



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 06:08 PM JST

PDB ID : 6LNH  
Title : Crystal structure of IDO from *Bacillus thuringiensis*  
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Deposited on : 2019-12-30  
Resolution : 2.34 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

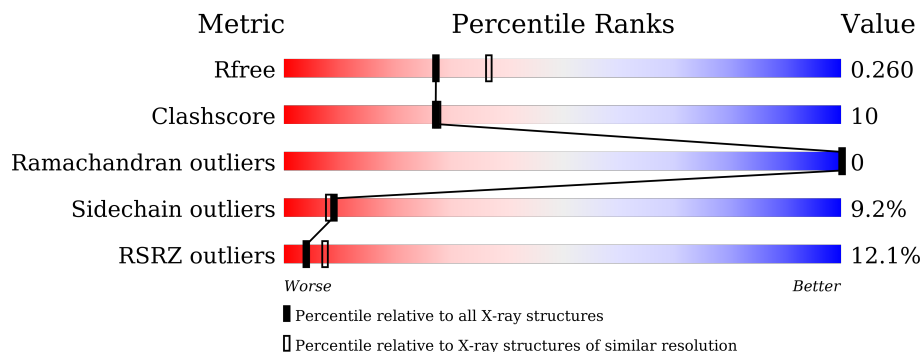
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	251	<div> <div>17%</div> <div> <div>69%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	251	<div> <div>8%</div> <div> <div>63%</div> <div>20%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	251	<div> <div>10%</div> <div> <div>71%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	251	<div> <div>7%</div> <div> <div>67%</div> <div>17%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7393 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 L-isoleucine-4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1841	1178	299	358	6			
1	B	223	Total	C	N	O	S	0	0	0
			1825	1164	301	356	4			
1	C	228	Total	C	N	O	S	0	0	0
			1872	1196	306	364	6			
1	D	211	Total	C	N	O	S	0	0	0
			1730	1108	282	336	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP E2GIN1
A	2	ALA	-	expression tag	UNP E2GIN1
A	3	GLY	-	expression tag	UNP E2GIN1
A	4	ALA	-	expression tag	UNP E2GIN1
A	5	GLY	-	expression tag	UNP E2GIN1
A	6	ALA	-	expression tag	UNP E2GIN1
A	7	GLY	-	expression tag	UNP E2GIN1
A	8	ALA	-	expression tag	UNP E2GIN1
A	9	GLY	-	expression tag	UNP E2GIN1
A	10	GLU	-	expression tag	UNP E2GIN1
A	11	PHE	-	expression tag	UNP E2GIN1
B	1	GLY	-	expression tag	UNP E2GIN1
B	2	ALA	-	expression tag	UNP E2GIN1
B	3	GLY	-	expression tag	UNP E2GIN1
B	4	ALA	-	expression tag	UNP E2GIN1
B	5	GLY	-	expression tag	UNP E2GIN1
B	6	ALA	-	expression tag	UNP E2GIN1
B	7	GLY	-	expression tag	UNP E2GIN1
B	8	ALA	-	expression tag	UNP E2GIN1
B	9	GLY	-	expression tag	UNP E2GIN1
B	10	GLU	-	expression tag	UNP E2GIN1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	PHE	-	expression tag	UNP E2GIN1
C	1	GLY	-	expression tag	UNP E2GIN1
C	2	ALA	-	expression tag	UNP E2GIN1
C	3	GLY	-	expression tag	UNP E2GIN1
C	4	ALA	-	expression tag	UNP E2GIN1
C	5	GLY	-	expression tag	UNP E2GIN1
C	6	ALA	-	expression tag	UNP E2GIN1
C	7	GLY	-	expression tag	UNP E2GIN1
C	8	ALA	-	expression tag	UNP E2GIN1
C	9	GLY	-	expression tag	UNP E2GIN1
C	10	GLU	-	expression tag	UNP E2GIN1
C	11	PHE	-	expression tag	UNP E2GIN1
D	1	GLY	-	expression tag	UNP E2GIN1
D	2	ALA	-	expression tag	UNP E2GIN1
D	3	GLY	-	expression tag	UNP E2GIN1
D	4	ALA	-	expression tag	UNP E2GIN1
D	5	GLY	-	expression tag	UNP E2GIN1
D	6	ALA	-	expression tag	UNP E2GIN1
D	7	GLY	-	expression tag	UNP E2GIN1
D	8	ALA	-	expression tag	UNP E2GIN1
D	9	GLY	-	expression tag	UNP E2GIN1
D	10	GLU	-	expression tag	UNP E2GIN1
D	11	PHE	-	expression tag	UNP E2GIN1

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Hg 3 3	0	0
2	A	3	Total Hg 3 3	0	0
2	D	1	Total Hg 1 1	0	0

