	1.46
2	A	501	FCE	C13-C4	3.75	1.62	1.52
2	B	501	FCE	C1-N7	3.62	1.41	1.33
2	A	501	FCE	C8-N4	3.59	1.41	1.34
2	B	501	FCE	C13-C4	3.44	1.61	1.52
2	A	501	FCE	C7-N3	3.37	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FCE	C1-N7	3.37	1.41	1.33
2	A	501	FCE	C32-N6	3.37	1.52	1.46
2	B	501	FCE	C7-N3	3.32	1.41	1.34
2	B	501	FCE	C4-N1	3.32	1.41	1.34
2	C	501	FCE	C7-N3	3.28	1.41	1.34
2	D	501	FCE	C30-N5	3.27	1.52	1.46
2	C	501	FCE	C1-N7	3.26	1.40	1.33
2	A	501	FCE	C4-N1	3.21	1.41	1.34
2	A	501	FCE	C34-N8	3.20	1.52	1.46
2	A	501	FCE	C24-C16	3.15	1.60	1.53
2	D	501	FCE	C1-N7	3.13	1.40	1.33
2	C	501	FCE	C32-N6	3.09	1.52	1.46
2	C	501	FCE	C13-C4	3.08	1.60	1.52
2	C	501	FCE	C4-N1	3.07	1.40	1.34
2	A	501	FCE	C16-C7	3.02	1.60	1.52
2	C	501	FCE	C2-N9	3.01	1.40	1.33
2	D	501	FCE	C4-N1	2.98	1.40	1.34
2	A	501	FCE	C2-N9	2.94	1.40	1.33
2	C	501	FCE	C16-C7	2.94	1.60	1.52
2	D	501	FCE	C8-N4	2.91	1.40	1.34
2	D	501	FCE	C2-N9	2.88	1.39	1.33
2	B	501	FCE	C16-C7	2.88	1.60	1.52
2	A	501	FCE	C13-N3	2.80	1.51	1.45
2	B	501	FCE	C30-N5	2.77	1.51	1.46
2	A	501	FCE	C16-N4	2.74	1.51	1.45
2	D	501	FCE	C7-N3	2.72	1.40	1.34
2	C	501	FCE	C8-N4	2.71	1.39	1.34
2	B	501	FCE	C2-N9	2.68	1.39	1.33
2	B	501	FCE	C13-N3	2.66	1.51	1.45
2	B	501	FCE	C32-N6	2.58	1.51	1.46
2	D	501	FCE	C5-N2	2.53	1.39	1.33
2	B	501	FCE	C24-C16	2.51	1.59	1.53
2	D	501	FCE	C32-N6	2.51	1.51	1.46
2	C	501	FCE	C30-N5	2.41	1.50	1.46
2	A	501	FCE	C5-N2	2.41	1.38	1.33
2	C	501	FCE	C13-N3	2.39	1.50	1.45
2	D	501	FCE	C13-C4	2.28	1.58	1.52
2	C	501	FCE	C5-N2	2.25	1.38	1.33
2	D	501	FCE	C16-C7	2.08	1.58	1.52
2	A	501	FCE	C10-C1	2.05	1.58	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FCE	C13-C4-N1	6.26	130.42	116.70
2	C	501	FCE	C13-C4-N1	6.17	130.23	116.70
2	A	501	FCE	C13-C4-N1	6.09	130.06	116.70
2	B	501	FCE	C29-C34-N8	5.51	122.50	111.06
2	B	501	FCE	O4-C4-N1	-3.95	115.61	122.93
2	C	501	FCE	O4-C4-N1	-3.87	115.76	122.93
2	A	501	FCE	O4-C4-N1	-3.79	115.92	122.93
2	B	501	FCE	C25-C30-N5	3.71	118.76	111.06
2	D	501	FCE	C13-C4-N1	3.70	124.81	116.70
2	A	501	FCE	C10-C1-N7	3.64	123.87	116.54
2	A	501	FCE	C29-C34-N8	3.64	118.61	111.06
2	D	501	FCE	C29-C34-N8	3.59	118.52	111.06
2	D	501	FCE	C25-C30-N5	3.47	118.25	111.06
2	C	501	FCE	C25-C30-N5	3.21	117.72	111.06
2	C	501	FCE	C29-C34-N8	3.10	117.49	111.06
2	B	501	FCE	O4-C4-C13	-3.09	113.96	120.45
2	C	501	FCE	O4-C4-C13	-3.06	114.01	120.45
2	A	501	FCE	O4-C4-C13	-3.06	114.02	120.45
2	D	501	FCE	C10-C1-N7	3.05	122.70	116.54
2	A	501	FCE	C25-C30-N5	3.02	117.32	111.06
2	C	501	FCE	C10-C1-N7	2.87	122.34	116.54
2	A	501	FCE	C4-C13-N3	2.84	118.88	111.16
2	B	501	FCE	C16-C7-N3	2.83	122.91	116.70
2	B	501	FCE	C10-C1-N7	2.75	122.09	116.54
2	B	501	FCE	O7-C7-N3	-2.75	117.84	122.93
2	A	501	FCE	C18-C10-C1	2.68	116.45	110.20
2	B	501	FCE	C10-N1-C4	2.67	127.40	121.67
2	C	501	FCE	C10-N1-C4	2.66	127.36	121.67
2	B	501	FCE	C2-C11-N2	-2.63	105.79	113.17
2	D	501	FCE	O4-C4-N1	-2.57	118.17	122.93
2	C	501	FCE	O7-C7-N3	-2.56	118.19	122.93
2	A	501	FCE	C24-C16-C7	2.50	116.04	110.20
2	A	501	FCE	O7-C7-N3	-2.35	118.57	122.93
2	C	501	FCE	C16-C7-N3	2.34	121.83	116.70
2	C	501	FCE	C5-C14-N7	-2.34	106.61	113.17
2	B	501	FCE	C24-C16-C7	2.33	115.65	110.20
2	C	501	FCE	C4-C13-N3	2.26	117.30	111.16
2	A	501	FCE	C16-C7-N3	2.22	121.58	116.70
2	C	501	FCE	C2-C11-N2	-2.21	106.96	113.17
2	C	501	FCE	C17-C8-N4	2.21	121.36	116.10
2	B	501	FCE	C5-C14-N7	-2.20	107.00	113.17
2	A	501	FCE	C2-C11-N2	-2.20	107.00	113.17
2	B	501	FCE	C4-C13-N3	2.17	117.05	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FCE	C8-C17-N9	-2.16	107.10	113.17
2	A	501	FCE	C1-C10-N1	-2.10	105.43	111.16
2	D	501	FCE	C7-C16-N4	-2.07	105.52	111.16
2	C	501	FCE	C8-C17-N9	-2.07	107.37	113.17
2	A	501	FCE	O1-C1-N7	-2.07	118.56	122.99

