



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 06:08 pm GMT

PDB ID : 9HRP / pdb\_00009hrp  
Title : Structure of YIUA from Yersinia ruckeri with iron  
Authors : Thompson, S.; Thomsen, E.; Duhme-Klair, A.; Butler, A.; Grogan, G.  
Deposited on : 2024-12-18  
Resolution : 2.32 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](mailto: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>.

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

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

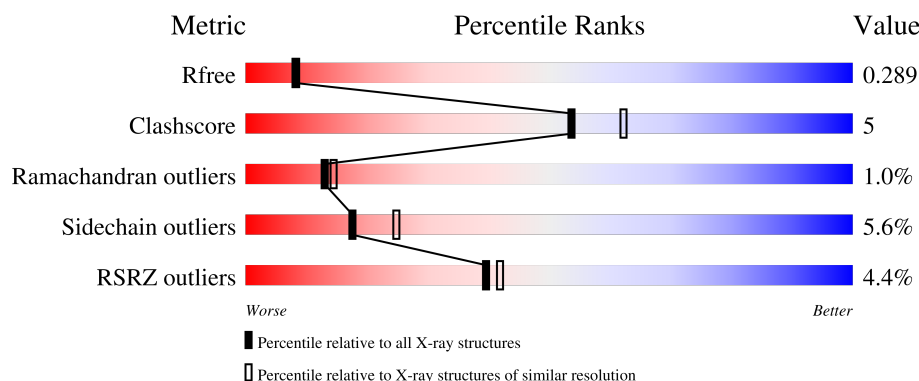
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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  $\geq 3$ , 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	349	 2% 82% 9% .. 5%
1	B	349	 3% 83% 9% .. 5%
1	C	349	 7% 83% 11% ..
1	D	349	 5% 86% 8% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10288 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 Periplasmic substrate-binding transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2512	1610	417	477	8			
1	B	330	Total	C	N	O	S	0	1	0
			2521	1614	423	477	7			
1	C	335	Total	C	N	O	S	0	1	0
			2529	1623	427	472	7			
1	D	334	Total	C	N	O	S	0	2	0
			2526	1613	430	476	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	ALA	conflict	UNP A0A085U4N5
A	12	VAL	ALA	conflict	UNP A0A085U4N5
A	233	THR	ALA	conflict	UNP A0A085U4N5
A	262	GLU	ALA	conflict	UNP A0A085U4N5
A	315	GLN	GLU	conflict	UNP A0A085U4N5
A	324	ASN	LYS	conflict	UNP A0A085U4N5
B	0	SER	ALA	conflict	UNP A0A085U4N5
B	12	VAL	ALA	conflict	UNP A0A085U4N5
B	233	THR	ALA	conflict	UNP A0A085U4N5
B	262	GLU	ALA	conflict	UNP A0A085U4N5
B	315	GLN	GLU	conflict	UNP A0A085U4N5
B	324	ASN	LYS	conflict	UNP A0A085U4N5
C	0	SER	ALA	conflict	UNP A0A085U4N5
C	12	VAL	ALA	conflict	UNP A0A085U4N5
C	233	THR	ALA	conflict	UNP A0A085U4N5
C	262	GLU	ALA	conflict	UNP A0A085U4N5
C	315	GLN	GLU	conflict	UNP A0A085U4N5
C	324	ASN	LYS	conflict	UNP A0A085U4N5
D	0	SER	ALA	conflict	UNP A0A085U4N5
D	12	VAL	ALA	conflict	UNP A0A085U4N5
D	233	THR	ALA	conflict	UNP A0A085U4N5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	262	GLU	ALA	conflict	UNP A0A085U4N5
D	315	GLN	GLU	conflict	UNP A0A085U4N5
D	324	ASN	LYS	conflict	UNP A0A085U4N5

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

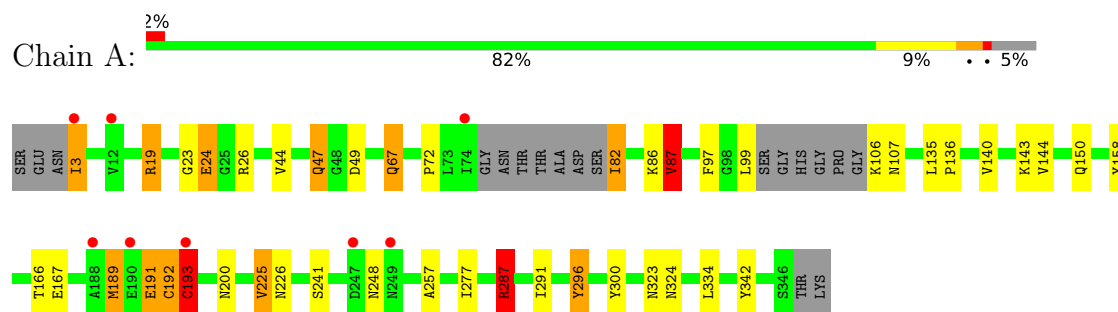
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	48	Total O 48 48	0	0
3	C	43	Total O 43 43	0	0
3	D	59	Total O 59 59	0	0