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

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

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

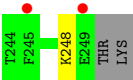
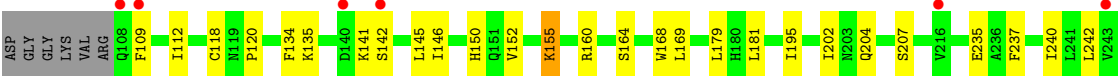
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	32	Total 32	O 32	0	0
4	C	38	Total 38	O 38	0	0
4	D	25	Total 25	O 25	0	0





● Molecule 1: L-isoleucine-4-hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.42Å 120.97Å 81.72Å 90.00° 108.11° 90.00°	Depositor
Resolution (Å)	24.86 – 2.34 24.85 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.6 (24.86-2.34) 97.6 (24.85-2.34)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.228 , 0.264 0.233 , 0.260	Depositor DCC
$R_{free}$ test set	1998 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, HG

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	0.45	0/1881	0.62	0/2539
1	B	0.44	0/1863	0.60	0/2516
1	C	0.41	0/1912	0.55	0/2580
1	D	0.47	0/1767	0.57	0/2389
All	All	0.44	0/7423	0.58	0/10024

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	1841	0	1772	33	0
1	B	1825	0	1766	53	0
1	C	1872	0	1807	35	0
1	D	1730	0	1677	29	0
2	A	3	0	0	0	0
2	B	3	0	0	1	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	19	0	0	0	0
4	B	32	0	0	1	0
4	C	38	0	0	2	0
4	D	25	0	0	0	0
All	All	7393	0	7022	144	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 10.