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	FCE	C10
2	A	501	FCE	N6
2	A	501	FCE	N5
2	A	501	FCE	C16
2	A	501	FCE	N8
2	B	501	FCE	N8
2	B	501	FCE	N6
2	B	501	FCE	N5
2	B	501	FCE	C10
2	C	501	FCE	N8
2	C	501	FCE	N6
2	C	501	FCE	N5
2	C	501	FCE	C10
2	D	501	FCE	N8
2	D	501	FCE	N6
2	D	501	FCE	N5

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FCE	C25-C30-N5-C3
2	A	501	FCE	C25-C30-N5-O10
2	A	501	FCE	C29-C34-N8-O14
2	A	501	FCE	C21-C27-C32-N6
2	B	501	FCE	C25-C30-N5-C3
2	B	501	FCE	C25-C30-N5-O10
2	B	501	FCE	C29-C34-N8-O14
2	B	501	FCE	C21-C27-C32-N6
2	B	501	FCE	C24-C29-C34-N8
2	C	501	FCE	C25-C30-N5-C3
2	C	501	FCE	C25-C30-N5-O10
2	C	501	FCE	C29-C34-N8-O14
2	C	501	FCE	C21-C27-C32-N6

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Mol	Chain	Res	Type	Atoms
2	D	501	FCE	C25-C30-N5-C3
2	D	501	FCE	C25-C30-N5-O10
2	D	501	FCE	C27-C32-N6-O11
2	D	501	FCE	C29-C34-N8-C9
2	D	501	FCE	C29-C34-N8-O14
2	D	501	FCE	C18-C25-C30-N5
2	D	501	FCE	C21-C27-C32-N6
2	A	501	FCE	C24-C16-N4-C8
2	B	501	FCE	C13-C4-N1-C10
2	C	501	FCE	C13-C4-N1-C10
2	A	501	FCE	C13-C4-N1-C10
2	A	501	FCE	O4-C4-N1-C10
2	B	501	FCE	O4-C4-N1-C10
2	C	501	FCE	O4-C4-N1-C10
2	A	501	FCE	C13-C21-C27-C32
2	B	501	FCE	C13-C21-C27-C32
2	C	501	FCE	C13-C21-C27-C32
2	A	501	FCE	O1-C1-C10-C18
2	D	501	FCE	C13-C21-C27-C32
2	D	501	FCE	C16-C24-C29-C34
2	B	501	FCE	N7-C14-C5-O5
2	B	501	FCE	N7-C14-C5-N2
2	A	501	FCE	C10-C18-C25-C30
2	B	501	FCE	C16-C24-C29-C34
2	C	501	FCE	C10-C18-C25-C30
2	A	501	FCE	N7-C1-C10-C18
2	D	501	FCE	C10-C18-C25-C30
2	C	501	FCE	N4-C16-C24-C29
2	B	501	FCE	C10-C18-C25-C30
2	C	501	FCE	N7-C14-C5-N2
2	C	501	FCE	C24-C29-C34-N8
2	A	501	FCE	N7-C1-C10-N1
2	C	501	FCE	N7-C14-C5-O5
2	A	501	FCE	O1-C1-C10-N1
2	B	501	FCE	O1-C1-C10-N1
2	C	501	FCE	O1-C1-C10-N1
2	C	501	FCE	N7-C1-C10-N1
2	B	501	FCE	O1-C1-C10-C18
2	B	501	FCE	N7-C1-C10-C18
2	B	501	FCE	N7-C1-C10-N1
2	C	501	FCE	O1-C1-C10-C18
2	C	501	FCE	N7-C1-C10-C18

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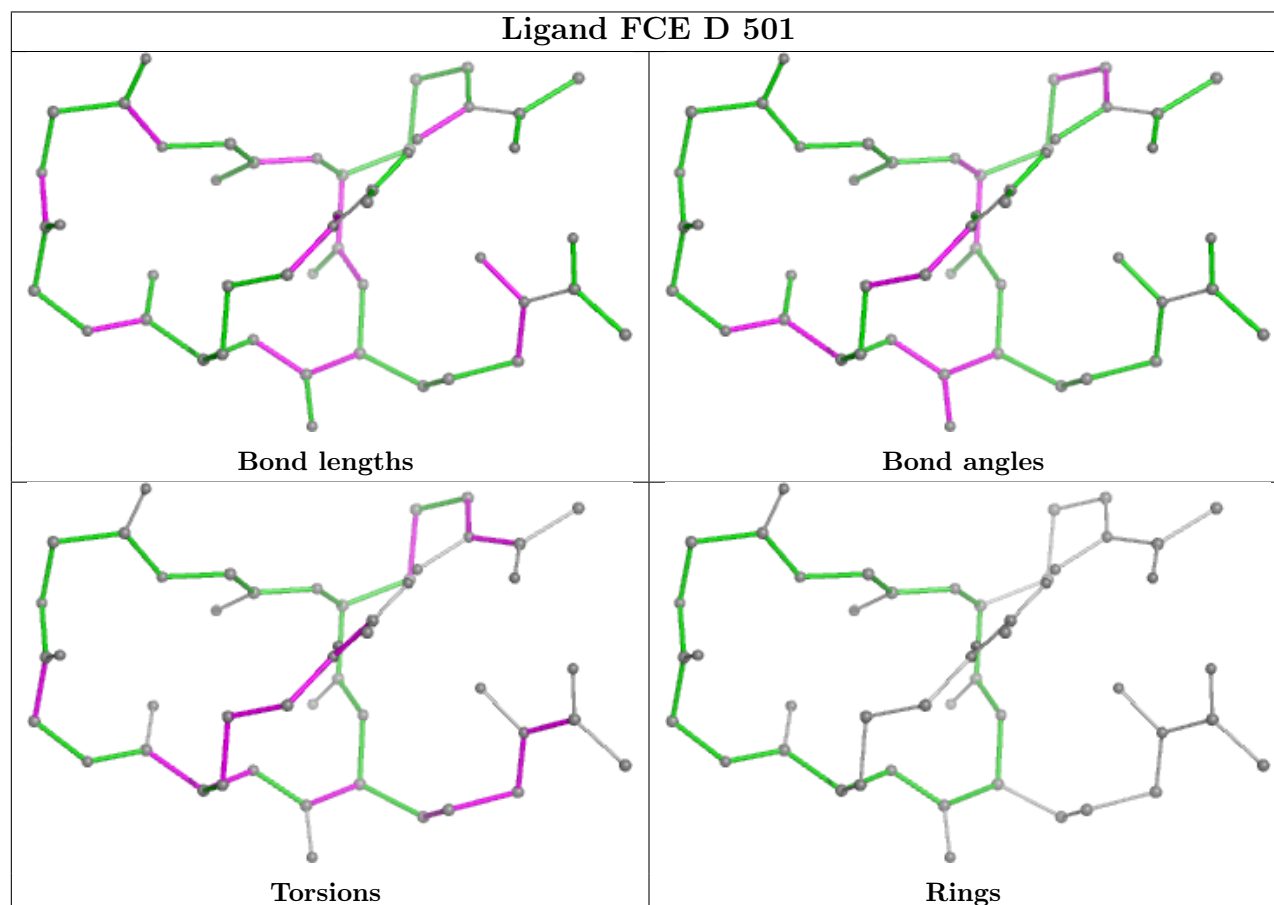
Mol	Chain	Res	Type	Atoms
2	B	501	FCE	C27-C32-N6-C6
2	B	501	FCE	C29-C34-N8-C9
2	C	501	FCE	C29-C34-N8-C9
2	D	501	FCE	C27-C32-N6-C6
2	C	501	FCE	C16-C24-C29-C34
2	A	501	FCE	C16-C24-C29-C34
2	D	501	FCE	O1-C1-C10-N1
2	D	501	FCE	N7-C1-C10-N1
2	D	501	FCE	N7-C14-C5-N2
2	A	501	FCE	C27-C32-N6-C6
2	C	501	FCE	C27-C32-N6-C6
2	A	501	FCE	C36-C3-N5-O10
2	A	501	FCE	C35-C6-N6-O11
2	A	501	FCE	C37-C9-N8-O14
2	B	501	FCE	C36-C3-N5-O10
2	B	501	FCE	C35-C6-N6-O11
2	B	501	FCE	C37-C9-N8-O14
2	C	501	FCE	C36-C3-N5-O10
2	C	501	FCE	C35-C6-N6-O11
2	C	501	FCE	C37-C9-N8-O14
2	D	501	FCE	C36-C3-N5-O10
2	D	501	FCE	C35-C6-N6-O11
2	D	501	FCE	C37-C9-N8-O14
2	A	501	FCE	O3-C3-N5-O10
2	A	501	FCE	O6-C6-N6-O11
2	A	501	FCE	O8-C9-N8-O14
2	B	501	FCE	O3-C3-N5-O10
2	B	501	FCE	O6-C6-N6-O11
2	B	501	FCE	O8-C9-N8-O14
2	C	501	FCE	O3-C3-N5-O10
2	C	501	FCE	O6-C6-N6-O11
2	C	501	FCE	O8-C9-N8-O14
2	D	501	FCE	O3-C3-N5-O10
2	D	501	FCE	O6-C6-N6-O11
2	D	501	FCE	O8-C9-N8-O14
2	A	501	FCE	C4-C13-C21-C27
2	D	501	FCE	C1-C10-N1-C4
2	D	501	FCE	C21-C13-C4-O4
2	B	501	FCE	C8-C17-N9-C2
2	C	501	FCE	C8-C17-N9-C2