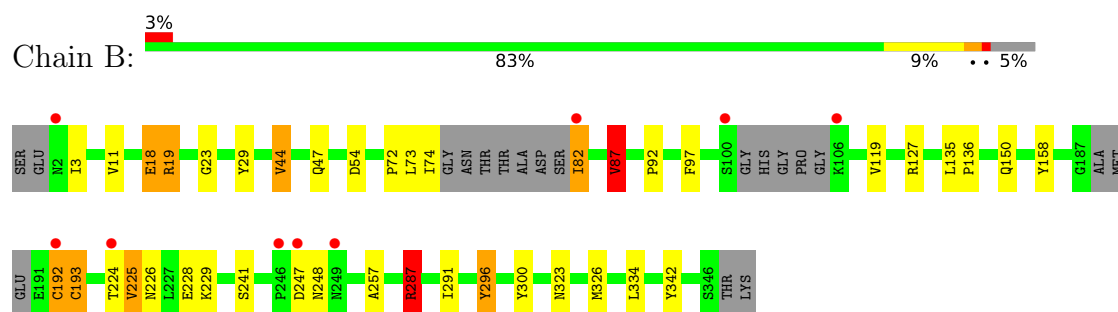
### 3 Residue-property plots [i](#)

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.

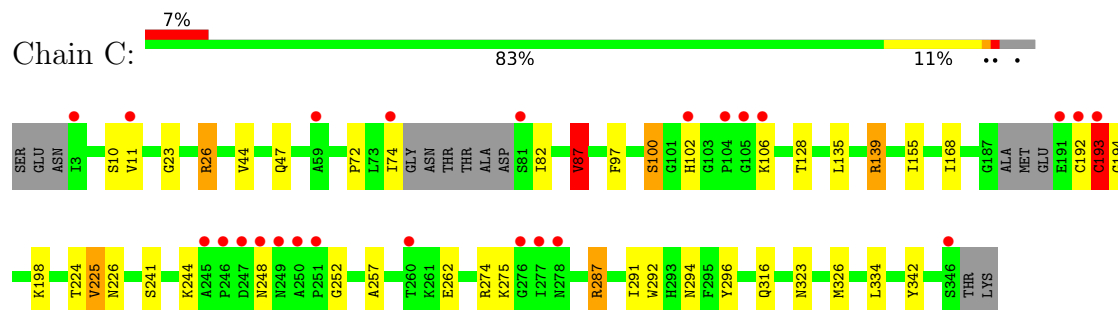
- Molecule 1: Periplasmic substrate-binding transport protein



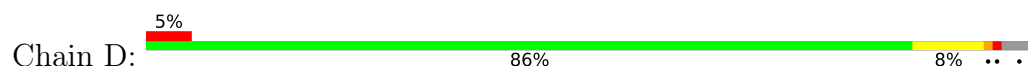
- Molecule 1: Periplasmic substrate-binding transport protein

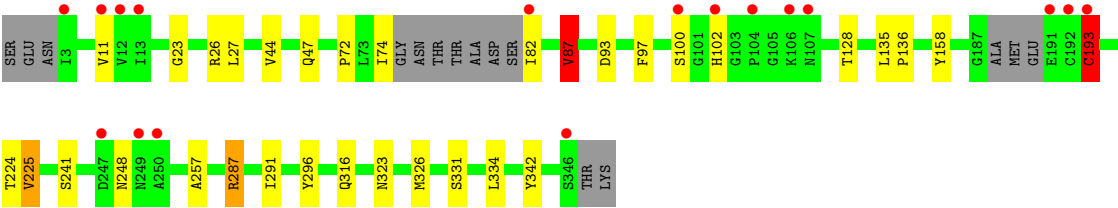


- Molecule 1: Periplasmic substrate-binding transport protein



- Molecule 1: Periplasmic substrate-binding transport protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.49Å 76.23Å 99.93Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	60.59 – 2.32 60.59 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.59-2.32) 99.9 (60.59-2.32)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.244 , 0.287 0.250 , 0.289	Depositor DCC
$R_{free}$ test set	2944 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.79 % 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 4.0629e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE

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	0.62	0/2567	1.10	5/3496 (0.1%)
1	B	0.69	2/2576 (0.1%)	1.13	8/3503 (0.2%)
1	C	0.62	0/2587	1.10	5/3520 (0.1%)
1	D	0.60	0/2587	1.09	4/3524 (0.1%)
All	All	0.63	2/10317 (0.0%)	1.10	22/14043 (0.2%)