All (144) 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:B:150:HIS:HB2	1:B:242:LEU:HB2	1.56	0.87
1:B:118:CYS:SG	2:B:303:HG:HG	1.94	0.86
1:B:155:LYS:HZ1	1:B:235:GLU:CD	1.83	0.81
1:A:90:ASN:ND2	1:A:90:ASN:O	2.14	0.79
1:A:202:ILE:HG12	1:B:167:ILE:HD11	1.64	0.78
1:A:153:ARG:HD3	1:A:239:ASP:OD1	1.84	0.78
1:A:146:ILE:HD11	1:A:248:LYS:HG3	1.65	0.77
1:B:155:LYS:HZ2	1:B:235:GLU:HB3	1.50	0.76
1:D:155:LYS:HE2	1:D:235:GLU:CD	2.07	0.74
1:B:160:ARG:HH21	1:B:160:ARG:HG3	1.51	0.74
1:B:139:ILE:HG23	1:B:145:LEU:HD21	1.67	0.74
1:B:141:LYS:O	1:B:141:LYS:HG2	1.89	0.72
1:B:143:LYS:O	1:B:145:LEU:HD12	1.90	0.71
1:B:155:LYS:NZ	1:B:235:GLU:CB	2.54	0.70
1:B:155:LYS:HZ2	1:B:235:GLU:CB	2.05	0.70
1:C:90:ASN:ND2	1:C:109:PHE:O	2.22	0.70
1:D:134:PHE:HE1	1:D:145:LEU:HD12	1.56	0.70
1:A:10:GLU:HA	1:A:10:GLU:OE2	1.92	0.68
1:B:155:LYS:NZ	1:B:235:GLU:HB3	2.09	0.68
1:C:70:ARG:NH2	1:C:150:HIS:ND1	2.41	0.68
1:B:153:ARG:HG3	1:B:153:ARG:O	1.93	0.68
1:C:108:GLN:CD	1:C:108:GLN:H	1.97	0.67
1:D:179:LEU:HD11	1:D:240:ILE:HG12	1.77	0.67
1:B:159:GLU:OE2	1:B:159:GLU:N	2.27	0.67
1:D:155:LYS:HD3	1:D:237:PHE:HE1	1.62	0.65
1:C:150:HIS:HB2	1:C:242:LEU:HB2	1.80	0.64
1:D:152:VAL:HB	1:D:240:ILE:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD22	1:C:217:PHE:CE1	2.34	0.63
1:B:195:ILE:HB	1:B:204:GLN:HB2	1.81	0.63
1:C:19:ILE:HD12	1:C:19:ILE:N	2.13	0.63
1:A:175:PRO:HA	1:A:219:GLN:HE21	1.64	0.62
1:B:68:ARG:NH2	1:B:163:PHE:O	2.32	0.61
1:D:155:LYS:O	1:D:160:ARG:NH1	2.33	0.61
1:A:180:HIS:CE1	1:A:214:THR:HG21	2.37	0.60
1:D:19:ILE:O	1:D:19:ILE:HG22	2.02	0.60
1:B:160:ARG:NH2	1:B:160:ARG:HG3	2.16	0.59
1:B:197:ASN:HA	1:B:221:VAL:HG12	1.85	0.58
1:A:108:GLN:HG2	1:A:108:GLN:O	2.04	0.57
1:C:108:GLN:N	1:C:108:GLN:OE1	2.32	0.57
1:C:32:LEU:HB3	1:C:216:VAL:HG22	1.87	0.57
1:B:233:SER:OG	1:D:37:GLU:OE2	2.22	0.57
1:D:79:VAL:HG13	1:D:141:LYS:O	2.05	0.56
1:D:76:ILE:HG13	1:D:87:ASP:HB2	1.88	0.56
1:C:27:GLU:HG2	1:C:138:ILE:HD11	1.88	0.55
1:A:157:THR:HG22	1:A:159:GLU:H	1.72	0.55
1:A:153:ARG:HG3	1:A:153:ARG:O	2.07	0.55
1:B:139:ILE:CG2	1:B:145:LEU:HD21	2.35	0.55
1:C:62:ASP:OD1	1:C:63:ALA:N	2.40	0.54
1:C:215:LEU:HD23	1:C:216:VAL:N	2.23	0.54
1:A:155:LYS:O	1:A:162:SER:HB2	2.08	0.54
1:D:48:LEU:HD22	1:D:120:PRO:HD2	1.88	0.54
1:C:134:PHE:HE1	1:C:145:LEU:HD22	1.73	0.54
1:D:70:ARG:HD3	1:D:109:PHE:CZ	2.43	0.54
1:D:17:PHE:N	1:D:17:PHE:CD2	2.76	0.53
1:D:73:SER:HB2	1:D:112:ILE:HD12	1.91	0.53
1:B:103:GLY:HA2	1:B:105:LYS:HE3	1.91	0.53
1:A:146:ILE:CD1	1:A:248:LYS:HG3	2.38	0.52
1:A:180:HIS:CE1	1:A:214:THR:CG2	2.92	0.52
1:D:195:ILE:HB	1:D:204:GLN:HB3	1.91	0.52
1:C:167:ILE:HD11	1:D:202:ILE:HG12	1.90	0.52
1:A:150:HIS:HB2	1:A:242:LEU:HB2	1.91	0.51
1:A:202:ILE:CG1	1:B:167:ILE:HD11	2.39	0.51
1:A:215:LEU:HD13	1:A:217:PHE:CZ	2.45	0.51
1:C:19:ILE:CD1	1:C:19:ILE:N	2.73	0.50
1:C:158:LYS:NZ	4:C:407:HOH:O	2.38	0.50
1:D:150:HIS:HB2	1:D:242:LEU:HB2	1.94	0.50
1:A:155:LYS:O	1:A:160:ARG:NH1	2.42	0.50
1:B:237:PHE:C	1:B:237:PHE:CD1	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG21	1:B:135:LYS:HB2	1.94	0.50
1:D:168:TRP:CG	1:D:169:LEU:N	2.77	0.49
1:C:107:ARG:NH1	1:C:107:ARG:HG2	2.28	0.49
1:B:34:ILE:HB	1:B:214:THR:HB	1.93	0.49
1:C:200:ARG:HD2	1:C:200:ARG:O	2.13	0.49
1:D:17:PHE:N	1:D:17:PHE:HD2	2.10	0.49
1:A:81:SER:HB3	1:A:82:PRO:HD2	1.95	0.49
1:C:215:LEU:CD2	1:C:217:PHE:CE1	2.96	0.48
1:B:210:GLU:O	1:B:213:GLU:HG3	2.13	0.48