All (1) ring outliers are listed below:

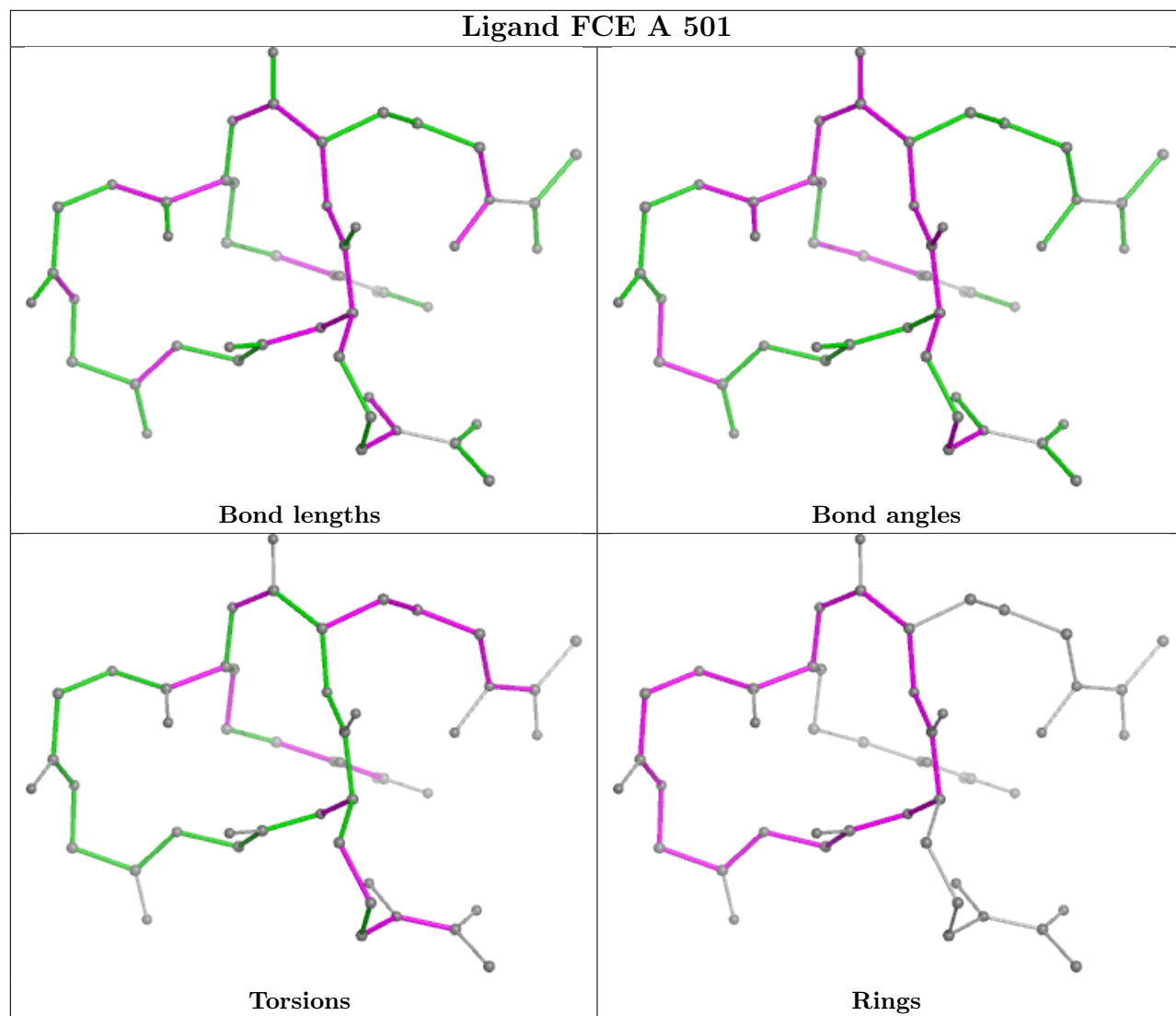
Mol	Chain	Res	Type	Atoms
2	A	501	FCE	C1-C10-C11-C13-C14-C16-C17-C2-C4-C5-C7-C8-N1-N2-N3-N4-N7-N9