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	B	0	2
1	C	0	2
1	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19[A]	ARG	C-O	10.59	1.35	1.23
1	B	19[B]	ARG	C-O	10.59	1.35	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	CYS	CB-CA-C	8.82	127.97	110.42
1	B	19[A]	ARG	CA-C-O	8.19	131.90	120.52
1	B	19[B]	ARG	CA-C-O	8.19	131.90	120.52
1	A	193	CYS	CB-CA-C	7.42	125.18	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	CYS	CB-CA-C	7.18	124.72	110.42
1	D	224	THR	CA-CB-OG1	-6.48	99.88	109.60
1	C	224	THR	CA-CB-OG1	-6.34	100.09	109.60
1	B	18	GLU	N-CA-C	-6.19	105.42	114.39
1	B	224	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	226	ASN	CB-CA-C	5.88	119.47	109.53
1	B	87	VAL	N-CA-CB	5.60	120.91	110.77
1	A	287	ARG	CG-CD-NE	5.55	124.22	112.00
1	C	226	ASN	CB-CA-C	5.51	118.84	109.53
1	A	192	CYS	N-CA-C	5.49	118.68	109.95
1	C	87	VAL	N-CA-CB	5.39	120.53	110.77
1	A	87	VAL	N-CA-CB	5.35	120.45	110.77
1	B	19[A]	ARG	O-C-N	-5.35	114.86	122.99
1	B	19[B]	ARG	O-C-N	-5.35	114.86	122.99
1	D	27	LEU	N-CA-C	-5.34	106.72	113.18
1	C	194	GLY	N-CA-C	-5.29	104.34	111.54
1	D	87	VAL	N-CA-CB	5.25	120.28	110.77
1	B	287	ARG	CG-CD-NE	5.25	123.56	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19[A]	ARG	Sidechain
1	B	19[B]	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	26	ARG	Sidechain
1	D	26	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2512	0	2427	32	0
1	B	2521	0	2460	24	0
1	C	2529	0	2461	23	0
1	D	2526	0	2444	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	46	0	0	3	0
3	B	48	0	0	0	0
3	C	43	0	0	4	0
3	D	59	0	0	1	0
All	All	10288	0	9792	93	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 5.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ARG:HH11	1:D:287:ARG:HG2	1.38	0.88
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.41	0.86
1:C:287:ARG:HG2	1:C:287:ARG:HH11	1.42	0.85
1:B:287:ARG:HG2	1:B:287:ARG:HH11	1.42	0.84
1:A:143:LYS:CD	1:A:143:LYS:NZ	2.43	0.81
1:C:100:SER:HB2	3:C:525:HOH:O	1.80	0.81
1:B:127:ARG:NH2	1:B:296:TYR:OH	2.13	0.79
1:C:100:SER:HB3	3:C:531:HOH:O	1.83	0.78
1:B:192:CYS:HG	1:B:193:CYS:HG	1.40	0.67
1:B:193:CYS:HB2	1:B:225:VAL:O	1.98	0.64
1:A:47:GLN:HG3	1:A:49:ASP:OD1	2.01	0.60
1:C:135:LEU:HD13	1:C:155:ILE:HG23	1.84	0.60
1:C:168:ILE:HG21	1:C:316:GLN:HG2	1.83	0.59
1:A:82:ILE:HG22	1:A:87:VAL:HG12	1.84	0.59
1:C:193:CYS:HB2	1:C:225:VAL:O	2.02	0.59
1:A:189:MET:HE1	1:A:277:ILE:HG12	1.85	0.58
1:C:287:ARG:HH11	1:C:287:ARG:CG	2.15	0.58
1:A:23:GLY:HA3	1:A:97:PHE:CE1	2.40	0.57
1:A:189:MET:O	1:A:189:MET:HG3	2.05	0.57
1:B:23:GLY:HA3	1:B:97:PHE:CE1	2.40	0.56
1:A:192:CYS:SG	1:A:193:CYS:N	2.78	0.56
1:A:47:GLN:CG	1:A:49:ASP:OD1	2.53	0.56
1:D:287:ARG:HH11	1:D:287:ARG:CG	2.14	0.56
1:A:24:GLU:HA	1:A:47:GLN:HG2	1.88	0.56
1:A:287:ARG:HH11	1:A:287:ARG:CG	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:VAL:O	1:B:72:PRO:HD2	2.07	0.54
1:C:326:MET:HE1	1:C:342:TYR:CD2	2.42	0.54
1:B:127:ARG:HD2	1:B:296:TYR:CE2	2.43	0.54
1:A:193:CYS:HB2	1:A:225:VAL:O	2.09	0.53
1:B:73:LEU:C	1:B:74:ILE:HD12	2.36	0.51
1:B:287:ARG:HH11	1:B:287:ARG:CG	2.15	0.51
1:D:23:GLY:HA3	1:D:97:PHE:CE1	2.45	0.51