1:A:155:LYS:HE3	1:A:235:GLU:OE2	2.13	0.48
1:A:180:HIS:ND1	1:A:214:THR:HG23	2.29	0.47
1:D:155:LYS:HE2	1:D:235:GLU:CG	2.42	0.47
1:D:181:LEU:HA	1:D:240:ILE:HD12	1.96	0.47
1:B:67:CYS:HB2	1:B:68:ARG:HH21	1.79	0.47
1:B:131:GLU:O	1:B:135:LYS:HG2	2.14	0.47
1:C:24:HIS:C	1:C:24:HIS:HD1	2.18	0.47
1:A:47:SER:O	1:A:51:GLN:HG3	2.15	0.47
1:B:155:LYS:HZ1	1:B:235:GLU:CB	2.26	0.47
1:A:201:GLU:HA	1:B:163:PHE:CE2	2.50	0.47
1:B:106:VAL:HG12	1:B:108:GLN:N	2.30	0.47
1:B:51:GLN:O	4:B:401:HOH:O	2.20	0.46
1:B:200:ARG:HD3	1:B:200:ARG:O	2.16	0.46
1:D:78:TYR:HB2	1:D:81:SER:CB	2.45	0.46
1:A:168:TRP:CG	1:A:169:LEU:N	2.83	0.46
1:A:163:PHE:CZ	1:B:201:GLU:HB2	2.51	0.46
1:A:131:GLU:O	1:A:135:LYS:HG3	2.16	0.46
1:B:143:LYS:HE3	1:B:143:LYS:HB2	1.57	0.46
1:B:157:THR:HG22	1:B:160:ARG:H	1.81	0.46
1:D:146:ILE:HD11	1:D:248:LYS:HA	1.97	0.46
1:C:142:SER:OG	1:C:142:SER:O	2.31	0.45
1:A:22:LYS:HA	1:A:22:LYS:HD2	1.78	0.45
1:B:103:GLY:HA2	1:B:105:LYS:NZ	2.31	0.45
1:B:157:THR:HG22	1:B:160:ARG:N	2.32	0.45
1:B:56:TYR:CD2	1:B:239:ASP:HB3	2.52	0.45
1:C:27:GLU:HG2	1:C:138:ILE:CD1	2.47	0.44
1:B:155:LYS:NZ	1:B:235:GLU:OE1	2.42	0.44
1:A:160:ARG:HB3	1:A:160:ARG:CZ	2.46	0.44
1:A:67:CYS:SG	1:A:162:SER:HA	2.56	0.44
1:A:32:LEU:HB3	1:A:216:VAL:CG1	2.48	0.44
1:D:77:LYS:HG2	1:D:134:PHE:HZ	1.83	0.44
1:C:107:ARG:HH11	1:C:107:ARG:HG2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LYS:O	4:C:401:HOH:O	2.21	0.44
1:C:157:THR:HG23	1:C:159:GLU:H	1.83	0.43
1:B:103:GLY:HA2	1:B:105:LYS:CE	2.48	0.43
1:B:168:TRP:HA	1:B:168:TRP:CE3	2.52	0.43
1:C:215:LEU:HD13	1:C:217:PHE:CZ	2.53	0.43
1:C:143:LYS:O	1:C:145:LEU:HD12	2.18	0.43
1:A:155:LYS:HD3	1:A:160:ARG:NH2	2.34	0.43
1:A:78:TYR:HA	1:A:144:ASP:OD1	2.19	0.43
1:B:130:THR:HA	1:B:245:PHE:CE1	2.53	0.43
1:C:70:ARG:HD3	1:C:109:PHE:CE1	2.54	0.42
1:C:226:THR:HG23	1:C:227:PRO:HD2	2.01	0.42
1:C:70:ARG:HD3	1:C:109:PHE:HE1	1.84	0.42
1:D:155:LYS:HD3	1:D:237:PHE:CE1	2.49	0.42
1:C:210:GLU:H	1:C:210:GLU:HG2	1.73	0.42
1:D:70:ARG:HD3	1:D:109:PHE:CE2	2.54	0.42
1:B:155:LYS:NZ	1:B:235:GLU:HB2	2.31	0.42
1:B:155:LYS:NZ	1:B:235:GLU:CD	2.65	0.42
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.82	0.42
1:A:155:LYS:CE	1:A:235:GLU:OE2	2.67	0.42
1:C:107:ARG:CG	1:C:107:ARG:HH11	2.33	0.42
1:D:155:LYS:HD2	1:D:235:GLU:HB3	2.01	0.42
1:B:160:ARG:CG	1:B:160:ARG:NH2	2.82	0.41
1:A:146:ILE:CG1	1:A:248:LYS:HG3	2.51	0.41
1:C:181:LEU:HA	1:C:240:ILE:HD13	2.03	0.41
1:B:118:CYS:HA	1:B:123:GLN:HE21	1.85	0.41
1:B:189:ILE:HD12	1:B:230:THR:HA	2.03	0.41
1:B:185:SER:OG	1:B:237:PHE:CD2	2.74	0.41
1:B:31:PHE:HA	1:B:216:VAL:O	2.21	0.41
1:C:141:LYS:HD3	1:C:141:LYS:N	2.36	0.41
1:B:70:ARG:HD3	1:B:109:PHE:CE1	2.56	0.40
1:C:168:TRP:CG	1:C:169:LEU:N	2.86	0.40
1:B:166:PRO:HG2	1:B:170:HIS:CG	2.57	0.40
1:B:188:ALA:HB1	1:B:228:LEU:HD11	2.04	0.40
1:D:155:LYS:CD	1:D:237:PHE:HE1	2.33	0.40
1:C:41:GLN:OE1	1:C:41:GLN:HA	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	219/251 (87%)	209 (95%)	10 (5%)	0	100	100
1	B	217/251 (86%)	213 (98%)	4 (2%)	0	100	100
1	C	222/251 (88%)	217 (98%)	5 (2%)	0	100	100
1	D	205/251 (82%)	200 (98%)	5 (2%)	0	100	100
All	All	863/1004 (86%)	839 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	208/223 (93%)	188 (90%)	20 (10%)	8	7
1	B	207/223 (93%)	182 (88%)	25 (12%)	5	4
1	C	212/223 (95%)	190 (90%)	22 (10%)	7	6
1	D	197/223 (88%)	188 (95%)	9 (5%)	27	33
All	All	824/892 (92%)	748 (91%)	76 (9%)	9	8

