



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 04:27 PM JST

PDB ID : 7CUP
Title : Structure of 2,5-dihydroxypridine Dioxygenase from *Pseudomonas putida* KT2440
Authors : Liu, G.Q.; Tang, H.Z.
Deposited on : 2020-08-23
Resolution : 2.00 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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

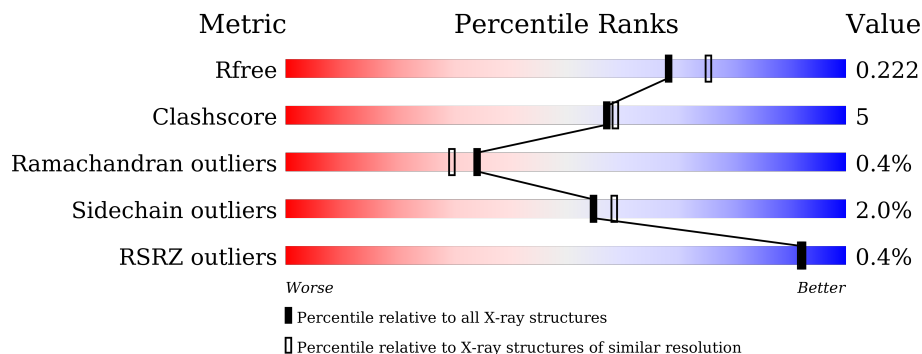
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	363	 83% 12% . .
1	B	363	 85% 9% . .
1	C	363	 87% 8% . .
1	D	363	 88% 7% .
1	E	363	 84% 11% . .
1	F	363	 86% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17845 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 2,5-dihydropyridine 5,6-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	2723	1720	472	515	16	0	0	0
1	B	348	2723	1720	472	515	16	0	0	0
1	C	348	2723	1720	472	515	16	0	0	0
1	D	348	2723	1720	472	515	16	0	0	0
1	E	347	2718	1717	471	514	16	0	0	0
1	F	347	2718	1717	471	514	16	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	LYS	-	expression tag	UNP Q88FY1
A	352	LEU	-	expression tag	UNP Q88FY1
A	353	ALA	-	expression tag	UNP Q88FY1
A	354	ALA	-	expression tag	UNP Q88FY1
A	355	ALA	-	expression tag	UNP Q88FY1
A	356	LEU	-	expression tag	UNP Q88FY1
A	357	GLU	-	expression tag	UNP Q88FY1
A	358	HIS	-	expression tag	UNP Q88FY1
A	359	HIS	-	expression tag	UNP Q88FY1
A	360	HIS	-	expression tag	UNP Q88FY1
A	361	HIS	-	expression tag	UNP Q88FY1
A	362	HIS	-	expression tag	UNP Q88FY1
A	363	HIS	-	expression tag	UNP Q88FY1
B	351	LYS	-	expression tag	UNP Q88FY1
B	352	LEU	-	expression tag	UNP Q88FY1
B	353	ALA	-	expression tag	UNP Q88FY1
B	354	ALA	-	expression tag	UNP Q88FY1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	355	ALA	-	expression tag	UNP Q88FY1
B	356	LEU	-	expression tag	UNP Q88FY1
B	357	GLU	-	expression tag	UNP Q88FY1
B	358	HIS	-	expression tag	UNP Q88FY1
B	359	HIS	-	expression tag	UNP Q88FY1
B	360	HIS	-	expression tag	UNP Q88FY1
B	361	HIS	-	expression tag	UNP Q88FY1
B	362	HIS	-	expression tag	UNP Q88FY1
B	363	HIS	-	expression tag	UNP Q88FY1
C	351	LYS	-	expression tag	UNP Q88FY1
C	352	LEU	-	expression tag	UNP Q88FY1
C	353	ALA	-	expression tag	UNP Q88FY1
C	354	ALA	-	expression tag	UNP Q88FY1
C	355	ALA	-	expression tag	UNP Q88FY1
C	356	LEU	-	expression tag	UNP Q88FY1
C	357	GLU	-	expression tag	UNP Q88FY1
C	358	HIS	-	expression tag	UNP Q88FY1
C	359	HIS	-	expression tag	UNP Q88FY1
C	360	HIS	-	expression tag	UNP Q88FY1
C	361	HIS	-	expression tag	UNP Q88FY1
C	362	HIS	-	expression tag	UNP Q88FY1
C	363	HIS	-	expression tag	UNP Q88FY1
D	351	LYS	-	expression tag	UNP Q88FY1
D	352	LEU	-	expression tag	UNP Q88FY1
D	353	ALA	-	expression tag	UNP Q88FY1
D	354	ALA	-	expression tag	UNP Q88FY1
D	355	ALA	-	expression tag	UNP Q88FY1
D	356	LEU	-	expression tag	UNP Q88FY1
D	357	GLU	-	expression tag	UNP Q88FY1
D	358	HIS	-	expression tag	UNP Q88FY1
D	359	HIS	-	expression tag	UNP Q88FY1
D	360	HIS	-	expression tag	UNP Q88FY1
D	361	HIS	-	expression tag	UNP Q88FY1
D	362	HIS	-	expression tag	UNP Q88FY1
D	363	HIS	-	expression tag	UNP Q88FY1
E	351	LYS	-	expression tag	UNP Q88FY1
E	352	LEU	-	expression tag	UNP Q88FY1
E	353	ALA	-	expression tag	UNP Q88FY1
E	354	ALA	-	expression tag	UNP Q88FY1
E	355	ALA	-	expression tag	UNP Q88FY1
E	356	LEU	-	expression tag	UNP Q88FY1
E	357	GLU	-	expression tag	UNP Q88FY1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	358	HIS	-	expression tag	UNP Q88FY1
E	359	HIS	-	expression tag	UNP Q88FY1
E	360	HIS	-	expression tag	UNP Q88FY1
E	361	HIS	-	expression tag	UNP Q88FY1
E	362	HIS	-	expression tag	UNP Q88FY1
E	363	HIS	-	expression tag	UNP Q88FY1
F	351	LYS	-	expression tag	UNP Q88FY1
F	352	LEU	-	expression tag	UNP Q88FY1
F	353	ALA	-	expression tag	UNP Q88FY1
F	354	ALA	-	expression tag	UNP Q88FY1
F	355	ALA	-	expression tag	UNP Q88FY1
F	356	LEU	-	expression tag	UNP Q88FY1
F	357	GLU	-	expression tag	UNP Q88FY1
F	358	HIS	-	expression tag	UNP Q88FY1
F	359	HIS	-	expression tag	UNP Q88FY1
F	360	HIS	-	expression tag	UNP Q88FY1
F	361	HIS	-	expression tag	UNP Q88FY1
F	362	HIS	-	expression tag	UNP Q88FY1
F	363	HIS	-	expression tag	UNP Q88FY1