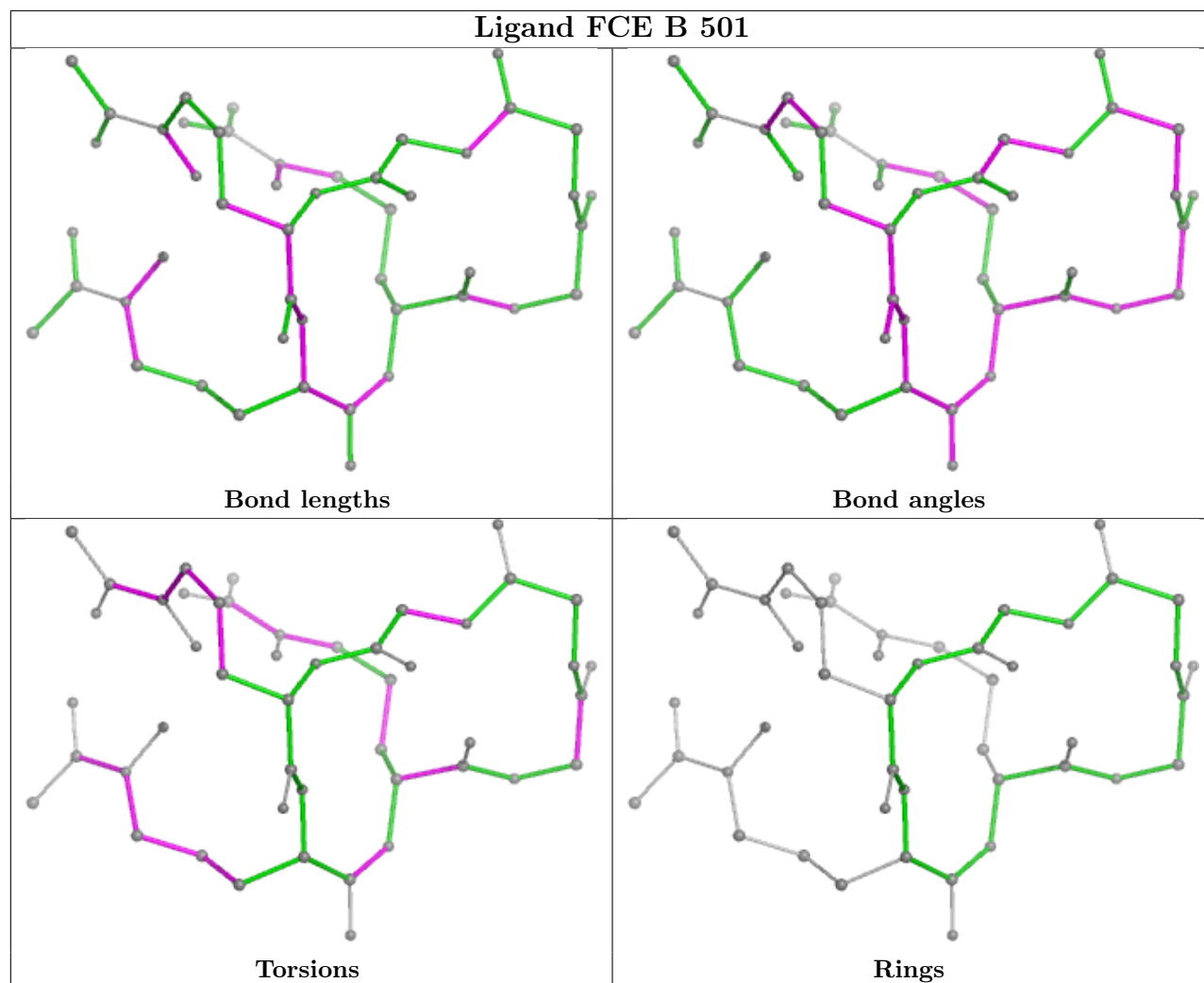
No monomer is involved in short contacts.

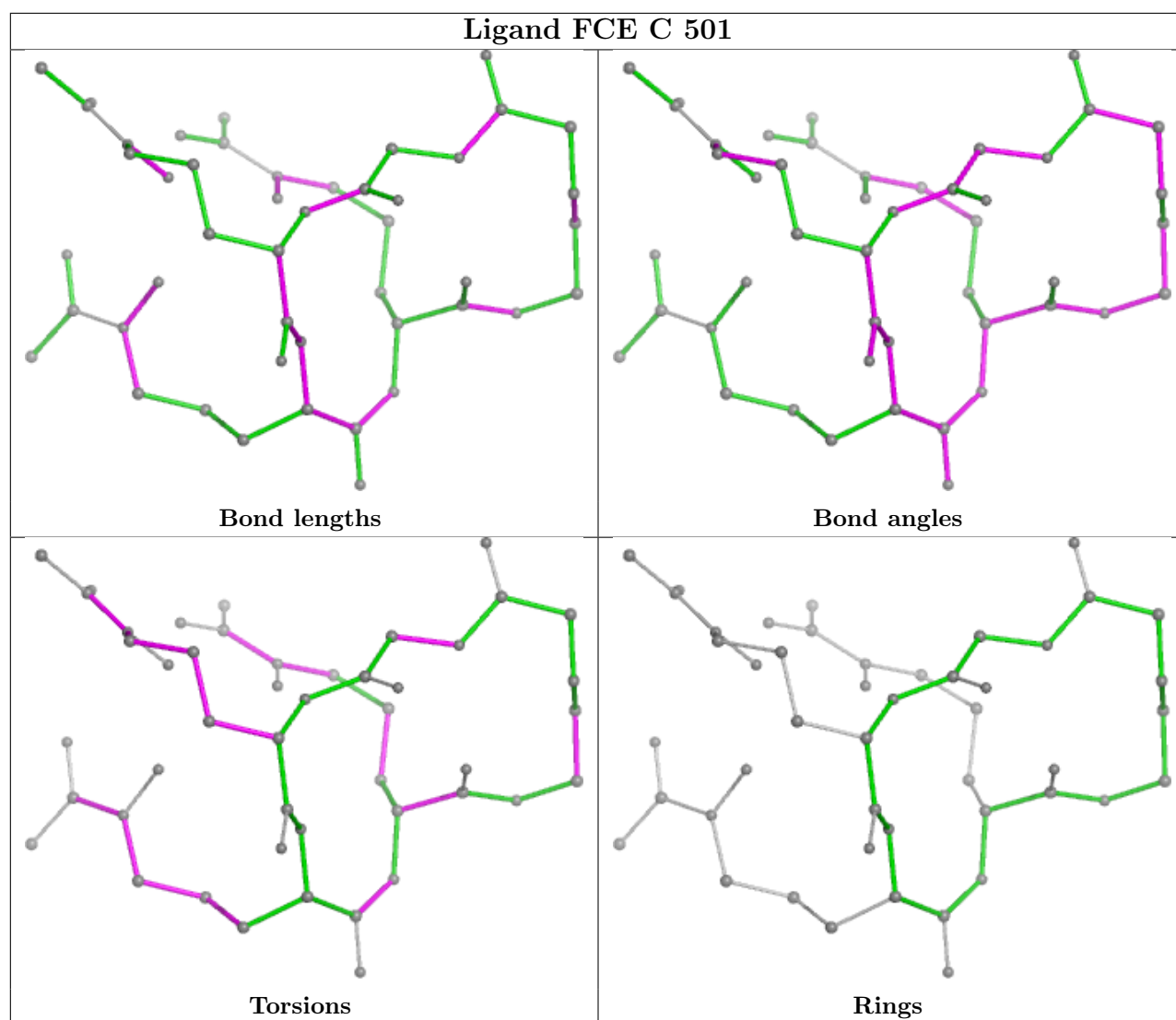
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FCE A 501