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	14	MET
1	A	15	SER
1	A	18	SER
1	A	22	LYS
1	A	24	HIS
1	A	35	SER
1	A	38	ILE
1	A	67	CYS
1	A	88	ASN
1	A	89	SER
1	A	90	ASN
1	A	153	ARG
1	A	155	LYS
1	A	164	SER
1	A	165	SER
1	A	200	ARG
1	A	207	SER
1	A	215	LEU
1	B	35	SER
1	B	61	ASP
1	B	66	GLU
1	B	68	ARG
1	B	70	ARG
1	B	81	SER
1	B	91	ASP
1	B	96	LYS
1	B	105	LYS
1	B	108	GLN
1	B	131	GLU
1	B	141	LYS
1	B	142	SER
1	B	143	LYS
1	B	153	ARG
1	B	155	LYS
1	B	157	THR
1	B	158	LYS
1	B	160	ARG
1	B	164	SER
1	B	168	TRP
1	B	198	SER
1	B	200	ARG
1	B	235	GLU

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Mol	Chain	Res	Type
1	B	240	ILE
1	C	14	MET
1	C	17	PHE
1	C	18	SER
1	C	20	GLU
1	C	21	GLU
1	C	32	LEU
1	C	37	GLU
1	C	43	GLU
1	C	44	GLU
1	C	47	SER
1	C	68	ARG
1	C	89	SER
1	C	91	ASP
1	C	96	LYS
1	C	107	ARG
1	C	108	GLN
1	C	127	ARG
1	C	141	LYS
1	C	142	SER
1	C	165	SER
1	C	200	ARG
1	C	201	GLU
1	D	18	SER
1	D	68	ARG
1	D	71	SER
1	D	118	CYS
1	D	135	LYS
1	D	142	SER
1	D	155	LYS
1	D	164	SER
1	D	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	45	ASN
1	C	204	GLN
1	D	45	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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	225/251 (89%)	1.07	43 (19%) <b>1</b> <b>2</b>	37, 57, 99, 119	0
1	B	223/251 (88%)	0.67	21 (9%) <b>8</b> <b>13</b>	37, 51, 88, 125	0
1	C	228/251 (90%)	0.63	26 (11%) <b>5</b> <b>8</b>	33, 47, 87, 104	0
1	D	211/251 (84%)	0.53	17 (8%) <b>12</b> <b>18</b>	35, 49, 83, 111	0
All	All	887/1004 (88%)	0.73	107 (12%) <b>4</b> <b>7</b>	33, 51, 91, 125	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	PHE	9.5
1	A	14	MET	8.7
1	A	17	PHE	8.2
1	A	80	ASP	7.0
1	B	62	ASP	6.7
1	D	67	CYS	6.5
1	A	81	SER	6.3
1	B	106	VAL	5.9
1	A	94	GLN	5.6
1	D	79	VAL	5.6
1	A	65	GLY	5.2
1	C	63	ALA	4.8
1	C	108	GLN	4.8
1	C	60	GLU	4.5
1	A	66	GLU	4.5
1	A	11	PHE	4.5
1	A	109	PHE	4.5
1	A	9	GLY	4.3
1	D	109	PHE	4.3
1	A	243	VAL	4.2
1	C	67	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	16	GLY	4.1
1	A	15	SER	4.1
1	C	200	ARG	4.0
1	C	62	ASP	3.9
1	D	108	GLN	3.8
1	C	17	PHE	3.8
1	B	61	ASP	3.7
1	D	17	PHE	3.7
1	B	243	VAL	3.7
1	B	80	ASP	3.6
1	A	108	GLN	3.5
1	C	95	SER	3.5
1	C	107	ARG	3.5
1	A	126	VAL	3.5
1	B	18	SER	3.4
1	B	41	GLN	3.4
1	A	249	GLU	3.4
1	B	107	ARG	3.4
1	A	91	ASP	3.4
1	A	37	GLU	3.4
1	C	97	GLU	3.3
1	C	243	VAL	3.3
1	D	249	GLU	3.3
1	A	149	LEU	3.2
1	D	19	ILE	3.2
1	D	80	ASP	3.1
1	B	94	GLN	3.0
1	B	60	GLU	3.0
1	C	15	SER	3.0
1	B	93	PHE	2.9
1	A	160	ARG	2.9
1	A	242	LEU	2.8
1	C	14	MET	2.8
1	D	37	GLU	2.8
1	C	42	GLU	2.8
1	A	179	LEU	2.8
1	D	140	ASP	2.8
1	A	92	TYR	2.8
1	B	108	GLN	2.7
1	A	231	GLU	2.7
1	C	241	LEU	2.7
1	C	12	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	180	HIS	2.6
1	A	79	VAL	2.6
1	C	13	LYS	2.6
1	D	243	VAL	2.6
1	D	88	ASN	2.6
1	C	20	GLU	2.6
1	B	241	LEU	2.5
1	A	142	SER	2.5
1	B	163	PHE	2.5
1	D	142	SER	2.5
1	A	241	LEU	2.5
1	A	244	THR	2.5
1	A	82	PRO	2.5
1	B	44	GLU	2.5
1	C	18	SER	2.5
1	C	10	GLU	2.4
1	C	21	GLU	2.4
1	B	95	SER	2.4
1	D	245	PHE	2.4
1	B	147	ILE	2.4
1	A	42	GLU	2.4
1	C	240	ILE	2.3
1	B	96	LYS	2.3
1	D	68	ARG	2.3
1	A	60	GLU	2.3
1	A	41	GLN	2.3
1	A	248	LYS	2.3
1	A	130	THR	2.3
1	D	216	VAL	2.3
1	A	144	ASP	2.3
1	D	61	ASP	2.2
1	B	178	PHE	2.2
1	B	200	ARG	2.2
1	A	177	VAL	2.2
1	B	79	VAL	2.2
1	A	125	ILE	2.1
1	C	89	SER	2.1
1	A	178	PHE	2.1
1	C	148	GLY	2.1
1	C	37	GLU	2.1
1	A	24	HIS	2.0
1	A	140	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	200	ARG	2.0
1	A	237	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