- Molecule 2 is FE (III) ION (three-letter code: 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
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	229	Total O 229 229	0	0

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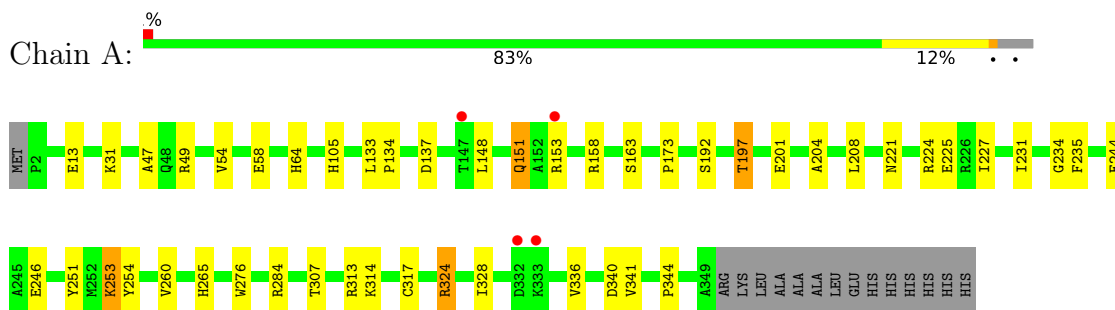
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	266	Total 266	O 266	0	0
3	C	251	Total 251	O 251	0	0
3	D	283	Total 283	O 283	0	0
3	E	246	Total 246	O 246	0	0
3	F	236	Total 236	O 236	0	0

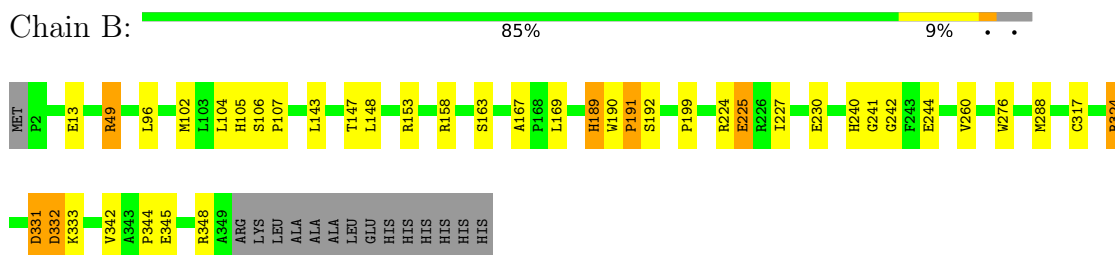
3 Residue-property plots [i](#)

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.

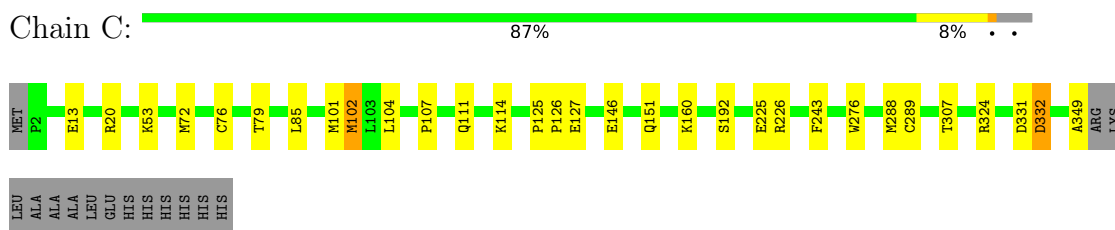
- Molecule 1: 2,5-dihydroxypyridine 5,6-dioxygenase



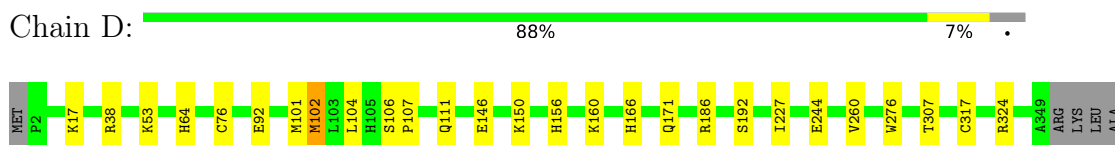
- Molecule 1: 2,5-dihydroxypyridine 5,6-dioxygenase



- Molecule 1: 2,5-dihydroxypyridine 5,6-dioxygenase




- Molecule 1: 2,5-dihydroxypyridine 5,6-dioxygenase



ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS


• Molecule 1: 2,5-dihydropyridine 5,6-dioxygenase

Chain E:  84% 11%

MET P2 D22 E23 T24 Q25 S26 E45 R49 K63 L59 C76 A87 Q88 L96 L104 H105 S106 P107 Q111 R118 R140 R153 R158 S163 W190 P191 S192 D202 S203 A204 I227 K233 G234 F235 I236 E244 E259

I263 W276 H282 N285 G310 T315 P316 R324 D331 D332 R348 ALA ARG LYS LEU LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: 2,5-dihydropyridine 5,6-dioxygenase

Chain F:  86% 9%

MET P2 V3 S4 N5 L8 M11 R38 Q48 K53 C76 H105 S106 P107 Q111 D138 V142 L148 Q151 R158 P168 W190 P191 S192 N200 A204 P218 N221 R226 I227 G234 E244 V260 G310 K314

T315 P316 C317 R324 D331 D332 R348 ALA ARG LYS LEU LEU ALA ALA LEU LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.96Å 143.75Å 118.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.00 47.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.41-2.00) 96.7 (47.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.171 , 0.213 0.182 , 0.222	Depositor DCC
R_{free} test set	2013 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	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	17845	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 43.38 % 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 1.7777e-04. 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: 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	0.70	0/2788	0.86	2/3788 (0.1%)
1	B	0.74	0/2788	0.89	4/3788 (0.1%)
1	C	0.75	1/2788 (0.0%)	0.90	0/3788
1	D	0.75	0/2788	0.88	1/3788 (0.0%)
1	E	0.72	1/2783 (0.0%)	0.89	3/3781 (0.1%)
1	F	0.71	0/2783	0.87	2/3781 (0.1%)
All	All	0.73	2/16718 (0.0%)	0.88	12/22714 (0.1%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	GLU	CD-OE1	5.39	1.31	1.25
1	E	26	SER	CA-CB	-5.05	1.45	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	B	324	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	A	324	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	332	ASP	CB-CA-C	-6.33	97.73	110.40
1	E	324	ARG	NE-CZ-NH1	6.05	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	E	105	HIS	CB-CA-C	5.76	121.92	110.40
1	E	332	ASP	CB-CA-C	-5.45	99.51	110.40
1	D	38	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	F	324	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	331	ASP	CB-CA-C	-5.07	100.26	110.40
1	F	105	HIS	CB-CA-C	5.04	120.48	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	332	ASP	Peptide