1:C:82:ILE:HG13	1:C:87:VAL:HG12	1.93	0.51
1:C:23:GLY:HA3	1:C:97:PHE:CE1	2.46	0.50
1:A:82:ILE:HG23	1:A:86:LYS:HB3	1.92	0.50
1:D:193:CYS:HB2	1:D:225:VAL:O	2.11	0.49
1:A:19[A]:ARG:HB3	1:A:44:VAL:HG11	1.94	0.49
1:A:324:ASN:ND2	3:A:504:HOH:O	2.46	0.49
1:B:92:PRO:HG2	1:B:119:VAL:HG21	1.93	0.49
1:C:168:ILE:HG21	1:C:316:GLN:CG	2.44	0.48
1:A:135:LEU:HD21	1:A:158:TYR:CD1	2.50	0.47
1:B:287:ARG:HG2	1:B:287:ARG:NH1	2.21	0.47
1:C:192:CYS:SG	1:C:193:CYS:N	2.90	0.45
1:B:3:ILE:C	1:B:3:ILE:HD12	2.40	0.45
1:B:226:ASN:ND2	1:B:228:GLU:HB2	2.31	0.45
1:A:106:LYS:HG2	1:A:107:ASN:N	2.32	0.45
1:A:135:LEU:HB2	1:A:136:PRO:HD3	1.99	0.45
1:A:166:THR:CB	3:A:501:HOH:O	2.64	0.45
1:B:135:LEU:HD21	1:B:158:TYR:CD1	2.51	0.45
1:D:135:LEU:HD21	1:D:158:TYR:CD1	2.52	0.45
1:C:244:LYS:HE2	1:C:252:GLY:N	2.32	0.44
1:A:72:PRO:HB3	1:A:82:ILE:HD12	1.99	0.44
1:C:274:ARG:O	1:C:275:LYS:C	2.60	0.44
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.20	0.44
1:B:29:TYR:OH	1:B:54:ASP:OD2	2.33	0.44
1:A:44:VAL:O	1:A:72:PRO:HD2	2.17	0.44
1:C:10:SER:HB3	3:C:523:HOH:O	2.18	0.44
1:A:3:ILE:HD12	1:A:140:VAL:HG22	1.99	0.44
1:A:67:GLN:H	1:A:67:GLN:HG3	1.48	0.43
1:C:292:TRP:CH2	1:C:294:ASN:HB2	2.53	0.43
1:D:287:ARG:HG2	1:D:287:ARG:NH1	2.17	0.43
1:B:135:LEU:HB2	1:B:136:PRO:HD3	1.99	0.43
1:D:326:MET:HE1	1:D:342:TYR:CD1	2.54	0.43
1:B:326:MET:HE1	1:B:342:TYR:CD1	2.53	0.43
1:A:257:ALA:HB2	1:A:342:TYR:OH	2.19	0.43
1:B:257:ALA:HB2	1:B:342:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:O	1:D:72:PRO:HD2	2.18	0.42
1:C:244:LYS:CE	1:C:252:GLY:O	2.68	0.42
1:A:3:ILE:HG13	1:A:144:VAL:HG13	2.01	0.42
1:A:3:ILE:HD13	1:A:3:ILE:HA	1.79	0.42
1:D:82:ILE:HG13	1:D:87:VAL:HG12	2.02	0.42
1:D:135:LEU:HB2	1:D:136:PRO:HD3	2.01	0.42
1:B:226:ASN:HD21	1:B:228:GLU:HB2	1.85	0.42
1:C:257:ALA:HB2	1:C:342:TYR:OH	2.20	0.42
1:D:257:ALA:HB2	1:D:342:TYR:OH	2.20	0.42
1:A:191:GLU:H	1:A:191:GLU:HG3	1.67	0.42
1:D:23:GLY:HA3	1:D:97:PHE:CD1	2.55	0.42
1:C:23:GLY:HA3	1:C:97:PHE:CD1	2.55	0.41
1:B:229:LYS:HA	1:B:229:LYS:HD2	1.92	0.41
1:C:44:VAL:O	1:C:72:PRO:HD2	2.21	0.41
1:A:23:GLY:HA3	1:A:97:PHE:CD1	2.54	0.41
1:B:241:SER:HA	1:B:291:ILE:O	2.20	0.41
1:C:10:SER:CB	3:C:523:HOH:O	2.68	0.41
1:C:241:SER:HA	1:C:291:ILE:O	2.20	0.41
1:B:23:GLY:HA3	1:B:97:PHE:CD1	2.55	0.41
1:A:26:ARG:HB2	3:A:503:HOH:O	2.20	0.41
1:B:3:ILE:HD11	1:B:11:VAL:HB	2.03	0.41
1:B:82:ILE:HG22	1:B:87:VAL:HG12	2.01	0.41
1:A:241:SER:HA	1:A:291:ILE:O	2.21	0.41
1:D:241:SER:HA	1:D:291:ILE:O	2.21	0.41
1:A:200:ASN:HD21	1:A:296:TYR:HB2	1.85	0.41
1:D:93:ASP:HA	3:D:525:HOH:O	2.20	0.41
1:C:287:ARG:HG2	1:C:287:ARG:NH1	2.19	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	326/349 (93%)	313 (96%)	11 (3%)	2 (1%)	22	26
1	B	323/349 (93%)	309 (96%)	11 (3%)	3 (1%)	14	17
1	C	330/349 (95%)	314 (95%)	12 (4%)	4 (1%)	11	11
1	D	330/349 (95%)	313 (95%)	13 (4%)	4 (1%)	11	11
All	All	1309/1396 (94%)	1249 (95%)	47 (4%)	13 (1%)	13	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	CYS
1	A	193	CYS
1	C	193	CYS
1	D	102	HIS
1	D	248	ASN
1	B	248	ASN
1	C	100	SER
1	C	102	HIS
1	C	248	ASN
1	D	193	CYS
1	B	192	CYS
1	D	100	SER
1	A	248	ASN