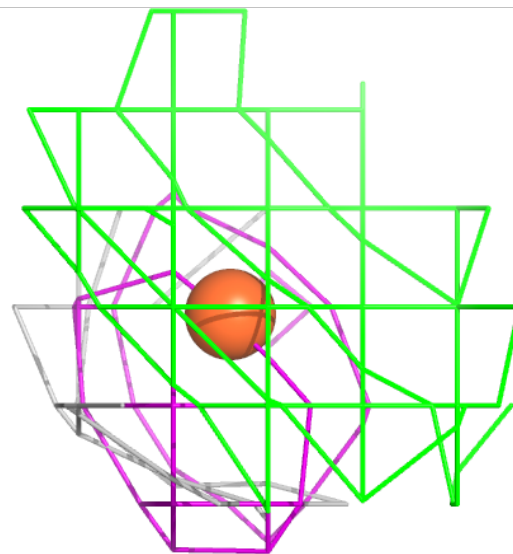
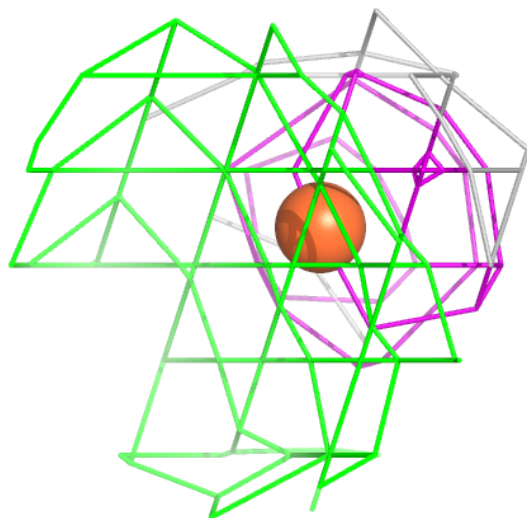
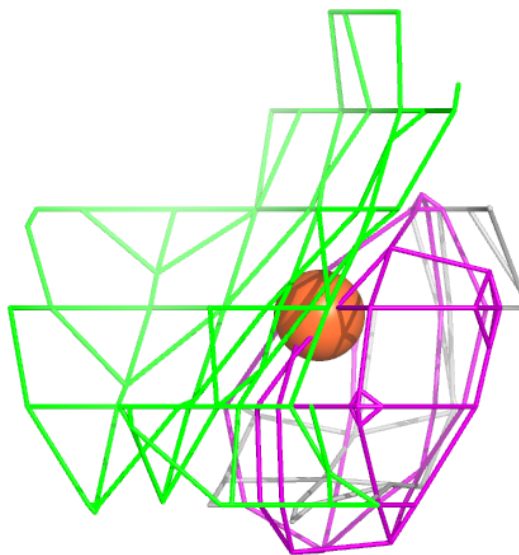
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FE	C	301	1/1	-0.02	0.25	48,48,48,48	0
2	HG	B	303	1/1	0.68	0.28	291,291,291,291	0
2	HG	A	303	1/1	0.77	0.15	141,141,141,141	0
2	HG	D	301	1/1	0.87	0.15	87,87,87,87	0
2	HG	A	301	1/1	0.87	0.12	167,167,167,167	0
3	FE	A	304	1/1	0.89	0.14	60,60,60,60	0
3	FE	B	304	1/1	0.91	0.21	48,48,48,48	0
2	HG	A	302	1/1	0.92	0.06	85,85,85,85	0
2	HG	B	302	1/1	0.93	0.21	224,224,224,224	0
2	HG	B	301	1/1	0.96	0.10	86,86,86,86	0
3	FE	D	302	1/1	0.97	0.10	58,58,58,58	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.