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	2723	0	2653	34	0
1	B	2723	0	2653	27	0
1	C	2723	0	2653	29	0
1	D	2723	0	2653	22	0
1	E	2718	0	2648	27	0
1	F	2718	0	2648	23	0
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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	229	0	0	5	0
3	B	266	0	0	7	0
3	C	251	0	0	10	0
3	D	283	0	0	9	0
3	E	246	0	0	5	0
3	F	236	0	0	5	0
All	All	17845	0	15908	157	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 (157) 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:C:289:CYS:HB2	3:C:727:HOH:O	1.34	1.26
1:F:348:ARG:C	3:F:504:HOH:O	1.96	1.03
1:E:348:ARG:C	3:E:508:HOH:O	1.95	1.02
1:F:8:LEU:HA	1:F:11:MET:HE3	1.45	0.97
1:B:241:GLY:O	3:B:502:HOH:O	1.85	0.93
1:D:107:PRO:O	1:D:111:GLN:HG2	1.68	0.92
1:E:22:ASP:OD1	1:E:24:THR:HG22	1.69	0.91
1:A:227:ILE:HD11	1:A:244:GLU:HB3	1.54	0.87
1:B:242:GLY:N	3:B:501:HOH:O	1.84	0.86
1:C:13:GLU:OE2	1:E:49:ARG:NH2	2.08	0.86
1:B:227:ILE:HD11	1:B:244:GLU:HB3	1.56	0.85
1:F:221:ASN:ND2	3:F:501:HOH:O	2.12	0.83
1:D:227:ILE:HD11	1:D:244:GLU:HB3	1.66	0.77
1:C:349:ALA:O	3:C:501:HOH:O	2.02	0.77
1:D:186:ARG:HB3	3:D:622:HOH:O	1.84	0.76
1:F:8:LEU:HA	1:F:11:MET:CE	2.19	0.73
1:D:186:ARG:HG3	3:D:716:HOH:O	1.88	0.73
1:E:331:ASP:O	1:E:332:ASP:HB2	1.86	0.72
1:A:153:ARG:NH1	3:A:501:HOH:O	2.22	0.72
1:C:225:GLU:OE1	3:C:502:HOH:O	2.10	0.69
1:D:171:GLN:OE1	3:D:501:HOH:O	2.11	0.68
1:B:148:LEU:HD22	1:B:344:PRO:HD3	1.75	0.68
1:E:331:ASP:O	1:E:332:ASP:CB	2.42	0.68
1:E:227:ILE:HD11	1:E:244:GLU:HB3	1.75	0.67
1:A:246:GLU:OE1	1:C:324:ARG:NH1	2.20	0.66
1:C:76:CYS:HA	1:C:104:LEU:HD13	1.77	0.65
1:D:76:CYS:HA	1:D:104:LEU:HD13	1.77	0.65
1:B:240:HIS:HD2	3:B:724:HOH:O	1.79	0.65
1:B:225:GLU:HG3	1:B:244:GLU:OE2	1.98	0.64
1:D:92:GLU:OE2	3:D:502:HOH:O	2.15	0.64
1:F:227:ILE:HD11	1:F:244:GLU:HB3	1.81	0.62
1:C:226:ARG:NH2	3:C:505:HOH:O	2.27	0.62
1:D:156:HIS:HE1	3:D:743:HOH:O	1.82	0.61
1:C:349:ALA:C	3:C:501:HOH:O	2.37	0.61
1:B:189:HIS:HE1	3:B:536:HOH:O	1.82	0.61
1:E:25:GLN:NE2	1:E:118:ARG:HH12	1.99	0.61
1:A:173:PRO:O	1:A:197:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ARG:HD2	3:E:604:HOH:O	2.02	0.60
1:A:204:ALA:HB3	1:A:234:GLY:HA2	1.84	0.58
1:C:102:MET:CE	1:C:288:MET:CE	2.81	0.58
1:E:88:GLN:HE22	1:E:111:GLN:HE21	1.49	0.58
1:B:331:ASP:O	1:B:332:ASP:CB	2.52	0.58
1:F:158:ARG:NH1	3:F:502:HOH:O	2.17	0.57
1:E:282:HIS:HE1	3:E:634:HOH:O	1.87	0.57
1:A:49:ARG:NH2	1:B:13:GLU:OE1	2.32	0.56
1:F:3:VAL:HG11	1:F:11:MET:HE1	1.87	0.56
1:C:20:ARG:NH1	3:C:514:HOH:O	2.39	0.56
1:A:13:GLU:OE2	1:B:49:ARG:NH2	2.39	0.55
1:E:107:PRO:O	1:E:111:GLN:HG3	2.07	0.55
1:F:3:VAL:HG11	1:F:11:MET:CE	2.36	0.55
1:F:48:GLN:NE2	3:F:507:HOH:O	2.34	0.55
1:C:101:MET:O	1:C:102:MET:HB3	2.06	0.55
1:D:107:PRO:O	1:D:111:GLN:CG	2.49	0.54
1:B:189:HIS:HD2	3:B:586:HOH:O	1.90	0.54
1:B:331:ASP:O	1:B:332:ASP:HB2	2.08	0.54
1:E:76:CYS:O	1:E:316:PRO:HA	2.08	0.54
1:D:156:HIS:HB2	3:D:701:HOH:O	2.07	0.54
1:B:241:GLY:CA	3:B:501:HOH:O	2.58	0.52
1:D:101:MET:O	1:D:102:MET:HB3	2.09	0.52
1:A:49:ARG:CZ	1:B:49:ARG:HD2	2.40	0.52
1:A:47:ALA:HB3	1:A:54:VAL:HG11	1.93	0.50
1:D:260:VAL:HG12	1:D:317:CYS:HB3	1.92	0.50
1:D:166:HIS:HB2	3:D:743:HOH:O	2.11	0.50
1:B:276:TRP:CE2	1:B:324:ARG:HD2	2.45	0.50
1:A:64:HIS:HD2	3:A:713:HOH:O	1.94	0.50
1:C:349:ALA:C	3:C:713:HOH:O	2.48	0.50
1:A:148:LEU:HD12	1:A:344:PRO:HD3	1.93	0.50
1:E:236:ILE:HD11	1:E:263:ILE:HD11	1.94	0.49
1:E:158:ARG:HA	1:E:163:SER:O	2.12	0.49
1:A:224:ARG:HD3	3:A:614:HOH:O	2.13	0.49
1:D:276:TRP:CE2	1:D:324:ARG:HD3	2.48	0.48
1:C:102:MET:CE	1:C:288:MET:HE2	2.43	0.48
1:A:148:LEU:HD12	1:A:344:PRO:HG3	1.95	0.48
1:E:45:GLU:HB2	3:E:636:HOH:O	2.13	0.48
1:B:102:MET:SD	1:B:288:MET:HE1	2.54	0.48
1:F:8:LEU:CA	1:F:11:MET:HE3	2.29	0.48
1:A:151:GLN:OE1	1:A:151:GLN:C	2.51	0.48
1:B:158:ARG:HA	1:B:163:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:MET:CE	1:C:288:MET:HE1	2.44	0.47