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	375/414 (90%)	0.52	7 (1%) 66 51	34, 48, 68, 95	0
1	B	377/414 (91%)	0.57	9 (2%) 59 44	33, 52, 71, 94	0
1	C	376/414 (90%)	0.64	7 (1%) 66 51	32, 49, 71, 100	0
1	D	381/414 (92%)	0.55	15 (3%) 44 32	32, 47, 71, 87	0
All	All	1509/1656 (91%)	0.57	38 (2%) 58 43	32, 49, 71, 100	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	PRO	3.7
1	A	93	LEU	3.1
1	C	125	THR	3.1
1	D	216	PRO	2.9
1	D	269	ALA	2.7
1	D	359	ALA	2.6
1	A	169	PRO	2.6
1	C	56	THR	2.6
1	D	57	ALA	2.6
1	B	373	SER	2.5
1	D	87	VAL	2.4
1	C	59	GLU	2.4
1	A	273	ILE	2.4
1	D	253	SER	2.4
1	A	216	PRO	2.3
1	C	299	ILE	2.3
1	D	411	HIS	2.3
1	D	358	ALA	2.3
1	D	407	LEU	2.3
1	D	401	GLY	2.3
1	D	171	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	2.2
1	B	311	VAL	2.2
1	B	400	GLY	2.2
1	B	282	ASP	2.2
1	A	222	THR	2.2
1	D	86	THR	2.2
1	D	169	PRO	2.2
1	B	215	TYR	2.2
1	B	90	ILE	2.1
1	D	340	VAL	2.1
1	C	359	ALA	2.1
1	A	109	LEU	2.1
1	C	217	ASP	2.0
1	A	55	VAL	2.0
1	B	105	ALA	2.0
1	D	101	ILE	2.0
1	C	57	ALA	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FCE	A	501	48/49	0.82	0.16	34,48,57,66	0
2	FCE	B	501	48/49	0.82	0.16	45,53,64,71	0
2	FCE	D	501	48/49	0.84	0.16	34,41,53,66	0
2	FCE	C	501	48/49	0.85	0.16	30,43,58,65	0
3	FE	A	502	1/1	0.99	0.08	37,37,37,37	0
3	FE	B	502	1/1	0.99	0.03	53,53,53,53	0

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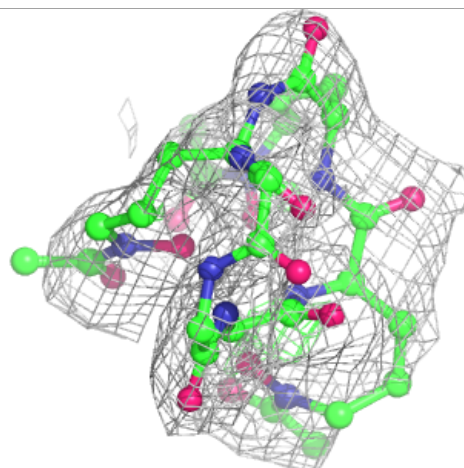
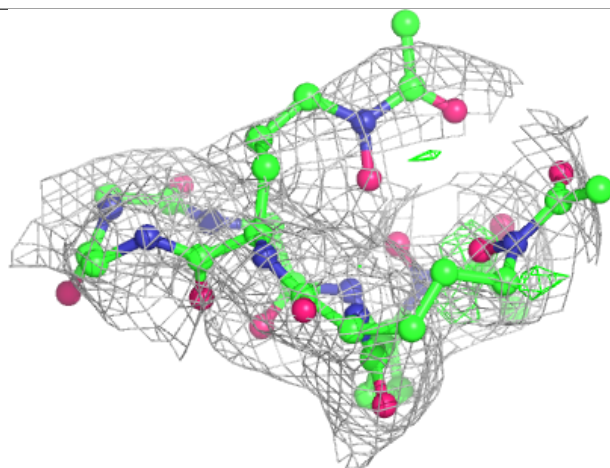
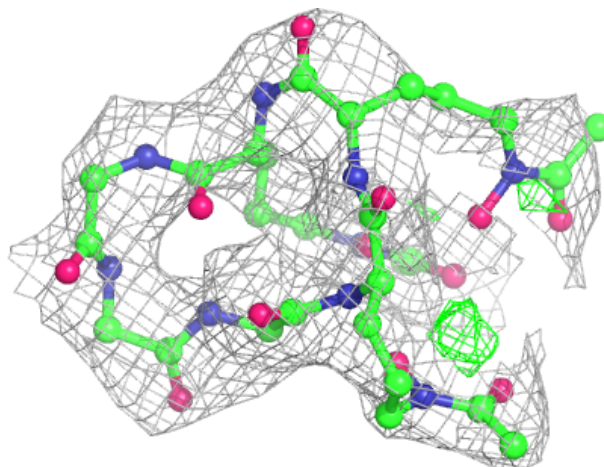
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FE	C	502	1/1	0.99	0.04	48,48,48,48	0
3	FE	D	502	1/1	0.99	0.03	35,35,35,35	0

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.

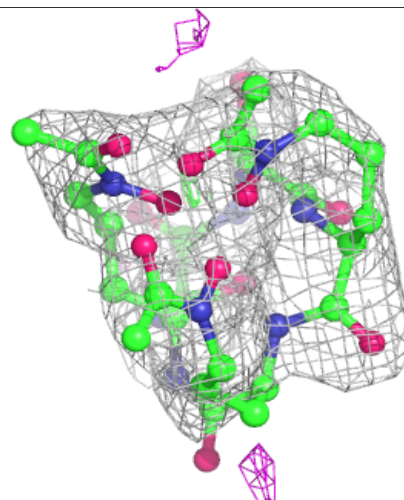
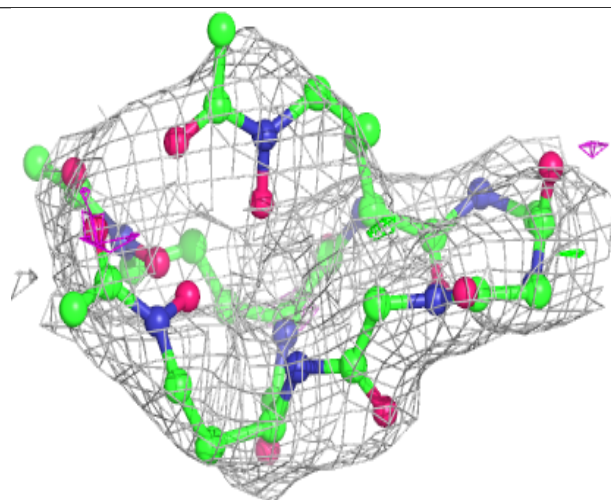
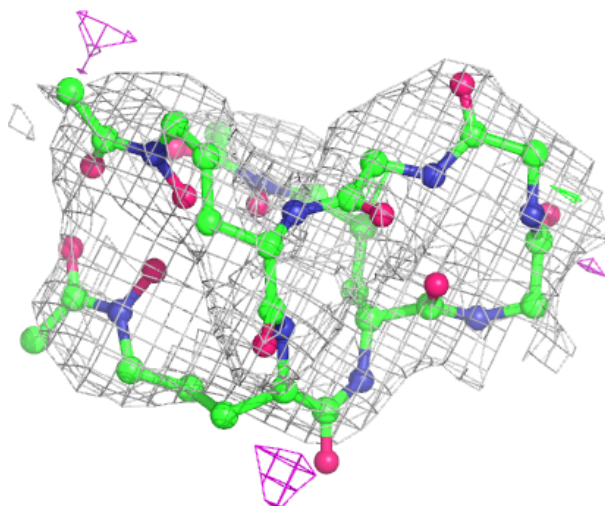
Electron density around FCE A 501:

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



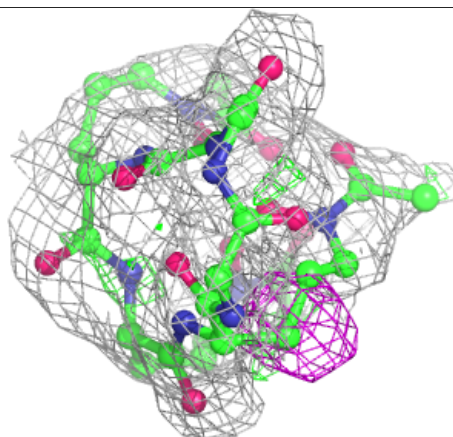
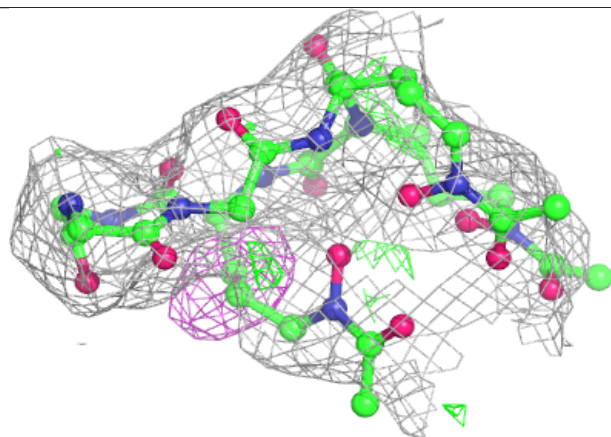
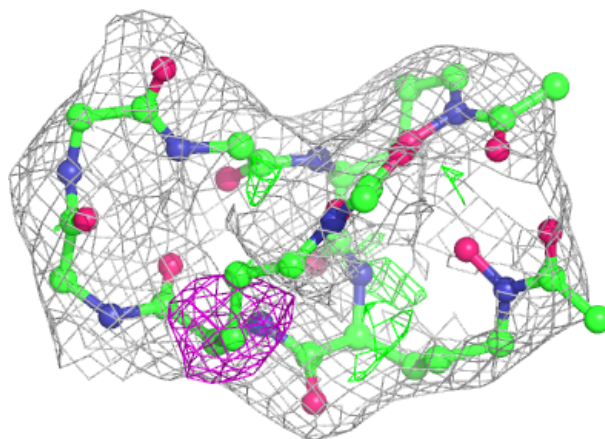
Electron density around FCE B 501:

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



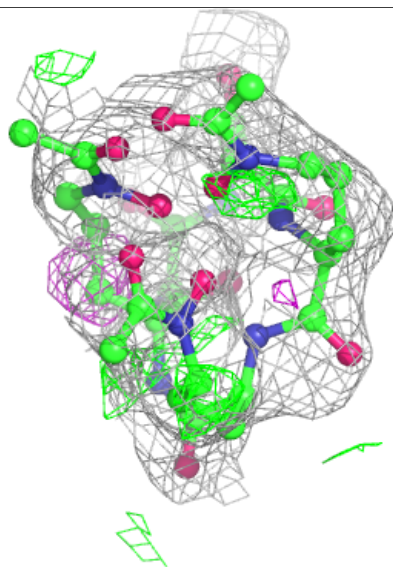
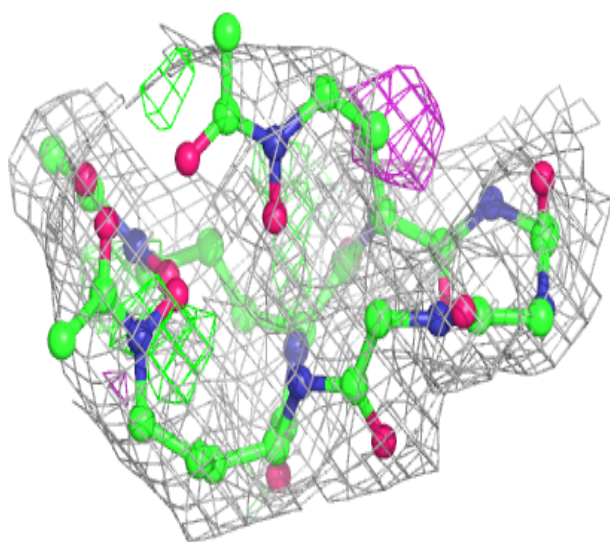
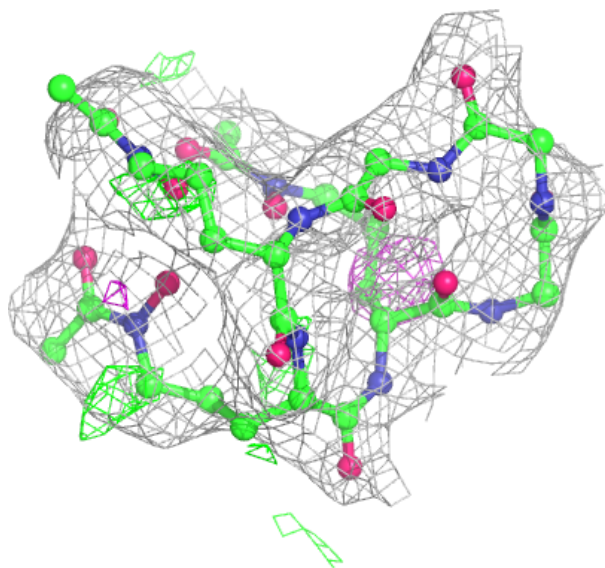
Electron density around FCE D 501:

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



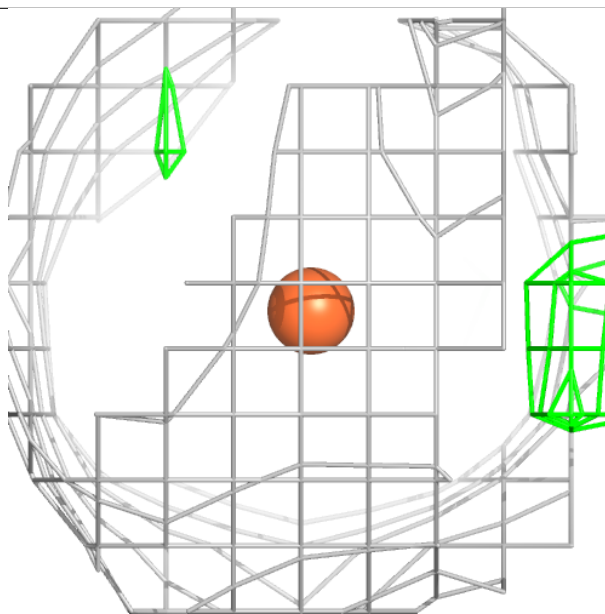
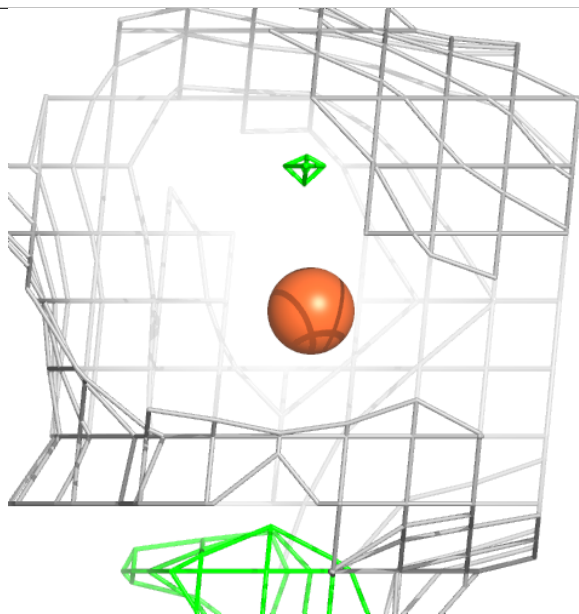
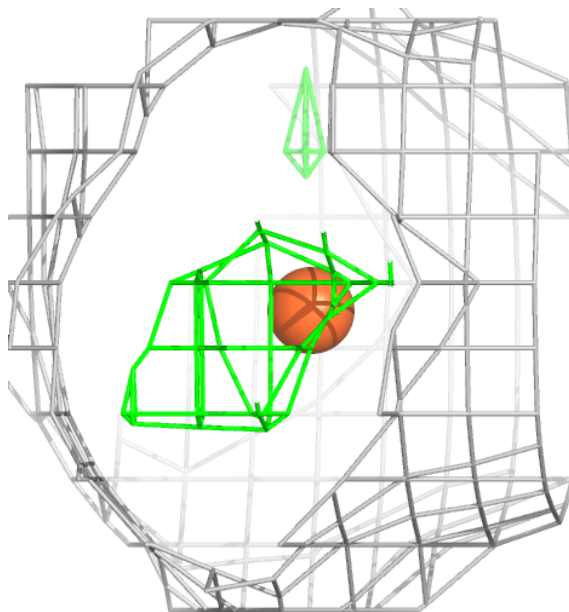
Electron density around FCE C 501:

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



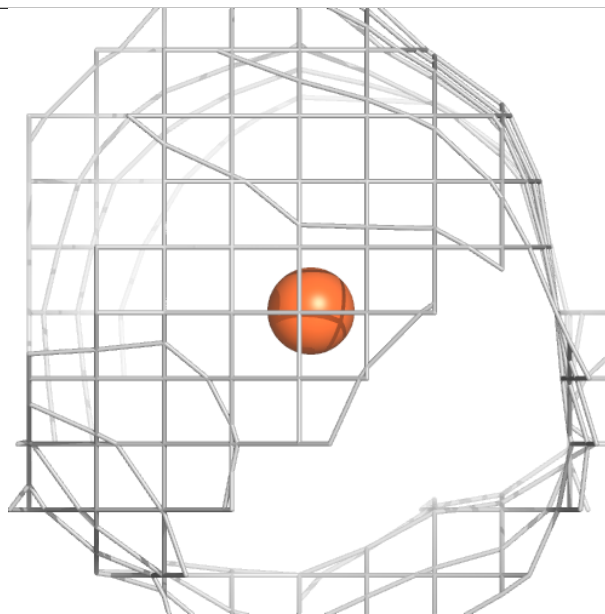
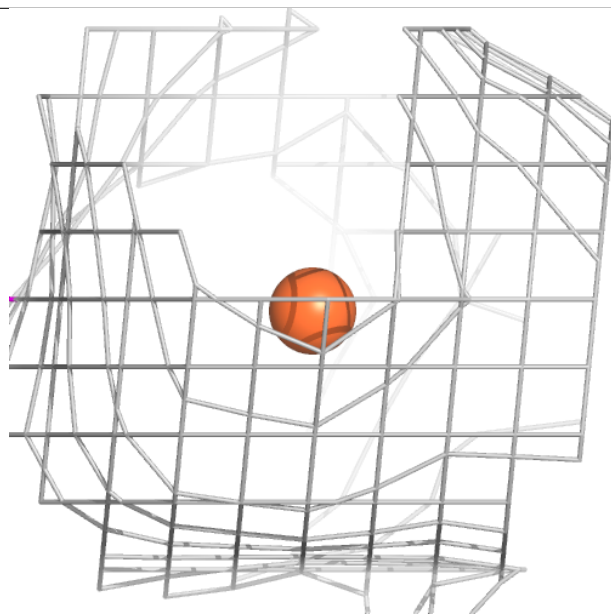
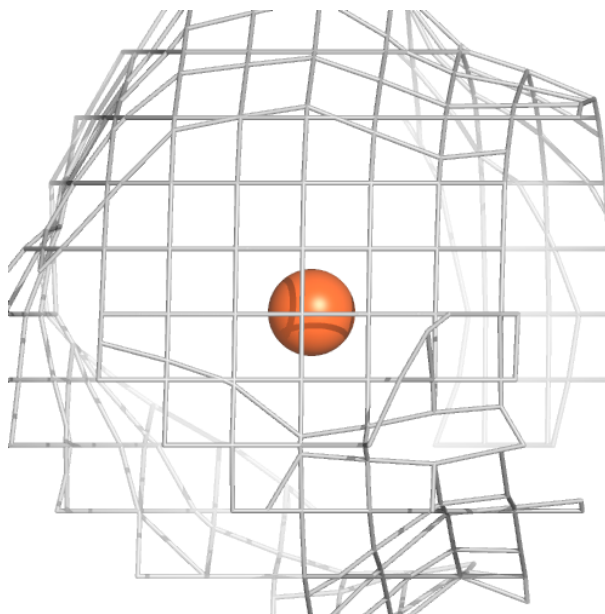
Electron density around FE A 502:

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



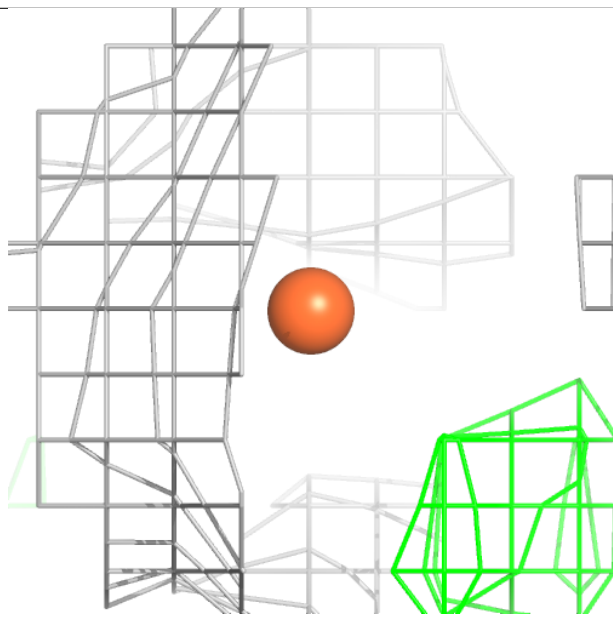
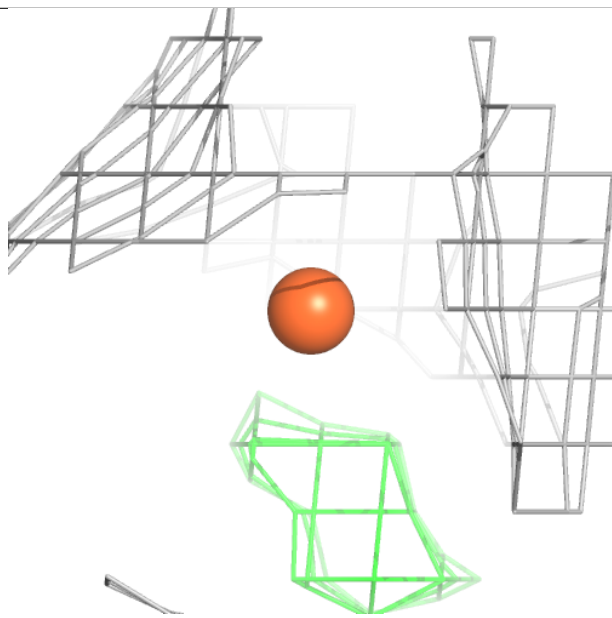
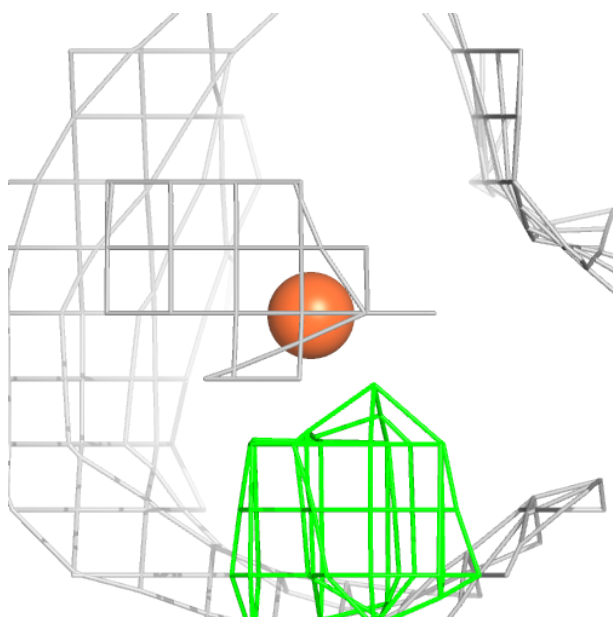
Electron density around FE B 502:

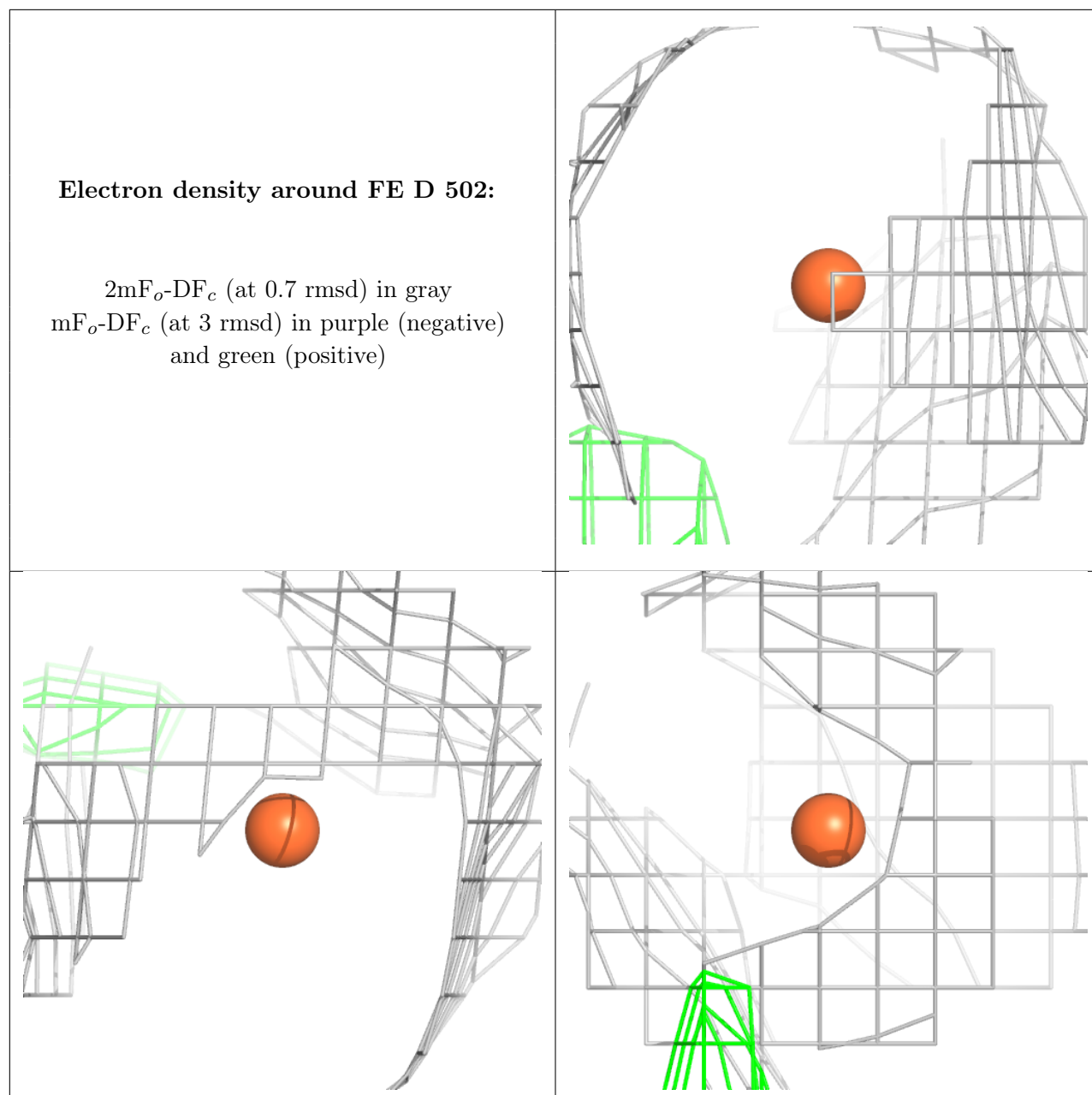
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE C 502:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.