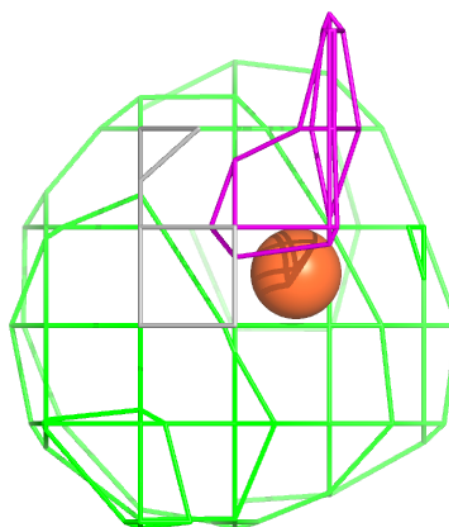
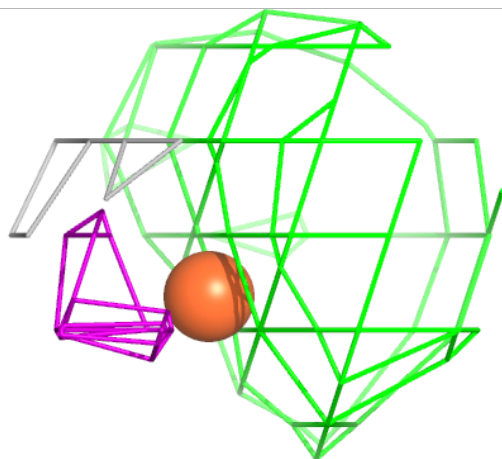
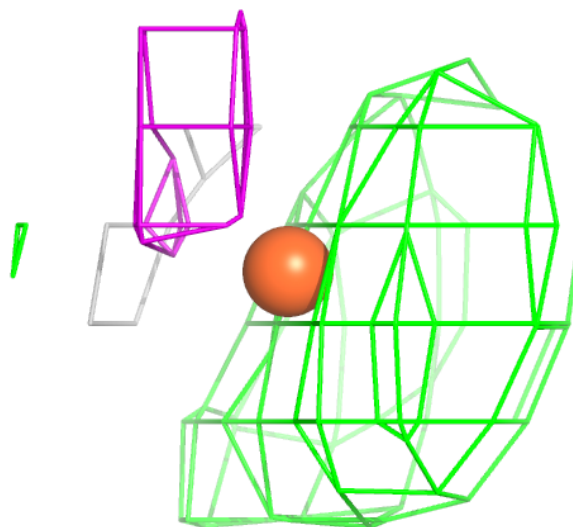
**Electron density around FE C 301:**

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



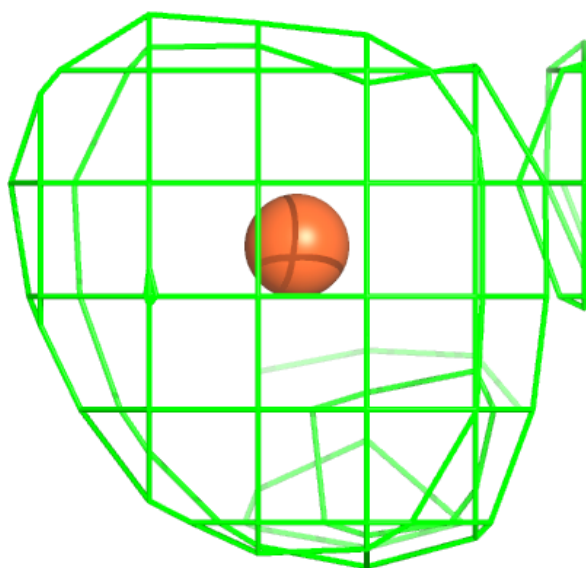
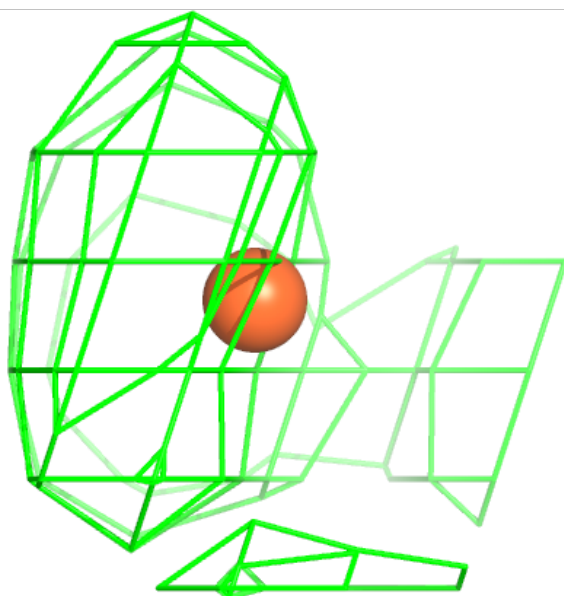
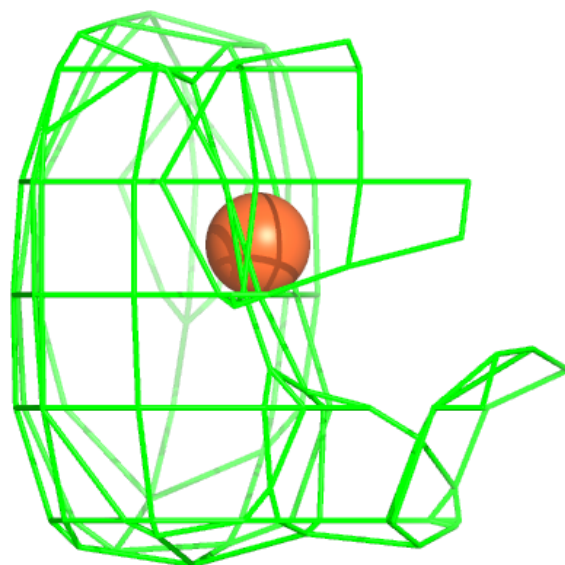
**Electron density around FE A 304:**