1:C:276:TRP:CD2	1:C:324:ARG:HD3	2.49	0.47
1:C:243:PHE:N	3:C:502:HOH:O	2.47	0.47
1:A:328:ILE:HD12	1:A:336:VAL:HG21	1.95	0.47
1:A:158:ARG:HA	1:A:163:SER:O	2.14	0.47
1:B:106:SER:HB2	1:B:107:PRO:HD2	1.97	0.47
1:A:253:LYS:HD2	1:A:253:LYS:C	2.36	0.47
1:C:79:THR:HG22	1:C:104:LEU:HD12	1.96	0.46
1:A:276:TRP:CE2	1:A:324:ARG:HD2	2.50	0.46
1:E:96:LEU:HD12	1:E:118:ARG:HG3	1.96	0.46
1:E:285:ASN:HB2	3:E:638:HOH:O	2.14	0.46
1:A:201:GLU:CG	3:A:533:HOH:O	2.63	0.46
1:C:72:MET:HB3	1:C:102:MET:HG2	1.98	0.46
1:C:102:MET:HE2	1:C:288:MET:CE	2.44	0.46
1:A:197:THR:O	1:A:265:HIS:HA	2.16	0.45
1:B:260:VAL:HG12	1:B:317:CYS:HB3	1.98	0.45
1:C:72:MET:CB	1:C:102:MET:HG2	2.46	0.45
1:C:276:TRP:CE2	1:C:324:ARG:HD3	2.51	0.45
1:E:25:GLN:HE22	1:E:118:ARG:HH12	1.64	0.45
1:A:307:THR:HG23	1:A:313:ARG:O	2.17	0.45
1:D:156:HIS:CE1	3:D:743:HOH:O	2.63	0.45
1:B:342:VAL:HA	1:B:348:ARG:HH11	1.81	0.45
1:A:231:ILE:HA	1:A:235:PHE:O	2.17	0.44
1:E:236:ILE:CD1	1:E:263:ILE:HD11	2.47	0.44
1:F:168:PRO:HB2	1:F:200:ASN:ND2	2.32	0.44
1:A:148:LEU:HD12	1:A:344:PRO:CD	2.47	0.44
1:D:146:GLU:HG2	1:D:150:LYS:HE2	1.99	0.44
1:A:251:TYR:O	1:A:254:TYR:HB3	2.17	0.44
1:D:276:TRP:CD1	1:D:324:ARG:HD3	2.52	0.44
1:D:276:TRP:CD2	1:D:324:ARG:HD3	2.53	0.44
1:F:76:CYS:O	1:F:316:PRO:HA	2.17	0.44
1:C:107:PRO:O	1:C:111:GLN:OE1	2.36	0.44
1:F:107:PRO:O	1:F:111:GLN:HG3	2.17	0.44
1:F:168:PRO:HB2	1:F:200:ASN:HD22	1.83	0.44
1:A:173:PRO:O	1:A:197:THR:CG2	2.66	0.43
1:B:167:ALA:HB1	1:B:199:PRO:HB3	2.00	0.43
1:E:202:ASP:O	1:E:233:LYS:HA	2.18	0.43
1:B:224:ARG:HD3	3:B:513:HOH:O	2.17	0.43
1:F:5:ASN:OD1	1:F:38:ARG:HD2	2.18	0.43
1:A:340:ASP:OD1	1:A:341:VAL:N	2.52	0.43
1:E:158:ARG:HB3	1:E:158:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:TRP:CE2	1:E:324:ARG:HD2	2.53	0.43
1:A:31:LYS:O	1:A:58:GLU:HA	2.19	0.43
1:A:276:TRP:NE1	1:A:324:ARG:HD2	2.34	0.43
1:F:204:ALA:HB3	1:F:234:GLY:HA2	2.01	0.43
1:F:148:LEU:HD12	1:F:148:LEU:HA	1.90	0.43
1:E:76:CYS:HA	1:E:104:LEU:HD13	2.01	0.42
1:D:276:TRP:CG	1:D:324:ARG:HD3	2.55	0.42
1:B:148:LEU:HD13	1:B:344:PRO:HG3	2.01	0.42
1:D:260:VAL:CG1	1:D:317:CYS:HB3	2.49	0.42
1:C:102:MET:HE2	1:C:288:MET:HE1	2.02	0.42
1:B:230:GLU:OE1	1:B:240:HIS:HE1	2.03	0.42
1:D:102:MET:O	1:D:102:MET:HG3	2.20	0.42
1:F:226:ARG:NE	3:F:522:HOH:O	2.52	0.42
1:C:102:MET:O	1:C:102:MET:HG3	2.20	0.41
1:C:125:PRO:HA	1:C:126:PRO:HD3	1.96	0.41
1:C:146:GLU:OE2	3:C:504:HOH:O	2.21	0.41
1:E:59:LEU:HD21	1:E:87:ALA:HB1	2.02	0.41
1:F:138:ASP:O	1:F:142:VAL:HG23	2.20	0.41
1:B:143:LEU:O	1:B:147:THR:HG23	2.20	0.41
1:F:260:VAL:HG12	1:F:317:CYS:HB3	2.00	0.41
1:A:208:LEU:HD12	1:A:231:ILE:HD11	2.02	0.41
1:A:133:LEU:HA	1:A:134:PRO:HD3	1.95	0.41
1:A:221:ASN:HD21	1:A:284:ARG:HH21	1.68	0.41
1:B:190:TRP:HA	1:B:191:PRO:HA	1.87	0.41
1:B:345:GLU:HA	1:B:348:ARG:HD3	2.03	0.41
1:F:331:ASP:O	1:F:332:ASP:CG	2.59	0.41
1:A:201:GLU:HG2	3:A:533:HOH:O	2.21	0.41
1:E:190:TRP:HA	1:E:191:PRO:HA	1.88	0.41
1:E:204:ALA:HB3	1:E:234:GLY:HA2	2.03	0.41
1:A:276:TRP:CD1	1:A:324:ARG:HD2	2.56	0.41
1:D:64:HIS:HE1	3:D:747:HOH:O	2.02	0.41
1:F:190:TRP:HA	1:F:191:PRO:HA	1.89	0.40
1:A:260:VAL:HG12	1:A:317:CYS:HB3	2.03	0.40
1:C:20:ARG:HG2	3:C:514:HOH:O	2.21	0.40
1:C:331:ASP:O	1:C:332:ASP:OD1	2.40	0.40
1:E:259:GLU:HB2	1:E:315:THR:HB	2.04	0.40
1:C:151:GLN:HE21	1:C:151:GLN:HB2	1.68	0.40
1:F:3:VAL:CG1	1:F:11:MET:HE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/363 (95%)	331 (96%)	14 (4%)	1 (0%)	41	37
1	B	346/363 (95%)	332 (96%)	13 (4%)	1 (0%)	41	37
1	C	346/363 (95%)	333 (96%)	11 (3%)	2 (1%)	25	19
1	D	346/363 (95%)	330 (95%)	14 (4%)	2 (1%)	25	19
1	E	345/363 (95%)	330 (96%)	13 (4%)	2 (1%)	25	19
1	F	345/363 (95%)	332 (96%)	12 (4%)	1 (0%)	41	37
All	All	2074/2178 (95%)	1988 (96%)	77 (4%)	9 (0%)	34	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	332	ASP
1	B	192	SER
1	D	192	SER
1	A	192	SER
1	C	102	MET
1	C	192	SER
1	E	192	SER
1	D	102	MET
1	F	192	SER