### 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	259/293 (88%)	240 (93%)	19 (7%)	11	15
1	B	264/293 (90%)	251 (95%)	13 (5%)	21	30
1	C	259/293 (88%)	244 (94%)	15 (6%)	17	23
1	D	262/293 (89%)	250 (95%)	12 (5%)	23	33
All	All	1044/1172 (89%)	985 (94%)	59 (6%)	17	24

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	19[A]	ARG
1	A	19[B]	ARG
1	A	24	GLU
1	A	47	GLN
1	A	67	GLN
1	A	82	ILE
1	A	87	VAL
1	A	99	LEU
1	A	150	GLN
1	A	167	GLU
1	A	189	MET
1	A	191	GLU
1	A	225	VAL
1	A	287	ARG
1	A	296	TYR
1	A	300	TYR
1	A	323	ASN
1	A	334	LEU
1	B	18	GLU
1	B	44	VAL
1	B	47	GLN
1	B	82	ILE
1	B	87	VAL
1	B	150	GLN
1	B	225	VAL
1	B	247	ASP
1	B	287	ARG
1	B	296	TYR
1	B	300	TYR
1	B	323	ASN
1	B	334	LEU
1	C	11	VAL
1	C	26	ARG
1	C	47	GLN
1	C	74	ILE
1	C	87	VAL
1	C	106	LYS
1	C	128	THR
1	C	139	ARG
1	C	198	LYS
1	C	225	VAL
1	C	262	GLU

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Mol	Chain	Res	Type
1	C	287	ARG
1	C	296	TYR
1	C	323	ASN
1	C	334	LEU
1	D	11	VAL
1	D	47	GLN
1	D	74	ILE
1	D	87	VAL
1	D	128	THR
1	D	225	VAL
1	D	287	ARG
1	D	296	TYR
1	D	316	GLN
1	D	323	ASN
1	D	331	SER
1	D	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	200	ASN
1	A	216	ASN
1	A	258	GLN
1	A	324	ASN
1	B	47	GLN
1	B	91	ASN
1	B	107	ASN
1	B	200	ASN
1	B	216	ASN
1	B	258	GLN
1	C	200	ASN
1	C	216	ASN
1	C	258	GLN
1	D	113	GLN
1	D	152	ASN
1	D	200	ASN
1	D	216	ASN
1	D	258	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/349 (94%)	0.37	8 (2%) 59 61	19, 42, 69, 99	1 (0%)
1	B	330/349 (94%)	0.17	9 (2%) 56 58	18, 37, 59, 88	1 (0%)
1	C	335/349 (95%)	0.63	24 (7%) 23 25	20, 45, 71, 115	1 (0%)
1	D	334/349 (95%)	0.36	17 (5%) 34 37	20, 40, 69, 96	2 (0%)
All	All	1330/1396 (95%)	0.38	58 (4%) 39 42	18, 41, 68, 115	5 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	VAL	4.7
1	C	247	ASP	4.7
1	C	74	ILE	3.9
1	C	81	SER	3.8
1	C	249	ASN	3.6
1	B	100	SER	3.5
1	A	249	ASN	3.5
1	A	188	ALA	3.4
1	C	191	GLU	3.4
1	C	260	THR	3.3
1	D	247	ASP	3.3
1	D	104	PRO	3.2
1	C	251	PRO	3.2
1	C	346	SER	3.2
1	A	74	ILE	3.1
1	C	104	PRO	3.1
1	D	11	VAL	2.9
1	B	247	ASP	2.9
1	C	102	HIS	2.8
1	D	193	CYS	2.7
1	B	224	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	11	VAL	2.7
1	C	105	GLY	2.7
1	A	12	VAL	2.7
1	B	192	CYS	2.6
1	D	346	SER	2.5
1	C	245	ALA	2.5
1	C	192	CYS	2.5
1	A	3	ILE	2.5
1	C	106	LYS	2.5
1	D	106	LYS	2.5
1	D	102	HIS	2.5
1	C	193	CYS	2.4
1	B	106	LYS	2.4
1	D	249	ASN	2.4
1	C	246	PRO	2.4
1	D	3	ILE	2.4
1	A	193	CYS	2.4
1	D	100	SER	2.4
1	B	2	ASN	2.4
1	B	249	ASN	2.4
1	C	250	ALA	2.4
1	C	278	ASN	2.3
1	C	3	ILE	2.3
1	A	190	GLU	2.3
1	D	107	ASN	2.3
1	C	277	ILE	2.3
1	B	246	PRO	2.2
1	D	250	ALA	2.2
1	C	59	ALA	2.2
1	D	192	CYS	2.2
1	C	276	GLY	2.1
1	D	13	ILE	2.1
1	C	248	ASN	2.1
1	D	191	GLU	2.0
1	A	247	ASP	2.0
1	B	82	ILE	2.0
1	D	82	ILE	2.0