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

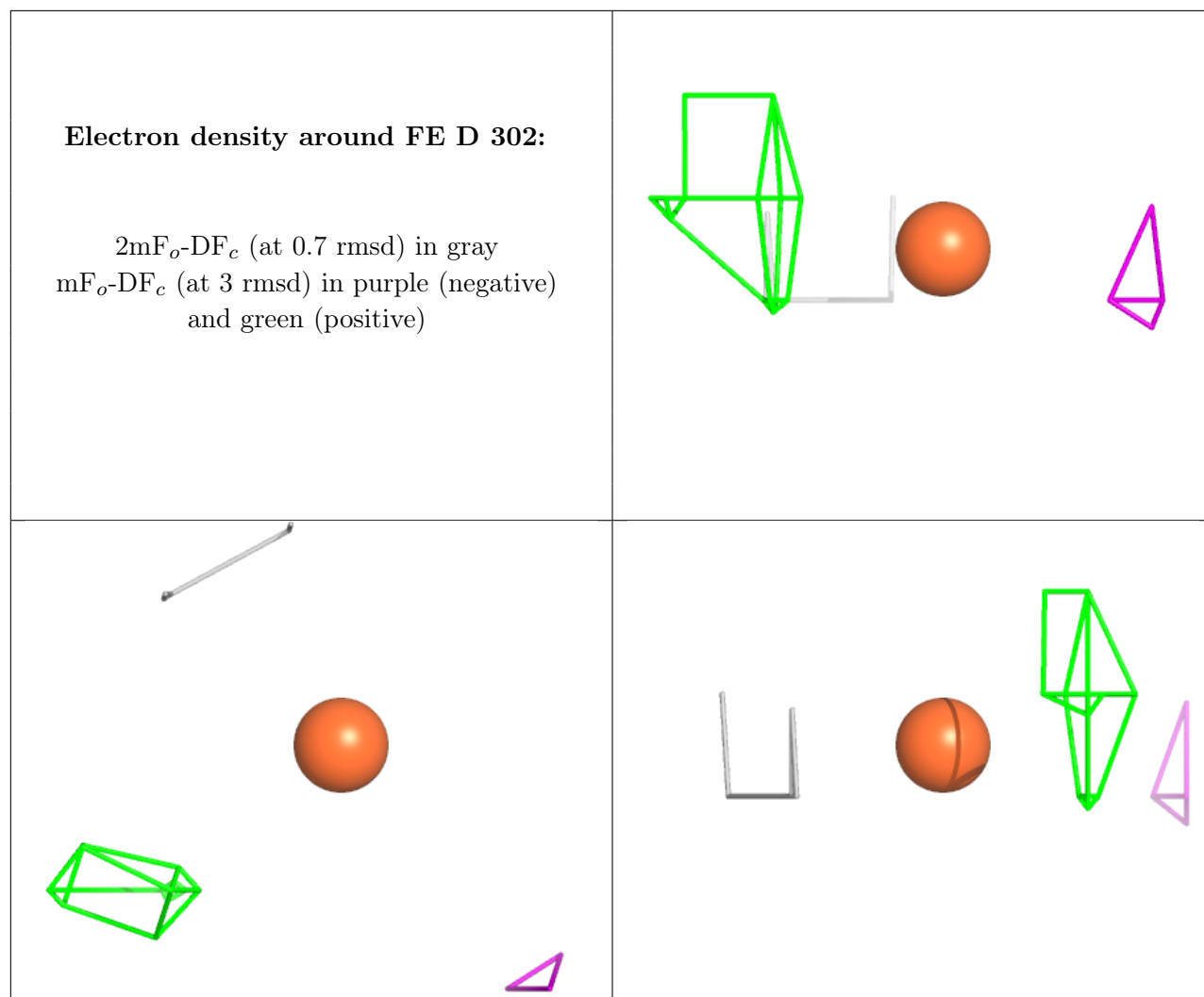


**Electron density around FE B 304:**

$2mF_o-DF_c$  (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.