5.3.2 Protein sidechains [i](#)

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	287/299 (96%)	280 (98%)	7 (2%)	49	51
1	B	287/299 (96%)	277 (96%)	10 (4%)	36	35
1	C	287/299 (96%)	282 (98%)	5 (2%)	60	65
1	D	287/299 (96%)	282 (98%)	5 (2%)	60	65
1	E	287/299 (96%)	284 (99%)	3 (1%)	76	81
1	F	287/299 (96%)	283 (99%)	4 (1%)	67	72
All	All	1722/1794 (96%)	1688 (98%)	34 (2%)	55	58

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	137	ASP
1	A	151	GLN
1	A	197	THR
1	A	225	GLU
1	A	253	LYS
1	A	314	LYS
1	B	49	ARG
1	B	96	LEU
1	B	104	LEU
1	B	105	HIS
1	B	153	ARG
1	B	169	LEU
1	B	189	HIS
1	B	191	PRO
1	B	225	GLU
1	B	333	LYS
1	C	53	LYS
1	C	85	LEU
1	C	114	LYS
1	C	160	LYS
1	C	307	THR
1	D	17	LYS
1	D	53	LYS
1	D	106	SER
1	D	160	LYS
1	D	307	THR
1	E	53	LYS
1	E	96	LEU
1	E	153	ARG

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Mol	Chain	Res	Type
1	F	53	LYS
1	F	218	PRO
1	F	221	ASN
1	F	314	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	221	ASN
1	A	240	HIS
1	A	256	ASN
1	B	189	HIS
1	B	240	HIS
1	C	48	GLN
1	C	151	GLN
1	D	109	GLN
1	D	221	ASN
1	E	25	GLN
1	E	111	GLN
1	E	282	HIS
1	F	221	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 6 ligands modelled in this entry, 6 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 [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	348/363 (95%)	-0.27	4 (1%) 80 79	18, 30, 50, 69	0
1	B	348/363 (95%)	-0.39	0 100 100	17, 26, 44, 60	0
1	C	348/363 (95%)	-0.29	0 100 100	18, 26, 46, 82	0
1	D	348/363 (95%)	-0.29	0 100 100	16, 24, 42, 74	0
1	E	347/363 (95%)	-0.39	1 (0%) 94 93	17, 27, 47, 59	0
1	F	347/363 (95%)	-0.37	3 (0%) 84 83	17, 28, 47, 67	0
All	All	2086/2178 (95%)	-0.33	8 (0%) 92 92	16, 27, 47, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	ASP	2.7
1	F	332	ASP	2.7
1	F	310	GLY	2.5
1	F	151	GLN	2.4
1	A	333	LYS	2.2
1	E	310	GLY	2.2
1	A	153	ARG	2.1
1	A	147	THR	2.1

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

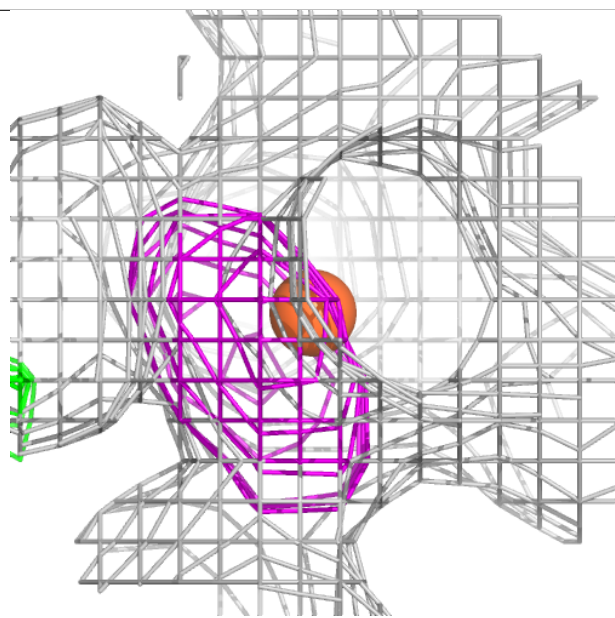
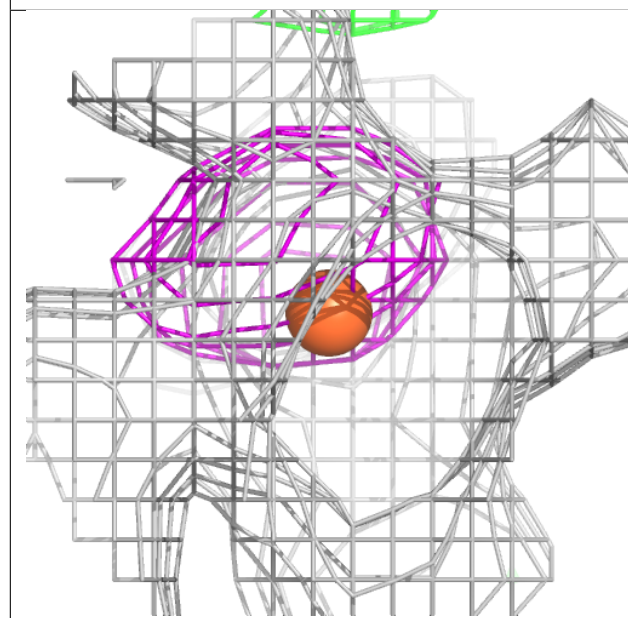
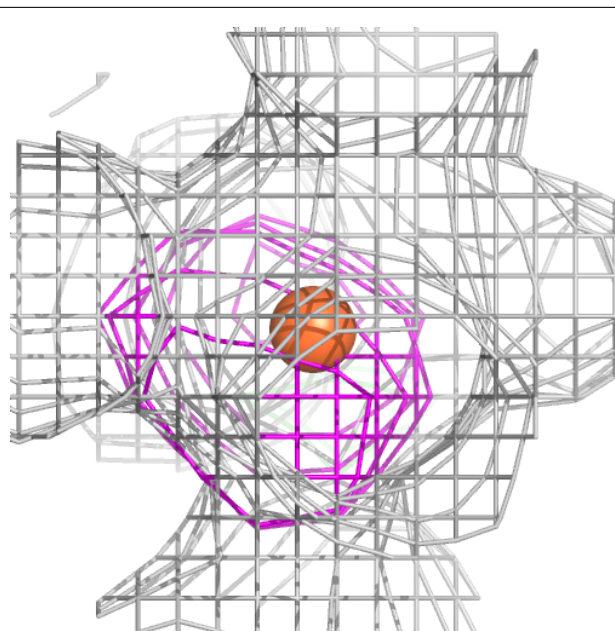
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FE	A	401	1/1	0.80	0.08	43,43,43,43	0
2	FE	D	401	1/1	0.84	0.09	36,36,36,36	0
2	FE	F	401	1/1	0.85	0.11	44,44,44,44	0
2	FE	C	401	1/1	0.86	0.12	39,39,39,39	0
2	FE	B	401	1/1	0.88	0.11	38,38,38,38	0
2	FE	E	401	1/1	0.97	0.08	38,38,38,38	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.