## 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 [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

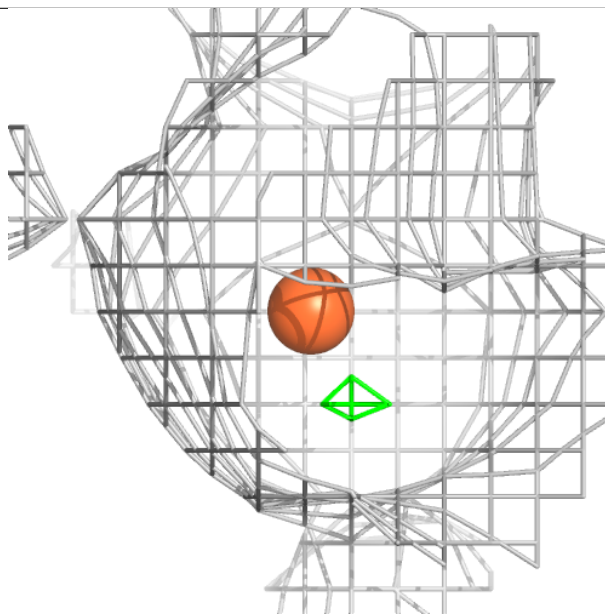
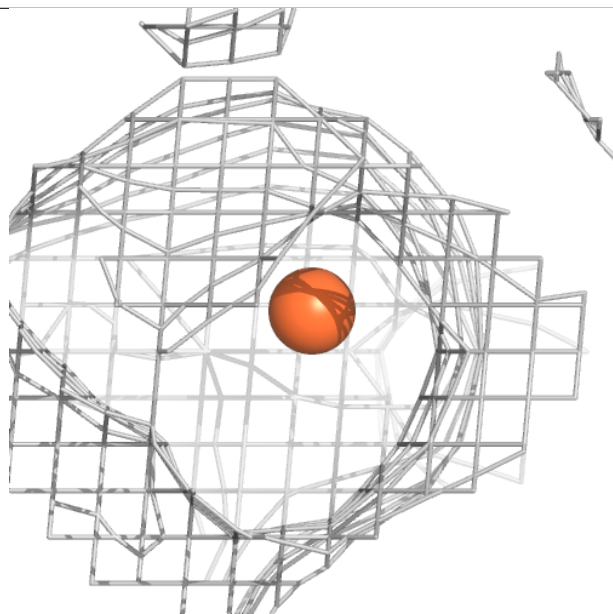
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	C	401	1/1	0.90	0.10	82,82,82,82	0
2	FE	D	401	1/1	0.90	0.09	80,80,80,80	0
2	FE	A	401	1/1	0.93	0.09	69,69,69,69	0
2	FE	B	401	1/1	0.98	0.09	59,59,59,59	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.

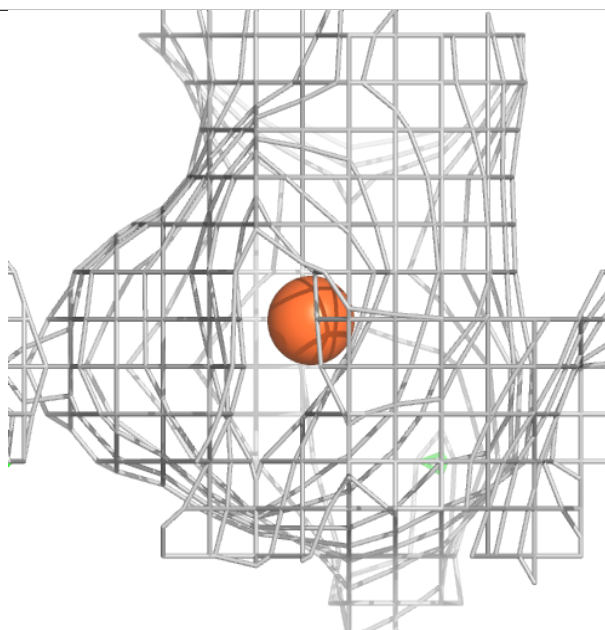
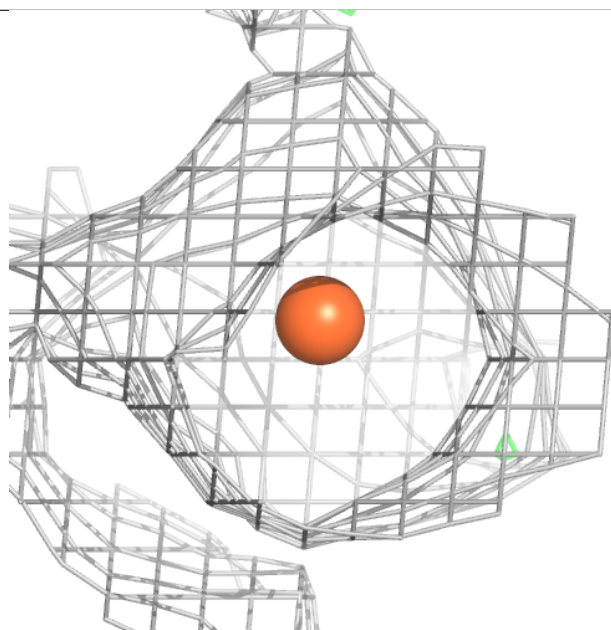
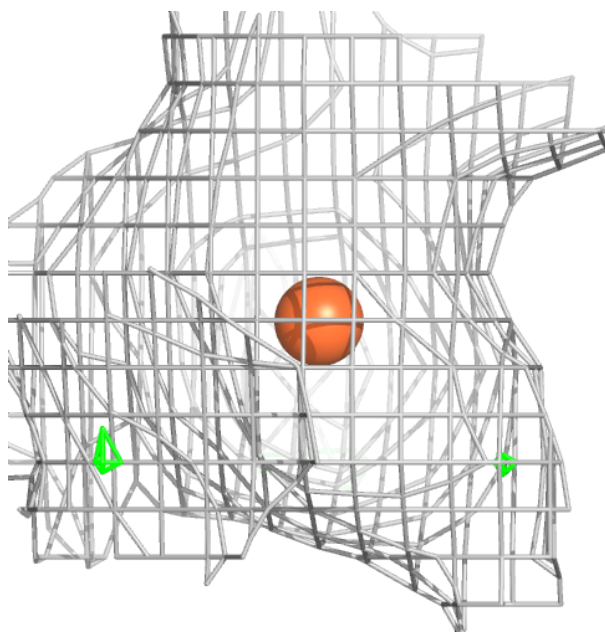
**Electron density around FE C 401:**

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



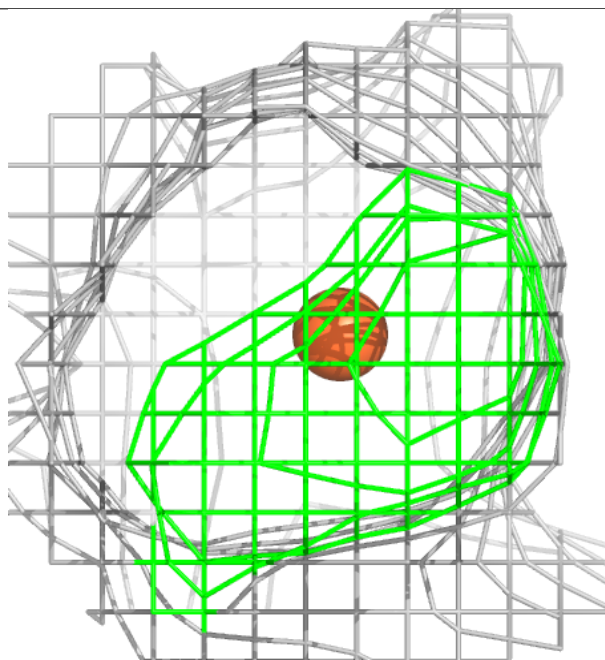
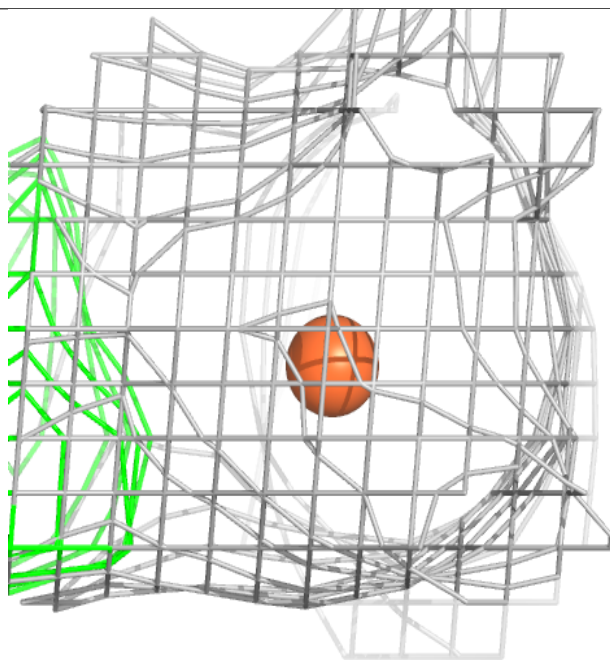
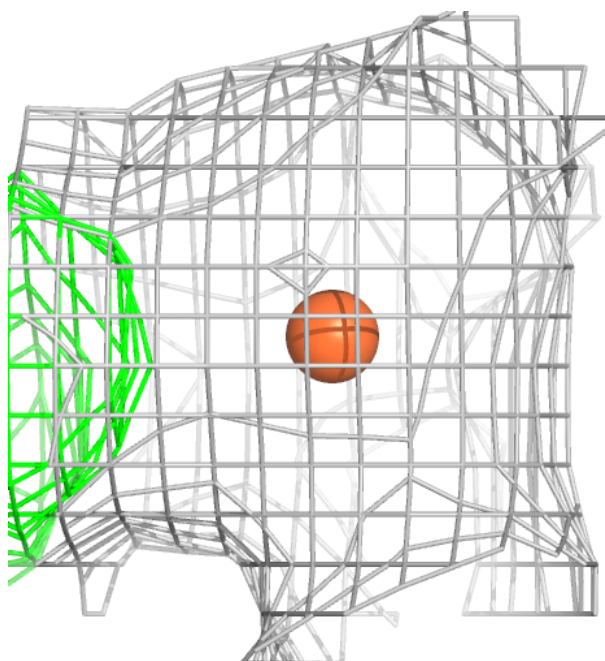
**Electron density around FE D 401:**