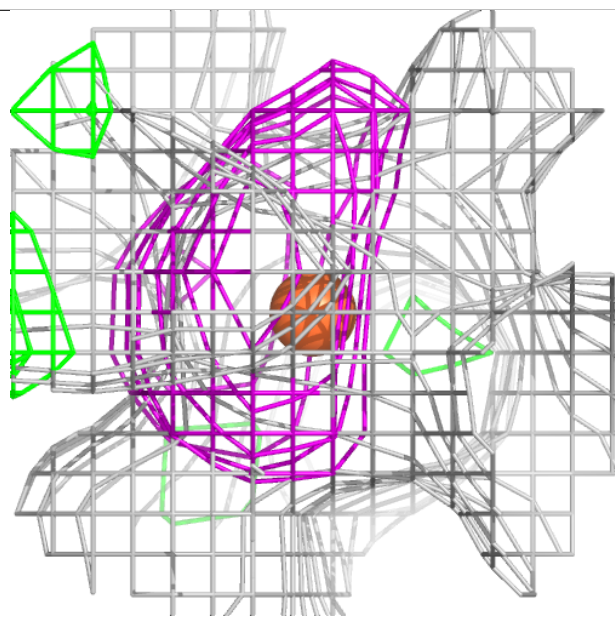
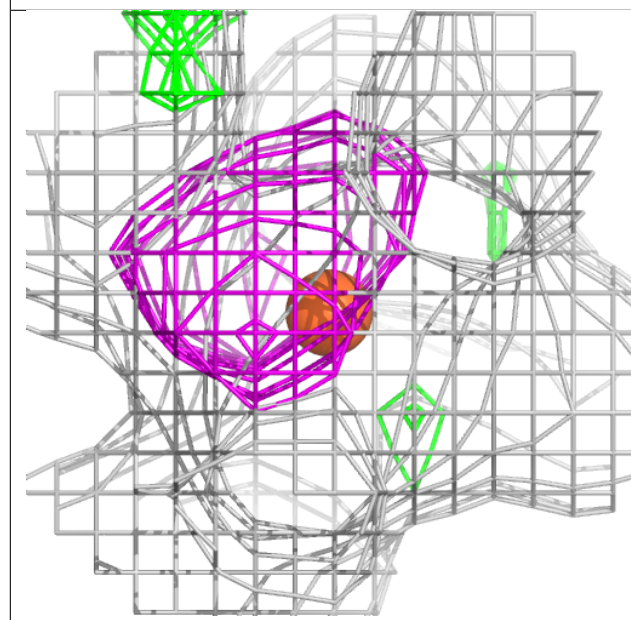
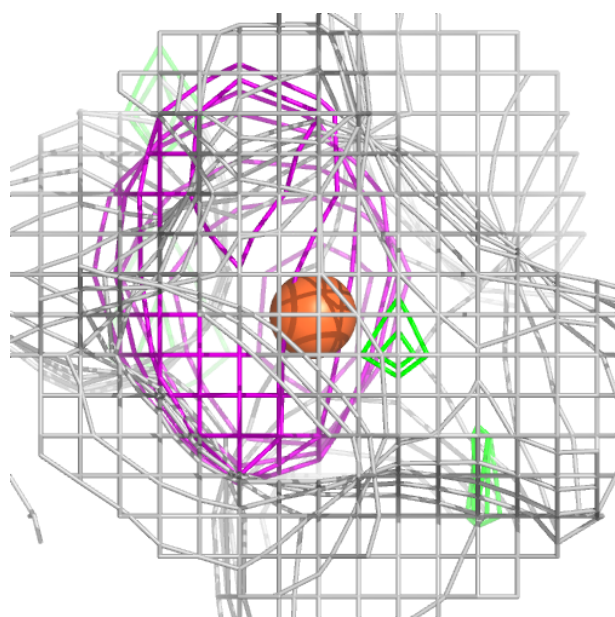
Electron density around FE A 401:

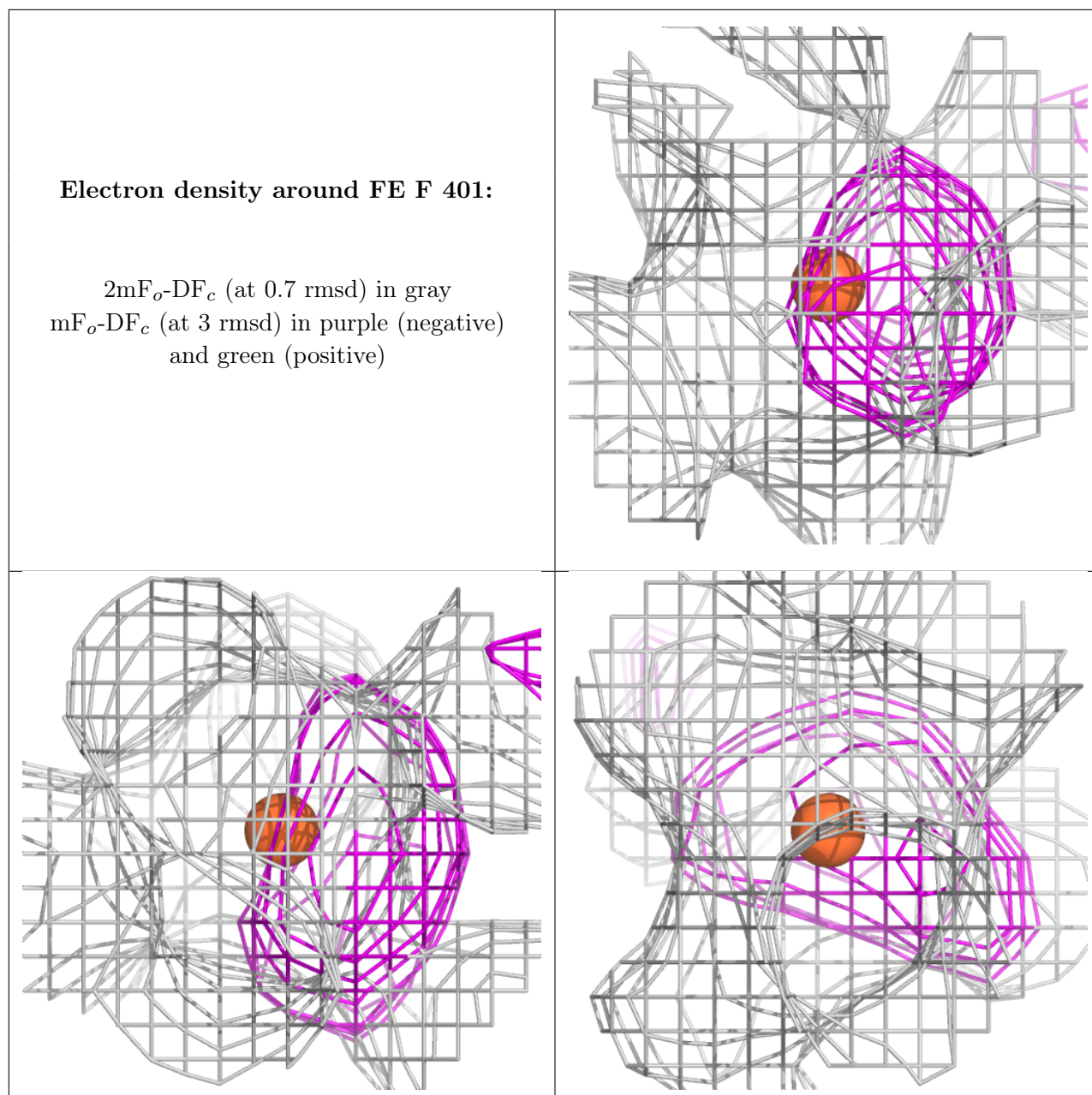
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE D 401:

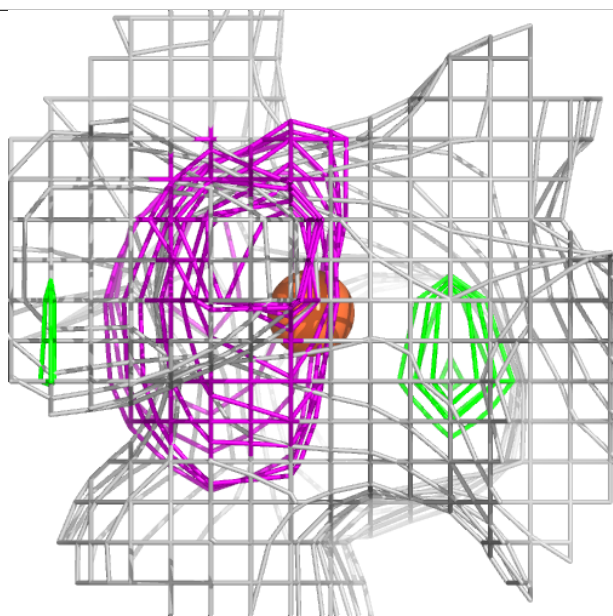
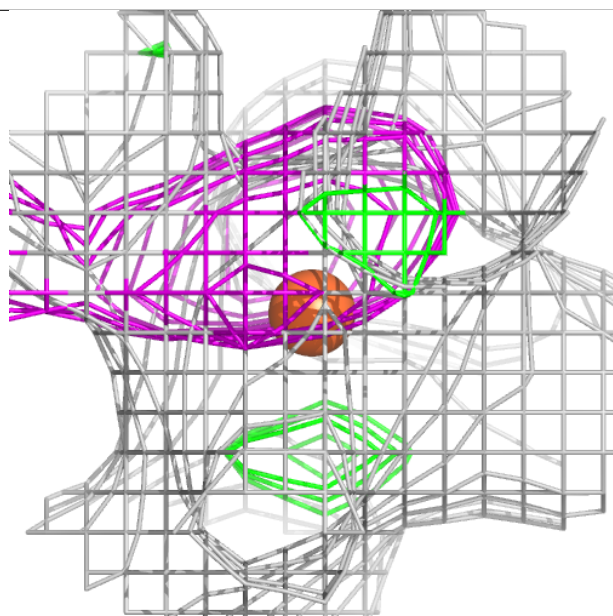
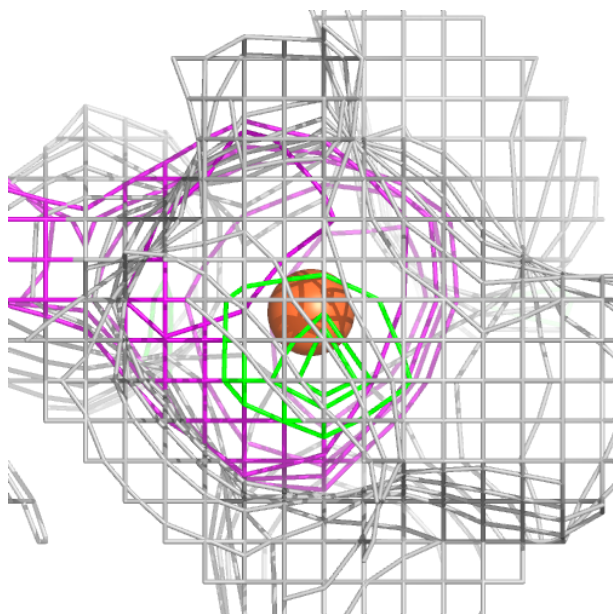
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