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

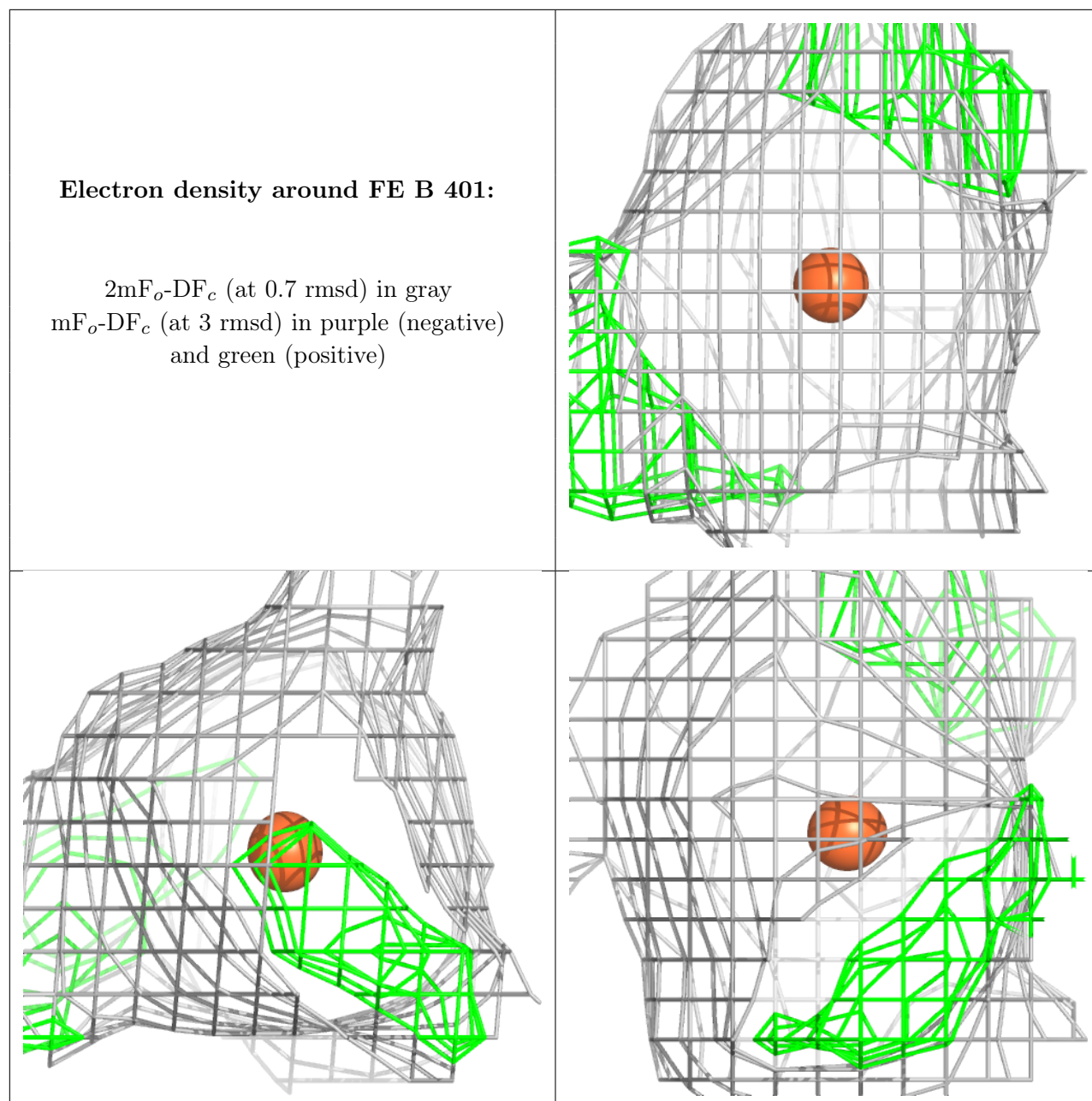


**Electron density around FE A 401:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.