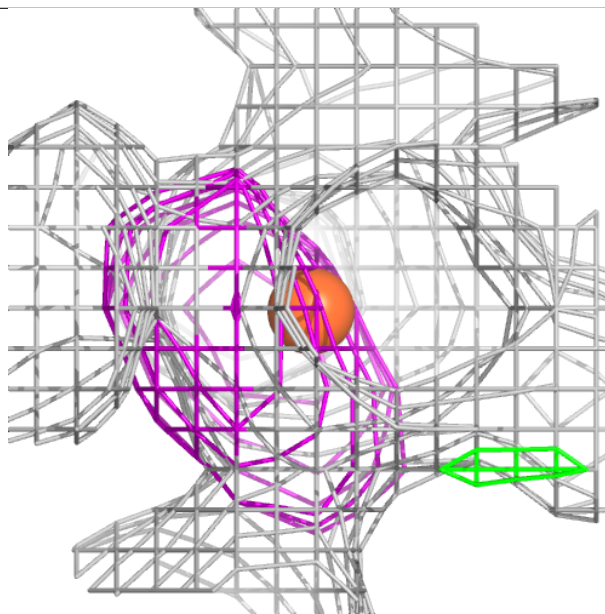
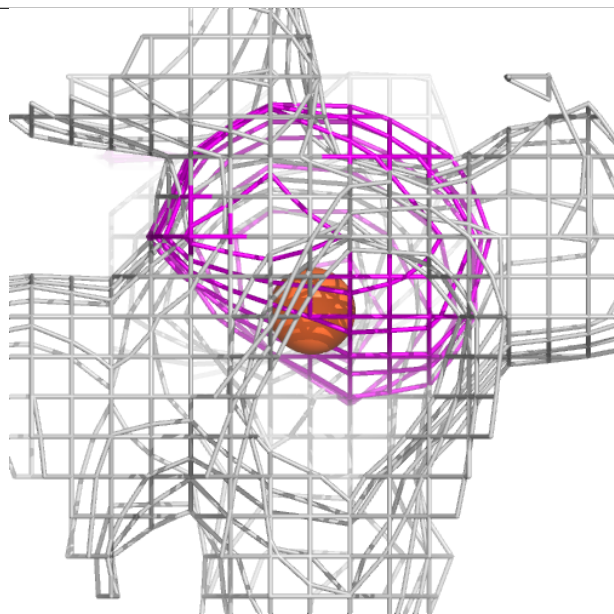
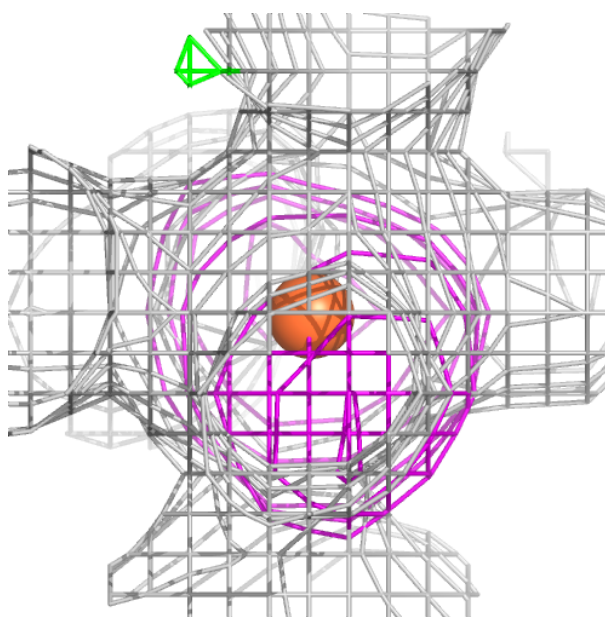
Electron density around FE C 401:

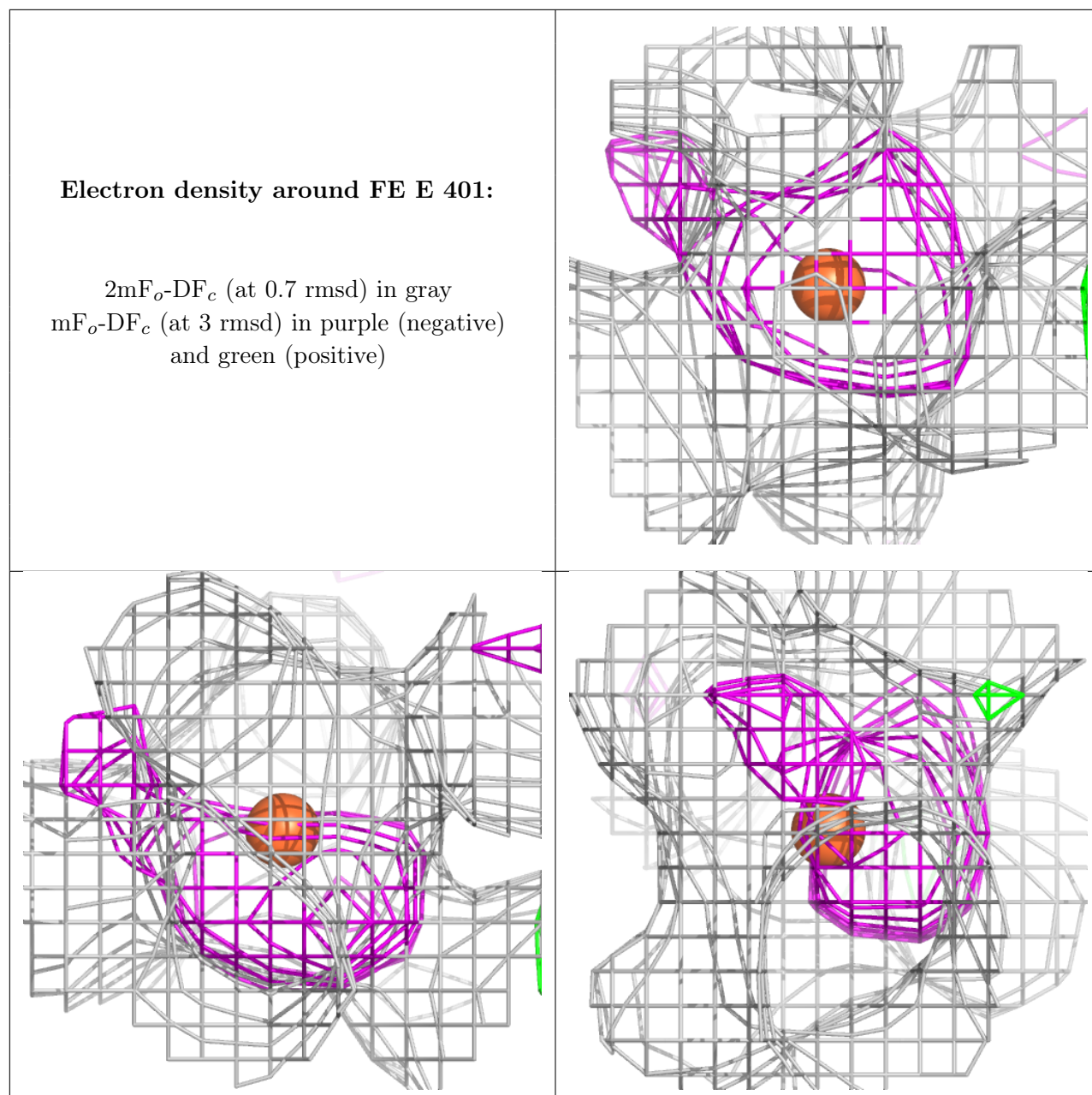
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE B 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.